CONVEX ANALYSIS 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 [10] applied it in the analysis of the transient initial-boundary value problem. Gajewski [6], [8] 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. It is a very attractive quantity with both the properties. In the case of variable temperature, however, the free energy is no convex functional. In [2], [3] we have started to set up an analogous frame for an investigation of the energy model of semiconductor devices in a similar way as Gajewski and Gröger dealt with the drift-diffusion model. The present paper is a self-contained continuation of [2].

Two versions of the energy model are presented. In both cases

- we consider balance equations for the carrier densities n and p and a balance equation for a (generalized) energy density,
- the current equations are formulated in the conjugate variables of the densities,
- the current equations reflect the Onsager symmetry and the positivity of the entropy production,
- there are convex thermodynamic potentials which allow us to apply the convex (functional) analysis.

In our opinion these physically motivated properties will be advantageous in the mathematical analysis of the problems as well as in numerical evaluations.

The difference of the two versions consists in the fact that the generalized density u of the total energy is balanced in the first version, but the density u_i of the interior energy is balanced in the second version. In the first version the boundary value problem for the Poisson equation for the electrostatic potential Ψ is considered as a state equation. The non-local electrostatic interaction implies some thermodynamic consequences which has been surprising for us, but which has been neither rejected nor confirmed in some discussions with experts. These consequences seem to be, moreover, unpleasant from the mathematical point of view. Therefore we prefer a second way which is completely equivalent to the generally accepted energy model. The second version can be considered as a Gummel iteration technique adapted to the energy model. It is possible, because the total energy is the sum of the interior energy and of the electrostatic energy. This splitting is possible, because we assume that the dielectric permittivity ϵ is independent of the temperature and the heat capacity of the lattice c_L is independent of the electric field. These assumptions are generally accepted in the simulation practice. We have included also the first version, because the arising questions might be of interest beyond the field of semiconductor theory in fields, where a non-local interaction like the electrostatic one plays a role.

In contrast to [2] we do not only formally discuss the subject, but we introduce function spaces and investigate the functionals on such function spaces. In this way we build a bridge to the modern mathematical theories of evolution equations or of the convex analysis. We present our approach on the half way, because

- we believe that the approach is worthwhile to be introduced,

- colleagues are invited to overcome the remaining problems on the way to the proof of existence and uniqueness of solutions,
- the approach should also be introduced to non-mathmaticians which are interested in this subject or in similar subjects, but which are not so much interested in the mathematical difficulties and techniques.

The paper is organized as follows. The basic notation and assumptions are introduced in section 2. In this section the free energy as a function of n, p and of the temperature T is also introduced, because this thermodynamic potential seems to be the most familiar one and because it represents the assumptions in the most illustrative way. Furthermore the conjugate variables (ξ, η, τ) of (n, p, u) and the corresponding thermodynamic potential $H(\xi, \eta, \tau)$ are derived in a formal way. The non-local terms in the equations (2.12) arise quite naturally; they causes the questions and the modifications of the energy model mentioned above. In the section 3 it is shown that the potential H is a concave F-differentiable functional on an open convex subset of the affine Banach space $z^D + H_0^1 \times H_0^1 \times (H_0^1 \cap L_\infty) \equiv z^D + Z_\infty$. In this section we take advantage of the moderate growth of Fermi integrals compared to the exponential function, i.e. we restrict us onto the Fermi-Dirac statistics. Some remarks which concern the convex analysis are gathered in section 4 in order to relate the properties of the energy model to properties on which the mathematical theory is founded. In the following two sections the approach based on the convex analysis is presented for the modified energy model and for the conventional energy model. These sections end with a first a priori estimate for solutions of evolution equations which are discretized in the time. These physically motivated a priori estimates are main results of this paper. We hope that they will be useful tools in the proof of existence (and uniqueness). As mentioned above the mathematical problems of proving suitable a priori estimates which guarantee the existence of solutions and other mathematical problems remain open, but the basis for a precise formulation of the problems is given. In the section 7 we discuss an oversimplified test example to illustrate our intentions. In an appendix we show that the approach to the energy model is closely related to the thermodynamics of ideal Fermi gases.

2. Notation and assumptions

We consider a simple, but generally accepted energy model of semiconductor devices. The device occupies a bounded open region $\Omega \subset R^m$ in the Euclidean space of dimension $m = 2$ or 3. Let $L_p(\Omega)$ with $1 \leq p \leq \infty$ denote the Banach space of measurable functions ϕ on Ω for which $|\phi|_p := \int |\phi|^p \, d\Omega^{1/p} < \infty$ $(p < \infty)$ or which are a.e. bounded with the least upper bound $|\phi|_\infty$ of $|\phi|$. Let L_∞^+ denote the open convex set

$$L_\infty^+ := \{\tau \in L_\infty(\Omega) : \; 0 < \underline{\tau} \leq \tau \quad \text{a.e. } \} \subset L_\infty(\Omega)$$

of strictly positive bounded measurable functions on Ω. Furthermore, $H^1(\Omega)$ denotes the space of square integrable functions $\phi \in L_2(\Omega)$ which have square integrable partial derivatives in the sense of distributions. The boundary $\partial\Omega$ is assumed to be a regular Lipschitz boundary, which is decomposed in a regular way into a proper part $\Gamma \subset \partial\Omega$ and its complement. Let denote H_0^1 the Banach space

$$H_0^1 := \{\phi \in H^1(\Omega) : \; \phi = 0 \quad \text{on} \quad \partial\Omega \setminus \Gamma \,\}$$

with the norm $\|\phi\| := \int |\nabla\phi|^2 d\Omega^{\ 1/2}$. Its dual space is denoted by $H^{-1} := (H_0^1)'$. The norm $\|.\|$ is equivalent to the H^1 norm on H_0^1, as we consider a measurable subset Γ of the boundary with the surface measure $|\Gamma| < |\partial\Omega|$.

The energy model which will be considered is, mathematically spoken, a system of four partial differential equations with suitable boundary conditions and with suitable initial conditions. The energy model is a phenomenological model. The states of the semiconductor device are described by three independent state variables, which are functions or generalized functions on the closure $\bar{\Omega}$ of Ω, e.g. the densities n and p of electrons and holes and the temperature T. Instead of T the density u of the total energy can be considered. The evolution of the state is described by a system of three balance equations and by the Poisson equation for the electrostatic potential Ψ, which describes the electrostatic interaction. The three balance equations are the continuity equations

$$\dot{n} + \nabla\cdot j_n = -R \quad \text{and} \quad \dot{p} + \nabla\cdot j_p = -R \tag{2.1}$$

with the net recombination rate R and the conservation law

$$\dot{u} + \nabla\cdot j_u = 0 \tag{2.2}$$

for the total energy. The Poisson equation reads

$$-\nabla\cdot(\epsilon\nabla\Psi) = d + p - n \tag{2.3}$$

with the dielectric permittivity $\epsilon \in L_\infty^+$ and with a fixed doping profile d. The mixed boundary conditions are Dirichlet conditions on $\partial\Omega\setminus\Gamma$, homogeneous natural conditions

$$\nu\cdot j_n = \nu\cdot j_p = 0 \quad \text{and} \quad \nu\cdot j_u = 0 \quad \text{on} \quad \Gamma \tag{2.4}$$

with the outward normal unit vector ν for the balance equations and a boundary condition of third type

$$\epsilon\partial_\nu\Psi + b\Psi = g \quad \text{on} \quad \Gamma \tag{2.5}$$

for the Poisson equation with given functions $0 \le b \in L_\infty(\Gamma)$ and g. The mixed boundary value problem for the Poisson equation is considered as a state equation. Instead of specifying d and g we write $\Psi = \Psi^D + \psi$, where $\Psi^D \in H^1 \cap L_\infty$ is the given 'exterior' electrostatic potential due to the doping profile and due to the boundary values, whereas $\psi = \psi_{p-n} \in H_0^1$ is the solution of the corresponding boundary value problem

$$\langle \mathbf{P}\psi, \phi\rangle := \int \epsilon\nabla\psi\nabla\phi\; d\Omega + \int_\Gamma b\psi\phi\; d\Gamma = \int (p-n)\phi\; d\Omega \tag{2.6}$$

($\phi \in H_0^1$) with homogeneous boundary conditions. This equation is briefly written as an equation $\mathbf{P}\psi = [p-n]$ in H^{-1}. The Green function of this problem is denoted by P, i.e. $\psi(x) = \int_\Omega P(x,y)[p(y)-n(y)]\; dy$. For arbitrary functions $\tau \in L_\infty^+ \cap H^1$, $\phi \in H^1$ and $\chi \in H_0^1$ we introduce the notation

$$\langle \mathbf{P}(\tau)\phi, \chi\rangle := \int \tau\epsilon\nabla\phi\nabla\chi\; d\Omega + \int_\Gamma \tau b\phi\chi\; d\Gamma =: \int \tau p[\phi,\chi]\; d(\Omega\cup\Gamma)$$

and the generalized density

$$u_e(\phi) = \frac{1}{2}\left[\epsilon|\nabla\phi|^2 + b\phi^2\delta_\Gamma\right]$$

of the electrostatic energy of the lattice with an electrostatic potential ϕ. The boundary term in (2.6) is responsible for the fact that we have to deal with generalized densities like u_e on $\bar{\Omega}$ or on $\Omega \cup \Gamma$.

Initial values for n, p, and u are n_0, p_0, and u_0. This initial-boundary value problem has to be supplemented by current equations and by specifying the net recombination rate. These specifications are given later.

A basic assumption of the energy model is that the principle of partial local equilibrium can be applied, i.e. in particular

- thermodynamic quantities like the temperature T, the electrochemical potentials v of electrons and w of holes are defined,
- they are (generalized) functions on $\bar{\Omega}$, which may also depend on the time t and
- at any point $x \in \Omega$ (and at any time t) thermodynamic relations hold like the state equations

$$(2.7) \qquad n = N_c \mathcal{F}_{1/2}\left[\frac{1}{T}(v + \Psi - E_c)\right] \quad \text{and} \quad p = N_v \mathcal{F}_{1/2}\left[\frac{1}{T}(E_v - w - \Psi)\right] .$$

The densities of state N_c and N_v and the band edges E_c and E_v are given material laws and $\mathcal{F}_{1/2}$ is one of the Fermi integrals

$$\mathcal{F}_\alpha(r) = \frac{1}{\Gamma(\alpha+1)} \int_0^\infty \frac{s^\alpha}{1+e^{s-r}}\, ds \qquad (\alpha > -1) .$$

Since the expressions for electrons and for holes are almost the same, we will often omit the expressions for holes, in particular, in proofs we often consider devices only with electrons.

The functions N_i and E_i $(i = c, v)$ are functions

$$N_i : \Omega \times R_+ \mapsto R_+ \quad \text{and} \quad E_i : \Omega \times R_+ \mapsto R ,$$

where $R_+ :=]0, \infty[$ denotes the open real half-line. The functions are assumed to be measurable in the first argument $x \in \Omega$, but twice continuously differentiable in the second argument $T \in R_+$. They and their derivatives with respect to the second argument are assumed to satisfy the estimates

$$\begin{aligned} 0 < \underline{N}_a^b \le N_i \le \bar{N}_a^b < \infty \quad &\text{and} \quad |E_i| \le E_a^b < \infty , \\ 0 \le \partial_T N_i \le \bar{N}_a^b < \infty \quad &\text{and} \quad |\partial_T E_i| \le E_a^b < \infty , \\ |\partial_T^2 N_i| \le \bar{N}_a^b < \infty \quad &\text{and} \quad |\partial_T^2 E_i| \le E_a^b < \infty \end{aligned}$$

a.e. on $\Omega \times [a, b]$ for any bounded closed interval $[a, b]$. It will be convenient to write briefly $N_i(T)$ instead of $N_i(., T)$ or instead of $N_i[., T(.)]$ and $N_i'(T)$ instead of $\partial_T N_i(., T)$. We write also $N_i \circ T$ instead of $N_i[., T(.)]$. Let us, moreover, introduce the notation $\mathcal{N}_i(1/T) := N_i(T)$ $(i = c, v)$, $E_n(T) := E_c(T) - \Psi$, $E_p(T) := E_v(T) - \Psi$, $\mathcal{E}_i(1/T) := E_i(T)/T$ $(i = c, n, p, v)$, and the functions

$$(2.8) \qquad h_j(s, \tau) = \mathcal{N}_c(\tau) \mathcal{F}_{1/2}[-s - \mathcal{E}_j(\tau)] \qquad (j = c, n)$$

and $h_k(s, \tau) = \mathcal{N}_v(\tau) \mathcal{F}_{1/2}[\mathcal{E}_k(\tau) - s]$ $(k = p, v)$ on $R \times R_+$. We assume, furthermore, that the material functions N_c and E_c (and, correspondingly, N_v and E_v) satisfy the following inequalities

$$\mathcal{N}_c{}''\mathcal{F}_{3/2} - \mathcal{N}_c\mathcal{E}_c{}''(\tau)\mathcal{F}_{1/2} > \frac{[\mathcal{N}_c'\mathcal{F}_{1/2}]^2}{\mathcal{N}_c\mathcal{F}_{-1/2}} \tag{2.9}$$

for all $(s,\tau) \in R \times R_+$ and for almost all $x \in \Omega$. This assumption guarantees the convexity of the functions h_j on $R \times R_+$ for a.a. $x \in \Omega$. The assumptions concerning N_c and E_j $(j = c, n)$ (or, correspondingly, N_v and E_k $(k = v, p)$) are satisfied in the model case

$$N_c(T) = N_c^+ T^{3/2} \quad \text{with} \quad N_c^+ \in L_\infty^+ \quad \text{and} \quad E_c(T) = E_c \in L_\infty(\Omega) \ .$$

A proof and the thermodynamic background are described in the Appendix.

Further material laws are the generalized density f_L of the free energy of the lattice, i.e. the semiconductor device without the carriers, and the density c_L of the heat capacity of the lattice. The function $c_L : \Omega \times R_+ \mapsto R_+$ is assumed to satisfy $c_L(.,T) \in L_\infty^+$ for all $T \in R_+$ and to increase monotonely and continuously in the second argument for a.a. $x \in \Omega$. As it is commonly done in simulation practice we assume that the dielectric permittivity does not depend on the temperature and that the heat capacity of the lattice does not depend on the electric field. As a consequence the total energy of the system is a sum of the 'interior' energy and of the electrostatic energy. Thus the generalized density f_L is

$$f_L(.,T) = f_L^i(.,T) + u_e(\Psi^D)$$

with a function $f_L^i : \Omega \times R_+ \mapsto R$ which is related to c_L by $\int^T c_L(s)\ ds = f_L^i(T) - T\partial_T f_L^i(T)$.

The state space of the energy model is physically described by an expression for the free energy. We choose

$$\begin{aligned} F(n,p,T) \ &:= \ \int f_L \circ T \ d\Omega \\ &+ \ \int nT\mathcal{F}_{1/2}^{-1}\left(\frac{n}{N_c \circ T}\right) - TN_c(T)\mathcal{F}_{3/2} \circ \mathcal{F}_{1/2}^{-1}\left(\frac{n}{N_c \circ T}\right) + nE_c(T)\ d\Omega \\ &+ \ \int pT\mathcal{F}_{1/2}^{-1}\left(\frac{p}{N_v \circ T}\right) - TN_v(T)\mathcal{F}_{3/2} \circ \mathcal{F}_{1/2}^{-1}\left(\frac{p}{N_v \circ T}\right) - pE_v(T)\ d\Omega \\ &+ \ \int \Psi^D(p-n) + \frac{1}{2}\epsilon|\nabla\psi|^2\ d\Omega + \frac{1}{2}\int_\Gamma b\psi^2\ d\Gamma \ =: \ \int f(n,p,T)\ d\Omega \end{aligned} \tag{2.10}$$

with a generalized density $f(n,p,T)$.

The following theorem and its proof are not stringent in the mathematical sense, but yield a thermodynamically motivated description of the semiconductor device as a system with a non-local electrostatic interaction, i.e. one of the state equations is a boundary value problem. The thermodynamic background (without electrostatic interaction) is also described in the Appendix. The theorem is the basis for an approach to the analysis of the energy model suggested in this paper. Let z denote the triple (ξ, η, τ) of state variables which will be introduced in the theorem.

Theorem 2.1. *The state equations* (2.7) *are compatible with the definition* (2.10) *of the free energy, i.e. the functional partial derivatives* $\partial_n F$ *and* $\partial_p F$ *satisfy*

$$\langle \partial_n F(n,p,T), \delta n\rangle = \int v\delta n \; d\Omega \quad \text{and} \quad \langle \partial_p F(n,p,T), \delta p\rangle = -\int w\delta p \; d\Omega \; .$$

The entropy $S := -\langle \partial_T F(n,p,T), 1\rangle$ *with the density* $s = -\partial_T f(n,p,T) =: s_f(n,p,T)$, *considered as a functional of the densities* n, p, *and*

$$u = u_f(n,p,T) := f(n,p,T) - T\partial_T f(n,p,T) \; , \tag{2.11}$$

is a concave functional. The conjugate variables of n, p, *and* u *are the state variables*

$$\begin{aligned} \xi = -\frac{v}{T} &- \int \left[\frac{1}{T} - \frac{1}{T(y)}\right] \epsilon(y)\nabla\psi(y)\nabla_y P(y,.) \; d\Omega(y) \\ &- \int_\Gamma \left[\frac{1}{T} - \frac{1}{T(y)}\right] b(y)\psi(y)P(y,.) \; d\Gamma(y) \; , \\ \eta = \frac{w}{T} &+ \int \left[\frac{1}{T} - \frac{1}{T(y)}\right] \epsilon(y)\nabla\psi(y)\nabla_y P(y,.) \; d\Omega(y) \\ &+ \int_\Gamma \left[\frac{1}{T} - \frac{1}{T(y)}\right] b(y)\psi(y)P(y,.) \; d\Gamma(y) \; , \end{aligned} \tag{2.12}$$

and $\tau = 1/T$.
The operators $\Pi_h(z) : H_0^1 \mapsto H^{-1}$ *defined by*

$$\Pi_h(\xi,\eta,\tau)\zeta := \mathbf{P}\mathbf{P}(\tau)^{-1}\mathbf{P}\zeta \quad - \quad \partial_\zeta[h_n(\xi-\zeta,\tau) - h_p(-\eta-\zeta,\tau)]$$

are strongly monotone operators.
The conjugate potential H *of* S *reads (up to an additive constant)*

$$H(\xi,\eta,\tau) = \int h_i(\xi,\eta,\tau,\zeta) \; d\Omega - \frac{1}{2}\langle \mathbf{P}\zeta, \mathbf{P}(\tau)^{-1}\mathbf{P}\zeta\rangle + \frac{1}{2}\langle \mathbf{P}\zeta^*, \zeta^*\rangle \tag{2.13}$$

with the integrand

$$\begin{aligned} h_i(\xi,\eta,\tau,\zeta) = \int_1^\tau \int^{1/\sigma} c_L(s) \; ds \; d\sigma + (\tau-1)u_e(\Psi^D) \\ - h_n(\xi-\zeta,\tau) + h_n(-\zeta^*,1) - h_p(\eta+\zeta,\tau) + h_p(\zeta^*,1) \end{aligned}$$

and with the solutions $\zeta = \zeta_h(z)$ *of the equation* $\Pi_h(z)\zeta = 0$ *and* ζ^* *of the equation* $\Pi_h(0,0,1)\zeta^* = 0$.

We consider state variables z which are triples of functions ξ, $\eta \in H^1(\Omega)$ and $\tau \in L_\infty^+ \cap H^1(\Omega)$. The boundary values on $\partial\Omega\setminus\Gamma$ are given by functions ξ^D, $\eta^D \in H^1(\Omega)$ and $\tau^D \in L_\infty^+ \cap H^1(\Omega)$. Let denote

$$Z_\infty^D := (\xi^D + H_0^1) \times (\eta^D + H_0^1) \times [(\tau^D + H_0^1) \cap L_\infty^+]$$

and $Z_\infty := H_0^1 \times H_0^1 \times (H_0^1 \cap L_\infty)$. Notice that $Z_\infty = Z'$ is the dual space of the Banach space $Z = H^{-1} \times H^{-1} \times (H^{-1} + L_1)$ and that there is an open convex neighbourhood Z^+ of $0 \in Z_\infty$ such that $Z_\infty^D = z^D + Z^+$ ($z^D = (\xi^D, \eta^D, \tau^D)$).

Proof of Theorem 2.1 (for electrons only). Let δn and δT denote arbitrary variations of n and of T. Formal differentiation of $F(n,T)$, the identity $\psi_{-n-\delta n} = \psi - \psi_{\delta n}$, and the Poisson equation (2.6) for $\psi_{\delta n}$ with the test function $\psi = \psi_{-n}$ yield

$$\langle \partial_n F(n,T), \delta n \rangle = \int T \left[\mathcal{F}_{1/2}^{-1}\left(\frac{n}{N_c}\right) + \frac{1}{T}(E_n - \psi) \right] \delta n \; d\Omega \; .$$

The left-hand side is $\int v \delta n \; d\Omega$ according to (2.7).

The assumption (2.9) and $c_L > 0$ guarantee the inequality $\partial_T u_f(n,T) > 0$ (cf. Appendix). The identity (2.11) implies $\partial_T u_f = T \partial_T s_f$. Therefore the entropy S can be considered as a functional of n and u. Eliminating δT by $\delta u = \partial_n u_f \delta n + \partial_T u_f \delta T$ one obtains

$$\delta s = (\partial_n s_f - \frac{1}{T}\partial_n u_f)\delta n + \frac{1}{T}\delta u =: \xi_f(n,T)\delta n + \frac{1}{T}\delta u$$

with

$$\begin{aligned} \xi_f(n,T)\delta n = -\frac{1}{T}\partial_n f(n,T)\delta n &= -\left[\mathcal{F}_{1/2}^{-1}\left(\frac{n}{N_c \circ T}\right) + \frac{1}{T}E_n(T) \right] \delta n \\ &+ \frac{\epsilon}{T}\nabla\psi\nabla\psi_{\delta n} + \frac{b}{T}\psi\psi_{\delta n}\delta_\Gamma \; . \end{aligned}$$

The functional partial derivative with respect to n is defined by

$$\langle \partial_n S(n,u), \delta n \rangle = \int \xi_f(n,T)\delta n \; d\Omega \; .$$

The conjugate variable ξ is obtained from the right-hand side.

We consider the quadratic form

$$\delta^2 s := \partial_n \xi_f(n,T)\delta' n \otimes \delta n + \partial_T \xi_f(n,T)\delta' T \otimes \delta n - \frac{1}{T^2}\delta' T \otimes \delta u$$

and observe that

$$\delta^2 s = -\frac{\epsilon}{T}\nabla\psi_{\delta' n}\nabla \otimes \psi_{\delta n} - \frac{b}{T}\psi_{\delta' n} \otimes \psi_{\delta n}\delta_\Gamma - \frac{\delta' n \otimes \delta n}{N_c \mathcal{F}_{-1/2}} - \frac{\partial_T u_f}{T^2}\delta' T \otimes \delta T \; ,$$

i.e. the functional $S = S(n,u)$ is a concave functional.

Since $\mathcal{F}_{1/2}$ is a monotone function the strong monotony of $\Pi_h(z)$ follows easily from

$$\langle \Pi_h(z)\zeta_2 - \Pi_h(z)\zeta_1, \zeta \rangle \geq \langle \mathbf{P}\mathbf{P}(\tau)^{-1}\mathbf{P}\zeta, \zeta \rangle \geq \mathrm{const}(\tau)\|\zeta\|^2$$

$(\zeta \equiv \zeta_2 - \zeta_1)$. Since equations with continuous strongly monotone operators have an unique solution, we denote $\zeta = \zeta_h(z)$ the solutions of the equations $\Pi_h(z)\zeta = 0$.

The conjugate potential of $S(n,u)$ is defined by

$$\tilde{H}(\xi,\tau) := \int \xi n + \tau u \; d\Omega - S(n,u) = \int \xi n + \frac{1}{T}f(n,T) \; d\Omega \; .$$

We get an explicit expression if we eliminate n and T on the right-hand side by ξ and $\tau = 1/T$. The integration of the initial value problem

$$-T\partial_T f_L^i(T) + f_L^i(T) = \int^T c_L(y)dy$$

with the initial value $f_L^i(1)$ at $T = 1$ yields

$$\frac{1}{T}f_L^i(T) = f_L^i(1) + \int_1^\tau \int^{1/\sigma} c_L(y)dy \; d\sigma \; .$$

The summand

$$\tilde{\zeta} := \int \frac{1}{T(y)}\epsilon(y)\nabla\psi(y)\nabla_y P(y,.)\ d\Omega(y) + \int_\Gamma \frac{1}{T(y)} b(y)\psi(y)P(y,.)\ d\Gamma(y)$$

in (2.12) satisfies

$$\int \tilde{\zeta}\delta n\ d\Omega = \langle \mathbf{P}(\tau)\psi, \psi_{\delta n}\rangle = \int \mathbf{P}^{-1}\mathbf{P}(\tau)\psi\delta n\ d\Omega\ ,$$

i.e. $\mathbf{P}\tilde{\zeta} = \mathbf{P}(\tau)\psi$ and thus

$$\mathbf{P}\mathbf{P}(\tau)^{-1}\mathbf{P}\tilde{\zeta} = \mathbf{P}\psi = -[n] = -[\mathcal{N}_c\mathcal{F}_{1/2}(-\xi + \tilde{\zeta} - \mathcal{E}_n)]\ ,$$

i.e. $\tilde{\zeta} = \zeta_h(\xi,\tau) \equiv \zeta$. So far we obtain

$$\begin{aligned}\tilde{H}(\xi,\tau) = \frac{1}{2}\langle \mathbf{P}(\tau)\Psi, \Psi\rangle + \int f_L^i(1)\ d\Omega + \int\int_1^\tau \int^{1/\sigma} c_L(y)dy\ d\sigma\ d\Omega \\ - \int \mathcal{N}_c(\tau)\mathcal{F}_{3/2}[-\xi + \zeta - \mathcal{E}_n(\tau)]\ d\Omega + \int n\zeta\ d\Omega + \frac{1}{2}\langle \mathbf{P}(\tau)\psi, \psi\rangle\ .\end{aligned}$$

The last two summands on the right-hand side can be transformed according to

$$\int n\zeta\ d\Omega + \frac{1}{2}\langle \mathbf{P}(\tau)\psi,\psi\rangle = -\langle \mathbf{P}\psi, \zeta\rangle + \frac{1}{2}\langle \mathbf{P}\zeta, \psi\rangle = -\frac{1}{2}\langle \mathbf{P}\zeta, \mathbf{P}(\tau)^{-1}\mathbf{P}\zeta\rangle\ .$$

Since an additive constant does not play an essential role, we set

$$H(\xi,\tau) := \tilde{H}(\xi,\tau) - \tilde{H}(0,1)\ .$$

This completes the proof of the Theorem 2.1.

3. The state space of the energy model

The aim of this section is to establish the functional H of Theorem 2.1 and its properties on the open convex set $Z_\infty^D \subset z^D + Z_\infty$. We start with an elementary lemma which, from the mathematical point of view, illustrates some advantages of the Fermi-Dirac statistics compared with the Boltzmann statistics.

Lemma 3.1. *The following estimates with real numbers $\alpha > -1$, $p \geq 1$ hold for functions $\mathcal{E} \in L_\infty(\Omega)$, $w \in H^1(\Omega)$ or $u \in L_p(\Omega)$:*

$$\frac{1}{2^{\alpha+1}}\mathcal{F}_\alpha(r) \leq 1 + \frac{1}{\Gamma(\alpha+2)}\max(0,r)^{\alpha+1} \quad (r \in R), \tag{3.1}$$

$$|\mathcal{F}_\alpha(u-\mathcal{E})|_{p/(\alpha+1)} \leq A_{p,\alpha} + B_\alpha |u|_p^{\alpha+1}\ , \tag{3.2}$$

$$|\mathcal{F}_\alpha(w-\mathcal{E})|_{6/(\alpha+1)} \leq A_\alpha + B_\alpha \|w\|^{\alpha+1}\ . \tag{3.3}$$

The constant $B_\alpha > 2^{\alpha+1}/\Gamma(\alpha+2)$ can be arbitrarily chosen, but the constants $A_{p,\alpha}$ depend on $|\mathcal{E}|_\infty$ and on the choice of B_α.

Proof. The first inequality follows from the estimates

$$\begin{aligned}\int_0^{ar} \frac{s^\alpha}{1+e^{s-r}}\ ds + \int_{ar}^\infty \frac{s^\alpha}{1+e^{s-r}}\ ds \ &\leq\ \frac{(ar)^{\alpha+1}}{\alpha+1} + a^{\alpha+1}\int_r^\infty \frac{s^\alpha}{1+e^{(a-1)s+s-r}}\ ds \\ &\leq\ \frac{(ar)^{\alpha+1}}{\alpha+1} + \left(\frac{a}{a-1}\right)^{\alpha+1}\end{aligned}$$

$(0 < r,\ 1 < a)$ with $a = 2$.

To prove the other inequalities, we observe that the function $r \mapsto \beta^{p-1} - (r+a)^p + c$ on the closed positive real half-line with parameters $p,\ \beta > 1$ has only one extremal point and that the function attains its minimal value there. This fact implies the estimate

$$(r+a)^p \leq \beta^{p-1} r^p + \left(\frac{\beta}{\beta - 1}\right)^{p-1} \tag{3.4}$$

$(r \geq 0)$. Now we apply (3.1), i.e.

$$|\mathcal{F}_\alpha(u - \mathcal{E})| \leq c + c \max{(u - \mathcal{E}, 0)}^{\alpha+1} \leq c + c(|u| + |\mathcal{E}|)^{\alpha+1}$$

and

$$|\mathcal{F}_\alpha(u - \mathcal{E})|_{p/(\alpha+1)} \leq c|\Omega|^{(\alpha+1)/p} + c(|u|_p + |\mathcal{E}|_p)^{\alpha+1} \ .$$

The estimate (3.4) applied to the second summand on the right-hand side yields the second assertion. The last assertion is a consequence of the Sobolev imbedding theorem. □

Lemma 3.2. *The operators $\Pi_h(z)$ $(z \in Z^D_\infty)$ introduced in the Theorem 2.1 maps H^1_0 into H^{-1}; they are hemicontinuous and strongly monotone.*

Proof. The operators $\mathbf{P}(\sigma)$ $(\sigma \in L^+_\infty)$ are linear isomorphisms between H^1_0 and H^{-1}. The functions $\mathcal{N}_c \mathcal{F}_{1/2}(-\xi + \bar{\zeta} - \mathcal{E}_n)$ belong to $L_{6/5} \hookrightarrow H^{-1}$ according to the preceding lemma. Therefore $\Pi_h(z)$ maps H^1_0 into H^{-1} and is strongly monotone. To prove the hemicontinuity we consider

$$[\mathcal{F}_{1/2}(u + t\chi) - \mathcal{F}_{1/2}(u + s\chi)]\phi = \chi\phi \int_s^t \mathcal{F}_{-1/2}(u + y\chi)\ dy$$

for arbitrary $u \in H^1_0 + L_\infty$, $\chi,\ \phi \in H^1_0$ and $t \geq s$. The Hölder inequality for three factors can be applied to the right-hand side. Choosing $p = 12$, $q = r = 24/11$ we obtain

$$|\chi\phi \int_s^t \mathcal{F}_{-1/2}(u + y\chi)\ dy|_1 \leq |\chi|_q |\phi|_q \int_s^t |\mathcal{F}_{-1/2}(u + y\chi)|_p\ dy = O(|t - s|)$$

according to (3.1) and (3.3), i.e. the function $t \mapsto \langle \Pi_h(z)(\bar{\zeta} + t\chi), \phi \rangle$ $(\bar{\zeta} \in H^1_0)$ is continuous on $[0, 1]$. □

We remember that the equations $\Pi_h(z)\zeta = 0$ in H^{-1} have uniquely determined solutions $\zeta = \zeta_h(z)$ (cf. e.g. [19]).

Theorem 3.1. *The expression (2.13) in the Theorem 2.1 defines an F-differentiable functional H on Z^D_∞ the differential of which satisfies*

$$\langle dH(z_2) - dH(z_1), \delta z \rangle < 0 \qquad (\delta z :\equiv z_2 - z_1 \neq 0)\ .$$

Proof. The proof is carried out for a system with electrons only. Let y_i $(i = 1, 2)$ denote the value of any state variable y in the state (ξ_i, τ_i) and $\delta y := y_2 - y_1$. The functions $\zeta_i,\ \zeta^* \in H^1_0$ are well defined. Let ω_i denote briefly the argument $-\xi_i + \zeta_i - \mathcal{E}_n(\tau_i)$ in the Fermi integrals. The integrability of the functions $\mathcal{N}_c(\tau_i)\mathcal{F}_{1/2}(\omega_i)$ and $N_c(1)\mathcal{F}_{3/2}[\zeta^* - E_n(1)]$ follows from Lemma 3.1, i.e. the expression (2.13) is defined on Z_∞^D. We have already differentiated the functional H in a formal way, i.e. we already know the expression dH, but we have still to prove that the expression

$$F := H_2 - H_1 - \int \delta\xi n_1 + \delta\tau u_f(n_1, 1/\tau_1)\ d\Omega$$

satisfies $F = o(\|\delta\xi\| + \|\delta\tau\| + |\delta\tau|_\infty)$ and $F < 0$ if $\delta\xi \oplus \delta\tau \neq 0$.
We have

$$\begin{aligned} F = & \int\int_0^{\delta\tau}\int_{1/\tau_1}^{1/(\sigma+\tau_1)} c_L(s)\ ds\ d\sigma\ d\Omega \\ & - \int \mathcal{N}_c(\tau_2)\mathcal{F}_{3/2}(\omega_2) - \mathcal{N}_c(\tau_1)\mathcal{F}_{3/2}(\omega_1) \\ & \quad + \delta\xi n_1 - \delta\tau\mathcal{N}_c'(\tau_1)\mathcal{F}_{3/2}(\omega_1) + \delta\tau\mathcal{E}_n'(\tau_1)n_1\ d\Omega \\ & - \frac{1}{2}\langle \mathbf{P}\zeta_2, \mathbf{P}(\tau_2)^{-1}\mathbf{P}\zeta_2\rangle + \frac{1}{2}\langle \mathbf{P}\zeta_1, \mathbf{P}(\tau_1)^{-1}\mathbf{P}\zeta_1\rangle - \frac{1}{2}\langle \mathbf{P}(\delta\tau)\psi_1, \psi_1\rangle\ . \end{aligned}$$

We add the identity

$$0 = \int \delta\zeta n_1\ d\Omega + \langle \mathbf{P}\psi_1, \delta\zeta\rangle = \int \delta\zeta n_1\ d\Omega + \langle \mathbf{P}(\tau_2)\psi_2 - \mathbf{P}(\tau_1)\psi_1, \psi_1\rangle$$

and obtain

$$\begin{aligned} F = & \int\int_0^{\delta\tau}\int_{1/\tau_1}^{1/(\sigma+\tau_1)} c_L(s)\ ds\ d\sigma\ d\Omega \\ & - \int [\mathcal{N}_c(\tau_2) - \mathcal{N}_c(\tau_1) - \delta\tau\mathcal{N}_c'(\tau_1)]\mathcal{F}_{3/2}(\omega_2)\ d\Omega \\ & - \int \mathcal{N}_c(\tau_1)\left[\mathcal{F}_{3/2}(\omega_2) - \mathcal{F}_{3/2}(\omega_1) - \delta\omega\mathcal{F}_{1/2}(\omega_1)\right]\ d\Omega \\ & + \int [\delta\mathcal{E}_n - \delta\tau\mathcal{E}_n'(\tau_1)]n_1\ d\Omega \\ & - \frac{1}{2}\langle \mathbf{P}(\tau_2)\psi_2, \psi_2\rangle + \langle \mathbf{P}(\tau_1)\psi_2, \psi_1\rangle - \frac{1}{2}\langle \mathbf{P}(\tau_2)\psi_1, \psi_1\rangle \\ \\ = & -\int\int_0^{\delta\tau}\int_0^{\sigma} c_L\left(\frac{1}{z+\tau_1}\right)\frac{1}{(z+\tau_1)^2}\ dz\ d\sigma\ d\Omega \\ & - \int (\delta\tau)^2\int_0^1\int_0^y \mathcal{N}_c''(\tau_1 + z\delta\tau)\ dz\ dy\mathcal{F}_{3/2}(\omega_2)\ d\Omega \\ & - \int \mathcal{N}_c(\tau_1)\delta\omega\int_0^1\left[\mathcal{F}_{1/2}(\omega_1 + y\delta\omega) - \mathcal{F}_{1/2}(\omega_1)\right]\ dy\ d\Omega \\ & + \int (\delta\tau)^2 n_1\int_0^1\int_0^y \mathcal{E}_n''(\tau_1 + z\delta\tau)\ dz\ dy\ d\Omega \\ & - \frac{1}{2}\langle \mathbf{P}(\tau_2)\delta\psi, \delta\psi\rangle\ . \end{aligned}$$

The identity

$$\begin{aligned}
&\Pi_h(\xi_1,\tau_1)\zeta_2 - \Pi_h(\xi_1,\tau_1)\zeta_1 \\
&= \mathbf{P}[\mathbf{P}(\tau_1)^{-1} - \mathbf{P}(\tau_2)^{-1}]\mathbf{P}\zeta_2 \\
&\quad + \left[\mathcal{N}_c(\tau_1)\mathcal{F}_{1/2}(\omega_2 + \delta\xi + \delta\mathcal{E}) - \mathcal{N}_c(\tau_2)\mathcal{F}_{1/2}(\omega_2)\right] \\
&= \mathbf{P}\mathbf{P}(\tau_1)^{-1}\mathbf{P}(\delta\tau)\mathbf{P}(\tau_2)^{-1}\mathbf{P}\zeta_2 \\
&\quad + \left[\mathcal{N}_c(\tau_1)(\delta\mathcal{E} + \delta\xi)\int_0^{\delta\mathcal{E}+\delta\xi} \mathcal{F}_{-1/2}[\omega_2 + y(\delta\mathcal{E} + \delta\xi)]\ dy - \delta\mathcal{N}_c\mathcal{F}_{1/2}(\omega_2)\right]
\end{aligned}$$

with $\mathbf{P}(\tau_2)^{-1}\mathbf{P}\zeta_2 = \psi_2$ yields an estimate for $\delta\zeta$, since the inverse of the strongly monotone operator $\Pi_h(\xi_1,\tau_1)$ is Lipschitz continuous. We have , indeed,

$$\|\delta\zeta\| \le c\|\Pi_h(\xi_1,\tau_1)\zeta_2 - \Pi_h(\xi_1,\tau_1)\zeta_1\|_{H^{-1}}$$

and

$$\begin{aligned}
\|\mathbf{P}\mathbf{P}(\tau_1)^{-1}\mathbf{P}(\delta\tau)\psi_2\|_{H^{-1}} &\le c\|\mathbf{P}(\delta\tau)\psi_2\|_{H^{-1}} \\
&\le c \sup_{\|\chi\|\le 1}\langle\mathbf{P}(\delta\tau)\psi_2,\chi\rangle = \frac{c}{\|\psi_2\|}\langle\mathbf{P}(\delta\tau)\psi_2,\psi_2\rangle \le c|\delta\tau|_\infty\|\psi_2\| \ .
\end{aligned}$$

The other summands can be estimated as in the proof of the preceding lemma. In this way we see that any summand is bounded from above by a bound, which contains a factor like $\|\delta\xi\|$, $\|\delta\tau\|$, or $|\delta\tau|_\infty$.

An estimate for $\delta\psi$ is obtained in a similar way. There is the identity

$$\begin{aligned}
&\Pi_h(\xi_1,\tau_1)\mathbf{P}^{-1}\mathbf{P}(\tau_1)\psi_2 - \Pi_h(\xi_1,\tau_1)\mathbf{P}^{-1}\mathbf{P}(\tau_1)\psi_1 \\
&= \mathbf{P}\psi_2 + \left[\mathcal{N}_c(\tau_1)\mathcal{F}_{1/2}[\omega_1 + \mathbf{P}^{-1}\mathbf{P}(\tau_1)\psi_2 - \zeta_1]\right] \\
&= \left[\mathcal{N}_c(\tau_1)\mathcal{F}_{1/2}[\omega_2 + \delta\mathcal{E} + \delta\xi + \mathbf{P}^{-1}\mathbf{P}(\tau_1)\psi_2 - \zeta_2] - \mathcal{N}_c(\tau_2)\mathcal{F}_{1/2}(\omega_2)\right] \\
&= \left[\mathcal{N}_c(\tau_1)\left(\mathcal{F}_{1/2}(\omega_2 + \delta\mathcal{E} + \delta\xi) - \mathcal{F}_{1/2}(\omega_2)\right) - \delta\mathcal{N}_c\mathcal{F}_{1/2}(\omega_2)\right. \\
&\quad \left. + \mathcal{N}_c(\tau_1)\left(\mathcal{F}_{1/2}[\tilde\omega - \mathbf{P}^{-1}\mathbf{P}(\delta\tau)\psi_2] - \mathcal{F}_{1/2}(\tilde\omega)\right)\right]
\end{aligned}$$

with $\zeta_2 - \mathbf{P}^{-1}\mathbf{P}(\tau_1)\psi_2 = \mathbf{P}^{-1}\mathbf{P}(\delta\tau)\psi_2$ and $\tilde\omega := \omega_2 + \delta\mathcal{E} + \delta\xi$.

As in the proof of the preceding lemma we get upper bounds for the absolute values of the diverse summands of the sum F such that each bound is quadratic in the small terms $\|\delta\xi\|$, $\|\delta\tau\|$, or $|\delta\tau|_\infty$.

We set $\chi_i :\equiv \xi_i - \zeta_i$. The difference F can be written in the form

$$\begin{aligned}
F = &- \int\int_0^{\delta\tau}\int_0^{\sigma} c_L\left(\frac{1}{z+\tau_1}\right)\frac{1}{(z+\tau_1)^2}\ dz\ d\sigma\ d\Omega \\
&- \int\left[h_n(\chi_2,\tau_2) - h_n(\chi_1,\tau_1) - \delta\tau\partial_\tau h_n(\chi_1,\tau_1) - \delta\chi\partial_\chi h_n(\chi_1,\tau_1)\right]\ d\Omega \\
&- \frac{1}{2}\langle\mathbf{P}(\tau_2)\delta\psi,\delta\psi\rangle\ ,
\end{aligned}$$

such that $F < 0$ obviously holds because of the assumption (2.9). $\square$

4. Convex analysis

The convex analysis is often presented in connection with proper convex lsc functionals on real reflexive Banach spaces (lsc means lower semicontinuous) or with monotone operators which map a real reflexive Banach space into its dual space, and many statements rest on the fact that bounded closed convex sets in reflexive Banach spaces are weakly compact. The theory can partially be carried over to proper convex w*lsc functionals on the dual space E' of a real Banach space E or to monotone operators which map E' into E, because the bounded closed convex sets in E' are weakly* compact.

Let, e.g., ϕ_0 denote a convex F-differentiable functional on an open convex subset U in an affine dual space $f_0 + E'$ of a real Banach space E such that the F-derivative $d\phi_0$ maps U in E. The functional $-H$ on Z_∞^D in the preceding section is an example. The functionals $f \mapsto \phi_0(g) + \langle f - g, d\phi_0(g)\rangle$ ($g \in U$ fix) are weakly* continuous affine functionals on $f_0 + E'$ which satisfy $\phi_0(f) \geq \phi_0(g) + \langle f - g, \partial\phi_0(g)\rangle$ for all $g \in U$. Therefore

$$\phi(f) := \sup_{g \in U} [\ \phi_0(g) + \langle f - g, d\phi_0(g)\rangle\ ]$$

defines a proper convex w*lsc extension of ϕ_0 onto the whole affine Banach space $f_0 + E'$. Let ϕ' denote the conjugate functional

$$\phi'(x) := \sup_{f \in f_0 + E'} \{\langle f - f_0, x\rangle - \phi(f)\}\ .$$

The biconjugate functional on $f_0 + E'$,

$$\phi"(f) := \sup_{x \in E} \{\langle f - f_0, x\rangle - \phi'(x)\} = \phi(f)\ ,$$

coincides with ϕ, since ϕ is the upper envelope of a family of weakly* continuous affine functions. Therefore the relations

$$x \in \partial\phi(f) \quad \Leftrightarrow \quad f - f_0 \in \partial\phi'(x) \quad \Leftrightarrow \quad \phi'(x) = \langle f - f_0, x\rangle - \phi(f) \tag{4.1}$$

hold. In particular, for $f - f_0 \in U$ the equivalence

$$x = d\phi_0(f) \quad \Leftrightarrow \quad f - f_0 \in \partial\phi'(x)$$

holds. Let H_- denote the corresponding extension of $-H$ from Z_∞^D onto the whole affine Banach space $z^D + Z_\infty$. The subdifferential ∂H_- coincides on Z_∞^D with the F-derivative $-dH$. The following proposition is adapted from a well known result (cf [4], Prop 2.13, p.41).

Proposition 4.1. *Let E be a real Banach space and E' its dual space. For any proper convex w*lsc functional F on E' the subdifferential $\partial F \subset E' \times E$ is surjective if and only if*

$$\lim_{||f|| \to \infty} [\ F(f) - \langle f, x\rangle\ ] = \infty$$

for any $x \in E$.

Proof. 1) If the condition is satisfied, then the functional $F(f) - \langle f, x\rangle$ attains its minimum in some point f_0, since w*lsc functionals attain their infimum on weakly* compact sets. Thus $F(f) - \langle f, x\rangle \geq F(f_0) - \langle f_0, x\rangle$, i.e. $x \in \partial F(f_0)$.

2) Let ∂F be surjective, but let us assume that there is an unbounded sequence (f_n) in E' for which there is an $x \in E$ such that $F(f_n) - \langle f_n, x \rangle \leq a < \infty$ holds for all n. As a consequence of the 'resonance theorem' ([17]) there is a $z \in E$ such that $\langle f_n, z \rangle \to \infty$. There is an $g \in E'$ such that $x + z \in \partial F(g)$ because of the surjectivity. Therefore the inequality $F(f_n) \geq F(g) + \langle f_n - g, x + z \rangle$ holds in contradiction to the unboundedness of $(\langle f_n, z \rangle)$, namely,

$$\langle f_n, z \rangle \leq F(f_n) - \langle f_n, x \rangle - F(g) + \langle g, x + z \rangle \leq a - F(g) + \langle g, x + z \rangle \ .$$

□

The space Z_∞ is densely and continuously imbedded into $\mathbf{H} = L_2(\Omega) \times L_2(\Omega) \times L_2(\Omega)$. Thus we have an evolution triple $Z_\infty \hookrightarrow \mathbf{H} \hookrightarrow Z$, which allows to introduce the Banach space

$$W(S) = \{ \ z \in L_2(S, Z_\infty) \ : \ \dot{z} \in L_2(S, Z) \ \} \hookrightarrow C(S, \mathbf{H})$$

on any compact interval S of time with the norm $\|.\|_W$ defined by

$$\|z\|_W^2 = \|z\|^2_{L_2(S,Z_\infty)} + \|\dot{z}\|^2_{L_2(S,Z)} \ .$$

In contrast to the usual evolution triples $V \hookrightarrow \mathbf{H} \hookrightarrow V'$, the Banach space Z_∞ is not reflexive, but we have $V = Z'$ and $V' = Z$ such that the weak* compactness substitutes the weak compactness in some sense. (We consider also the possibility to substitute the third factor of H by the direct sum $L_2(\Omega) \oplus L_2(\Gamma)$. The choice of one of the two alternatives seems to be related to the formulation of the boundary value problem for the Poisson equation and the choice of $\mathbf{P}$. The choice is relevant with respect to the initial-value problem, because the initial values are naturally chosen in $\mathbf{H}$!)

5. The energy model, time discretization and regularization

The current equations of the energy model are

$$\begin{aligned} j_n &= -D_n n(\nabla v + P_n \nabla T), \\ j_p &= \quad D_p p(\nabla w - P_p \nabla T), \\ j_u &= -\kappa \nabla T + (TP_n + v) j_n + (TP_p - w) j_p, \end{aligned}$$

with the diffusion coefficient (or, as a matter of scaling, the carrier mobility) D_i, the thermoelectric power P_i and 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. [15] or [16]). The electrochemical potentials v and w have the opposite sign as the quasi-Fermi levels φ_n and φ_p in [15]. These current equations can be written in a more symmetric form, namely,

$$\begin{pmatrix} j_n \\ j_p \\ j_u \end{pmatrix} = \mathbf{D} \nabla \begin{pmatrix} -v/T \\ w/T \\ 1/T \end{pmatrix} \tag{5.1}$$

with

$$\mathbf{D} = \begin{pmatrix} nTD_n & 0 & nT^2D_n\left(P_n + \frac{v}{T}\right) \\ 0 & pTD_p & pT^2D_p\left(P_p - \frac{w}{T}\right) \\ nT^2D_n\left(P_n + \frac{v}{T}\right) & pT^2D_p\left(P_p - \frac{w}{T}\right) & \mathcal{D} \end{pmatrix}$$

and

$$\mathcal{D} = T^2\kappa + nT^3D_n\left(P_n + \frac{v}{T}\right)^2 + pT^3D_p\left(P_p - \frac{w}{T}\right)^2 .$$

We do not yet specify the coefficients, which are state variables, but we remark that the matrix $\mathbf{D}$ is a symmetric positive semi-definite matrix in accordance with the Onsager principle. As a model case we mention the material functions $D_n = D_{\beta_n}T^{\beta_n}$, e.g. $\beta_n = -1/2$, and then

$$P_n + \frac{v}{T} = \frac{5}{2} + \beta_n + \tau(E_c - \Psi)$$

and, similarly,

$$P_p - \frac{w}{T} = \frac{5}{2} + \beta_p - \tau(E_v - \Psi)$$

(cf [13]).

We observe the discrepancy between the thermodynamic forces in (5.1) and the conjugate variables (ξ, η, τ) of (n, p, u). If we derive, however, current equations from the entropy balance equation (a suggestion made by W. Muschik, Berlin) then we get the equation

$$\begin{pmatrix} j_n \\ j_p \\ j_u \end{pmatrix} = \mathbf{D}\nabla \begin{pmatrix} \xi \\ \eta \\ \tau \end{pmatrix} \tag{5.2}$$

in a similar way as the conjugate variables were determined in the preceding section. Therefore we suggest to modify the conventional energy model by substituting (5.1) by (5.2). We do not have the competence to decide which of the current equations (5.1) or (5.2) are the correct equations, but we believe that it is a reasonable question for experimenters and for more physically educated specialists.

Under suitable assumptions on the coefficient matrix $\mathbf{D}$ in the current equations a monotone potential operator $\partial_z A(n, p, T, .)$ is defined with the potential

$$A(z) \equiv A(n, p, T, z) := \frac{1}{2}\int \nabla z \cdot \mathbf{D}(n, p, T)\nabla z \; d\Omega .$$

The functions n, p, and T are not considered as the state variables related to z here, but they are considered as suitable measurable positive parameter functions. The potential is F-differentiable (with respect to z) and its derivative has values in Z.

Typical net recombination rates used in the drift-diffusion model are $R = r_+(n, p, T)(np - n_i^2)$ with the intrinsic carrier density n_i or $R = r_+(n, p, T)(e^{v-w} - 1)$ with a positive function $r_+ : R_+^3 \mapsto R_+$. As the temperature is more or less a scaling parameter in the drift-diffusion model, we also regard the net recombination rate

$$R \equiv r_+(n, p, T)\left[\; e^{(v-w)/T} - 1 \;\right] = r_+(n, p, T)(e^{-\xi-\eta} - 1) ,$$

which is advantageous in some sense as we will see below. The advantage of this expression is also preserved in the case

$$R \equiv r_+(n,p,T)(e^{v-w}-1) =: r_-(n,p,T)\frac{1}{T}e^{-(\xi+\eta)T} - r_+(n,p,T) \ .$$

If n, p, and T are positive real numbers, then

$$g_1(n,p,T,z) = r_+(n,p,T)(\xi+\eta+e^{-\xi-\eta})$$

or

$$g_2(n,p,T,z) = r_+(n,p,T)(\xi+\eta) + r_-(n,p,T)\frac{1}{T}e^{-(\xi+\eta)T}$$

are differentiable convex functions of $z=(\xi,\eta,\tau)\in R^3$ (,which do not depend on τ). Under suitable assumptions on r_+, r_- and on the parameter functions n, p, and T the convex differentiable functions $g(n,p,T,z)$ define proper convex lsc functionals $G(n,p,T,.)$ on $L_2(\Omega)^3$ by

$$G(n,p,T,z) = \int g[n(x),p(x),T(x),z(x)]\ d\Omega$$

($G(n,p,T,z)=\infty$ if the integrand is not integrable). Since z^D+Z_∞ is continuously imbedded in $L_2(\Omega)^3$, G is a proper convex lsc functional also on z^D+Z_∞, such that $\mathcal{G}(n,p,T,z) := \int_S G[n(t),p(t),T(t),z(t)]\ dt$ is also a proper convex lsc functional on $z^D+L_2(S,Z_\infty)$. The effective domains of definition of the functionals $G(n,p,T,.)$ and $\mathcal{G}(n,p,T,.)$ do not contain interior points, since there are L_2 functions u arbitrarily close to 0 such that e^{-u} is not integrable. Therefore we will regularize g by substituting the factors $e^{-\xi}$ and $e^{-\eta}$ by convex functions with bounded derivatives such that the regularized potentials $\tilde{G}(n,p,T,.)$ and $\tilde{\mathcal{G}}(n,p,T,.)$ are F-differentiable on the whole space and such that the derivative attains values in Z or in $L_2(S,Z)$.

The evolution equation

$$\partial_t \begin{pmatrix} n \\ p \\ u \end{pmatrix} + \nabla\cdot\left[\mathbf{D}\begin{pmatrix} \nabla\xi \\ \nabla\eta \\ \nabla\tau \end{pmatrix}\right] + \begin{pmatrix} \tilde{R} \\ \tilde{R} \\ 0 \end{pmatrix} = 0$$

with a regularized recombination term can be considered as an equation

$$\partial_t d\mathcal{H}_-(z) + \partial_z\mathcal{A}(n,p,T,z) + \partial_z\tilde{\mathcal{G}}(n,p,T,z) = 0 \tag{5.3}$$

in $L_2(S,Z)$ for functions $z\in z^D+L_2(S,Z_\infty)$ with values $z(t)\in Z^D_\infty$ for $a.a.\ t\in S$.

The initial-value problem for (5.3) on a finite closed time interval $S=[0,T^*]$ is discretized in time now. Let denote $t_k = kT^*/M$ discrete times ($k=0,\ 1,\ \ldots,M$), $\lambda_M = M/T^*$, y_k the value of a state variable y at time t_k (n_0, p_0 and u_0 or T_0 are given initial data) and $\Delta_k y := y_k - y_{k-1}$. A discrete version of the initial-value problem for the evolution equation (5.3) reads

(5.4)

$$dH_-(z_k) + \lambda_M\left[\ dA_{k-1}(z_k) + d\tilde{G}_{k-1}(z_k)\ \right] = dH_-(z_{k-1}) \qquad (k=1,\ 2,\ \ldots,\ M)$$

with $A_{k-1}(z_k) := A(n_{k-1},p_{k-1},T_{k-1},z_k)$. The sum rule can be applied to the functionals H_-, A_{k-1} and $\tilde{G}_{k-1}$ such that we have a finite sequence of minimum problems with the proper convex w*lsc functionals $H_- + \lambda(A_{k-1}+\tilde{G}_{k-1})$. Notice that the minimum problems generalizes the equations (5.4) in so far as the F-derivative dH_-

is substituted by its multivalued subdifferential extension. A priori estimates will be necessary which guarantee that the τ_k are strictly positive. The functionals satisfy the surjectivity condition in the Proposition 4.1 such that a generalized regularized solution of the discretized problem exist (details have to be checked yet!).

We are interested in the question, whether the conjugate functional of the convex extension H_- can be applied to get first a priori estimates as in the case of the drift-diffusion model.

For any (affine) Banach space X let $L_2^M(S,X) \subset L_2(S,X)$ denote the space of step functions u which are constant u_k on $]t_{k-1},t_k]$, and $C_M(S,X) \subset C(S,X) \cap H^1(S,X)$ the space of continuous functions with the values u_k at the discrete times t_k which are affine between the discrete times. We define discrete time derivatives $\partial_M^{u_0} u \in L_2^M(S,X)$ for functions $u \in L_2^M(S,X)$ with initial values $u_0 \in X$, namely $\partial_M^{u_0} u = \lambda_M(u_k - u_{k-1})$ on $]t_{k-1},t_k]$. The integral of this function with respect to time with the initial value u_0 is just $L_M^{u_0} u \in C_M(S,X)$ with the values u_k. We introduce, moreover, the map $\mathbf{T}_M^{u_0} : L_2^M(S,X) \mapsto L_2^M(S,X)$ by $[\mathbf{T}_M^{u_0} u]_k := u_{k-1}$. The discretized problem (5.4) can be considered as the problem

$$\partial_M^{u_0} d\mathcal{H}_-(z) + \partial_z \mathcal{A}(\mathbf{T}_M^{n_0} n, \mathbf{T}_M^{p_0} p, \mathbf{T}_M^{T_0} T, z) + \partial_z \tilde{\mathcal{G}}(\mathbf{T}_M^{n_0} n, \mathbf{T}_M^{p_0} p, \mathbf{T}_M^{T_0} T, z) = 0 \tag{5.5}$$

in $L_2(S,Z)$ for functions $z \in z^D + L_2^M(S,Z_\infty)$. Let us assume that we would have a solution $z^M \in z^D + L_2^M(S,Z_\infty)$ with $\rho^M = d\mathcal{H}_-(z^M)$ for each large natural number M. What about upper bounds

$$\sup_M \max \left[\ \|z^M - z^D\|_{L_2(S,Z_\infty)} \ , \ \|\partial_M^{\rho_0} \rho^M\|_{L_2(S,Z)} \ , \ \|L_M^{\rho_0} \rho^M\|_{C(S,\mathbf{H})} \ \right] \quad ? \tag{5.6}$$

Let S_- denote the conjugate functional on Z of H_-,

$$S_-(\rho) = \sup_{z \in z^D + Z_\infty} \{ \ \langle \rho, z - z^D \rangle - H_-(z) \ \} \ .$$

The biconjugate functional H_-" of H_- coincides with H_-, because H_- is an upper envelope of weakly* continuous affine functions on $z^D + Z_\infty$. Moreover, the relations

$$\rho \in \partial H_-(z) \quad \Leftrightarrow \quad z - z^D \in \partial S_-(\rho) \quad \Leftrightarrow \quad S_-(\rho) = \langle \rho, z - z^D \rangle - H_-(z)$$

hold, in particular, we have

$$\rho = dH_-(z) \quad \Leftrightarrow \quad z - z^D \in \partial S_-(\rho) \quad \Leftrightarrow \quad S_-(\rho) = \langle dH_-(z), z - z^D \rangle - H_-(z)$$

for $z \in Z_\infty^D$. The definition of the subgradient yields

$$\begin{aligned} S_-(\rho_k) - S_-(\rho_{k-1}) &\leq \langle \rho_k - \rho_{k-1}, z_k - z^D \rangle \\ &= -\lambda \langle dA_{k-1}(z_k) + d\tilde{G}_{k-1}(z_k), z_k - z^D \rangle \end{aligned}$$

for solutions $z_k - z^D \in Z_\infty$ of the equation

$$\partial \{ \ H_-(z_k) + \lambda [A_{k-1}(z_k) + \tilde{G}_{k-1}(z_k)] \ \} \ni \rho_{k-1}$$

and for $\rho_k \in \partial H_-(z_k)$. Summing up the estimates for a single time step, we get the physically motivated a priori estimates

$$S_-(\rho_k) + \lambda_M \sum_1^k \langle [dA_{j-1}(z_j) - dA_{j-1}(z^D)] + [d\tilde{G}_{j-1}(z_j) - d\tilde{G}_{j-1}(z^D)], z_j - z^D \rangle$$

$$\leq S_-(\rho_0) - \lambda_M \sum_1^k \langle dA_{j-1}(z^D) + d\tilde{G}_{j-1}(z^D), z_j - z^D \rangle \tag{5.7}$$

$(k = 1, ..., M)$, which we had in mind from the beginning. Note that all the summands on the left-hand side are non-negative, but sharper estimates from below will be necessary for finding upper bounds (5.6).

6. The conventional energy model

The fact that the total energy is the sum of the electrostatic energy and of the interior energy allows still another approach. We change the notation in this section slightly.

The state variables n, p, T, v, w, $\tau = 1/T$, N_c, $\mathcal{N}_c$, ..., E_v, and $\mathcal{E}_v$ have the same meaning as before, but u denotes the density of the interior energy. We set $\xi := -v/T$, $\eta := w/T$, and we introduce $\zeta_n = \xi - \tau\Psi$ and $\zeta_p = \eta + \tau\Psi$. We consider $z :\equiv (\zeta_n, \zeta_p, \tau) \equiv: (\zeta, \tau)$ as independent state variables. The carrier densities read $n = \mathcal{N}_c(\tau)\mathcal{F}_{1/2}[-\zeta_n - \mathcal{E}_c(\tau)]$ and $p = \mathcal{N}_v(\tau)\mathcal{F}_{1/2}[\mathcal{E}_v(\tau) - \zeta_p]$ in these variables. The Dirichlet data on $\partial\Omega \setminus \Gamma$ are given now by functions $\zeta^D \in H^1(\Omega)^2$ and by Ψ^D, τ^D as above. As before there is an open convex set $\mathcal{Z}^+ \subset Z_\infty$ such that

$$\mathcal{Z}_\infty^D := [\zeta^D + (H_0^1)^2] \times [(\tau^D + H_0^1) \cap L_\infty^+] = z^D + \mathcal{Z}^+$$

holds. The evolution equation of the energy model with the (conventional) current equation (5.1) reads

$$\partial_t \begin{pmatrix} n \\ p \\ u \end{pmatrix} + \nabla \cdot \left[\mathbf{D} \begin{pmatrix} \nabla\xi \\ \nabla\eta \\ \nabla\tau \end{pmatrix} \right] = \begin{pmatrix} -R \\ -R \\ \Psi\nabla\cdot(j_p - j_n) \end{pmatrix} . \tag{6.1}$$

We test the equation with functions $\bar{z}$. Since

$$\begin{aligned} & \langle \nabla\cdot j_n, \bar{\zeta}_n \rangle + \langle \nabla\cdot j_p, \bar{\zeta}_p \rangle \;+\; \langle \nabla\cdot j_u, \bar{\tau} \rangle - \langle \Psi\nabla\cdot(j_p - j_n), \bar{\tau} \rangle \\ = \; & \langle \nabla\cdot j_n, \bar{\zeta}_n + \Psi\bar{\tau} \rangle + \langle \nabla\cdot j_p, \bar{\zeta}_p - \Psi\bar{\tau} \rangle \;+\; \langle \nabla\cdot j_u, \bar{\tau} \rangle \, , \end{aligned}$$

we get

$$\begin{aligned} & \langle \dot{n}, \bar{\zeta}_n \rangle + \langle \dot{p}, \bar{\zeta}_p \rangle + \langle \dot{u}, \bar{\tau} \rangle \;+\; \int R(\bar{\zeta}_n + \bar{\zeta}_p)\, d\Omega \\ & - \int \nabla \begin{pmatrix} \bar{\zeta}_n + \Psi\bar{\tau} \\ \bar{\zeta}_p - \Psi\bar{\tau} \\ \bar{\tau} \end{pmatrix} \cdot \mathbf{D}\nabla \begin{pmatrix} \xi \\ \eta \\ \tau \end{pmatrix} d\Omega \;=\; 0 \, . \end{aligned}$$

Before we discretize the evolution equation with respect to time, we introduce a convex function h_- on the open half-space $R \times R \times R_+$. This function is defined for any point $z = (\zeta_n, \zeta_p, \tau) \in R \times R \times R_+$ by

$$
\begin{aligned}
h_-(z) \;=\; -\int_{\tau^D}^{\tau}\int^{1/\sigma} c_L(s)\ ds\ d\sigma + h_n(\zeta_n,\tau) - h_n(\zeta_n^D,\tau^D)\\
+ h_p(\zeta_p,\tau) - h_p(\zeta_p^D,\tau^D)
\end{aligned}
\tag{6.2}
$$

with a fixed point $z^D \in R \times R \times R_+$. We notice that the partial derivatives are just $-\nabla h_-(z) = (n, p, u)$ according to the state equations used in this preprint. This function is extended to a proper convex lsc functional on R^3 by

$$
h_-(\zeta,\tau) := \sup_{(y,s)\in R^2\times R_+} [\ h_-(y,s) + (\zeta - y)\partial_y h_(y,s) + (\tau - s)\partial_s h_(y,s)\ ]\ . \tag{6.3}
$$

We set

$$
H_-(z) = \int_\Omega h_-[z(x)]\ dx \equiv \int h_-[z]\ d\Omega
$$

for functions $z \in L_2(\Omega)^3$, if $h_- \circ z \in L_1(\Omega)$, but $+\infty$ elsewhere.

Theorem 6.1. *The functional H_- on $\mathcal{Z}_\infty^D$ is convex and F-differentiable with $dH_-(z) \in Z$.*

Proof. The proof is carried out for a system of electrons only. Let y_i $(i = 1, 2)$ denote the value of any state variable y in the state (ζ_i, τ_i) and $\delta y := y_2 - y_1$. The integrability of the functions h_{-i} follows from the estimate (3.3) in Lemma 3.1 with $w = \zeta_i$, $\mathcal{E} = \mathcal{E}_c(\tau_i)$. We already know the derivatives of h_- such that we have to prove that

$$
0 < F := H_{-2} - H_{-1} + \int \delta\zeta n_1 + \delta\tau u_{if}(n_1, T_1)\ d\Omega = o(\|\delta\zeta\| + \|\delta\tau\| + |\delta\tau|_\infty)
$$

for small $\delta\zeta \oplus \delta\tau \neq 0$. The following formula, in which d^2h_n denotes the matrix of the second-order partial derivatives of the function h_n on $R \times R_+$, is checked at the end of the Appendix (if z^D and z are identified there with z_2 and z_1, respectively).

$$
\begin{aligned}
F = \int\int_{\tau_2}^{\tau_1}\int_\sigma^{\tau_1} c_L(\frac{1}{y})\frac{1}{y^2}\ dy\ d\sigma\ d\Omega\\
+ \int \begin{pmatrix}\delta\zeta\\ \delta\tau\end{pmatrix} \cdot \int_0^1\int_0^t d^2h_n(\zeta_1 + s\delta\zeta, \tau_1 + s\delta\tau)\ ds\ dt \begin{pmatrix}\delta\zeta\\ \delta\tau\end{pmatrix}\ d\Omega\ .
\end{aligned}
\tag{6.4}
$$

Since there are bounds $0 < \underline{\tau} \leq \tau_i \leq \bar{\tau}$, we have an upper bound $C|\delta\tau|_\infty^2/\underline{\tau}^2$ for the first summand on the left-hand side of (6.4). According to our assumptions on the material laws N_a and E_a the non-negative second summand can be estimated by a sum of terms

$$
C\int |\delta\zeta|^j|\delta\tau|^{2-j}\int_0^1\int_0^t \mathcal{F}_{3/2-k}[-\zeta_1 - s\delta\zeta - \mathcal{E}(\tau_1 + s\delta\tau)]\ ds\ dt\ d\Omega
$$

$(j,\ k \in \{0, 1, 2\})$. The summands can be estimated from above by

$$
C|\delta\tau|_\infty^{2-j}|\delta\zeta|_6^j\int_0^1\int_0^t |\mathcal{F}_{3/2-k}[-\zeta_1 - s\delta\zeta - \mathcal{E}(\tau_1 + s\delta\tau)]|_{p_j}\ ds\ dt
$$

$(p_0 = 1\ ,\quad p_1 = 6/5\ ,\quad p_2 = 3/2)$. According to Lemma 3.1 we have

$$
|\mathcal{F}_{3/2-k}(-\zeta - \mathcal{E})|_{2q_j/(5-2k)} \leq A_{q_j,3/2-k} + B_{3/2-k}|\zeta|_{q_j}^{5/2-k}\ .
$$

These estimates imply the assertions of the theorem, because

$$q_j = (\frac{5}{2} - k)p_j \leq (\frac{5}{2} - k)\frac{3}{2} \leq \frac{15}{4} < 6 \ .$$

□

The potentials $\tilde{g}(n,p,T,z)$ on R^3, $\tilde{G}(n,p,T,z)$ on $L_2(\Omega)^3$ and $\tilde{\mathcal{G}}(n,p,T,z)$ on $L_2[S, L_2(\Omega)^3]$ of the preceding section are used here with ζ instead of (ξ, η) there. This change is possible, because the potentials depend on z via the sum $\zeta_n + \zeta_p = \xi + \eta$. We have to find, moreover, a suitable function space on which the potential

$$b(n,p,T,\psi,z) = \frac{1}{2}\int \nabla \begin{pmatrix} \zeta_n + \Psi\tau \\ \zeta_p - \Psi\tau \\ \tau \end{pmatrix} \cdot \mathbf{D}(n,p,T)\nabla \begin{pmatrix} \zeta_n + \Psi\tau \\ \zeta_p - \Psi\tau \\ \tau \end{pmatrix} \ d\Omega$$

in $z = (\zeta, \tau)$ is well defined for measurable positive parameter functions n, p, T, and for parameter functions Ψ which are solutions of the Poisson equation $\mathbf{P}\Psi(t) = [d - n(t) + p(t)]$ in H^{-1} for functions $\Psi(t) \in \Psi^D + H_0^1$ with the operator

$$\langle \mathbf{P}\chi, \phi \rangle := \int \epsilon \nabla\chi \cdot \nabla\phi \ d\Omega + \int_\Gamma (b\chi - g)\phi \ d\Gamma \ .$$

The functions Ψ will belong to the space $\Psi^D + V_p$, where $V_p := \{u \in W_p^1(\Omega) : u|_{\partial\Omega\setminus\Gamma} = 0\}$ is chosen with a parameter $p > 2$ (cf [12]). Therefore the function spaces $\Psi \in \Psi^D + V_p \cap L_q$ and $\tau \in \tau^D + V_p \cap L_q$ with a reflexive function space $V_p \cap L_q$ instead of $H_0^1 \cap L_\infty$, where the parameter p near 2 and a large q are chosen such that $\frac{1}{q} + \frac{1}{p} \leq \frac{1}{2}$, might be reasonable candidates (cf [9], [12]).

The evolution equation (6.1) with the regularized net recombination rate $\tilde{R}$ instead of R reads

(6.5)

$$\partial_t dH_-[z(t)] + \partial_z B[n(t), p(t), T(t), \Psi(t), z(t)] + \partial_z \tilde{G}[n(t), p(t), T(t), z(t)] = 0 \ .$$

The system of equations which arises if this equation is discretized in the time reads

(6.6) $$\partial\{ \ H_-(z_k) + \lambda_M[B_{k-1}(z_k) + \tilde{G}_{k-1}(z_k)] \ \} \ni \rho_{k-1} \qquad (\rho_{k-1} \in \partial H_-(z_{k-1}))$$

($k = 1, \ \ldots, \ M$), but it has to be supplemented by the Poisson equation $\mathbf{P}\Psi_k = [d - n_k + p_k]$ ($k = 0, 1, \ \ldots, \ m$) in H^{-1} for functions $\Psi \in \Psi^D + H_0^1$. It might be advantageous to apply the non-linear Poisson equations $\mathbf{P}\Psi_k = [d - n_k e^{\Psi_k - \Psi_{k-1}} + p_k e^{\Psi_{k-1} - \Psi_k}]$ instead of the linear ones.

The density u of the interior energy of the system as a function of n, p and T reads

$$\begin{aligned} u \ \equiv \ u_{if}(n,p,T) \ = \ \int^T c_L(y)dy \ &+ \ n\mathcal{E}_c'(1/T) + T^2 N_c'(T)\mathcal{F}_{3/2} \circ \mathcal{F}_{1/2}^{-1}\left[\frac{n}{N_c(T)}\right] \\ &- \ p\mathcal{E}_v'(1/T) + T^2 N_v'(T)\mathcal{F}_{3/2} \circ \mathcal{F}_{1/2}^{-1}\left[\frac{p}{N_v(T)}\right] \end{aligned}$$

($\mathcal{E}_c'(1/T) = E_c(T) - TE_c'(T)$). The conjugate function

(6.7) $$s_-(\rho) = \sup_{z \in R^2 \times R_+} \{ \ \langle \rho, z - z^D \rangle - h_-(z) \ \} \geq 0$$

of h_- can be alternatively described on the domain

$$\Delta := \left\{ \rho = -\begin{pmatrix} n \\ p \\ u_{if}(n,p,T) \end{pmatrix} \ : \ 0 < n,p,T \right\} \subset R^3$$

by means of the conjugate variables. The identity

$$s_-(\rho) = (\tau - \tau^D)^2 \int_0^1 \int_0^t \frac{1}{[\tau + s(\tau^D - \tau)]^2} c_L \left[\frac{1}{\tau + s(\tau^D - \tau)} \right] \ ds \ dt$$

$$+ \sum_a \begin{pmatrix} \zeta_a - \zeta_a^D \\ \tau - \tau^D \end{pmatrix} \cdot \int_0^1 \int_0^s d^2 h_a[(\zeta_a, \tau) + t(\zeta_a^D - \zeta_a, \tau^D - \tau)] \ ds \ dt \begin{pmatrix} \zeta_a - \zeta_a^D \\ \tau - \tau^D \end{pmatrix}$$

on Δ is checked at the end of the Appendix. It holds analogously to the equation (6.4) in the proof of Theorem 6.1. Analogous properties has the conjugate functional S_- of H_- on $L_2(\Omega, R^3)$ which is also defined by $S_-(\rho) = \int_\Omega s_-[\rho(x)] \ dx$ if $s_- \circ \rho \in L_1(\Omega)$, but $S_-(\rho) = \infty$ elsewhere (cf [4]).

As in the preceding section we get the physically motivated a priori estimates

$$S_-(\rho_k) + \lambda_M \sum_1^k \langle [dB_{j-1}(z_j) - dB_{j-1}(z^D)] + [d\tilde{G}_{j-1}(z_j) - d\tilde{G}_{j-1}(z^D)], z_j - z^D \rangle$$

$$\leq S_-(\rho_0) - \lambda_M \sum_1^k \langle dB_{j-1}(z^D) + d\tilde{G}_{j-1}(z^D), z_j - z^D \rangle \tag{6.8}$$

$(k = 1, ..., M)$ for solutions $z^M = (z_1^M, ..., z_M^M)$ of the discretized equation (6.6).

7. An illustrative test example

Let us consider the problem

$$(\dot{n} + R, \dot{p} + R, \dot{u}) = 0, \quad \rho(0) = \rho_0 \ .$$

We discuss a model case only, i.e. the material laws are $c_L(y) = c_L > 0$ constant, $\mathcal{N}_a(\tau) = N_a \tau^{-3/2}$ and $\mathcal{E}_a(\tau) = \tau E_a$ with constants $N_a > 0$ and $E_c > E_v$, $r(n,p,T) = r_1 T^3 e^{-E_g/T} \equiv: r_1 n_i(T)^2$ with a positive constant $r_1 > 0$ and with the gap width $E_g = E_c - E_v > 0$. Even this simple example is fairly illustrative. Our approach requires some ideas from [10], although a lot of technical problems are avoided.

Let us consider the problem more directly, before we apply the calculus of the preceding section. We introduce the sum $Z := \zeta_n + \zeta_p$. The carrier densities n and p changes in a (short) time interval according to $\delta n = \delta p = -r(e^{-Z} - 1)$, i.e. Z and the change $\delta n = \delta p$ have the same sign. Because of both the inequalities $\partial_T u_{if} \geq c_L > 0$ and $\partial_n u_{if} + \partial_p u_{if} \geq E_c - E_v \equiv E_g > 0$ the change δn is connected with a change δT of the opposite sign and with a change $\delta Z = A\delta T - B\delta n$ with coefficients $A > E_g/T^2$ and $B > 0$. The change δZ has the opposite sign as Z, i.e. $Z \to 0$ in a monotone way.

In this example there is no reason to prefer the Fermi-Dirac statistics to the Boltzmann statistics, and we will take sometimes the last one, because formulas are more transparent. The following arguments show (in the case of Boltzmann statistics) that the initial-value problem has an unique solution. The charge and the energy are conserved, i.e.

$$p - n = p_0 - n_0 =: Q_0 \ , \tag{7.1}$$

$$c_L T + \frac{1}{2}(E_g + 3T)(n+p) = u_0 + \frac{1}{2}(E_c + E_v) Q_0 \ . \tag{7.2}$$

We consider the case of Boltzmann statistics and introduce the variable $Y = e^{-Z}$. The two conservation laws admit exactly one state for each $Y \in [\min(1, e^{-Z_0}), \max(1, e^{-Z_0})]$. To see this, we set $X = N_c e^{\zeta_n}$ and substitute the state equations in the conservation laws. The conservation of charge yields

$$n = \sqrt{Y n_i(T)^2 + Q_0^2/4} - Q_0/2 \ .$$

The conservation of energy reads then

$$\sqrt{Y n_i(T)^2 + Q_0^2/4} = -\frac{1}{3} c_L + \frac{u_0 + (E_c + E_v)Q_0/2 + c_L E_g/3}{E_g + 3T}$$

for $T > 0$. Since $u_0 + (E_c + E_v)Q_0/2 > 0$, the equation has exactly one solution if and only if

$$E_g \sqrt{Y n_i(0)^2 + Q_0^2/4} \le u_0 + (E_c + E_v)Q_0/2 \ .$$

This condition is fulfilled, since

$$u_0 + (E_c + E_v)Q_0/2 = c_L T_0 + (3T_0 + E_g)\sqrt{Y_0 n_i(T_0)^2 + Q_0^2/4} > \frac{1}{2} E_g |Q_0| \ .$$

This fact guarantees the uniqu solvability.

It is interesting to see that the conservation of the energy and of the charge do not yield too much a priori estimates. We have seen only three non-trivial bounds, namely,

$$T < \frac{1}{c_L}[u_0 + (E_c + E_v)Q_0/2] \ , \quad n+p < \frac{2}{E_g}[u_0 + (E_c + E_v)Q_0/2] \ , \quad |Q_0| < \max(n,p) \ .$$

Of course, there are more bounds in connection with $0 \le |Z| \le |Z_0|$, but the question is to have bounds which are easily evaluated.

With the potentials h_- and g which were introduced in the preceding sections the initial-value problem can be written in the form

$$\dot{\rho} + \partial_z g(T, z) = 0 \ , \quad \rho = dh_-(z) \ , \quad \rho(0) = \rho_0 \ . \tag{7.3}$$

The evolution equation can be considered as a family of problems

$$\partial_t dh_-[z(t)] + \partial_z g[T(t), z(t)] = 0 \ , \quad z(0) = z_0 \tag{7.4}$$

depending on a parameter $x \in \Omega$. The problem is compatible with the Dirichlet data on $\partial\Omega \setminus \Gamma$ if and only if $R = R^D = 0$ there. This condition is satisfied if the electron-hole equilibrium is assumed to hold on the Dirichlet boundary (in the simulation practice this equilibrium is accepted on the Dirichlet contacts). We start with a regularized problem

$$\partial_t dh_-[z(t)] + \partial_z \tilde{g}[T(t), z(t)] = 0 \ , \quad z(0) = z_0 \ . \tag{7.5}$$

Let $0 < \underline{T} < \bar{T} < \infty$ be suitable bounds for the temperature, $\underline{n} := n_i(\underline{T})$ and $\bar{n} := n_i(\bar{T})$, and let e_K denote the convex differentiable function which coincides with the exponential function e^Z on the interval $[-K, K]$ and which is affine on either side of the interval. We set

$$\tilde{g}(T,z) := r_1 \max\{\underline{n}, \min[n_i(T), \bar{n}]\}^2 [Z + e_{2|Z_0|}(-Z)] =: \tilde{r}(T)[Z + e_{2|Z_0|}(-Z)] \ .$$

The regularization does not concern neither the conservation of charge, the conservation of energy nor our argumentation above. A solution $\tilde{z}$ of the regularized problem (7.5) is therefore also a solution of the problem (7.4), if the bounds $\underline{T}$ and $\bar{T}$ are suitably chosen.

The time discretization of the regularized test problem (7.5) with M equidistant discrete times $t_k > 0 \equiv t_0$ reads

$$d[\ h_-(z_k) + \lambda_M \tilde{g}_{k-1}(z_k)\ ] = dh_-(z_{k-1}) \qquad (k = 1, ..., M) \ . \tag{7.6}$$

The existence of solutions of the discretized test problem is guaranteed, at least in case of Boltzmann statistics, as

$$\lim_{\max(\tau, 1/\tau, |\zeta|) \to \infty} h_-(\zeta, \tau) + \lambda \tilde{g}(T_0, \zeta) + \langle \rho_0, z \rangle = +\infty$$

is satisfied for any positive parameters λ, T_0, n_0, and p_0 (cf Proposition 4.1). This can be seen from

$$\begin{aligned} B :\equiv h_-(\zeta,\tau) + \lambda\tilde{g}(T_0,\zeta) + \langle\rho_0, z\rangle \ &= \ B_1 + c_L(\tau - \log\tau) + \tilde{r}_0(Z + e_{2|Z_0|}(-Z) \\ + \left[N_c \tau^{-3/2} e^{-\zeta_n - E_c\tau} + n_0(\zeta_n + E_c\tau) + \frac{3}{2} n_0 \tau + n_0 \max\left(0, \log\frac{n_0}{N_c} - \frac{3}{2}\right)\right] \\ + \left[N_v \tau^{-3/2} e^{E_v\tau - \zeta_p} + p_0(\zeta_p - E_v\tau) + \frac{3}{2} p_0 \tau + p_0 \max\left(0, \log\frac{p_0}{N_v} - \frac{3}{2}\right)\right] \end{aligned}$$

with constants B_1 and $\tilde{r}_0 > 0$. The difference $B - B_1$ is a sum of four non-negative summands $B_\tau + B_Z + B_n + B_p$ with $\lim_{\max(\tau,1/\tau)\to\infty} B_\tau = \infty$ and $\lim_{|Z|\to\infty} B_Z = \infty$; if $\max(\tau, 1/\tau)$ and Z remain bounded, but $\zeta \to \infty$, then either $\zeta_n + E_c\tau \to +\infty$ or $\zeta_p - E_v\tau \to +\infty$.

The definition of the subgradient yields the estimates

$$\begin{aligned} s_-(\rho_k) - s_-(\rho_{k-1}) &\leq \langle dh_-(z_k) - dh_-(z_{k-1}), z_k - z^D\rangle \\ &= -\lambda_M \langle d\tilde{g}_{k-1}(z_k) - d\tilde{g}_{k-1}(z^D), z_k - z^D\rangle \\ &\quad - \lambda_M \langle d\tilde{g}_{k-1}(z^D), z_k - z^D\rangle \end{aligned} \tag{7.7}$$

$(k = 1,\ ...,\ M,\ \lambda_M = T^*/M)$.

In the following we prove the convergence of Rothe's method of discretizing the time, i.e. we give an existence proof. The proof is based on these physically motivated estimates and on a coercivity estimate

$$\langle \partial_z \tilde{g}(T,z) - \partial_z \tilde{g}(T,w), z - w\rangle \geq \gamma |Z - W|^2 \tag{7.8}$$

with a positive constant γ. Such an estimate holds with a constant $\gamma = \tilde{\gamma}(\underline{T}, \bar{T}, |Z_0|)$. The solutions of (7.6) are considered as step functions $z^M \in L_2^M(S, R^3)$. We use the notation $\mathcal{H}_-(z^M) = \int_0^{T^*} h_-[z^M(t)]\ dt$ etc as in section 5.

Lemma 7.1. *Let $z^M \in L_2^M(S, R^3)$ be a solution of the equation (7.6). Then the following estimates hold uniformly with respect to M, i.e. with positive constants $c_j(S)$ which do not depend on M:*

$$\begin{array}{rcll} |Z^M|_{L_2(S)} & \leq & s_-(\rho_0) + c_1(S) \ , & \\ |\partial_M^{\rho_0}\rho^M|_{L_2(S,R^3)} & \leq & c_2(S) \ , & \\ n_k^M, \ p_k^M, \ |u_k^M| & \leq & c_3(S) & (k = 1, \ ..., \ M) \ , \\ 0 < c_5(S) \leq \tau_k^M & \leq & c_6(S) & (k = 1, \ ..., \ M) \ , \\ \left[\zeta_{nk}^M\right]_- , \ \left[\zeta_{pk}^M\right]_- & \leq & c_7(S) & (k = 1, \ ..., \ M) \ , \\ |\zeta_n^M|_{L_2(S)}, \ |\zeta_p^M|_{L_2(S)} & \leq & c_8(S) \ . & \end{array}$$

Proof. Summing up the corresponding estimates (7.7) one gets the estimates

$$\begin{array}{rl} & s_-(\rho_k) + \lambda_M \sum_1^k \langle d\tilde{g}_{j-1}(z_j) - d\tilde{g}_{j-1}(z^D), z_j - z^D \rangle \\ \leq & s_-(\rho_0) - \lambda_M \sum_1^k \langle d\tilde{g}_{j-1}(z^D), z_j - z^D \rangle \end{array} \tag{7.9}$$

□

$(k = 1, ..., M)$. We regard $s_- \geq 0$ and apply the coercivity estimate to the second summand on the left-hand side and Young's inequality to the right-hand side. Thus we get the first estimate. The second estimate, which obviously implies the third one, is an immediate consequence of the equation $\partial_M^{\rho_0}\rho^M = -\partial_z\tilde{\mathcal{G}}(\sigma_-^M T^M, z^M)$ with $\sigma_-^M T^M = T_{k-1}^M$ on $]t_{k-1}, t_k]$. From the first estimate follows, in particular, that the right-hand side of (7.9) is bounded from above by a constant $s_-(\rho_0) + C_4(S)$. Therefore the estimates

$$c_L \left[\log \frac{\tau_k^M}{\tau^D} - 1 + \frac{\tau^D}{\tau_k^M}\right] \leq s_-(\rho_k^M) \leq s_-(\rho_0) + c_4(S) \qquad (k = 1, \ ..., \ M)$$

hold, which imply the fourth estimate. The fifth estimate is a consequence of the last two preceding ones and of the state equations for the densities n and p. The last estimate follows from the first one and from the preceding one, since

$$|Z|_{L_2} \geq |[\zeta_a]_+|_{L_2} - |[\zeta_n]_-|_{L_2} - |[\zeta_p]_-|_{L_2}$$

and $|\zeta_a|_{L_2}^2 = |[\zeta_a]_+|_{L_2}^2 + |[\zeta_a]_-|_{L_2}^2$.

Lemma 7.2. *There is a solution $z \in L_2(S, R^3)$ of the initial-value problem* (7.5).

Proof. Since the sequences (z^M), $(\partial_M^{\rho_0}\rho^M)$ in $L_2(S, R^3)$ and $(L_{\rho_0}^M\rho^M)$ in $C(\bar{S}, R^3)$ are bounded, there is a subsequence (M_l) such that the sequences

- $z^{M_l} \equiv z_l \rightharpoonup z^*$ in $L_2(S, R^3)$ and $L_{\rho_0}^{M_l}\rho^{M_l} \equiv \omega_l \rightharpoonup \omega^*$ in $H^1(S, R^3)$

weakly converge. Since the Dirac measures on S belong to $H^1(S)'$ the convergence

- $\omega_l(t) \to \omega^*(t) \qquad (t \in \bar{S})$

holds. We get also

- $\rho^{M_l}(t) \equiv \rho_l(t) \to \omega^*(t) \quad a.e.$ on S

because $|L^M_{\rho_0}\rho^M - \rho^M|_{L_2(S,R^3)} \leq \Delta^M|\partial^{\rho_0}_M \rho^M|$. Since $H^1(S)$ is compactly imbedded into $L_2(S, R^3)$

- $\rho_l,\ \omega_l \to \omega^*$ in $L_2(S, R^3)$.

Let be $[a,b] \subset \bar{S}$ any subinterval and $\bar{\rho}$ any element of the effective domain of s_-. Then the estimate

$$\begin{aligned} \int_a^b \langle \bar{\rho} - \omega^*(t), z^*(t) - z^D \rangle \, dt &= \lim_{l\to\infty} \int_a^b \langle \bar{\rho} - \omega_l(t), z_l(t) - z^D \rangle \, dt \\ \leq \quad \limsup_l \int_a^b [s_-(\bar{\rho}) - s_-[\rho_l(t)]] \, dt &\leq \int_a^b [s_-(\bar{\rho}) - s_-[\omega^*(t)]] \, dt \end{aligned}$$

holds because of the lower semi-continuity of s_-. This estimate with an arbitrary subinterval implies the pointwise estimate

$$\langle \bar{\rho} - \omega^*(t), z^*(t) - z^D \rangle \leq s_-(\bar{\rho}) - s_-[\omega^*(t)]$$

$a.e.$ on S, i.e. $z^*(t) - z^D \in \partial s_-[\omega^*(t)]$ $a.e.$ on S and the identity

$$s_-[\omega^*(t)] - s_-(\rho_0) = \int_0^t \langle \dot{\omega}^*(s), z^*(s) - z^D \rangle \, ds \tag{7.10}$$

for all $t \in \bar{S}$.

The identity

$$\begin{aligned} 0 &= \lim_{l\to\infty} \int_S \langle \partial^{\rho_0}_{M_l} \rho^{M_l} + d\tilde{g}[z_l(t)], z_l(t) - z^*(t) \rangle \, dt \\ &= \lim_{l\to\infty} \int_S [\ \langle \partial^{\rho_0}_{M_l} \rho^{M_l}, z_l(t) - z^D \rangle \\ &\quad + \langle \dot{\omega}^*(t), z^*(t) - z^D \rangle + \langle d\tilde{g}[z_l(t)] - d\tilde{g}[z^*(t)], z_l(t) - z^*(t) \rangle\ ] \ dt \\ &\leq \limsup_{l\to\infty} \left\{ s_-[\omega_l(T^*)] - s_-(\rho_0) + \int_S \langle \dot{\omega}^*(t), z^*(t) - z^D \rangle \, dt + \gamma|\zeta_{nl} + \zeta_{pl} - \zeta^*_n - \zeta^*_p|_{L_2(S)} \right\} \\ &\leq \limsup_{l\to\infty} \left\{ s_-[\omega^*(T^*)] - s_-(\rho_0) + \int_S \langle \dot{\omega}^*(t), z^*(t) - z^D \rangle \, dt + \gamma|\zeta_{nl} + \zeta_{pl} - \zeta^*_n - \zeta^*_p|_{L_2(S)} \right\} \end{aligned}$$

yields the convergence of the sums

- $\zeta_{nl} + \zeta_{pl} \to \zeta^*_n + \zeta^*_p$ in $L_2(S)$

i.e. the convergence of the gradients

- $d\tilde{G}(z_l) \to d\tilde{G}(z^*)$ in $L_2(S, R^3)$.

Using the convergence properties the limit $l \to \infty$ can be taken in the problem $\partial^{\rho_0}_{M_l} \rho^{M_l} + d\tilde{G}(z_l) = 0$ and in the relation $\rho^{M_l} = dH_-(z_l)$, i.e. z^* is a solution of the problem (7.5) and thus of the problem (7.3). □

Let us mention Gajewski's method of proving the uniqueness. Its starting point is the identity

$$\begin{aligned} & s_-[\rho_1(t)] + s_-[\rho_2(t)] - 2s_-[\rho(t)] \\ &= \int_0^t [\langle \dot\rho_1(s), z_1(s) - z(s)\rangle + \langle \dot\rho_2(s), z_2(s) - z(s)\rangle] \ ds \\ &= -\int_0^t [\ \langle dg[z_1(s)], z_1(s) - z(s)\rangle + \langle dg[z_2(s)], z_2(s) - z(s)\rangle\ ] \ ds \ , \end{aligned}$$

where z_1 and z_2 denote two solutions of the initial-value problem (7.3) with the same initial value, ρ denotes the arithmetic mean of the ρ_i and $z(s) = z^D + d\rho(s)$. Notice that $z_1(s) - z(s) \approx -[z_2(s) - z(s)]$. The idea of the method is to use the convexity of s_- or h_- and of g to get an estimate from below on the left-hand side and an estimate of the integrand from above on the right-hand side and to apply Gronwall's lemma.

We have not checked whether this method is applicable to this example, but we have some doubts because the quadratic form $d^2 g$ is rather degenerated.

8. Appendix

Lemma 8.1. *Let two real functions $0 < \mathcal{N} \in C^2(R_+)$ and $\mathcal{E} \in C^2(R_+)$ be given. The function $h_n(x,\tau) = \mathcal{N}(t)\mathcal{F}_{3/2}[-x - \mathcal{E}(t)]$ on $R \times R_+$ is convex if and only if $\mathcal{E}$ and $\mathcal{N}$ satisfy the condition*

$$\mathcal{N}''\mathcal{F}_{3/2} - \mathcal{N}\mathcal{E}''\mathcal{F}_{1/2} \geq \frac{[\mathcal{N}'\mathcal{F}_{1/2}]^2}{\mathcal{N}\mathcal{F}_{-1/2}} \ . \tag{8.1}$$

Proof. The positivity $0 < \mathcal{N}$ guarantees $h_{nxx} > 0$. The condition (8.1) is just the inequality $h_{n\tau\tau} \geq h_{nx\tau}^2 / h_{nxx}$, which implies that the eigenvalues of the matrix $d^2 h_n$ of the second-order partial derivatives $\partial_u \partial_v h_n \equiv h_{nuv}$ are non-negative, i.e. the function h_n is convex. □

Let us denote the partial derivatives of h_n by $h_{nx} = -n$ and $h_{n\tau} = -u$. If we introduce the notation $T = 1/\tau$, $\mathcal{N}(\tau) = N(T)$ and $E(T) = T\mathcal{E}(1/T)$, then we see

$$\begin{aligned} n &= N(T)\mathcal{F}_{1/2}\left[-x - \frac{1}{T}E(T)\right] \ , \\ u &= nE(T) - nTE'(T) + T^2 N'(T)\mathcal{F}_{3/2} \circ \mathcal{F}_{1/2}^{-1}\left[\frac{n}{N(T)}\right] =: u_f(n,T) \ , \end{aligned}$$

i.e. h_n is a thermodynamic potential of a Fermi gas with a state density $N(T)$ of quasi-particles with the chemical potential $-x$ in a potential $E(T)$; n is particle density, and u is the energy density of the gas. The density of the free energy of such a gas is

$$f(n,T) = nT\mathcal{F}_{1/2}^{-1}\left[\frac{n}{N(T)}\right] - TN(T)\mathcal{F}_{3/2} \circ \mathcal{F}_{1/2}^{-1}\left[\frac{n}{N(T)}\right] + nE(T) \ .$$

The familiar thermodynamic relation $u_f(n,T) = f(n,T) - T\partial_T f(n,T)$ as well as the identities

$$(8.2)\qquad -s_f(n,T) = \partial_T f(n,T) = -nx - u\tau - h_n(x,\tau)|_{-(n,u)=(h_{nx},h_{nu})} \;,$$

$$T^2\partial_T u_f(n,T) = \mathcal{N}"\mathcal{F}_{3/2} - \mathcal{N}\mathcal{E}"\mathcal{F}_{1/2} - \frac{\left[\mathcal{N}'\mathcal{F}_{1/2}\right]^2}{\mathcal{N}\mathcal{F}_{-1/2}}$$

are checked by elementary calculations. According to the last identity, the condition (8.1) in the Lemma 8.1 means that the Fermi gas has a positive heat capacity. The identity (8.2) says that the negative entropy considered as a function of the densities n and u is a convex function and the thermodynamic potential which is conjugate to h_n.

In the model case $N(T) = NT^{3/2}$ and $\mathcal{E}(\tau) = E\tau$ with real constants $N > 0$ and E the heat capacity is

$$\partial_T u_f(n,T) = \frac{9}{4}N(T)\left(\frac{5}{3}\mathcal{F}_{3/2} - \frac{\mathcal{F}_{1/2}^2}{\mathcal{F}_{-1/2}}\right) \;.$$

The following lemma, the proof of which has been given by my colleague H. Stephan, shows that the condition (8.1) of the Lemma 8.1 is fulfilled in the model case.

Lemma 8.2. *The inequality*

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

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^{th} derivative with respect to α. The Jensen inequality is applied with the convex function x^2, i.e.

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

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

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

i.e.

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

□

The inequality of the lemma can be written in the form

$$\frac{1}{\alpha+1}\mathcal{F}_{\alpha+1}\mathcal{F}'_\alpha \;>\; \mathcal{F}^2_\alpha - \mathcal{F}_{\alpha+1}\mathcal{F}'_\alpha \;=\; \mathcal{F}^2_\alpha[\frac{\mathcal{F}_{\alpha+1}}{\mathcal{F}_\alpha}]' \,.$$

The sign of the difference on the right-hand side of the inequality is also of interest (cf. [7]).

Lemma 8.3. *The inequalities*

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

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

Proof. The difference

$$A := (\alpha+1)e^{-u-v}\int_0^\infty \frac{t^\alpha e^{t-u}}{(1+e^{t-u})^2}dt\int_0^\infty \frac{t^\alpha e^{t-v}}{(1+e^{t-v})^2}dt[\frac{\mathcal{F}_\alpha(v)}{\mathcal{F}'_\alpha(v)} \;-\; \frac{\mathcal{F}_\alpha(u)}{\mathcal{F}'_\alpha(u)}]$$

can be written in the form

$$\begin{aligned} A &= \int_0^\infty \frac{t^\alpha e^t}{(e^u+e^t)^2}dt\int_0^\infty \frac{t^{\alpha+1}e^t}{(e^v+e^t)^2}dt \;-\; \int_0^\infty \frac{t^\alpha e^t}{(e^v+e^t)^2}dt\int_0^\infty \frac{t^{\alpha+1}e^t}{(e^u+e^t)^2}dt \\ &= \int [(e^v+e^x)^2(e^u+e^y)^2-(e^u+e^x)^2(e^v+e^y)^2]y\,d\mu \\ &= (e^v-e^u)\int (e^y-e^x)y\,d\lambda \;=\; (e^v-e^u)\int_{y>x}(e^y-e^x)(y-x)d\lambda \;>\; 0 \end{aligned}$$

with the measures

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

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_+. □

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

It might be desirable to have convex functions $\tilde{h}_n$ which are defined on the whole plane and which differs from h_n for large temperatures only. We have, however, the following 'no go' lemma.

Lemma 8.4. *There is no* C^2 *function* $\mathcal{N} > 0$ *on the real line such that* $\mathcal{N}' < 0$ *on* R *and that* $h_n(x,t) = \mathcal{N}(t)\mathcal{F}_{3/2}(-x-tE)$ *is convex on* R^2.

Proof. Let us assume that such a function $\mathcal{N}$ would exist. In the case $\mathcal{E}'' \equiv 0$ the condition (8.1) reads

$$0 \le (\mathcal{N}')^2\mathcal{F}_{-1/2}\mathcal{F}_{3/2}\left[\frac{\mathcal{N}\mathcal{N}''}{(\mathcal{N}')^2} - 1 + 1 - \frac{\mathcal{F}^2_{1/2}}{\mathcal{F}_{-1/2}\mathcal{F}_{3/2}}\right]$$

or, in other words,

$$\frac{\mathcal{F}^2_{1/2}}{\mathcal{F}_{-1/2}\mathcal{F}_{3/2}}\left(\frac{\mathcal{F}_{3/2}}{\mathcal{F}_{1/2}}\right)' \le \left(\frac{\mathcal{N}}{\mathcal{N}'}\right)^2\left[\frac{\mathcal{N}''}{\mathcal{N}} - \left(\frac{\mathcal{N}'}{\mathcal{N}}\right)^2\right] = -\left[\frac{1}{(\log\mathcal{N})'}\right]'$$

for all t and all x. With regard to the preceding lemma there is a constant $c > 0$ with $c < -[1/(\log \circ \mathcal{N})']'$ for all $t \geq t_0$. Let $t_1 > 0$ be fixed, $z_1 := (\log \circ \mathcal{N})'(t_1)$. Then the inequality

$$(\log \circ \mathcal{N})'(t) \leq \frac{z_1}{1 + cz_1(t_1 - t)} < 0$$

holds for $t < t_1$ and implies the inequality $\mathcal{N}(t) \geq \mathcal{N}(t_1)[1 + cz_1(t_1 - t)]^{-1/c}$ there, but the inequality contradicts the assumption. □

In the case of Boltzmann statistics the situation is quite different. The function $h_-(x,t) = \mathcal{N}(t)e^{x-\mathcal{E}(t)}$ with two real functions $0 < \mathcal{N} \in C^2(R_+)$ and $\mathcal{E} \in C^2(R_+)$ is convex if

$$\frac{\mathcal{N}''}{\mathcal{N}} - \mathcal{E}'' > \left(\frac{\mathcal{N}'}{\mathcal{N}}\right)^2 ,$$

i.e. if $(\log \circ \mathcal{N} - \mathcal{E})'' > 0$ holds. Let a real function $0 < \mathcal{N} \in C^2(R_+)$ satisfy $\mathcal{N}' < 0 < (\log \circ \mathcal{N})''$. Then there are functions $0 < \mathcal{N}_\beta \in C^2(R)$ for any $\beta \in]0,1[$ which is equal to $\mathcal{N}$ on the interval $t \geq \beta$ and satisfy $\mathcal{N}_\beta' < 0 < (\log \circ \mathcal{N}_\beta)''$ on R, such that $h_\beta(x,t) := \mathcal{N}_\beta(t)e^{x-tE}$ is a convex function on the whole plane. The function

$$(\log \circ \mathcal{N})_\beta(t) = \frac{z_2}{2}\left(t - \beta + \frac{z_1}{z_2}\right)^2 - \frac{z_1^2}{2z_2} + z_0$$

on the interval $t < \beta$ with $z_k := (\log \circ \mathcal{N})^{(k)}(\beta)$ $(k = 0,\ 1,\ 2)$ is a suitable continuation of $\log \circ \mathcal{N}$. For functions $\mathcal{E} \in C^2(R_+)$ instead of tE more technical refinements are necessary.

We bring the Appendix to an end with a proof of the formula (6.4) for a system with electrons only.

$$\begin{aligned}
s_-(\rho) &= \langle \rho, z - z^D \rangle - h_-(z)|_{\rho=-dh_-(z)=-(n,u)} \\
&= -n(\zeta - \zeta^D) - u(\tau - \tau^D) + \int_\tau^{\tau^D} \int^{1/\sigma} c_L(y)dyd\sigma - h_n(\zeta,\tau) + h_n(\zeta^D,\tau^D) \\
&= h_n(\zeta^D,\tau^D) - h_n(\zeta,\tau) - (\zeta^D - \zeta)\partial_\zeta h_n(\zeta,\tau) \\
&\quad + \int_\tau^{\tau^D} \int^{1/\sigma} c_L(y)dyd\sigma + (\tau - \tau^D)\partial_\tau h_n(\zeta,\tau) \\
&= \int_\tau^{\tau^D} \int_{1/\tau}^{1/\sigma} c_L(y)dyd\sigma \\
&\quad + h_n(\zeta^D,\tau^D) - h_n(\zeta,\tau) - (\zeta^D - \zeta)\partial_\zeta h_n(\zeta,\tau) - (\tau^D - \tau)\partial_\tau h_n(\zeta,\tau) \\
&= \int_{\tau^D}^\tau \int_\sigma^\tau \frac{1}{y^2} c_L\left(\frac{1}{y}\right)\ dy\ d\sigma \\
&\quad + (\zeta^D - \zeta)\int_0^1 \{\partial_\zeta h_n[\zeta + t(\zeta^D - \zeta), \tau + t(\tau^D - \tau)] - \partial_\zeta h_n(\zeta,\tau)\}\ dt \\
&\quad + (\tau^D - \tau)\int_0^1 \{\partial_\zeta h_n[\zeta + t(\zeta^D - \zeta), \tau + t(\tau^D - \tau)] - \partial_\zeta h_n(\zeta,\tau)\}\ dt\ ,
\end{aligned}$$

$$s_-(\rho) = \int_{\tau^D}^{\tau} \int_{\sigma}^{\tau} \frac{1}{y^2} c_L \left(\frac{1}{y}\right) \, dy \, d\sigma$$
$$+ \begin{pmatrix} \zeta^D - \zeta \\ \tau^D - \tau \end{pmatrix} \cdot \int_0^1 \int_0^t d^2 h_n[\zeta + s(\zeta^D - \zeta), \tau + s(\tau^D - \tau)] \, ds \, dt \begin{pmatrix} \zeta^D - \zeta \\ \tau^D - \tau \end{pmatrix} .$$

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