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On uniqueness of solutions to the drift–diffusion–model of semiconductor devices

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CONTENTS

ABSTRACT. We prove a uniqueness result for the drift–diffusion–model of semiconductor devices under weak regularity assumptions. Our proof rests on the convexity of the free energy functional and uses a new concavity argument.

1. Introduction

Since the drift–diffusion–model has been established by van Roosbroeck in 1950 [16] it has proven to be of fundamental significance for the mathematical describing and numerical simulation of carrier transport in semiconductor devices. The drift–diffusion–model is formed by a coupled system of a Poisson equation for the electrostatic potential and continuity equations for positive and negative carriers (holes and electrons). The existence of solutions to these device equations has been proved under natural assumptions (comp. [12, 3]). With respect to the uniqueness of solutions the situation is more complex. Whereas steady state solutions to the device equations in general cannot expected to be unique by physical reasons (comp. [11, 10]), uniqueness of transient solutions should hold in principle, but has been proved only under unpleasant restrictions up to now.

The first uniqueness result for the transient device equations was published by Mock [11] under strong regularity assumptions, excluding nonsmooth domains as well as mixed boundary conditions. More recently Gajewski & Gröger [2] have shown weak solutions to be unique, provided the semiconductor obeys Boltzmann statistics. Concerning the physically more realistic Fermi–Dirac statistics, these authors [3] proved uniqueness of solutions having bounded gradients. In a forthcoming paper Gröger & Rehberg [8] could relax this regularity condition essentially in the case of two space dimensions.

The main result of this paper is a uniqueness result which rests on a new concavity argument involving density and conductivity as functions of the chemical potentials of electrons and holes. This argument allows to remove all regularity assumptions except for a mild L_q–condition with respect to the gradient of the electrostatic potential. Our idea of proof is based on the convexity of the free energy functional, which induces a natural metric in the space of solutions to the device equations. This approach has been discussed in [1] in a more abstract way.

The plan of the paper is as follows: First we formulate the complete initial boundary value problem for the drift–diffusion–model. In Section 2 suitable function spaces, definitions and assumptions are introduced. The energy functional is discussed in Section 3. Section 4 is devoted to the proof of the uniqueness result. Finally, the assumptions are verified in Section 5.

2. The initial boundary value problem

Let be: $S = (0,T)$ a bounded time interval, $\Omega \subset \mathbb{R}^N, 1 \leq N \leq 3$, a bounded Lipschitzian domain and $Q = S \times \Omega$. We suppose that $\partial\Omega = \Gamma_D \cup \Gamma \cup \Gamma_N$, where the subsets $\Gamma_D, \Gamma, \Gamma_N$ are pairwise disjoint and Γ_D is closed and possesses positive surface measure. Moreover, $\nu(x_0)$ denotes the outer unit normal at $x_0 \in \partial\Omega$.

The transient carrier transport in a semiconductor occupying the domain Ω can be described by the following system of partial differential equations:

$$-\nabla(\cdot\varepsilon\nabla v_0) = D + u_p - u_n, \tag{2.1}$$

$$\frac{\partial}{\partial t}u_i + e_i\nabla\cdot J_i + r_i = 0, \quad i = n, p, \quad e_n = -1, e_p = +1. \tag{2.2}$$

Here and in what follows the subscript i stands for electrons $i = n$ (negative) resp. holes $i = p$ (positive). The physical meaning of the other quantities is:
v_0 – electrostatic potential,
v_i – chemical potential,
$u_i = f_i(v_i)$ – carrier density,
$J_i = J_i(x, v_i, z_i), z_i = \nabla(v_0 + e_i v_i)$ – current density,
ε – dielectric permittivity,
D – density of impurities,
$r_i = r_i(x, v), v = (v_l), l = 0, n, p$ – recombination/generation rate.
From the functional analytic point of view it turns out to be advantageous to replace the Poisson equation (2.1) by the current conservation equation

$$\nabla \cdot J + r_0 = 0, \quad J = -\varepsilon \nabla \frac{\partial v_0}{\partial t} + J_n + J_p, \quad r_0 = r_p - r_n - D_t, \tag{2.3}$$

which results from (2.1) after differentiating with respect to time and eliminating u_{it} from (2.2).
We complete (2.2)–(2.3) by initial conditions

$$v_l(0, \cdot) = v_{l0} \quad on\ \Omega \tag{2.4}$$

and boundary conditions

$$\begin{aligned} v_l = v_{l\Gamma} \quad & on\ S \times \Gamma_D, \\ \nu \cdot J = k_0 u_{0t} + \alpha, \quad v_i = v_{i\Gamma} \quad & on\ S \times \Gamma, \\ -\nu \cdot \nabla v_{0t} = k_0 u_{0t}, \quad \nu \cdot J_i = 0 \quad & on\ S \times \Gamma_N, \end{aligned} \tag{2.5}$$

where the functions $v_{l\Gamma}$ represent given boundary values and

$$u_0 = v_0 - v_{0\Gamma},$$
$$\alpha = exp(-k_1 t)(k_2 + k_3 \int_0^t exp(k_1 s) u_0(s)\, ds).$$

Remark. From the physical point of view Γ_D models Ohmic contacts. The condition on Γ describes interaction of the semiconductor with an outer electric circuit formed by inductivity ($L = \frac{1}{k_3}$), resistance ($R = \frac{k_1}{k_3}$) and parallely switched capacity ($C = k_0$). Finally, Γ_N can be interpreted as interface between semiconductor and an isolator.

3. Definitions and assumptions

We denote by $L_q, (\|\cdot\|_q, \|\cdot\| = \|\cdot\|_2)$, $1 \le q \le \infty$, H^1, H^{-1} the usual spaces of functions defined on Ω (comp. [4, 5, 17]). Additionally we introduce

$$V_0 = \{h \in H^1, h = 0\ on\ \Gamma_D\}, \quad V = \{h \in V_0,\ h = 0\ on\ \Gamma\},$$
$$H = \{v = (v_0, v_i),\ v_0 \in V_0,\ v_i \in L_2\}, \quad \|v\|_H^2 = \||\nabla v_0|\|^2 + \|v_n\|^2 + \|v_p\|^2.$$

If X is a Banach space, $L_q(S;X)$ is the space of Bochner measurable functions $t \to h(t) \in X$ such that

$$\int_0^T \|h(t)\|_X^q \, dt < \infty.$$

Definition 3.1. A function vector $v = (v_l), l = 0, n, p$, is called (weak) solution of (2.2)–(2.5), if:

(D1) $v_l \in L_\infty(Q) \cap L_2(S;H^1), \quad v_{0t} \in L_2(S;H^1), \quad v_{it} \in L_2(S;H^{-1})$;
(D2) $v_l(0) = v_{l0}$;
(D3) $v_0 = v_{0\Gamma}$ *on* $S \times \Gamma_D, \quad v_i = v_{i\Gamma},$ *on* $S \times (\Gamma_D \cup \Gamma)$;
(D4) for almost every $t \in S$ it holds

$$\int (J \cdot \nabla h + r_0 h) \, d\Omega = \int (k_0 u_{0t} + \alpha) h \, d\Gamma + \int k u_{0t} h \, d\Gamma_N, \quad \forall h \in V_0,$$

$$\int [(u_{it} + r_i)h - e_i J_i \cdot \nabla h] \, d\Omega = 0, \quad \forall h \in V.$$

Remark. The integral involving u_{it} has to be understood in the sense of distributions, that means as dual pairing between H^{-1} and V.

Definition 3.2. $\beta \in (\Omega \times \mathbb{R}^N \to \mathbb{R}^N)$ is called Carathéodory function if:

(i) the function $x \to \beta(x,z)$ is measurable for every $z \in \mathbb{R}^N$;
(ii) the function $z \to \beta(x,z)$ is continuous in $\mathbb{R}^N$ for almost every $x \in \Omega$;
(iii) $|\beta(x,z)| \le C(\beta_0(x) + |z|) \quad , \quad \beta_0 \in L_2$.

We suppose the current densities J_i to have the representation

$$J_i(x,s,z) = -(a_i(s)z + b_i(s)\beta_i(x,z) + f_i'(s)\gamma_i(x,z)). \tag{3.1}$$

Moreover, we suppose constants $K, \kappa > 0$ to exist such that for a. e. $x \in \Omega$, $\forall s, \forall s_j \in I = [-K, K]$, $0 < |s_1 - s_2| \le \kappa$, $\forall z_j \in \mathbb{R}^N$, $j = 1,2$, the following assumptions are satisfied:

(A1) $f_i \in C^1(I), \quad f_i'$ is Lipschitzian , $f_i'(s) > 0$;
(A2) $g_i = f_i' \circ f_i^{-1}$ is uniformly concave on I such that

$$G_i \ge c|f_i(s_1) - f_i(s_2)|^2, \; c > 0,$$

where

$$G_i = 2 - g_{i1} - g_{i2}, \quad g_{ij} = \frac{g_i(f_i(s_j))}{g_{im}}, \quad g_{im} = g_i\left(\frac{f_i(s_1) + f_i(s_2)}{2}\right);$$

(A3) $a_i \in C(I), \quad a_i(s) > 0$;
(A4)

$$\rho_i(s_1,s_2) = \frac{(g_{i1}a_{i2} - g_{i2}a_{i1})^2}{8G_i a_{i1} a_{i2}} < 1, \quad a_{ij} = a_i(s_j);$$

(A5) b_i is Lipschitzian on I, $\quad b_i(s) \ge 0$;
(A6) β_i is Carathéodory function such that

$$|\beta_i(x,z)| \le c_\beta, \; \beta_i(x,0) = 0, \quad (\beta_i(x,z_1) - \beta_i(x,z_2)) \cdot (z_1 - z_2) \ge 0;$$

(A7) γ_i is Carathéodory function such that

$$\gamma_i(x,0)=0,\ (\gamma_i(x,z_1)-\gamma_i(x,z_2))\cdot(z_1-z_2)\geq m_\gamma|z_1-z_2|^2,\quad m_\gamma>0;$$

(A8) $r_l(x,v)$, $l=0,n,p$, is Carathéodory function, locally Lipschitzian with respect to v;

(A9) $\varepsilon\in L_\infty$, $\varepsilon(x)\geq\varepsilon_0>0$, $0\leq k_0\in L_\infty(\Gamma_N)$, $0\leq k_1,k_2,k_3\in L_\infty(\Gamma)$;

(A10) $v_{l0}\in L_\infty(Q)$, $v_{l\Gamma}\in L_\infty(Q)\cap L_2(S;H^1)$, $v_{0\Gamma t}\in L_2(S;H^1)$.

Remark. The coefficients a_i, b_i and f_i' may be interpreted as electrical conductivities.

Remark. As a consequence of (A1), (A2) it holds

$$\begin{gathered}G_i\geq c|s_1-s_2|^2\geq c|g_{i1}-g_{i2}|^2,\\ \forall s_1,\forall s_2\in\mathbb{R},\ |s_j|\leq K,\ 0<|s_1-s_2|\leq\kappa,\end{gathered}\tag{3.2}$$

where G_i and g_{ij} are given by (A2).

4. Energy functional

For $u=(u_l)\in L_2(S;H)$ we define the energy functional

$$\begin{aligned}F(u)=&\int[\frac{\varepsilon}{2}|\nabla u_0|^2+\sum_{i=n}^{p}\Big(\int_0^{u_i}f_i^{-1}(s)\,ds-u_iv_{i\Gamma}\Big)]\,d\Omega\\&+\int[\frac{k_0}{2}u_0^2+\frac{\alpha^2}{2k_3}]\,d\Gamma+\int\frac{k_0}{2}u_0^2\,d\Gamma_N.\end{aligned}$$

For a solution v to (2.2)-(2.5) the function

$$t\to\phi(t)=F(Ev(t)),\quad Ev=u=(u_0,u_n,u_p),$$

is absolutely continuous. Moreover, for a. e. $t\in S$ we find by (D4)

$$\begin{aligned}\phi'(t)=&\int[\varepsilon\nabla v_{0t}\cdot\nabla u_0+\sum_{i=n}^{p}u_{it}(v_i-v_{i\Gamma})]\,d\Omega\\&+\int[(k_0u_{0t}+\alpha)u_0-\frac{k_1}{k_3}\alpha^2]\,d\Gamma+\int k_0u_{0t}u_0\,d\Gamma_N\\=&\int[-J\cdot\nabla u_0+\sum_{i=n}^{p}(J_i\cdot\nabla u_0+u_{it}(v_i-v_{i\Gamma}))]\,d\Omega\\&+\int[(k_0u_{0t}+\alpha)u_0-\frac{k_1}{k_3}\alpha^2]\,d\Gamma+\int k_0u_{0t}u_0\,d\Gamma_N\\=&\int[r_0u_0+\sum_{i=n}^{p}(J_i\cdot(z_i-z_{i\Gamma})-r_i(v_i-v_{i\Gamma}))]\,d\Omega-\int\frac{k_2}{k_3}\alpha^2\,d\Gamma,\end{aligned}\tag{4.1}$$

where $z_i=\nabla(v_0+e_iv_i)$, $z_{i\gamma}=\nabla(v_{0\gamma}+e_iv_{i\gamma})$.

Remark. From (4.1) it is clear, that ϕ can be looked at as Lyapunov function of (2.2)-(2.3) in some situations. Indeed, let for example $v_{0\Gamma} + e_i v_{i\Gamma} = r_0 = 0, r_i = exp(v_n + v_p) - 1$. Then, we infer from (4.1), using (3.1),(A3),(A5)-(A7),

$$\phi'(t) = \int [\sum_{i=n}^{p} J_i \cdot z_i - (exp(v_n + v_p) - 1)(v_n + v_p)] \, d\Omega \leq 0.$$

5. Uniqueness

In this section the uniqueness result will be proved. To this end let us suppose that we are given two solutions $v_j = (v_{lj})$, $j = 1, 2$, of (2.2)-(2.5) such that $\|v_{ij}\|_{L_\infty(Q)} \leq K$, $\|v_{i1} - v_{i2}\|_{L_\infty(Q)} \leq \kappa$. We introduce

$$d(t) = d(v_1(t), v_2(t)) = [F(Ev_1) + F(Ev_2) - 2F\left(\frac{Ev_1 + Ev_2}{2}\right)](t)$$

as a kind of distance between v_1 and v_2. Our aim is to show that

$$c_1 \|v(t)\|_H^2 \leq d(t) \leq c_2 \int_0^t \sigma(s) \|v(s)\|_H^2 \, ds, \quad t \in S, \quad v = v_1 - v_2,$$

where $\sigma \in L_1(S)$.

Lemma 5.1. *There exists a constant $c > 0$ such that*

$$c\|v(t)\|_H^2 \leq d(t).$$

Proof. Because of (A1) the function $\psi(y) = \int_0^y f_i^{-1}(s) \, ds$, $y \in \mathbb{R}$, is convex. Moreover, setting

$$c_0 = min\{f_i'(s), |s| \leq K\}, \quad c_1 = max\{f_i'(s), |s| \leq K\}, \tag{5.1}$$

we find by elementary calculations that for $y_j = f_i(s_j)$, $|s_j| \leq K$,

$$\psi(y_1) + \psi(y_2) - 2\psi\left(\frac{y_1 + y_2}{2}\right) \geq \frac{1}{4c_1}|y_1 - y_2|^2 \geq \frac{c_0}{4c_1}|s_1 - s_2|^2.$$

This estimate along with the uniform convexity of the energy functional F with respect to u_0 proves the lemma. $\square$

Lemma 5.2. *Suppose in addition to (D1) that the solutions v_i satisfy the regularity condition*

$$|\nabla v_{0j}| \in L_{2q/(q-N)}(S; L_q), \; j = 1, 2, \; q > N. \tag{5.2}$$

Then there exists a constant c such that

$$d(t) \leq c \int_0^t \sigma(s) \|v(s)\|_H^2 \, ds, \; \sigma(t) = 1 + \sum_{j=1}^{2} \|y_j(t)\|_q^{2q/(q-N)}, \quad y_j = \nabla v_{0j}. \tag{5.3}$$

Proof. Setting

$$
\begin{aligned}
&v_l = v_{l1} - v_{l2}, \quad v_{0m} = \frac{v_{01} + v_{02}}{2}, \quad v_{im} = f_i^{-1}\left(\frac{u_{i1} + u_{i2}}{2}\right), \quad u_{ij} = f_i(v_{ij}), \\
&y_j = \nabla v_{0j}, \quad z_{ij} = \nabla(v_{0j} + e_i v_{ij}), \quad z_{im} = \nabla(v_{0m} + e_i v_{im}), \\
&\alpha = \alpha_1 - \alpha_2, \quad J = J_1 - J_2, \quad r_l = r_{l1} - r_{l2},
\end{aligned}
$$

we infer from (4.1) and (A8)

$$
\begin{aligned}
d'(t) &= \int [\frac{1}{2} r_0 v_0 + \sum_{i,j=1}^{2} (J_{ij} \cdot (z_{ij} - z_{im}) - r_{ij}(v_{ij} - v_{im}))] \, d\Omega - \frac{1}{2} \int \frac{k_2}{k_3} \alpha^2 \, d\Gamma \\
&\leq \int \sum_{i,j=1}^{2} J_{ij} \cdot (z_{ij} - z_{im}) \, d\Omega + c\|v(t)\|_H^2.
\end{aligned} \tag{5.4}
$$

In view of (A2) we have

$$
\nabla v_{im} = \frac{1}{2} \sum_{j=1}^{2} g_{ij} \nabla v_{ij}
$$

and hence

$$
z_{im} = \frac{1}{2} \sum_{j=1}^{2} [g_{ij} z_{ij} + (1 - g_{ij}) y_j].
$$

Thus, setting $z_i = z_{i1} - z_{i2}, \quad y = y_1 - y_2$, we find

$$
\begin{aligned}
\sum_{i,j=1}^{2} J_{ij} \cdot (z_{ij} - z_{im}) = \frac{1}{2} [&\sum_{i,j=1}^{2} G_i J_{ij} \cdot z_{ij} \\
&+ \sum_{i=1}^{2} (g_{i2} J_{i1} - g_{i1} J_{i2}) \cdot z_i \\
&- \sum_{i=1}^{2} (J_{i1} + J_{i2}) \cdot \sum_{j=1}^{2} (1 - g_{ij}) y_j].
\end{aligned} \tag{5.5}
$$

We are now going to estimate the right-hand side of (5.5) term by term. To this end we drop the subscript i for convenience. From (3.1) (5.1) and (A1)-(A7) we see that

$$
G J_j \cdot z_j \leq -G(a_j + c_0 m_\gamma)|z_j|^2 = -G(a_j + \delta)|z_j|^2, \quad \delta > 0. \tag{5.6}
$$

Next, setting $g_m = g((u_1 + u_2)/2)$ and using (A6), (A7), we get

$$
\begin{aligned}
(g_2J_1 - g_1J_2)\cdot z &= -[g_2(a_1z_1 + b_1\beta_1 + g_m g_1\gamma_1) - g_1(a_2z_2 + b_2\beta_2 + g_m g_2\gamma_2)]\cdot z \\
&= -[g_2a_1z_1 - g_1a_2z_2 + \frac{1}{2}(g_2b_1 + g_1b_2)(\beta_1 - \beta_2) \\
&\quad + \frac{1}{2}(g_2b_1 - g_1b_2)(\beta_1 + \beta_2) + g_m g_1 g_2(\gamma_1 - \gamma_2)]\cdot z \\
&\le -(g_2a_1z_1 - g_1a_2z_2)\cdot z + c|v||z| - 2\delta|z|^2 \\
&\le -(g_2a_1z_1 - g_1a_2z_2)\cdot z + c|v|^2 - \delta|z|^2.
\end{aligned}
\tag{5.7}
$$

Now, setting

$$
A = (G+g_2)a_1, \quad B = (G+g_1)a_2, \quad C = g_2a_1 + g_1a_2,
$$

and noting that by (A4)

$$
4AB - C^2 = 8Ga_1a_2 - (g_1a_2 - g_2a_1)^2 \ge \delta G,
$$

we find by (A4)

$$
\begin{aligned}
G\sum_{j=1}^{2} a_j|z_j|^2 + (g_2a_1z_1 - g_1a_2z_2)\cdot z &= A|z_1|^2 + B|z_2|^2 - Cz_1\cdot z_2 \\
&\ge A|z_1|^2 + B|z_2|^2 - \frac{C}{2}((A/B)^{1/2}|z_1|^2 + (B/A)^{1/2}|z_2|^2) \\
&= \left(1 - (1 - \frac{4AB - C^2}{4AB})^{1/2}\right)(A|z_1|^2 + B|z_2|^2) \\
&\ge \frac{4AB - C^2}{8}(|z_1|^2/B + |z_2|^2/A) \\
&\ge \delta G(|z_1|^2 + |z_2|^2).
\end{aligned}
$$

Thus it follows from (5.6) and (5.7)

$$
G\sum_{j=1}^{2} J_j\cdot z_j + (g_2J_1 - g_1J_2)\cdot z \le c|v|^2 - \delta(G\sum_{j=1}^{2}|z_j|^2 + |z|^2). \tag{5.8}
$$

We turn now to the remaining term from (5.5). Using (3.2), (A6), (A7) and setting $g = g_1 - g_2$, we get

$$
\begin{aligned}
|(J_1+J_2)\cdot\sum_{j=1}^{2}(1-g_j)y_j| &= |\frac{1}{2}(J_1+J_2)\cdot(G\sum_{j=1}^{2}y_j-gy)| \\
&\le \frac{1}{2}|J_1+J_2|(G\sum_{j=1}^{2}|y_j|+|g||y|) \\
&\le c(1+|z_1|+|z_2|)(G\sum_{j=1}^{2}|y_j|+G^{1/2}|y|) \\
&\le \delta G(|z_1|^2+|z_2|^2)+c(\delta)(G(|y_1|^2+|y_2|^2)+|y|^2+|v|^2).
\end{aligned} \tag{5.9}
$$

Setting $\sigma = \sum_{j=1}^{2}\|y_j\|_q^{2q/(q-N)} \in L_1(S)$, we find by means of the inequalities of Hölder, Gagliardo-Nirenberg [13] and Young [9]

$$
\begin{aligned}
\int G|y_j|^2\,d\Omega &\le \|G\|_{q/(q-2)}\|y_j\|_q^2 \le c\|v\|_{2q/(q-2)}^2\|y_j\|_q^2 \\
&\le c\|\nabla v\|^{2N/q}\|v\|^{2(q-N)/q}\|y_j\|_q^2 \le \frac{\delta}{2}\|\nabla v\|^2+c(\delta)\sigma\|v\|^2 \\
&\le \delta(\|z\|^2+\|y\|^2)+c\sigma\|v\|^2.
\end{aligned} \tag{5.10}
$$

Now the lemma follows from (5.4), (5.5) and (5.8) – (5.10). □

We are now able to state our main result.

Theorem 5.1. *Let v_j, $j=1,2$, be (weak) solutions of (2.2)–(2.5) such that the regularity assumption (5.2) is satisfied. Let in addition*

$$
\|v_{ij}\|_{L_\infty(Q)} \le K, \quad \|v_{i1}-v_{i2}\|_{L_\infty(Q)} \le \kappa \tag{5.11}
$$

and (A1)–(A9) be satisfied. Then $v_1=v_2$.

Proof. The theorem is a consequence of Lemma 4.1, Lemma 4.2 and Gronwall's Lemma (comp. [9]). □

Remark. In view of the initial condition (2.4) the second part of (5.11) can be replaced by supposing the solutions v_j to be continuous in time and space.

6. Applications

As to the existence of solutions v in the sense of Definition 3.1, we refer to [3]. Further, the electrostatic potential $v_0(t), t>0$, turns out to be weak solution of Poisson's equation (2.1), provided the initial value $v(0)=(v_{l0})$ satisfies (2.1). Thus standard regularity results for weak solutions to linear elliptic equations can be applied to verify the condition (5.2). In particular, under quite general conditions it can be proved [6] that $|\nabla v_0(t)| \in L_q$ for some $q>2$. Concerning conditions guaranteeing $q>N=3$, we refer to [15]. Finally, results implying continuity of solutions to drift–diffusion–equations in the spatially two-dimensionally case can be found in [7].

We turn to the verification of the basic assumptions and restrict us to the most involved conditions (A2) and (A4).

Condition (A2)
A sufficient condition for (A2) is:

Lemma 6.1. *Let $f \in C^3(\mathbb{R})$ satisfy*

$$f' > 0, \quad f''^2 > f'f'''.$$

Then $g = f' \circ f^{-1}$ is uniformly concave.

Proof. For $s_1, s_2 \in \mathbb{R}$, $s = \frac{s_2 - s_1}{2}$, we have

$$2g\left(\frac{s_1+s_2}{2}\right) - g(s_1) - g(s_2) = -s^2 \int_0^1 \int_0^1 g''(s_1 + (\tau+\eta)s)\, d\tau\, d\eta.$$

Since

$$g''(s) = \frac{f'f''' - f''^2}{f'^3} \circ f^{-1},$$

the lemma follows. □

Using this lemma, it is easy to show that the function

$$f_a(s) = \eta^{3/2}\ ,\ \eta = c\log(1+\frac{\tau}{c})\ ,\ \tau = \exp(2s/3)\ ,\ c = \left(\frac{6}{\pi}\right)^{1/3}\ , \qquad (6.1)$$

satisfies (A2) for arbitrary $0 < \kappa, K < \infty$. f_a serves in some situations as simple but sufficient approximation of the Fermi function

$$f_i(s) = \mathcal{F}(s) = \frac{2}{\sqrt{\pi}} \int_0^\infty \frac{\sqrt{t}\, dt}{1+\exp(t-s)}\ , \qquad (6.2)$$

which is the favoured example from the physical point of view, since Fermi–Dirac statistics is based on it. Unfortunately, it seems to be difficult to prove rigorously that the Fermi function satisfies (A2). However, computer calculations make this evident (comp. [Fig. 1]).
In many physical situations Boltzmann statistics is considered as sufficient approximation for Fermi–Dirac statistics. Boltzmann statistics is based on

$$f_i(s) = f(s) = exp(s), \qquad (6.3)$$

which implies

$$g_i(s) = s, \quad G_i = 0. \qquad (6.4)$$

Thus (6.3) violates (A2) (and also (A4)) and can be looked at merely as (nonallowed) limit case. However, uniqueness results under Boltzmann statistics have been proved in [3] for the special case $\Gamma = \emptyset$, using only the chemical part of the energy functional, i. e.

$$F_c(u) = \int \sum_{i=n}^{p} \int_0^{u_i} f_i^{-1}(s)\, ds\, d\Omega$$

for defining a distance. Moreover, as a pleasant consequence of (6.4) even the regularity condition (5.2) could be removed in [3] .

Condition (A4)

There are different options for a_i. A first physically interesting choice is [14]

$$a_i = \mu_i f_i', \quad \mu_i = const.,$$

which verifies (A4) trivially with $\rho = 0$, provided g_i is strictly concave. A frequently used choice is [3]

$$a_i = \mu_i f_i, \quad \mu_i = const.. \tag{6.5}$$

Of course, both choices coincide under Boltzmann statistics.

By computing levels of the function $\rho(s_1, s_2)$ corresponding to (6.2) and (6.5) it can be made evident (comp. [Fig. 2]) that the condition (A4) holds for finite K and suitable κ. In particular, the trace of this function given by

$$\rho(s) = \lim_{s_2 \to s_1 = s} = \frac{(ff'' - f'^2)^2}{2f^2(f''^2 - f'f''')}(s) = \frac{-[(\log(\log f)')']^2}{2(\log f')''}(s),$$

satisfies

$$\rho(s) < 1, \quad s \in \mathbb{R}. \tag{6.6}$$

For the approximation (6.1), one gets rigorously

$$\lim_{s \to -\infty} = 0 < \rho_{f_a}(s) = \frac{(\tau - \eta)^2}{\tau(\tau - \eta + 2\eta^2/c)} < \lim_{s \to \infty} = 1.$$

Remark. The 'local' condition (6.6) along with the continuity of the function ρ imply the 'global' condition (A4) for sufficiently small κ.

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Fig. 1. g (s) , f = Fermi function

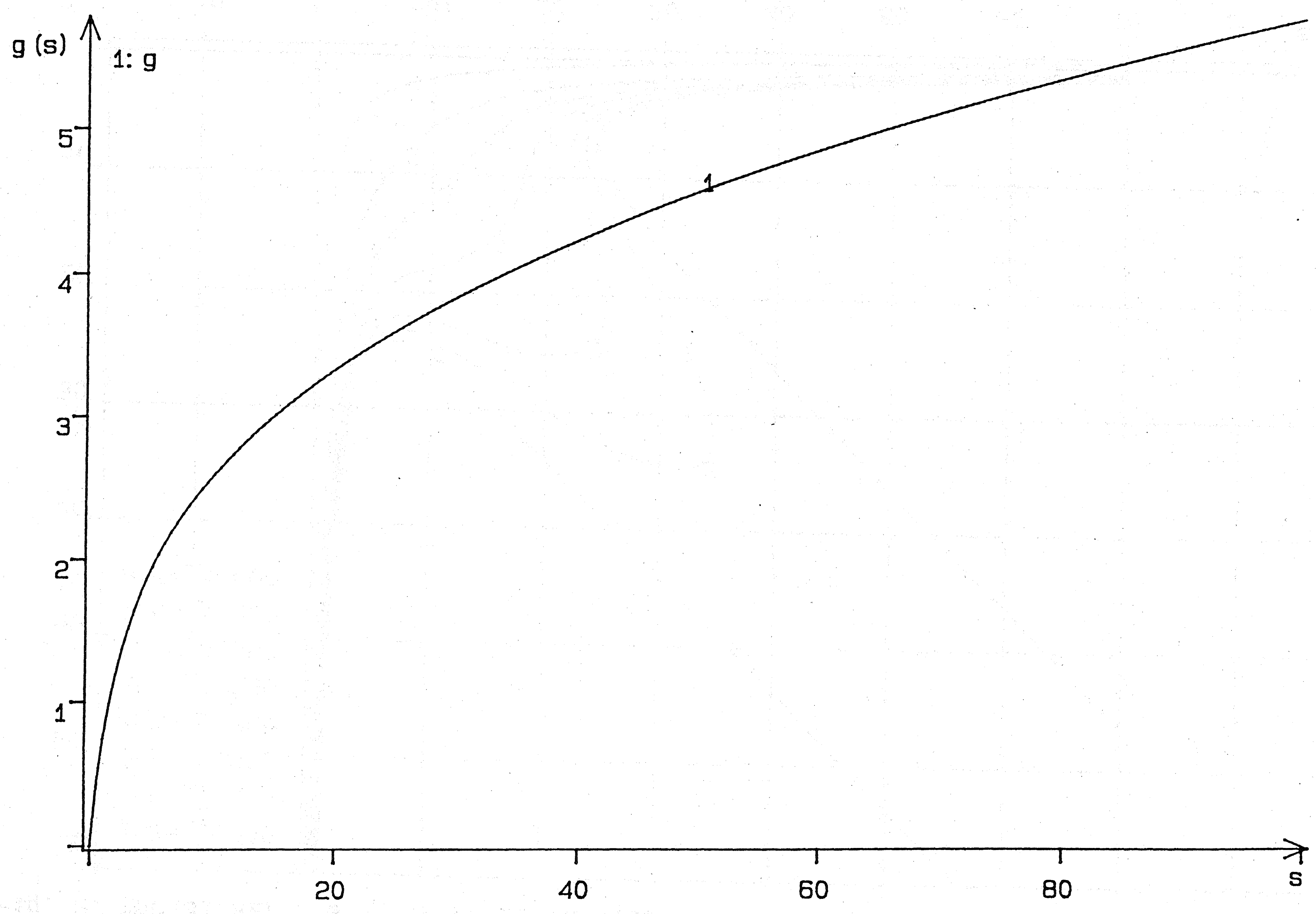
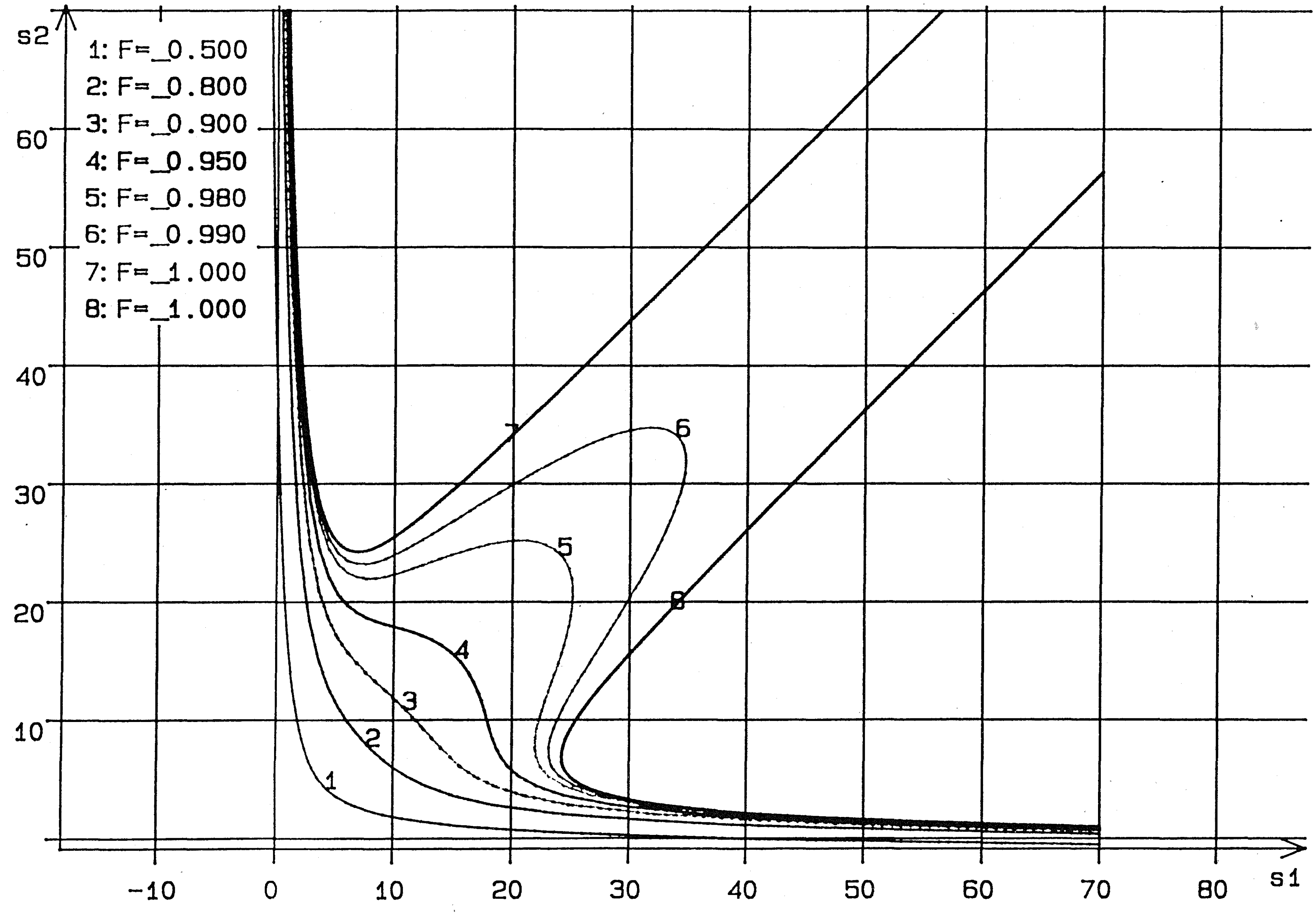


Fig. 2. rho(s1, s2) , a = f = Fermi function



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