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## A thermodynamically motivated formulation of the energy model of semiconductor devices

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## 1. INTRODUCTION

In the drift-diffusion model of semiconductor devices the free energy has turned out to be a very useful quantity. Gajewski and Gröger [7] applied it in the analysis of the transient initial-boundary value problem. Gajewski [3], [5] also used it to control the step width in the time discretization. Considered as a functional of the carrier densities, the free energy is a thermodynamic potential and a convex functional. With both the properties the free energy becomes a very attractive quantity. Moreover, as an integral quantity it is not too sensitive to local deviations of either the carrier densities or the electric field. In the case of variable temperature, however, the free energy is no convex functional.

The main topic of this paper is to set up a frame for an investigation of the energy model of semiconductor devices in a similar way as H. Gajewski and K. Gröger dealt with the drift-diffusion model. We formulate the energy model as a system of balance equations for the carrier densities  $n$  and  $p$  and for the density  $u$  of the total energy. The non-local electrostatic interaction of the carriers is described by a boundary value problem for the Poisson equation which includes mixed boundary conditions. Although function spaces are not specified yet, the thermodynamic calculus for a system of electrons and holes in a semiconductor device is developed with regard to functional analysis. We prove, in particular, that the negative entropy considered as a functional of the densities  $n$ ,  $p$  and  $u$  is a convex thermodynamic potential. The current densities  $j_n$  and  $j_p$  of carriers and  $j_u$  of the total energy are expressed in the conjugate variables  $X_n := \Phi_n/T$ ,  $X_p := \Phi_p/T$  and  $Y := 1/T$ , where  $T$  denotes the temperature and  $\Phi_n$  and  $\Phi_p$  denote the electro-chemical potentials. In this formulation a Lyapunov function for the system of evolution equations is defined, which is closely related to the negative entropy. The Lyapunov function also works in the cases of time discretization or space discretization. The intention to introduce a Lyapunov function forced us to describe quantities like energy rather explicitly. With regard to the simulation practice, material laws like effective masses are admitted to depend on the temperature. Both the variants, the case of Boltzmann statistics and the Fermi case, are treated as well as the case of a non-parabolic band structure.

The paper is organized as follows. Our basic notation is introduced in section 2. Moreover, the electrostatic energy of the system is specified and its functional derivatives are evaluated. In section 3 the total energy is defined starting from the free energy or from an other suitable thermodynamic potential. Customary versions of the energy model are derived from the energy balance equation. In section 4 the energy model is formulated in the variables  $\Phi_n/T$ ,  $\Phi_p/T$  and  $1/T$ , which we consider as the natural ones. In section 5 a Lyapunov function related to the entropy is constructed for the energy model. In section 6 the spatial discretization is described. The calculus is quite analogous. In section 7 the case of a general dispersion is studied. This case is a little bit different from the cases of parabolic band structure, because the state equations are more implicit. The convexity of the potential  $U(n, p, s)$  is proved also in this case. In contrast to  $d^2U$  the quadratic form  $d^2G$  of the conjugate potential  $G(\Phi_n, \Phi_p, T)$  is the difference  $d_n^2G - d_p^2G$  of two positive semidefinite quadratic forms.

## 2. NOTATION. ELECTROSTATIC ENERGY

The device occupies a bounded region  $\Omega$  with the boundary  $\partial\Omega$  in the Euclidean space of two or three dimensions. Let  $q$ ,  $k_B$  and  $T^*$  denote the elementary charge, the Boltzmann constant and a fixed reference temperature in *Kelvin*. Let  $V = q\psi/k_B T^*$  denote the (dimension-less) potential of a hole in the electrostatic potential  $\psi$ . Then the Poisson equation in a semiconductor device with given completely ionized doping profile  $qd$  reads

$$-\nabla(\epsilon\nabla V) = d + p - n,$$

where  $\epsilon$  denotes the scaled dielectric permittivity. The boundary conditions are the Dirichlet condition  $V = V_D$  on some part  $\Gamma_D$  of the boundary, a boundary condition of the third kind,

$$\epsilon\partial_\nu V + \beta V = \beta V_G,$$

on some other part  $\Gamma_G$  of the boundary and the homogeneous Neumann conditions everywhere else on the boundary. Although function spaces are not specified yet in this paper, we mention the space  $H^1(\Omega)$  of quadratic integrable functions which have quadratic integrable derivatives and the space  $H_0^1 := H_0^1(\Omega \setminus \Gamma_D)$  of functions  $\chi \in H^1(\Omega)$  which vanish on  $\Gamma_D$ . The boundary value problem for the Poisson equation is written as an variational equation

$$\int \epsilon\nabla V \cdot \nabla \chi d\Omega + \int_{\Gamma_G} \beta V \chi d\Gamma = \int (d + p - n)\chi d\Omega + \int_{\Gamma_G} \beta V_G \chi d\Gamma$$

( $\chi \in H_0^1$ ) for a function  $V \in V_D + H_0^1$ , where  $V_D \in H^1(\Omega)$  represents the Dirichlet data on  $\Gamma_D$ . We assume that the dielectric permittivity is independent of the temperature and that the heat capacities of the lattice and of the carrier densities  $n$  and  $p$  do not depend on the electric field. Thus the total energy  $U$  of the device model is a sum of its interior energy  $U^i$  and of its electrostatic energy  $U^e$ .

Quantities like energy are functionals of the state represented by a set of independent state variables and of some parameters like  $d$ ,  $V_D$  or  $V_G$ . In our discussions the parameters are assumed to be fixed and thus the dependence of the quantities on them is not indicated. The state can be described by several sets of state variables, e.g. by  $n$ ,  $p$  and  $T$  or by  $n$ ,  $p$  and the entropy density  $s$ . Therefore we distinguish the functionals by an index,

$$U \equiv U(n, p, s) \equiv U_1(n, p, T) = U_1^i(n, p, T) + U^e(p - n).$$

The index is omitted at the thermodynamic potentials.

There are several possibilities to define a functional  $U^e$ . We prefer the choice

$$U^e(p - n) = \int V^*(p - n)d\Omega + \frac{1}{2} \int \epsilon(\nabla V_{p-n})^2 d\Omega + \frac{1}{2} \int_{\Gamma_G} \beta V_{p-n}^2 d\Gamma,$$

where  $V = V^* + V_{p-n}$  and where  $V_p \in H_0^1$  denotes the solution of

$$(2.1) \quad \int \epsilon\nabla V_p \cdot \nabla \chi d\Omega + \int_{\Gamma_G} \beta V_p \chi d\Gamma = \int \rho \chi d\Omega \quad (\chi \in H_0^1).$$

Regarding this integral identity we have

$$U^e(p - n + \delta\rho) = U^e(p - n) + \int V \delta\rho d\Omega + \int \epsilon (\nabla \delta\rho)^2 d\Omega + \int_{\Gamma_G} \beta (\delta\rho)^2 d\Gamma,$$

i.e.

$$\begin{aligned} \langle dU^e(p - n), \delta\rho \rangle &= \int V \delta\rho d\Omega, \\ \langle d^2U^e(p - n), \delta\rho_1 \otimes \delta\rho_2 \rangle &= \int \epsilon \nabla V_{\delta\rho_1} \cdot \nabla V_{\delta\rho_2} d\Omega + \int_{\Gamma_G} \beta V_{\delta\rho_1} V_{\delta\rho_2} d\Gamma. \end{aligned}$$

Sometimes the physically intuitive formal notation with densities is used in the paper, i.e.  $U^e(p - n) = \int u^e(p - n) d\Omega$  with the generalized density and its derivatives,

$$\begin{aligned} u^e(\rho) &= V^* \rho + \frac{1}{2} \epsilon (\nabla V_\rho)^2 + \frac{1}{2} \beta V_\rho^2 \delta_{\Gamma_G}, \\ (u^e)'(p - n) &= V, \\ (u^e)''(p - n) \delta\rho_1 \delta\rho_2 &= \epsilon \nabla V_{\delta\rho_1} \cdot \nabla V_{\delta\rho_2} + \beta V_{\delta\rho_1} V_{\delta\rho_2} \delta_{\Gamma_G}. \end{aligned}$$

The differentiation of the density has a symbolic meaning only.

An alternative choice of the electrostatic energy would be

$$\tilde{U}^e(p - n) = \int \epsilon \nabla (V - \frac{1}{2} V_{p-n}) \cdot \nabla V_{p-n} d\Omega + \int_{\Gamma_G} \beta (V - \frac{1}{2} V_{p-n}) V_{p-n} d\Gamma.$$

The second order derivative of this functional coincides with that of  $U^e$ , but its first order derivative contains an additional boundary term

$$\langle d\tilde{U}^e(p - n), \delta\rho \rangle = \int V \delta\rho d\Omega + \int_{\Gamma_D} V_D \epsilon \partial_\nu V_{\delta\rho} d\Gamma.$$

Let  $\Phi^*(T)$  denote the Fermi level of the semiconductor device in the equilibrium state at the constant temperature  $T$ . The electro-chemical potentials of the electrons or holes are chosen as  $\Phi_d(1) + \Phi_n$  and  $\Phi_d(1) + \Phi_p$ , respectively, but the additive constant  $\Phi_d(1)$  will be included into the potential  $V$ . The state equations are

$$(2.2) \quad n = N_c(T) \exp\left(-\frac{E_c(T)}{T}\right) \exp\left(\frac{\Phi_n + V}{T}\right) =: \mathcal{N}(T) \exp\left(\frac{\Phi_n + V}{T}\right),$$

$$(2.3) \quad p = N_v(T) \exp\left(\frac{E_v(T)}{T}\right) \exp\left(-\frac{\Phi_p + V}{T}\right) =: \mathcal{P}(T) \exp\left(-\frac{\Phi_p + V}{T}\right).$$

in the case  $B$  of Boltzmann statistics,

$$(2.4) \quad n := N_c(T) \mathcal{F}_{1/2} \left[ \frac{\Phi_n + V - E_c(T)}{T} \right],$$

$$(2.5) \quad p := N_v(T) \mathcal{F}_{1/2} \left[ -\frac{\Phi_p + V - E_v(T)}{T} \right].$$

in the case  $F$  of Fermi statistics, and

$$\begin{aligned} n &:= \int_0^\infty \frac{a_c(\omega, T)}{1 + \exp\left[-\frac{\Phi_n + V - E_c(T)}{T}\right]} d\omega \\ p &:= \int_0^\infty \frac{a_v(\omega, T)}{1 + \exp\left[\frac{\Phi_p + V - E_v(T)}{T}\right]} d\omega. \end{aligned}$$

in the case  $G$  of general dispersion. The state densities  $N_c$  and  $N_v$  are not necessarily proportional to  $T^{3/2}$ , since the effective masses, in the case of parabolic band structure, or the dispersions  $\omega_c$  or  $\omega_v$ , in general, may depend on  $T$ . Of course, the band edges  $E_c$ ,  $E_v$  and the other material functions may also explicitly depend on the spatial coordinates. Such a dependence is caused, e.g., by the doping profile or by a heterostructure. We will not indicate, however, such a dependence and use also the notation  $E_c(T) = E \circ T$  etc. The notation

$$\mathcal{F}_\alpha(x) = \frac{1}{\Gamma(\alpha+1)} F_\alpha(x) = \frac{1}{\Gamma(\alpha+1)} \int_0^\infty \frac{t^\alpha}{\exp(t-x)+1} dt$$

( $\alpha > -1$ ) is used for the Fermi integrals such that  $\mathcal{F}'_{\alpha+1} = \mathcal{F}_\alpha$  holds. In the case of general dispersions the numerators of the integrands denote the surface areas

$$a_b(\omega, T) = \int_{\omega_b(p, T) = \omega} d\sigma(p) \quad (b = c, v)$$

of the energy levels in the momentum space which are assumed to be finite.

An upper index  $C = B, F$  or  $G$  distinguishes the Boltzmann case, the Fermi case and the case of a general dispersion if a distinction is necessary. Some letters are used with several meanings, e.g., the letter  $n$  denotes the density of electrons and it is used as the lower index of state variables of the electrons. In section 6 the letter  $n$  is also used as lower index and as upper index for the components of grid vectors associated with the triangulation of the domain. We hope, however, that this multiple use does not cause any confusion.

The potentials  $\Phi_n$  and  $\Phi_p$  here have the opposite sign as the quasi-Fermi levels  $\varphi_n$  and  $\varphi_p$  in [14], [15]. Therefore the particle fluxes and the total heat flux are

$$(2.6) \quad j_n = -D_n n (\nabla \Phi_n + P_n \nabla T),$$

$$(2.7) \quad j_p = D_p p (\nabla \Phi_p - P_p \nabla T),$$

$$(2.8) \quad j^Q = -\kappa \nabla T + T P_n j_n + T P_p j_p,$$

respectively, with the total thermal conductivity

$$\kappa = \kappa_L + n(\lambda_n/T - D_n P_n^2 T) + p(\lambda_p/T - D_p P_p^2 T).$$

(cf. [14] or [15]). The heat flux is, of course, primarily an expression in terms of the thermodynamic forces, but it can be represented in the given form.

### 3. FREE ENERGY, TOTAL ENERGY AND THE ENERGY BALANCE EQUATION

We consider a system, which consists of electrons and holes and of a lattice with an unspecified density  $f_L(T)$  of its free energy. In analogy to the ideal gas the density of the free energy of the system is given by

$$\begin{aligned} f^B(n, p, T) &= u^e(p - n) + f_L(T) \\ &+ nT \log [n/\mathcal{N}(T)] - nT + pT \log [p/\mathcal{P}(T)] - pT. \end{aligned}$$

in the Boltzmann case. The third summand on the right-hand side and the fifth one contain, in particular, the interaction terms  $nE_c$  and  $pE_v$ .

In the Fermi case, one can start with the thermodynamic potential

$$\Omega(T, \mu) = -cT^{5/2} \mathcal{F}_{3/2}\left(\frac{\mu}{T}\right),$$

of a Fermi gas (cf. [10], (56.6)). The density of the gas and the density of its free energy are  $n = -\partial_\mu \Omega(T, \mu)$  and  $f(n, T) = n\mu + \Omega(T, \mu)$ . Accordingly, the density of the free energy of our system is given by

$$\begin{aligned} f^F(n, p, T) &= u^e(p - n) + f_L(T) \\ &+ nT \mathcal{F}_{1/2}^{-1}[n/N_c(T)] - TN_c(T) \mathcal{F}_{3/2} \circ \mathcal{F}_{1/2}^{-1}[n/N_c(T)] + nE_c(T) \\ &+ pT \mathcal{F}_{1/2}^{-1}[p/N_v(T)] - TN_v(T) \mathcal{F}_{3/2} \circ \mathcal{F}_{1/2}^{-1}[p/N_v(T)] - pE_v(T). \end{aligned}$$

The free energy  $F(n, p, T) = \int f(n, p, T) d\Omega$  as a functional of  $n$ ,  $p$  and  $T$  is a thermodynamic potential. Regarding  $(u^e)'(p - n) = V$  etc, one straightforward checks the usual thermodynamic relations like  $\partial_n f = \Phi_n$  and  $\partial_p f = -\Phi_p$ , meanwhile  $\partial_T f = -s$  defines the entropy density, namely,

$$(3.1) \quad \begin{aligned} s_1^B(n, p, T) &= -f'_L(T) - n \log[n/N(T)] + n + nTN'(T)/N(T) \\ &- p \log[p/P(T)] + p + pTP'(T)/P(T), \end{aligned}$$

$$(3.2) \quad \begin{aligned} s_1^F(n, p, T) &= -f'_L(T) - nE'_c(T) + pE'_v(T) \\ &- n\mathcal{F}_{1/2}^{-1}(n/N_c \circ T) + (TN_c \circ T)' \mathcal{F}_{3/2} \circ \mathcal{F}_{1/2}^{-1}(n/N_c \circ T) \\ &- p\mathcal{F}_{1/2}^{-1}(p/N_v \circ T) + (TN_v \circ T)' \mathcal{F}_{3/2} \circ \mathcal{F}_{1/2}^{-1}(p/N_v \circ T). \end{aligned}$$

The (generalized) density of the total energy of the system is the partial Legendre transform  $u(n, p, s) := f(n, p, T) + Ts$ , but more familiar is the density given as a function of  $n$ ,  $p$  and  $T$ ,

$$u_1^B(n, p, T) := u^e(p - n) + \int^T c_L + nT^2 \frac{N'(T)}{N(T)} + pT^2 \frac{P'(T)}{P(T)},$$

$$\begin{aligned} u_1^F(n, p, T) &= u^e(p - n) + \int^T c_L \\ &+ n[E_c(T) - TE'_c(T)] + T^2 N'_c(T) \mathcal{F}_{3/2} \circ \mathcal{F}_{1/2}^{-1}[n/N_c(T)] \\ &- p[E_v(T) - TE'_v(T)] + T^2 N'_v(T) \mathcal{F}_{3/2} \circ \mathcal{F}_{1/2}^{-1}[p/N_v(T)] \end{aligned}$$

with the notation  $\int^T c_L := f_L(T) - Tf'_L(T)$  for the interior energy of the lattice.

Following Wachutka the flux of total energy reads

$$j_u = -\kappa \nabla T + (TP_n + \Phi_n)j_n + (TP_p - \Phi_p)j_p$$

and the balance of the total energy  $\dot{u} + \nabla \cdot j_u = 0$  for a thermodynamic process in our system can be written as a heat equation

$$\partial_T u_1(n, p, T) \dot{T} - \nabla \cdot (\kappa \nabla T) = \mathcal{H}$$

with the right-hand side

$$\begin{aligned} \mathcal{H} &= -\nabla \cdot [(TP_n + \Phi_n)j_n + (TP_p - \Phi_p)j_p] - \partial_n u_1(n, p, T)\dot{n} - \partial_p u_1(n, p, T)\dot{p} \\ &= -\nabla \cdot [(TP_n + \Phi_n)j_n + (TP_p - \Phi_p)j_p] + \partial_n u_1(n, p, T)(\nabla \cdot j_n + R) \\ &\quad + \partial_p u_1(n, p, T)(\nabla \cdot j_p + R), \end{aligned}$$

where  $R$  denotes the net recombination rate.

The differential of the total energy for a fixed doping profile and fixed boundary values can also be written as

$$du = du_1^i(n, p, T) - Vdn + Vdp.$$

Thus the balance of the total energy becomes

$$\partial_t \{u_1^i[n(t), p(t), T(t)]\} + V(\dot{p} - \dot{n}) + \nabla \cdot j_u = 0,$$

where  $\{u_1^i[n(t), p(t), T(t)]\}$  indicates that the density of the interior energy of the system during a thermodynamic process is considered as a function on space and time. Regarding the continuity equations for the densities  $n$  and  $p$  we get just the balance equation of the interior energy

$$(3.3) \quad \begin{aligned} & \partial_t \{u_1^i[n(t), p(t), T(t)]\} + \\ & \nabla \cdot [-\kappa \nabla T + (TP_n + \Phi_n + V)j_n + (TP_p - \Phi_p - V)j_p] \\ & = \nabla V \cdot (j_n - j_p) \end{aligned}$$

with the conventional Joule heating term  $-\nabla \psi \cdot j_{el}$  on the right-hand side. This equation is in the spirit of [1] if the relations

$$\begin{aligned} P_n T + \Phi_n + V &= T \{P_n + \log [n/\mathcal{N}(T)]\}, \\ P_p T - \Phi_p - V &= T \{P_p + \log [p/\mathcal{P}(T)]\} \end{aligned}$$

are regarded.

*Remark 3.1.* If the functional  $\tilde{U}^e$  is chosen as the electrostatic energy, then an additional boundary term  $\int_{\Gamma_D} V_D \epsilon \partial_\nu V_{p-n}$  appears in the energy balance equation. As far as we know such boundary terms are not used in energy balance equations yet. The lack of the mentioned boundary terms might be a serious lack of the usual energy balance equations. The functional  $U^e$  is the correct one in connection with the energy balance equations used in simulation practice.

#### 4. NATURAL VARIABLES FOR THE ENERGY MODEL

The fundamental thermodynamic identity

$$(4.1) \quad du = \Phi_n dn - \Phi_p dp + T ds$$

(which is easily checked by applying the formulas  $u_1 = f - T \partial_T f = f + T s$ ,  $\partial_n f = \Phi_n$  and  $\partial_p f = -\Phi_p$ ) offers the possibility to substitute the energy balance equation by the entropy balance equation. This possibility looks attractively, since the gradients of  $\Phi_n$ ,  $\Phi_p$  and  $T$  are a basis in the space of thermodynamic forces and since  $s$  is a density like  $n$  and  $p$  (cf intensive and extensive state variables). There are deeper reasons to consider  $n$ ,  $p$  and  $s$  together with  $\Phi_n$ ,  $\Phi_p$  and  $T$  as 'natural coordinates' for the energy model. The coefficient matrix, which assigns the vector of the current densities with the components  $j_n$ ,  $j_p$  and  $j_s$  to the vector of the gradients of  $\Phi_n$ ,  $-\Phi_p$  and  $T$ , is symmetric positive semidefinite according to the Onsager symmetry. Moreover, the thermodynamic potential  $U(n, p, s)$  is a convex functional (cf below).



**Proposition 4.1.** *If the state equations are regarded, the system of equations*

$$(4.2) \quad \begin{aligned} \dot{n} + \nabla \cdot j_n &= -R \\ \dot{p} + \nabla \cdot j_p &= -R \\ \dot{u} + \nabla \cdot j_u &= 0 \end{aligned}$$

*is equivalent to the system of equations*

$$(4.3) \quad \begin{aligned} \dot{n} + \nabla \cdot j_n &= -R \\ \dot{p} + \nabla \cdot j_p &= -R \\ \dot{s} + \nabla \cdot j_s &= \frac{\Phi_n - \Phi_p}{T} R + \frac{1}{T} (-\nabla \Phi_n \cdot j_n + \nabla \Phi_p \cdot j_p - \nabla T \cdot j_s), \end{aligned}$$

where

$$\begin{pmatrix} j_n \\ j_p \\ j_s \end{pmatrix} = - \begin{pmatrix} nD_n & 0 & nD_n P_n \\ 0 & pD_p & pD_p P_p \\ nD_n P_n & pD_p P_p & \frac{\kappa}{T} + nD_n P_n^2 + pD_p P_p^2 \end{pmatrix} \begin{pmatrix} \nabla \Phi_n \\ -\nabla \Phi_p \\ \nabla T \end{pmatrix}.$$

*Proof.* The differentials in (4.1) may be substituted by the time derivatives of the corresponding state variables in a thermodynamic process. Thus we get

$$\begin{aligned} \dot{s} &= \frac{1}{T} (\dot{u} - \Phi_n \dot{n} + \Phi_p \dot{p}) \\ &= \frac{1}{T} [-\nabla \cdot j_u + \Phi_n (\nabla \cdot j_n + R) - \Phi_p (\nabla \cdot j_p + R)] \\ &= \frac{R}{T} (\Phi_n - \Phi_p) - \nabla \cdot \left[ \frac{1}{T} (j_u - \Phi_n j_n + \Phi_p j_p) \right] \\ &\quad + \frac{1}{T} (\nabla \Phi_p \cdot j_p - \nabla \Phi_n \cdot j_n) + \nabla \left( \frac{1}{T} \right) \cdot (j_u - \Phi_n j_n + \Phi_p j_p). \end{aligned}$$

The last identity is written as the entropy balance equation

$$\dot{s} + \nabla \cdot j_s = \frac{\Phi_n - \Phi_p}{T} R + \frac{1}{T} (-\nabla \Phi_n \cdot j_n + \nabla \Phi_p \cdot j_p - \nabla T \cdot j_s)$$

with the entropy flux

$$j_s := \frac{1}{T} j^Q = -\frac{\kappa}{T} \nabla T + P_n j_n + P_p j_p.$$

□

*Remark 4.1.* Both the systems of evolution equations have to be supplemented by initial conditions and by boundary conditions. Initial data might be  $n_0$ ,  $p_0$  and  $T_0$ . These data allow to evaluate  $u_0$  or  $s_0$ . Concerning the boundary conditions we have

$$\nu \cdot j_a = 0 \quad \text{on } \partial\Omega \setminus \Gamma_D \quad (a \in \{n, p, u \text{ or } s\})$$

in mind, meanwhile  $n$ ,  $p$  and  $T$  are prescribed on  $\Gamma_D$  by means of either  $\tilde{\Phi}_n$ ,  $\tilde{\Phi}_p$  and  $\tilde{T}$  or  $\tilde{X}_n$ ,  $\tilde{X}_p$  and  $\tilde{Y}$ , such that  $\Phi_n - \tilde{\Phi}_n \in H_0^1$  etc.

*Remark 4.2.* In the equivalent 'entropy model' (4.3) the Onsager symmetry is perfectly reflected. Moreover, the right-hand side of the entropy balance equation is the sum of the entropy production rates due to the recombination and due to the

fluxes. The entropy production rate of the fluxes can be written as the positive semidefinite quadratic form

$$\frac{1}{T} \left( \nabla \Phi_n \quad -\nabla \Phi_p \quad \nabla T \right) \times \begin{pmatrix} nD_n & 0 & nD_n P_n \\ 0 & pD_p & pD_p P_p \\ nD_n P_n & pD_p P_p & \frac{\kappa}{T} + nD_n P_n^2 + pD_p P_p^2 \end{pmatrix} \begin{pmatrix} \nabla \Phi_n \\ -\nabla \Phi_p \\ \nabla T \end{pmatrix}.$$

The entropy model provides an argument for choosing the opposite sign for the electro-chemical potential. This is a reason why we have not worried about the differing signs of our electro-chemical potentials and Wachutka's quasi-Fermi levels. The entropy model contains terms with products of the gradients of the sought functions. This seems to be a disadvantage of the entropy model compared with the energy model, at least from the point of view of partial differential equations. There is, however, the possibility to write also the energy model in a symmetric form.

The state variables  $s$  and  $u$  can exchange their roles. The identity  $ds = (1/T)du - (\Phi_n/T)dn + (\Phi_p/T)dp$  shows that the state variables  $-\Phi_n/T$ ,  $\Phi_p/T$  and  $1/T$  are the conjugate variables of  $n$ ,  $p$  and  $u$ . Choosing their gradients as a basis in the space of thermodynamic forces we get a symmetric version of the energy model. We have, indeed,

$$(4.4) \quad \begin{pmatrix} j_n \\ j_p \\ j_u \end{pmatrix} = \mathbf{D} \nabla \begin{pmatrix} -\Phi_n/T \\ \Phi_p/T \\ 1/T \end{pmatrix}$$

with

$$\mathbf{D} = \begin{pmatrix} nTD_n & 0 & nTD_n(TP_n + \Phi_n) \\ 0 & pTD_p & pTD_p(TP_p - \Phi_p) \\ nTD_n(TP_n + \Phi_n) & pTD_p(TP_p - \Phi_p) & \mathcal{D} \end{pmatrix}$$

and

$$\mathcal{D} = T^2 \kappa + nTD_n(TP_n + \Phi_n)^2 + pTD_p(TP_p - \Phi_p)^2.$$

The following theorem is of interest, since the identity  $\dot{u} = \Phi_n \dot{n} - \Phi_p \dot{p} + T \dot{s}$  holds for a thermodynamic process in our system. This identity makes the functionals  $U(n, p, s)$  or  $S(n, p, u)$  be candidates for Lyapunov functions of the entropy model (4.3) or of the energy model (4.2) in natural coordinates with the current densities (4.4).

**Theorem 4.1.** *The functional  $U = U(n, p, s)$  is convex and the functional  $S = S(n, p, u)$  is concave.*

*Proof.* The proofs of both the assertions are similar with the difference that energy and entropy exchange their roles. We will prove that the  $3 \times 3$  matrix  $\mathbf{U} = ((U_{ab}))$ ,

$$U_{ab} = \langle \partial_a \partial_b U(n, p, s), \delta a \otimes \delta b \rangle \quad (a, b \in \{n, p, s\}),$$

is positive semidefinite for any state  $(n, p, s)$  and arbitrary variations  $\delta n, \delta p, \delta s$ , meanwhile the analogous matrix  $\mathbf{S}$  is negative semidefinite. If no variation  $\delta a$  vanishes identically, the matrices are definite. The functionals  $U$  and  $S$  are given by

the densities  $u_1 = u^e + u_1^i$  or  $s_1$  from the section 3, respectively, but in wrong coordinates. We use the notation  $w_a$  for the partial derivative with respect to  $a \in \{n, p, T\}$  of any function  $w = w(n, p, T) = w(x, t, n, p, T)$ . We have

$$dU = \langle (U^e)'(p - n), \delta p - \delta n \rangle + \int (u_{1n}^i \delta n + u_{1p}^i \delta p + u_{1T}^i \delta T) d\Omega =: \int \delta u d\Omega,$$

$$\delta s = s_{1n} \delta n + s_{1p} \delta p + s_{1T} \delta T.$$

Because of  $T s_{1T} = u_{1T}$  the summand  $u_{1T} \delta T$  in  $dU$  can be substituted by

$$u_{1T} \delta T = T(\delta s - s_{1n} \delta n - s_{1p} \delta p)$$

and the summand  $s_{1T} \delta T$  in  $dS$  can be substituted by

$$s_{1T} \delta T = \frac{1}{T} [\delta u - u_{1n}^i \delta n - u_{1p}^i \delta p - V(\delta n - \delta p)].$$

Substituting  $\delta T$  in this way we get the well known identities

$$dU = \int (\Phi_n \delta n - \Phi_p \delta p + T \delta s) d\Omega =: U_n + U_p + U_s$$

and

$$dS = \int \left( -\frac{\Phi_n}{T} \delta n + \frac{\Phi_p}{T} \delta p + \frac{1}{T} \delta u \right) d\Omega =: S_n + S_p + S_u.$$

Considering  $dU$  and  $dS$  for fixed functions  $\delta n$ ,  $\delta p$ ,  $\delta s$ , or  $\delta u$  as functionals of  $n$ ,  $p$  and  $s$  or  $u$ , given in the coordinates  $n$ ,  $p$  and  $T$  we calculate  $d^2U$  and  $d^2S$  in the same way. As the coefficients of  $\delta T$  are different from  $u_{1T}$  or  $s_{1T}$ , we need the assumption  $u_{1T} > 0$ .

For a moment we consider the particular case that the band edges and the effective masses do not depend on  $T$ . In this model case we have  $u_{1T}^B = c_L(T) + \frac{3}{2}(n+p) > 0$ , meanwhile  $0 < u_{1T}^F$  is not so obvious, but it will be proved below in a lemma. In general,  $u_{1T} > 0$  is a reasonable condition on  $\mathcal{N}$  and  $\mathcal{P}$  or on  $N_c$ ,  $E_c$ ,  $N_v$ , and  $E_v$ , i.e. on the dependence of the band edges and of the effective masses from the temperature, since  $u_{1T}$  is the heat capacity of the system.

The calculations are straightforward excepted, maybe, the evaluation of an expression like  $\langle \partial_n \int \frac{V}{T} \delta n, \delta n \rangle$ , which arises in  $\langle \partial_n S_n, \delta n \rangle$ . To explain the result

$$- \langle \partial_n \int \frac{V}{T} \delta n, \delta n \rangle = \int \frac{1}{T} \epsilon (\nabla V_{\delta n})^2 d\Omega + \int_{\Gamma_G} \frac{1}{T} \beta (V_{\delta n})^2 d\Gamma,$$

we consider a differentiable map  $f : X \mapsto Y$  of a Banach space into a Banach space and a linear map  $A_u : Y \mapsto Z$  of  $Y$  into a Banach space ( $u$  might be a parameter from another Banach space). The differential  $df(x)$  of  $f$  and the differential  $dg(x)$  of the composite mapping  $g = A_u \circ f$  for a fixed  $x$  are linear mappings from  $X$  into  $Y$  or  $Z$ , respectively, for which  $\langle dg(x), \delta x \rangle = \langle A_u \circ df(x), \delta x \rangle = \langle A_u, \langle df(x), \delta x \rangle \rangle$  holds. In our case,  $V \in Y$  and  $A_u(V) = \int \frac{\delta n}{T} V d\Omega$ .

We consider  $d^2U(n, p, s; \delta n, \delta p, \delta s)$  as a quadratic form on the real three-dimensional linear space which is spanned by  $\delta n$ ,  $\delta p$  and  $\delta s$ . This form is represented by the  $3 \times 3$

matrix  $\mathbf{U}$ ,

$$\begin{aligned} \mathbf{U} = & \int \frac{1}{s_{1T}} \begin{pmatrix} (s_{1n}\delta n)^2 & s_{1n}\delta n s_{1p}\delta p & -s_{1n}\delta n\delta s \\ s_{1n}\delta n s_{1p}\delta p & (s_{1p}\delta p)^2 & -s_{1p}\delta p\delta s \\ -s_{1n}\delta n\delta s & -s_{1p}\delta p\delta s & (\delta s)^2 \end{pmatrix} d\Omega \\ & + \int \begin{pmatrix} \epsilon(\nabla V_{\delta n})^2 + \frac{T}{n}(\delta n)^2 & -\epsilon\nabla V_{\delta n} \cdot \nabla V_{\delta p} & 0 \\ -\epsilon\nabla V_{\delta p} \cdot \nabla V_{\delta n} & \epsilon(\nabla V_{\delta p})^2 + \frac{T}{p}(\delta p)^2 & 0 \\ 0 & 0 & 0 \end{pmatrix} d\Omega \\ & + \int_{\Gamma_\sigma} \beta \begin{pmatrix} V_{\delta n}^2 & -V_{\delta n}V_{\delta p} & 0 \\ -V_{\delta p}V_{\delta n} & V_{\delta p}^2 & 0 \\ 0 & 0 & 0 \end{pmatrix} d\Gamma. \end{aligned}$$

The matrix  $\mathbf{U}$  has obviously the structure

$$\mathbf{U} = \begin{pmatrix} xx + uu + \xi\xi & xy - uv & -xz \\ xy - uv & yy + vv + \eta\eta & -yz \\ -xz & -yz & zz \end{pmatrix}$$

with three different scalar products  $xy$ ,  $\xi\eta$  and  $uv$ .

$d^2S$  and  $\mathbf{S}$  are calculated quite analogously. The matrix has the same structure with the opposite sign.

The proof will be finished by the following lemma. □

**Lemma 4.1.** *The matrix  $\mathbf{U}$  has nonnegative eigenvalues only.*

*Proof.* The matrix can be considered as a quadratic form on the real three-dimensional linear space spanned by  $\delta n$ ,  $\delta p$ , and  $\delta s$ . Let us consider the restrictions of the quadratic form on each two dimensional subspace.

At first we consider the subspace spanned by  $\delta n \neq 0$  and  $\delta s \neq 0$ . The matrix corresponding to this restriction is

$$\begin{pmatrix} xx + uu + \xi\xi & -xz \\ -xz & zz \end{pmatrix}.$$

Their eigenvalues are positive, since

$$\begin{aligned} 0 &< xx + uu + \xi\xi + zz, \\ 0 &< \frac{1}{4}(xx + uu + \xi\xi - zz)^2 + (xz)^2 \\ &= \frac{1}{4}(xx + uu + \xi\xi + zz)^2 - (xx + uu + \xi\xi)zz + (xz)^2, \\ (xz)^2 &\leq (xx)(zz) < (xx + uu + \xi\xi)zz \\ &= \frac{1}{4}(xx + uu + \xi\xi + zz)^2 - \frac{1}{4}(xx + uu + \xi\xi - zz)^2. \end{aligned}$$

The same argument holds for the subspace spanned by  $\delta p \neq 0$  and  $\delta s \neq 0$ .

Finally we consider subspaces spanned by vectors satisfying

$$a\delta n + b\delta p - \delta s = 0$$

for arbitrary fixed real  $a$  and  $b$ . The matrix corresponding to this restriction is

$$\begin{aligned} & - \begin{pmatrix} xx + uu + \xi\xi - 2axz + a^2zz & xy - uv - ayz - bxz + abzz \\ xy - uv - ayz - bxz + abzz & yy + vv + \eta\eta - 2byz + b^2zz \end{pmatrix} \\ & = - \begin{pmatrix} (x - az, x - az) + uu + \xi\xi & (x - az, y - bz) - uv \\ (x - az, y - bz) - uv & (y - bz, y - bz) + vv + \eta\eta \end{pmatrix}. \end{aligned}$$

Similar arguments as in the first case hold again.  $\square$

*Remark 4.3.* The assertions of the theorem also hold for

$$\tilde{U}(n, p, s) := \int \tilde{u}_1(n, p, T) d\Omega \quad \text{and} \quad \tilde{S}(n, p, \tilde{u}) := \int s_1(n, p, T) d\Omega,$$

$\tilde{u} = \tilde{u}_1(n, p, T) = \tilde{u}^e(p - n) + u_1^i(n, p, T)$ . Using the functions  $\delta u$ ,  $\Phi_n$  and  $\Phi_p$  from above we get

$$d\tilde{U} = \int \delta u + \int_{\Gamma_D} V_D \epsilon \partial_\nu V_{\delta p - \delta n} d\Gamma,$$

$$d\tilde{S}(n, p, \tilde{u}; \delta n, \delta p, \delta u) = dS(n, p, u; \delta n, \delta p, \delta u) + \int_{\Gamma_D} \frac{1}{T} V_D \epsilon \partial_\nu V_{\delta p - \delta n} d\Gamma,$$

but  $d^2\tilde{U} = d^2U$  and  $d^2\tilde{S}(n, p, \tilde{u}) = d^2S(n, p, u)$ .

In the Fermi case the partial derivative  $s_{1T}^F$  of  $s_1^F$  with respect to  $T$  is

$$\begin{aligned} s_{1T}^F &= \frac{1}{T} u_{1T}^F = \frac{c_L \circ T}{T} - n E''_c(T) + p E''_v(T) \\ &+ (TN_c \circ T)'' \mathcal{F}_{3/2} \circ \mathcal{F}_{1/2}^{-1}(n/N_c \circ T) - T \frac{(nN'_c \circ T)^2}{N_c(T)^3} \frac{1}{\mathcal{F}_{-1/2} \circ \mathcal{F}_{1/2}^{-1}(n/N_c \circ T)} \\ &+ (TN_v \circ T)'' \mathcal{F}_{3/2} \circ \mathcal{F}_{1/2}^{-1}(p/N_v \circ T) - T \frac{(pN'_v \circ T)^2}{N_v(T)^3} \frac{1}{\mathcal{F}_{-1/2} \circ \mathcal{F}_{1/2}^{-1}(p/N_v \circ T)}. \end{aligned}$$

In the model case in which the band edges and the effective masses do not depend on  $T$  the inequalities  $s_T^F > 0$  and  $u_T^F > 0$  follow from the next lemma with  $\alpha = 1/2$  and with the argument  $u = \mathcal{F}_{1/2}^{-1}(n/c_n T^{3/2})$ , since

$$\begin{aligned} & \frac{15}{4} \frac{c_n T^{3/2}}{T} \mathcal{F}_{3/2} \circ \mathcal{F}_{1/2}^{-1}(n/c_n T^{3/2}) - \frac{9}{4} \frac{n^2}{c_n T^{5/2}} \frac{1}{\mathcal{F}_{-1/2} \circ \mathcal{F}_{1/2}^{-1}(n/c_n T^{3/2})} \\ &= \frac{9}{4} c_n T^{1/2} \left[ \frac{5}{3} \mathcal{F}_{3/2}(u) - \frac{\mathcal{F}_{1/2}(u)^2}{\mathcal{F}_{-1/2}(u)} \right]. \end{aligned}$$

The proof of the following lemma has been given by my colleague H. Stephan.

**Lemma 4.2.** *The inequality*

$$\left(1 + \frac{1}{\alpha + 1}\right) \mathcal{F}_{\alpha+1} - \frac{\mathcal{F}_\alpha^2}{\mathcal{F}'_\alpha} > 0$$

holds everywhere on the real line for any  $\alpha > -1$ .

*Proof.* Since  $\mathcal{F}'_\alpha > 0$  everywhere on the real line, the inequality is equivalent to

$$G(\alpha + 1)G(\alpha - 1) - G(\alpha)^2 > 0$$

with the function

$$G(\alpha) = (\alpha + 1) \int_0^\infty \frac{t^\alpha}{e^{t-u} + 1} dt = \int_0^\infty \frac{t^{\alpha+1} e^{t-u}}{1 + e^{t-u}} dt = \int dp_\alpha(t).$$

We observe  $G^{(k)}(\alpha) = \int (\log t)^k dp_\alpha(t)$  for the  $k^{\text{th}}$  derivative with respect to  $\alpha$ . The Jensen inequality is applied with the convex function  $x^2$ , i.e.

$$\left[ \int \log t dp_\alpha(t) / \int dp_\alpha(t) \right]^2 < \int (\log t)^2 dp_\alpha(t) / \int dp_\alpha(t),$$

i.e.  $G(\alpha)G''(\alpha) > G'(\alpha)^2$ . The function  $H(\alpha) := \log [G(\alpha)]$  satisfies

$$H''(\alpha) = \frac{1}{G''(\alpha)^2} [G(\alpha)G'''(\alpha) - G'(\alpha)^2] > 0,$$

i.e.

$$\log \left[ \frac{G(\alpha - 1)G(\alpha + 1)}{G(\alpha)^2} \right] > 0,$$

i.e. the assertion.  $\square$

We finish this section with a remark on Fermi integrals. The inequality of the lemma can be written in the form

$$\frac{1}{\alpha + 1} \mathcal{F}_{\alpha+1} \mathcal{F}'_\alpha > \mathcal{F}_\alpha^2 - \mathcal{F}_{\alpha+1} \mathcal{F}'_\alpha = \mathcal{F}_\alpha^2 \left[ \frac{\mathcal{F}_{\alpha+1}}{\mathcal{F}_\alpha} \right]'$$

The sign of the difference on the right-hand side of the inequality is also of interest (cf. [4]).

**Lemma 4.3.** *The inequalities*

$$\frac{\mathcal{F}_\alpha(v)}{\mathcal{F}'_\alpha(v)} > \frac{\mathcal{F}_\alpha(u)}{\mathcal{F}'_\alpha(u)} \quad (u < v)$$

hold for any Fermi integral  $\mathcal{F}_\alpha$ ,  $\alpha > -1$ .

*Proof.* Let us consider the difference

$$\begin{aligned} A &:= (\alpha + 1) e^{-u-v} \int_0^\infty \frac{t^\alpha e^{t-u}}{(1 + e^{t-u})^2} dt \int_0^\infty \frac{t^\alpha e^{t-v}}{(1 + e^{t-v})^2} dt \left[ \frac{\mathcal{F}_\alpha(v)}{\mathcal{F}'_\alpha(v)} - \frac{\mathcal{F}_\alpha(u)}{\mathcal{F}'_\alpha(u)} \right] \\ &= \int_0^\infty \frac{t^\alpha e^t}{(e^u + e^t)^2} dt \int_0^\infty \frac{t^{\alpha+1} e^t}{(e^v + e^t)^2} dt - \int_0^\infty \frac{t^\alpha e^t}{(e^v + e^t)^2} dt \int_0^\infty \frac{t^{\alpha+1} e^t}{(e^u + e^t)^2} dt \\ &= \int [(e^v + e^x)^2 (e^u + e^y)^2 - (e^u + e^x)^2 (e^v + e^y)^2] y d\mu \\ &= (e^v - e^u) \int (e^y - e^x) y d\lambda = (e^v - e^u) \int_{y>x} (e^y - e^x)(y - x) d\lambda > 0 \end{aligned}$$

with the measures

$$d\mu(x, y) = \frac{x^\alpha y^\alpha e^{x+y} dx dy}{(e^u + e^x)^2 (e^u + e^y)^2 (e^v + e^x)^2 (e^v + e^y)^2} = d\mu(y, x)$$

and  $d\lambda(x, y) = [(e^u + e^v)(e^y + e^x) + 2e^{u+v} + 2e^{x+y}] d\mu(x, y)$  on  $R_+^2$ .  $\square$

Since  $\mathcal{F}'_\alpha(u) > 0$  for any  $\alpha > -1$  the concavity of the functions  $\mathcal{F}_\alpha^{-1} \circ \mathcal{F}_{\alpha+1}$  is rigorously proved for any  $\alpha > -1$ .

## 5. A LYAPUNOV FUNCTION FOR THE ENERGY MODEL

In this section a Lyapunov function is constructed for the energy model (4.2) in natural coordinates  $n, p, u$  and  $X_n = \Phi_n/T$ ,  $X_p = \Phi_p/T$ , and  $Y = 1/T$ . To this aim we need the conjugate potential  $H(X_n, X_p, Y)$  of the entropy  $S(n, p, u)$ . A state variable like  $n$  will be denoted by  $n_i$ , if we want to emphasize that it is considered as a function of the intensive state variables  $(X_n, X_p, Y)$ . Sometimes it is more convenient to indicate the dependence of a state variable upon the electrostatic potential separately. The indicator will be the lower index 2, i.e.

$$n = n_i(X_n, X_p, Y) = n_2[X_n, X_p, Y, V_i(X_n, X_p, Y)],$$

where  $V_i(\cdot) \in H_0^1$  denotes the solution of the nonlinear Poisson equation

$$(5.1) \quad \int \epsilon \nabla W \cdot \nabla \chi d\Omega + \int_{\Gamma_G} \beta W \chi d\Gamma = \int [p_2(\cdot, W) - n_2(\cdot, W)] \chi d\Omega \quad (\chi \in H_0^1).$$

*Remark 5.1.* Let  $(H_0^1)'$  denote the dual space of  $H_0^1$  and let  $\mathbf{X}$  and  $\mathbf{Y}$  denote unspecified function spaces of either  $X_n$  or  $X_p$  and  $Y$ . The nonlinear operators  $P_2(X_n, X_p, Y, \cdot) : H_0^1 \mapsto (H_0^1)'$  defined by

$$\langle P_2(\cdot, W), \chi \rangle = \int \{ \epsilon \nabla W \cdot \nabla \chi d\Omega + [n_2(\cdot, W) - p_2(\cdot, W)] \chi \} d\Omega + \int_{\Gamma_G} \beta W \chi d\Gamma$$

are strongly monotone operators. The nice properties also appear in the linearized equations. The coefficient of the additional term on the left-hand side in each equation is a nonnegative function.

*Remark 5.2.* Let  $\mathcal{P}_i \subset \mathbf{X} \times \mathbf{X} \times \mathbf{Y} \times H_0^1$  denote the manifold of zeros of the map  $P_2 : \mathbf{X} \times \mathbf{X} \times \mathbf{Y} \times H_0^1 \mapsto (H_0^1)'$ . The projection  $\pi_i : \mathcal{P}_i \mapsto \mathbf{X} \times \mathbf{X} \times \mathbf{Y}$  is a chart map of the manifold and  $H_i = H_2 \circ \pi_i^{-1}$ .

Because of the identities

$$\partial_n s(n, p, u) = -X_n, \quad \partial_p s(n, p, u) = X_p \quad \text{and} \quad \partial_u s(n, p, u) = Y$$

the density of the conjugate potential  $H$  of  $S$  is defined by

$$h_0 = -nX_n + pX_p + uY - s = -nX_n + pX_p + f/T ,$$

$$h^B = -n_i^B - p_i^B + Yf_L(1/Y) + h^e ,$$

$$\begin{aligned} h^F &= -N_c(1/Y)\mathcal{F}_{3/2}[X_n + Y(V^* + V_i - E_c(1/Y))] \\ &\quad - N_v(1/Y)\mathcal{F}_{3/2}[-X_p - Y(V^* + V_i - E_v(1/Y))] \\ &\quad + Yf_L(1/Y) + h^e , \end{aligned}$$

$$h^e = Y \left[ \frac{1}{2}\epsilon(\nabla V_i)^2 + \frac{1}{2}\beta V_i^2 \delta_{\Gamma_G} - (p_i - n_i)V_i \right] .$$

Note that  $h^e$  also differs in both the cases  $B$  and  $F$  like  $n_i$ ,  $p_i$  and also  $V_i$  do.

We want to check the relations

$$\langle \partial_{X_n} H, \delta X_n \rangle = - \int n \delta X_n d\Omega, \quad \dots, \quad \langle \partial_Y H, \delta Y \rangle = \int u \delta Y d\Omega .$$

We start with the identities

$$\langle \partial_\alpha H, \delta \alpha \rangle = \int \delta \alpha \partial_\alpha h_2[\cdot, V_i(\cdot)] d\Omega + \int \langle \partial_\alpha V_i, \delta \alpha \rangle \partial_{V_i} h_2[\cdot, V_i(\cdot)] d\Omega$$

( $\alpha \in \{X_n, X_p, Y\}$ ). The function

$$\langle \partial_\alpha V_i, \delta \alpha \rangle =: \delta_\alpha V_i(X_n, X_p, Y)$$

in  $H_0^1$  is the solution of the linearized Poisson equation

$$\begin{aligned} \int [\epsilon \nabla W \cdot \nabla \chi + W \partial_{V_i}(n_2 - p_2) \chi] d\Omega + \int_{\Gamma_G} \beta W \chi d\Gamma \\ (5.2) \quad \quad \quad = \int \delta \alpha \partial_\alpha (p_2 - n_2) \chi d\Omega \quad (\chi \in H_0^1). \end{aligned}$$

Let us consider  $\langle \partial_W H_2(\cdot, W), \delta W \rangle$ . Since

$$\int \delta W \partial_W [n_2^B(\cdot, W) + p_2^B(\cdot, W)] d\Omega = \int \delta W Y [n_2^B(\cdot, W) - p_2^B(\cdot, W)] d\Omega$$

and

$$\begin{aligned} \int \delta W \partial_W [N_c \mathcal{F}_{3/2}(YW + \dots) + N_v \mathcal{F}_{3/2}(-YW - \dots)] d\Omega \\ = \int \delta W Y [n_2^F(\cdot, W) - p_2^F(\cdot, W)] d\Omega, \end{aligned}$$

the identity

$$\begin{aligned} \langle \partial_W H_2(\cdot, W), \delta W \rangle &= \int_{\Gamma_G} Y \beta W \delta W d\Gamma \\ &\quad + \int Y \{ \epsilon \nabla \delta W \cdot \nabla W - \delta W \partial_W [n_2(\cdot, W) - p_2(\cdot, W)] W \} d\Omega \end{aligned}$$



holds. The key of the proof is to understand that the variations  $\delta_\alpha V_i$ , which are solutions of (5.2) also satisfy

$$\langle \partial_{V_i} H_2(\cdot, V_i), \delta_\alpha V_i \rangle = \int Y \delta_\alpha \partial_\alpha [n_2(\cdot, V_i) - p_2(\cdot, V_i)] V_i d\Omega$$

because of  $H = H_2 \circ \pi_i^{-1}$  lives on the manifold  $\mathcal{P}_i$ . Then the relations follow easily from

$$\langle \partial_\alpha H, \delta_\alpha \rangle = \int \delta_\alpha \{ \partial_\alpha h_2[\cdot, V_i(\cdot)] + Y \partial_\alpha [n_2(\cdot, V_i) - p_2(\cdot, V_i)] V_i \} d\Omega.$$

*Remark 5.3.* We had to learn to deal with mappings into function spaces  $\mathbf{Z} \oplus \mathbf{Z}_\Gamma$  living on the domain  $\Omega$  as well as on a part of the boundary. The same situation occurs, of course, with the generalized energy density  $u$ . The same situation also occurs, if we start with the energy density  $\tilde{u} = u^i + \tilde{u}^e$ . We know from section 2 and from the third remark in section 4 that

$$\langle \partial_n \tilde{U}, \delta n \rangle = \int \Phi_n \delta n - \int_{\Gamma_D} V_D \epsilon \partial_\nu V \delta n d\Gamma.$$

In the case of the energy density  $\tilde{u}$  the corresponding electro-chemical potential  $\tilde{\Phi}_n$  is a functional living partially on a part of the boundary. This construction looks rather formally, of course, and one might be inclined to stick to the state variable  $\Phi_n$ . Doing so, however, the thermodynamic calculus is left.

According to our definition of  $\Phi_n$ ,  $\Phi_p$  and  $T$  the equilibrium state of our system is

$$\bar{\Phi}_n = \bar{\Phi}_p = 0, \quad \bar{T} = 1, \quad \text{or} \quad \bar{X}_n = \bar{X}_p = 0, \quad \bar{Y} = 1.$$

The electrostatic potential of the system in the equilibrium state is  $\bar{V} = V^* + \bar{V}_i$  with the solution  $\bar{V}_i$  of the nonlinear Poisson equation

$$\begin{aligned} \int \epsilon \nabla W \cdot \nabla \chi d\Omega + \int_{\Gamma_G} \beta W \chi d\Gamma &= \int [p_2(\cdot, W) - n_2(\cdot, W)] \chi d\Omega \\ &= \int [\bar{p}_2(\cdot, W) - \bar{n}_2(\cdot, W)] \chi d\Omega \end{aligned}$$

( $\chi \in H_0^1$ ). Note that  $\bar{V} = \bar{V}^C$  are different in the cases  $C = B$  or  $F$ .

For boundary values of  $X_n$ ,  $X_p$  and of  $Y$  on  $\Gamma_D$  which are compatible with the equilibrium state we set

$$\begin{aligned} \bar{S}_-(n, p, u) &:= \int [n(X_n - \bar{X}_n) - p(X_p - \bar{X}_p) - u(Y - \bar{Y})] d\Omega \\ &\quad + H(X_n, X_p, Y) - H(\bar{X}_n, \bar{X}_p, \bar{Y}). \end{aligned}$$

This functional is nonnegative and convex. If a solution of the system (4.2) satisfies boundary values on  $\Gamma_D$  which are compatible with the equilibrium state then the

estimate

$$\begin{aligned}
& \frac{d}{dt} \{ \bar{S}_-[n(t), p(t), u(t)] \} \\
&= \int \{ \dot{n}(t)[X_n(t) - \bar{X}_n] - \dot{p}(t)[X_p(t) - \bar{X}_p] - \dot{u}(t)[Y(t) - \bar{Y}] \} d\Omega \\
&= \int \{ j_n \cdot \nabla [X_n(t) - \bar{X}_n] - R[t][X_n(t) - \bar{X}_n] - j_p \cdot \nabla [X_p(t) - \bar{X}_p] \\
&\quad + R[t][X_p(t) - \bar{X}_p] - j_u \cdot \nabla [Y(t) - \bar{Y}] \} d\Omega \\
&= - \int \nabla \begin{pmatrix} -[X_n(t) - \bar{X}_n] \\ X_p(t) - \bar{X}_p \\ Y(t) - \bar{Y} \end{pmatrix} \cdot \mathbf{D} \nabla \begin{pmatrix} -[X_n(t) - \bar{X}_n] \\ X_p(t) - \bar{X}_p \\ Y(t) - \bar{Y} \end{pmatrix} d\Omega \\
&\quad - \int R[t][X_n(t) - \bar{X}_n - X_p(t) + \bar{X}_p] d\Omega \leq 0
\end{aligned}$$

is fulfilled. Here we used the properties  $\nabla X_n(t) = \nabla [X_n(t) - \bar{X}_n]$  and  $X_n(t) - \bar{X}_n \in H_0^1$  etc. The total dissipation rate on the right-hand side is the sum  $D = D_f + D_r$  of the dissipation rate  $D_f$  due to the flux and of that one due to the generation and recombination of carriers. The density  $R[t][X_n(t) - \bar{X}_n - X_p(t) + \bar{X}_p]$  of  $D_r$  already appeared in the entropy balance equation. It denotes the entropy production rate due to the recombination and generation of electrons and holes. Therefore the term has to be nonnegative. This property is easily proved in the Boltzmann case for typical net recombination rates like  $R = R_0(np - \mathcal{N}\mathcal{P})$ . At least, if this net recombination rate is written in the form  $R = \mathcal{R}(\exp(X_n - X_p) - 1)$  it has the property in the Fermi case, too.

The right-hand side of the estimate is the negative sum of the dissipation rates due to the fluxes and due to the recombination or generation of carriers. The estimate can also be written in the form

$$(5.3) \quad \bar{S}_-[n(t), p(t), u(t)] \leq \bar{S}_-[n(0), p(0), u(0)] - \int_0^t D[n(\tau), p(\tau), u(\tau)] d\tau.$$

The functional  $\bar{S}_-$  can also be used in the case of time discretization. Let  $t_0 = 0 < t_1 < \dots < t_K$  be given. Let denote  $\tau_k = 1/(t_k - t_{k-1})$  and  $\tau := \tau_k(t - t_{k-1})$ . We consider the system of equations

$$(5.4) \quad \begin{aligned} \tau_k(n_k - n_{k-1}) + \nabla \cdot j_n^k &= -R^k \\ \tau_k(p_k - p_{k-1}) + \nabla \cdot j_p^k &= -R^k \\ \tau_k(u_k - u_{k-1}) + \nabla \cdot j_u^k &= 0 \end{aligned}$$

for  $0 < k \leq K$  with given initial data  $n_0, p_0$  and  $u_0$  and with the current densities

$$(5.5) \quad \begin{pmatrix} j_n^k \\ j_p^k \\ j_u^k \end{pmatrix} = \mathbf{D}^k \nabla \begin{pmatrix} -(X_n)_k \\ (X_p)_k \\ Y_k \end{pmatrix}.$$

The unknown new values  $(X_n)_k, \dots, u_k$  are used as much as possible in the coefficients  $\mathbf{D}^k$  and right-hand sides  $R^k$  of the equations, but we will be forced to use the already

known values  $(X_n)_{k-1}, \dots, u_{k-1}$  in much places. We interpolate the densities  $n, p$  and  $u$  linearly, i.e.  $\tilde{n}(t) = n_{k-1} + \tau(n_k - n_{k-1}) \equiv n_{k-1} + \tau\Delta_k n$  etc on the interval  $S_k = ]t_{k-1}, t_k]$ . From these state variables we obtain the other ones like  $\tilde{Y}$  by the state equations (if we need these values at all!). We get, in particular,  $\tilde{S}_-[\tilde{n}(t), \tilde{p}(t), \tilde{u}(t)]$ . This function satisfies

$$\begin{aligned} & \frac{d}{dt} \{ \tilde{S}_-[\tilde{n}(t), \tilde{p}(t), \tilde{u}(t)] \} \\ &= \tau_k \int \{ \Delta_k n [\tilde{X}_n(t) - \bar{X}_n] - \Delta_k p [\tilde{X}_p(t) - \bar{X}_p] - \Delta_k u [\tilde{Y}(t) - \bar{Y}] \} d\Omega \\ &\leq \tau_k \int \{ \Delta_k n [(X_n)_k - \bar{X}_n] - \Delta_k p [(X_p)_k - \bar{X}_p] - \Delta_k u [Y_k - \bar{Y}] \} d\Omega \\ &= \int \{ j_n^k \cdot \nabla [(X_n)_k - \bar{X}_n] - R^k [(X_n)_k - \bar{X}_n] - j_p^k \cdot \nabla [(X_p)_k - \bar{X}_p] \\ &\quad + R^k [(X_p)_k - \bar{X}_p] - j_u^k \cdot \nabla [Y_k - \bar{Y}] \} d\Omega =: -D_f^k - D_r^k \leq 0. \end{aligned}$$

The first estimate is proved by a convexity argument, namely

$$\tilde{n}(t) - n_k = (\tau - 1)\Delta_k n$$

and thus

$$\begin{aligned} & \tau_k \int \{ \Delta_k n [\tilde{X}_n(t) - (X_n)_k] - \Delta_k p [\tilde{X}_p(t) - (X_p)_k] - \Delta_k u [\tilde{Y}(t) - Y_k] \} d\Omega \\ &= -\frac{\tau_k}{1-\tau} \int \{ [\tilde{n}(t) - n_k][\tilde{X}_n(t) - \bar{X}_n] - [\tilde{p}(t) - p_k][\tilde{X}_p(t) - \bar{X}_p] \\ &\quad - [\tilde{u}(t) - u_k][\tilde{Y}(t) - \bar{Y}] \} d\Omega \\ &= \frac{\tau_k}{1-\tau} \{ \langle \partial_{X_n} \tilde{H}[t] - \partial_{X_n} H^k, \tilde{X}_n(t) - \bar{X}_n \rangle + \langle \partial_{X_p} \tilde{H}[t] - \partial_{X_p} H^k, \tilde{X}_p(t) - \bar{X}_p \rangle \\ &\quad + \langle \partial_Y \tilde{H}[t] - \partial_Y H^k, \tilde{Y}(t) - \bar{Y} \rangle \} \leq 0, \end{aligned}$$

since the conjugate potential  $H$  of the concave potential  $S$  is also concave.

The estimates for  $\tilde{S}_-[t]$  and their discrete analogue are of interest in so far as they show that the mathematical model reflects the stability of the equilibrium state in some way. Initial-boundary value problems for (4.2) with Dirichlet data  $(\tilde{X}_n, \tilde{X}_p, \tilde{Y}) \neq (\bar{X}_n, \bar{X}_p, \bar{Y})$  are more realistic. In this case, the functional

$$\begin{aligned} \tilde{S}_-(n, p, u) &:= \int \left[ n(X_n - \tilde{X}_n) - p(X_p - \tilde{X}_p) - u(Y - \tilde{Y}) \right] d\Omega \\ &\quad + H(X_n, X_p, Y) - H(\tilde{X}_n, \tilde{X}_p, \tilde{Y}) \end{aligned}$$

satisfies the estimate

$$\begin{aligned}
& \frac{d}{dt} \{ \tilde{S}_- [n(t), p(t), u(t)] \} \\
&= \int \{ \dot{n}(t) [X_n(t) - \tilde{X}_n] - \dot{p}(t) [X_p(t) - \tilde{X}_p] - \dot{u}(t) [Y(t) - \tilde{Y}] \} d\Omega \\
&= \int \{ j_n \cdot \nabla [X_n(t) - \tilde{X}_n] - R[t] [X_n(t) - \tilde{X}_n] - j_p \cdot \nabla [X_p(t) - \tilde{X}_p] \\
&\quad + R[t] [X_p(t) - \tilde{X}_p] - j_u \cdot \nabla [Y(t) - \tilde{Y}] \} d\Omega \\
&= - \int \nabla \begin{pmatrix} -[X_n(t) - \tilde{X}_n] \\ X_p(t) - \tilde{X}_p \\ Y(t) - \tilde{Y} \end{pmatrix} \cdot \mathbf{D} \nabla \begin{pmatrix} -[X_n(t) - \tilde{X}_n] \\ X_p(t) - \tilde{X}_p \\ Y(t) - \tilde{Y} \end{pmatrix} d\Omega \\
&\quad - \int R[t] [X_n(t) - \tilde{X}_n - X_p(t) + \tilde{X}_p] d\Omega \\
&= - \int \nabla \begin{pmatrix} -[X_n(t) - \tilde{X}_n] \\ X_p(t) - \tilde{X}_p \\ Y(t) - \tilde{Y} \end{pmatrix} \cdot \mathbf{D} \nabla \begin{pmatrix} -\tilde{X}_n \\ \tilde{X}_p \\ \tilde{Y} \end{pmatrix} d\Omega \\
&\quad + \int R[t] [\tilde{X}_n(t) - \tilde{X}_n - \tilde{X}_p(t) + \tilde{X}_p] d\Omega.
\end{aligned}$$

The additional last term on the right-hand side is not definite in general, but linear in the gradients of  $\tilde{X}_n$  etc. Thus one can try to get an estimate for it by the dissipation rate. The chances that such an estimate hold are not so bad if the stationary problem with the boundary values  $(\tilde{X}_n, \tilde{X}_p, \tilde{Y})$  on  $\Gamma_D$  has an unique solution and if  $(\tilde{X}_n, \tilde{X}_p, \tilde{Y})$  is just this solution.

*Remark 5.4.* The Scharfetter-Gummel procedure, which has been successfully applied in the drift-diffusion model, has an analogue for the system (5.4) coupled with (5.1): The whole system at time  $t_k$  can iteratively be solved, solving (5.4) with the state equations  $n = n_2(X_n, Y, W_0)$  etc with frozen electrostatic potential in a first part of one iteration step, but (5.1) with the new values of  $X_n, X_p, Y$  in a second part.

## 6. SPATIAL DISCRETIZATION OF THE ENERGY MODEL DISCRETIZED IN TIME

We apply a box method to discretize the system of equations (5.4), (5.5) spatially. We consider a triangulation  $\mathcal{S}$  of the domain  $\Omega$  with the grid points  $\mathbf{r}_1, \dots, \mathbf{r}_N$ . Let  $\mathcal{S}_n$  ( $1 \leq n \leq N$ ) denote the ordered set simplices  $S^m \in \mathcal{S}$  which have one of their corners in  $\mathbf{r}_n$ . Let  $\mathcal{R}_n$  denote the set of all neighbours  $\mathbf{r}_l$ , i.e. the finite line from  $\mathbf{r}_n$  to  $\mathbf{r}_l$  is the edge of a simplex of the triangulation. Let

$$B^n := \{ \mathbf{r} \in \Omega : |\mathbf{r} - \mathbf{r}_n| = \min_{l=1}^N |\mathbf{r} - \mathbf{r}_l| \}$$

denote the box or Voronoi cell around  $\mathbf{r}_n$ . If the triangulation is sufficient regular (cf Delaunay property) the boundary  $\partial B^n$  consist of plane parts  $A_n^l$  such that  $\mathbf{r}_l - \mathbf{r}_n = d_{nl} \mathbf{n}_n^l$  with the exterior normal unit vector on  $A_n^l$  ( $\mathbf{r}_l \in \mathcal{R}_n$ ). For a density  $u$  on  $\Omega$  we set  $U^n = \int_{B^n} u d\Omega$ . Thus we get

$$\tau_k(U_k^n - U_{k-1}^n) = - \int_{B^n} \nabla \cdot \mathbf{j}_u^k d\Omega = - \sum_{\mathcal{R}_n} \int_{A_n^l} \mathbf{n}_n^l \cdot \mathbf{j}_u^k dA \approx \sum_{\mathcal{R}_n} d_{nl} I_u^k(nl).$$

for the last equation of the system (5.4). We need an expression for the current  $I_u^k(nl)$  in the edge from  $\mathbf{r}_n$  to  $\mathbf{r}_l$  during the  $k$ -th time step.

The one-dimensional current equation corresponding to (5.5) reads

$$\begin{aligned} aX_n' &+ rY' = I_n \\ bX_p' &+ sY' = I_p \\ rX_n' + sX_p' &+ cY' = I_u \end{aligned}$$

with constant right-hand sides. A rough approximation arises if the coefficients  $f$  are substituted by the average  $\bar{f}^{k-1} \equiv \frac{1}{2}(f_n^{k-1} + f_l^{k-1})$  of their values in the endpoints of the edge at the time  $t_{k-1}$ . A more refined approximation arises if the coefficients are considered as affine functions  $f(x) = f_n + f'x$  ( $0 < x, \Delta l$ ) on the edge. The full program

$$\begin{pmatrix} \Delta X_n \\ \Delta X_p \\ \Delta Y \end{pmatrix} = \int_0^l \frac{1}{abc - as^2 - br^2} \begin{pmatrix} bc - s^2 & rs & -br \\ rs & ac - r^2 & -as \\ -br & -as & ab \end{pmatrix} dx \cdot \begin{pmatrix} I_n \\ I_p \\ I_u \end{pmatrix},$$

however, will be too expensive. A lot of compromises can be suggested. Above all, coefficients with  $|f_n - f_l| \ll \bar{f}$  should be substituted by  $\bar{f}$ .

The coefficients of the spatially discretized thermodynamic forces  $\Delta X_n$  are state variables, which depend on the state variables in the endpoints of the edge. We have the possibility to choose the old values or the new unknown ones. A good choice will be characterized by the properties that the new values are taken as often as possible, but that the equations, which become nonlinear if unknown new values are regarded in the coefficients, have still a good behaviour. Summarizing all box balance equations we get a finite system of equations

$$\tau_k \begin{pmatrix} N_k - N_{k-1} \\ P_k - P_{k-1} \\ U_k - U_{k-1} \end{pmatrix} + \tilde{\mathbf{D}}^k \begin{pmatrix} -(X_n)_k \\ (X_p)_k \\ Y_k \end{pmatrix} = \begin{pmatrix} -\tilde{R}^k \\ -\tilde{R}^k \\ 0 \end{pmatrix}$$

( $0 < k \leq K$ ) for the grid vectors  $N_k, \dots, Y_k$  with given initial data  $N_0, P_0$  and  $U_0$ . This system has to be completed by the discretized Poisson equation

$$(6.1) \quad \mathbf{PW} = \mathbf{P} - \mathbf{N}$$

at each time step  $k$  and by state equations for  $N, P$  and  $U$ .

For grid vectors  $W = (W^n), Y$  with  $Y^n > 0$  and  $Z$  let  $(W, Z), W * Z$  and  $W/Y$  denote, respectively, the scalar product  $\sum_n W^n Z^n$  and the grid vectors with the components  $W^n Z^n$  or  $W^n/Y^n$ . Note that densities and functions have to be discretized. Accordingly, the discretized objects are extensive grid vectors like  $N$  or intensive ones like  $T$  or  $n \equiv N/|B|$ . The natural pairing is the scalar product of an intensive grid vector and an extensive one. For functions from the preceding

sections like  $p_2$  or  $u_1^i$  let  $p := p_2(X_p, Y, W)$  or  $u_1^i(n, p, T)$  denote the grid vectors with the components  $p_2(X_p^n, Y^n, W^n)$  or  $u_1^i(n^n, p^n, T^n)$  such that, e.g.,

$$N = |B| * n_2[X_n, Y, V_i(X_n, X_p, Y)],$$

where  $V_i$  denotes the solution of the discretized nonlinear Poisson equation

$$\mathbf{P}W = |B| * [p_2(X_p, Y, W) - n_2(X_n, Y, W)].$$

The discretized electrostatic energy is defined by

$$\mathcal{U}^e(p - n) = (V^*, P - N) + \frac{1}{2}(V_{p-n}, \mathbf{P}V_{p-n}),$$

where  $V_{p-n}$  denotes the solution  $W = \mathbf{P}^{-1}(P - N)$  of the Poisson equation (6.1), i.e.

$$\mathcal{U}^e(p - n) = (V^*, P - N) + \frac{1}{2}(P - N, \mathbf{P}^{-1}(P - N)),$$

and

$$u^e(p - n) = V^* * (p - n) + \frac{1}{2}(p - n) * \mathbf{P}^{-1}[|B| * (p - n)].$$

Under these conventions the identities

$$\langle d\mathcal{S}_1(n, p, T), \delta n \oplus \delta p \oplus \delta T \rangle = (\partial_n s_1, \delta N) + (\partial_p s_1, \delta P) + (|B|, \partial_T s_1 * \delta T),$$

$$\delta T = [\delta u - V * (\delta p - \delta n) - \partial_n u_1^i * \delta n - \partial_p u_1^i * \delta p] / \partial_T u_1^i,$$

and

$$\partial_T u_1^i = \partial_T u_1 = \partial_T (f - T \partial_T f) = -T \partial_T^2 f = T \partial_T s_1$$

hold. Thus we get

$$\begin{aligned} \langle d\mathcal{S}(n, p, u), \delta n \oplus \delta p \oplus \delta u \rangle &= (1/T, \delta U) + \\ &(\partial_n s_1 - (\partial_n u_1^i - V)/T, \delta N) + (\partial_p s_1 - (\partial_p u_1^i + V)/T, \delta P) \\ &= (-X_n, \delta N) + (X_p, \delta P) + (Y, \delta U). \end{aligned}$$

In the Boltzmann case, e.g.,

$$\begin{aligned} X_n &= \log \left[ \frac{n}{\mathcal{N}(T)} \right] - [V^* + \mathbf{P}^{-1}(P - N)]/T, \quad \dots \\ \delta T/T &= [\delta u/T - \delta n * a_n - \delta p * a_p] / \partial_T u_1^{iB}, \end{aligned}$$

with

$$a_n = T * \mathcal{N}'(T)/\mathcal{N}(T) - V/T \quad \text{and} \quad a_p = T * \mathcal{P}'(T)/\mathcal{P}(T) + V/T.$$

Therefore we have

$$\begin{aligned} &\langle d\{-\log[n/\mathcal{N}(T)], \delta N\} + (V^* + \mathbf{P}^{-1}(P - N), \delta N/T) \\ &\quad - \log[p/\mathcal{P}(T)], \delta P\} - (V^* + \mathbf{P}^{-1}(P - N), \delta P/T) + (1/T, \delta U) \rangle, \delta n \oplus \delta p \oplus \delta T \\ &= -(\delta N, \delta n/n) + (\mathbf{P}^{-1}(\delta P - \delta N), \delta n/T) + (\delta T/T, a_n * \delta N) \\ &\quad - (\delta P, \delta p/p) - (\mathbf{P}^{-1}(\delta P - \delta N), \delta p/T) + (\delta T/T, a_p * \delta P) - (\delta T/T, \delta U/T), \end{aligned}$$

i.e.

$$\begin{aligned} d^2 \mathcal{S}^B(n, p, u; \delta n, \delta p, \delta u) \\ = - (|B|, \delta n * \delta n/n + \delta p * \delta p/p) - (\mathbf{P}^{-1}(\delta P - \delta N), (\delta P - \delta N)/(T * |B|)) \\ - (|B|/\partial_T u_1^{iB}, (\delta n \ \delta p \ \delta u/T) * \mathbf{S}^B * (\delta n \ \delta p \ \delta u/T)') \end{aligned}$$

with the matrix

$$\mathbf{S}^B = \begin{pmatrix} a_n * a_n & a_n * a_p & -a_n \\ a_n * a_p & a_p * a_p & -a_p \\ -a_n & -a_p & 1 \end{pmatrix}.$$

The conjugate potential

$$\mathcal{H}(X_n, X_p, Y) := -(X_n, N) + (X_p, P) + (Y, U) - \mathcal{S}(n, p, u)$$

reads in the Boltzmann case, e.g.,

$$\begin{aligned} \mathcal{H}^B(X_n, X_p, Y) := (F_L(1/Y), Y) - (1, P_2^B[X_p, Y, V_i] + N_2^B[X_n, Y, V_i]) \\ - \frac{1}{2} (P_2^B[X_p, Y, V_i] - N_2^B[X_n, Y, V_i], V_i/Y). \end{aligned}$$

The discrete analogue

$$\begin{aligned} \bar{\mathcal{S}}_-(n, p, u) := (N, X_n - \bar{X}_n) - (P, X_p - \bar{X}_p)(U, Y - \bar{Y}) \\ + \mathcal{H}(X_n, X_p, Y) - \mathcal{H}(\bar{X}_n, \bar{X}_p, \bar{Y}) \end{aligned}$$

is a Lyapunov function for the problem discretized in time and space. The arguments are completely analogous, such that we do not repeat them here. The spatial discretization and the whole calculus can also be applied with continuous time.

## 7. GENERAL DISPERSION

The case  $C = G$  of general dispersions  $\omega_b(x, p, T)$  ( $b = c, v$ ) is a little bit more complicate. In this case, we will not write down the full program, but we only proof the convexity of the potential  $U(n, p, s)$ . We consider also the conjugate potential  $G(\Phi_n, \Phi_p, T)$ , which is also convex. We are surprised that  $d^2G$  is the difference of two semidefinite forms, meanwhile  $d^2U$  is a sum of semidefinite forms as in the cases  $B$  and  $F$ .

We assume that the Lebesgue measure of the surfaces  $\omega_b(x, \cdot, T) = \omega$  in the momentum space are finite, i.e.

$$a_b(\omega, T) \equiv a_b(x, \omega, T) := \int_{\omega_b(x, p, T) = \omega} d\sigma(p) < \infty.$$

It will be convenient to introduce the chemical potentials  $Y_b = \Phi_b + V \equiv \Phi_b + V^* + V_l^G$  ( $b = n, p$ ) and to abbreviate  $z_n \equiv \frac{1}{T}(Y_n - E_c - \omega)$ ,  $z_p \equiv \frac{1}{T}(Y_p - E_v + \omega)$ . The carrier

densities are

$$n = n_l^G(\Phi_n, \Phi_p, T) = n_3^G[\Phi_n, T, V_l^G(\Phi_n, \Phi_p, T)] = n^G(Y_n, T),$$

$$p = p_l^G(\Phi_n, \Phi_p, T) = p_3^G[\Phi_p, T, V_l^G(\Phi_n, \Phi_p, T)] = p^G(Y_p, T)$$

with

$$n^G(Y_n, T) = \int_0^\infty \frac{a_c(\omega, T)}{1 + \exp[-\frac{1}{T}(Y_n - E_c - \omega)]} d\omega,$$

$$p^G(Y_p, T) = \int_0^\infty \frac{a_v(\omega, T)}{1 + \exp[\frac{1}{T}(Y_p - E_v + \omega)]} d\omega,$$

where  $V_l^G$  is the solution of the nonlinear Poisson equation

$$\begin{aligned} \int \epsilon \nabla W \cdot \nabla \chi \, d\Omega + \int_{\Gamma_G} \beta W \chi \, d\Gamma \\ = \int [p_3^G(\Phi_p, T, W) - n_3^G(\Phi_n, T, W)] \chi \, d\Omega \end{aligned}$$

( $\chi \in H_0^1$ ) in  $H_0^1$ . The expression

$$f^G(n, p, T) := f_L(T) + \Omega_n + Y_n n + \Omega_p - Y_p p + u^e(p^G - n^G)$$

with these  $Y_n, Y_p, V$  and with the quantities

$$\Omega_n(Y_n, T) = -T \int_0^\infty a_c(\omega, T) \log [1 + \exp \frac{1}{T}(Y_n - E_c - \omega)] d\omega$$

and

$$\Omega_p(Y_p, T) = -T \int_0^\infty a_v(\omega, T) \log [1 + \exp \frac{-1}{T}(Y_p - E_v + \omega)] d\omega$$

is the density of the free energy.

We notice that the potential  $V$  is fixed for fixed  $n$  and  $p$ . Thus the density of entropy  $s$  is defined by

$$\begin{aligned} \partial_T f^G(n, p, T) &= f_L'(T) + \partial_T \Omega_n + \partial_{Y_n} \Omega_n \cdot (\partial_T Y_n)_{n,p} + n(\partial_T Y_n)_{n,p} \\ &\quad + \partial_T \Omega_{p3} + \partial_{Y_p} \Omega_{p3} \cdot (\partial_T Y_p)_{n,p} - p(\partial_T Y_p)_{n,p} \\ &= f_L'(T) + \partial_T \Omega_n(Y_n, T) + \partial_T \Omega_p(Y_p, T) = -s^G(Y_n, Y_p, T). \end{aligned}$$



The density  $u$  of the total energy is given by

$$\begin{aligned}
u(n, p, s) &= f(n, p, T) - T \partial_T f(n, p, T) = u^e(p - n) + f_L(T) - T f'_L(T) \\
&+ \Omega_n(Y_n, T) - T \partial_T \Omega_n(Y_n, T) + Y_n n^G(Y_n, T) \\
&+ \Omega_p(Y_p, T) - T \partial_T \Omega_p(Y_p, T) - Y_p p^G(Y_p, T) \\
&\equiv u^e(p^G - n^G) + u^{iG}(Y_n, Y_p, T) := u^e(p^G - n^G) + \int^T c_L \\
&+ T^2 \int_0^\infty \log(1 + e^{z_n}) \partial_T a_c(\omega, T) d\omega + \int_0^\infty \frac{Y_n - T(z_n + E'_c)}{1 + e^{-z_n}} a_c(\omega, T) d\omega \\
&+ T^2 \int_0^\infty \log(1 + e^{-z_p}) \partial_T a_v(\omega, T) d\omega - \int_0^\infty \frac{Y_p - T(z_p + E'_v)}{1 + e^{z_p}} a_v(\omega, T) d\omega
\end{aligned}$$

The partial derivatives of the functional  $U(n, p, s)$  are calculated with the partial derivatives of

$$u^G(Y_n, Y_p, T) = u^e [p^G(Y_n, T) - n^G(Y_n, T)] + u^{iG}(Y_n, Y_p, T)$$

by solving the linear system of differentials

$$\begin{aligned}
n^G Y_n dY_n &+ n^G_T dT = dn, \\
p^G_{Y_p} dY_p + p^G_T dT &= dp, \\
s^G_{Y_n} dY_n + s^G_{Y_p} dY_p + s^G_T dT &= ds.
\end{aligned}$$

The system is solvable if and only if its coefficient determinant

$$\mathcal{D} := n^G_{Y_n} [p^G_{Y_p} s^G_T - p^G_T s^G_{Y_p}] - n^G_T p^G_{Y_p} s^G_{Y_n} \neq 0.$$

It is convenient to introduce the measures

$$d\mu_b(\omega) = \frac{e^{-\delta_b z_b}}{[1 + e^{-\delta_b z_b}]^2} a_b(\omega, T) d\omega$$

( $\delta_c = 1$ , but  $\delta_v = -1$ ) and the notation

$$M_b^{(k)} = \int (z_{n_b} + \partial_T E_b)^k d\mu_b, \quad M_b = M_b^{(0)}, \quad M'_b = M_b^{(1)}, \quad M_b'' = M_b^{(2)},$$

$$\mathcal{M}'_b = M'_b - \delta_b T \int_0^\infty \frac{\partial_T a_b(\omega, T)}{1 + e^{-\delta_b z_{n_b}}} d\omega,$$

$$\begin{aligned}
\mathcal{M}_b'' &= M_b'' - T \int_0^\infty \frac{2(z_{n_b} + \partial_T E_b) \partial_T a_b(\omega, T) + a_c(\omega, T) \partial_T^2 E_b}{1 + e^{-\delta_b z_{n_b}}} d\omega \\
&+ T \int_0^\infty \log(1 + e^{\delta_b z_{n_b}}) [2 \partial_T a_b(\omega, T) + T \partial_T^2 a_b(\omega, T)] d\omega.
\end{aligned}$$

In the model case in which neither  $a_b(\omega)$  nor  $E_b$  depend on  $T$ , the determinant is

$$\begin{aligned} \mathcal{D} = & -\frac{1}{T^3} \left\{ c_L \circ T \int_0^1 d\mu_c(\omega) \int_0^1 d\mu_v(\omega) \right. \\ & + \left[ \int_0^1 z_p^2 d\mu_v(\omega) \int_0^1 d\mu_v(\omega) - \left( \int_0^1 z_p d\mu_v(\omega) \right)^2 \right] \int_0^1 d\mu_c(\omega) \\ & \left. + \left[ \int_0^1 z_n^2 d\mu_c(\omega) \int_0^1 d\mu_c(\omega) - \left( \int_0^1 z_n d\mu_c(\omega) \right)^2 \right] \int_0^1 d\mu_v(\omega) \right\} < 0 \end{aligned}$$

because of Jensen's inequality.

**Theorem 7.1.** *The functional*

$$U = U(n, p, s) := U^e(p - n) + \int u_3^{iG}(Y_n, Y_p, T) d\Omega,$$

where  $Y_b \equiv \Phi_b + V^* + V_b^G(\Phi_n, \Phi_p, T)$  ( $b = n, p$ ) and  $T$  satisfy  $n = n^G(Y_n, T)$ ,  $p = p^G(Y_p, T)$  and  $s = s^G(Y_n, Y_p, T)$ , is convex if the conditions

$$M_b \mathcal{M}_b'' > (\mathcal{M}_b')^2 \quad (b = c, v)$$

are satisfied.

Notice that the assumptions of the theorem are fulfilled in the model case.

*Proof.* We have

$$\begin{aligned} DdY_n &= (p_Y s_T - p_T s_{Y_p}) dn + s_{Y_p} n_T dp - p_Y n_T ds, \\ DdY_p &= p_T s_{Y_n} dn + (n_Y s_T - s_{Y_n} n_T) dp - n_Y p_T ds, \\ DdT &= -p_Y s_{Y_n} dn - s_{Y_p} n_Y dp + n_Y p_Y ds. \end{aligned}$$

(here the upper index  $G$  has been omitted and  $n_{Y_n} \equiv n_Y$  etc) and

$$\begin{aligned} \partial_n u(n, p, s) &= -V + \frac{u_{Y_n}^i}{\mathcal{D}} (p_Y s_T - p_T s_{Y_p}) + \frac{u_{Y_p}^i}{\mathcal{D}} p_T s_{Y_n} - \frac{u_T^i}{\mathcal{D}} p_Y s_{Y_n}, \\ \partial_p u(n, p, s) &= V + \frac{u_{Y_n}^i}{\mathcal{D}} n_T s_{Y_p} + \frac{u_{Y_p}^i}{\mathcal{D}} (n_Y s_T - n_T s_{Y_n}) - \frac{u_T^i}{\mathcal{D}} n_Y s_{Y_p}, \\ \partial_s u(n, p, s) &= -\frac{u_{Y_n}^i}{\mathcal{D}} n_T p_Y - \frac{u_{Y_p}^i}{\mathcal{D}} n_Y p_T - \frac{u_T^i}{\mathcal{D}} n_Y p_Y. \end{aligned}$$

The relations  $\partial_n u(n, p, s) = \Phi_n = Y_n - V$  etc. can be checked by straightforward calculations. We calculate the  $3 \times 3$  matrix  $U = ((U_{ab}))$  starting from

$$\begin{aligned} dU(n, p, s, \delta n, \delta p, \delta s) &= \int (\Phi_n \delta n - \Phi_p \delta p + T \delta s) d\Omega \\ &= \int (-V \delta n + Y_n \delta n + V \delta p - Y_p \delta p + T \delta s) d\Omega. \end{aligned}$$

The matrix has the same structure as in the proof of the Theorem 4.1 with the same electrical part, but with

$$zz = \int \frac{1}{T^2 |\mathcal{D}|} (\delta s \sqrt{M_c M_v})^2, \quad \dots \quad xx = \int \frac{1}{T^2 |\mathcal{D}|} (\mathcal{M}'_c \delta n)^2,$$

$$\xi\xi = \int \frac{1}{T^2 |\mathcal{D}|} \left\{ M_v c_L(T) + [M_v \mathcal{M}_v'' - (\mathcal{M}'_v)^2] + \frac{M_v}{M_c} [M_c \mathcal{M}_c'' - (\mathcal{M}'_c)^2] \right\} (\delta n)^2.$$

The proof is finished by Lemma 4.1.  $\square$

Because the state variables  $(\Phi_n, \Phi_p, T)$  are directly available, we consider the conjugate potential of the energy. A generalized density  $g_0$  of it is defined by  $g_0 = n\Phi_n - p\Phi_p + Ts - u$ . Because of the Poisson equation (2.1), this generalized density with boundary terms can be substituted by an actual density. We set

$$g_3^G(Y_n, Y_p, T, W) := -f_L(T) - \Omega_n(Y_n, T) - \Omega_p(Y_p, T) + \frac{1}{2}W[p^G(Y_p, T) - n^G(Y_n, T)]$$

and

$$g^G(\Phi_n, \Phi_p, T) := g_3^G[\Phi_n + V^* + V_i^G, \Phi_p + V^* + V_i^G, T, V_i^G].$$

The state variable  $G^G(\Phi_n, \Phi_p, T) = \int g^G(\Phi_n, \Phi_p, T) d\Omega$  is, indeed, the conjugate potential of the total energy. The relations  $\partial_{\Phi_n} G = n$  etc are checked similarly as in section 4, e.g.,

$$\begin{aligned} \langle \partial_T \int g^G d\Omega, \delta T \rangle &= - \int \{ \delta T \partial_T (f_L + \Omega_n + \Omega_p) + \delta_T V_i^G (\partial_{Y_n} \Omega_n + \partial_{Y_p} \Omega_p) \} d\Omega \\ &+ \frac{1}{2} \int \{ \delta_T V_i^G (p^G - n^G) + V_i^G [\delta T \partial_T (p^G - n^G) + \delta_T V_i^G (\partial_{Y_p} p^G - \partial_{Y_n} n^G)] \} d\Omega \\ &= \int s^G \delta T d\Omega + \frac{1}{2} \int \{ -(p - n) \delta_T V_i^G \\ &\quad + V_i^G [\delta_T V_i^G (\partial_{Y_p} p^G - \partial_{Y_n} n^G) + \delta T V_i^G \partial_T (p^G - n^G)] \} d\Omega \\ &= \int s^G \delta T d\Omega. \end{aligned}$$

Thus we have

$$\begin{aligned} dG^G(\Phi_n, \Phi_p, T; \delta\Phi_n, \delta\Phi_p, \delta T) &= \int \{ n^G [\Phi_n + V^* + V_i^G, T] \delta\Phi_n \\ &\quad - p^G [\Phi_p + V^* + V_i^G, T] \delta\Phi_p + s^G [\Phi_n + V^* + V_i^G, \Phi_p + V^* + V_i^G, T] \delta T \} d\Omega. \end{aligned}$$

and

$$d^2 G = d_i^2 G + d_e^2 G \quad \text{with}$$

$$\begin{aligned} d_i^2 G &= \int (\delta\Phi_n, \delta\Phi_p, \delta T) \begin{pmatrix} \partial_{Yn} & 0 & \partial_{Tn} \\ 0 & -\partial_{Yp} & -\partial_{Tp} \\ \partial_{Yn}s & \partial_{Yp}s & \partial_{Ts} \end{pmatrix} \begin{pmatrix} \delta\Phi_n \\ \delta\Phi_p \\ \delta T \end{pmatrix} d\Omega \\ &= \int \frac{1}{T} (\delta\Phi_n, \delta\Phi_p, \delta T) \begin{pmatrix} M_c & 0 & -\mathcal{M}'_c \\ 0 & M_v & -\mathcal{M}'_v \\ -\mathcal{M}'_c & -\mathcal{M}'_v & c_L(T) + \mathcal{M}_c'' + \mathcal{M}_v'' \end{pmatrix} \begin{pmatrix} \delta\Phi_n \\ \delta\Phi_p \\ \delta T \end{pmatrix}, \\ d_e^2 G &= \int (\delta\Phi_n, \delta\Phi_p, \delta T) d\Omega \begin{pmatrix} \partial_{Yn} & \partial_{Yn} & \partial_{Yn} \\ -\partial_{Yp} & -\partial_{Yp} & -\partial_{Yp} \\ \partial_{Yn}s & \partial_{Yp}s & (\partial_{Yn} + \partial_{Yp})s \end{pmatrix} \begin{pmatrix} \delta_n V_l^G \\ \delta_p V_l^G \\ \delta_T V_l^G \end{pmatrix} d\Omega. \end{aligned}$$

Because of (5.2) the electrical part is

$$d_e^2 G = -[\delta_n V_l^G + \delta_p V_l^G + \delta_T V_l^G, \delta_n V_l^G + \delta_p V_l^G + \delta_T V_l^G]$$

with the scalar product

$$[\chi, W] := \int [\epsilon \nabla \chi \cdot \nabla W + \frac{1}{T} (M_c + M_v) \chi W] d\Omega + \int_{\Gamma_G} \beta \chi W d\Gamma.$$

The symmetric matrix  $\mathbf{G}$  which corresponds to the quadratic form generated by  $d^2 G$  on the three-dimensional linear space spanned by the arbitrary, but fixed functions  $\delta\Phi_n$ ,  $\delta\Phi_p$ , and  $\delta T$  is the difference of two positive definite symmetric matrices  $\mathbf{G}_i$  and  $\mathbf{G}_e$ . As the functional  $G$  is the conjugate functional of the convex functional  $U$ , it is a convex functional, i.e. the quadratic form  $d_e^2 G$  is dominated by the quadratic form  $d_i^2 G$ . The question is, whether this dominance is a trivial consequence of well known a-priori estimates for solutions of elliptic boundary value problems or whether the dominance is an particular type of an a-priori estimate.

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