The Thermal Equilibrium State of Semiconductor Devices

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Abstract—The thermal equilibrium state of two oppositely charged gases confined to a bounded domain $\Omega \subset \mathbb{R}^m$, $m = 1, 2$ or $m = 3$, is entirely described by the gases’ particle densities $p, n$ minimizing the total energy $E(p, n)$. It is shown that for given $P, N > 0$ the energy functional $E$ admits a unique minimizer in $\{(p, n) \in L^2(\Omega) \times L^2(\Omega) : p, n \geq 0, \int_\Omega p = P, \int_\Omega n = N\}$ and that $p, n \in C(\Omega) \cap L^\infty(\Omega)$.

The analysis is applied to the hydrodynamic semiconductor device equations. These equations in general possess more than one thermal equilibrium solution, but only the unique solution of the corresponding variational problem minimizes the total energy. It is equivalent to prescribe boundary data for electrostatic potential and particle densities satisfying the usual compatibility relations and to prescribe $V^e$ and $P, N$ for the variational problem.

Keywords—Thermal equilibrium state of mixture of charged gases, Variational inequalities, Minimization of total energy, Hydrodynamic semiconductor device model.

1. INTRODUCTION

In this paper, the thermal equilibrium state of a thermodynamic system is investigated. This system consists of two charged gases confined to a bounded domain $\Omega \subset \mathbb{R}^m$, $m = 1, 2$ or $m = 3$. $\partial \Omega$ splits into two disjoint sets $\Gamma_D$ and $\Gamma_N$ with $\text{meas}_{n-1}(\Gamma_D) > 0$. The outer unit normal vector $\nu$ is assumed to exist a.e. on $\Gamma_N$. In $\Omega$ an electrostatic potential $V^e(x), x \in \Omega$ is applied: $-\Delta V^e = C$ with $\nabla V^e \cdot \nu = 0$ on $\Gamma_N$ where $C$ represents a fixed charge distribution. The electrostatic potential generated by the charged gases is denoted by $V_0 = V_0(x)$, i.e., $-\Delta V_0 = \lambda_1 p - \lambda_2 n$ on $\Omega$. $p = p(x), n = n(x)$ are the nonnegative mass densities of the gases. $\lambda_1, -\lambda_2 \neq 0$ is the respective gas’ charge per particle expressed as multiple of the elementary charge. For the sake of simplicity, $\lambda_1 = \lambda_2 = 1$ is assumed. (The general case can be treated by obvious changes.) $V_0$ is subject to homogeneous, mixed boundary conditions: $V_0 = 0$ on $\Gamma_D$ and $\nabla V_0 \cdot \nu = 0$ on $\Gamma_N$. The total mass of each gas is assumed to be prescribed: $\int_\Omega p = P > 0, \int_\Omega n = N > 0$.

The thermodynamic description of this system does crucially depend on the constitutive law which determines the functional relation between the macroscopic quantities pressure, mass density and temperature. Both gases shall behave as ideal gases and the analysis is restricted to isentropic states. Then the total energy reads (see [1])

$$E(p, n) = \int_\Omega H(p) + \int_\Omega H(n) + \int_\Omega (p - n) V^e + \frac{1}{2} \int_\Omega |\nabla V_0 [p - n]|^2$$

with $H''(t) \equiv (r''(t))/t$ where $r(\rho)$ is the pressure function.

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In thermal equilibrium the total energy of the system is minimal. The corresponding mass densities \( p^* \) and \( n^* \) minimize \( \mathcal{E} \), i.e., \( (p^*, n^*) \) is expected to solve the variational problem
\[
\mathcal{E}(p^*, n^*) = \inf_{(p,n) \in C} \mathcal{E}(p, n)
\]
where \( C \) is a set of appropriately chosen mass densities.

The paper is organized as follows. At the beginning of Section 2 various regularity assumptions on the system’s data are stated. Then the precise formulation of the variational problem is given. The variational inequalities are equivalent to a semilinear elliptic differential equation in terms of the electrostatic potential. This equivalence allows us to deduce the main result of this paper: The variational problem admits for a very large class of pressure functions \( r \) (see assumption (A1) at the beginning of Section 2) a unique minimizer.

The Lagrange multipliers \( \alpha_1, \alpha_2 \) associated to the constraints \( p, n \geq 0, \int_\Omega p = P, \int_\Omega n = N \) are uniquely determined by \( P, N \) and that the map \( a : ((0, \infty))^2 \to \mathbb{R}^2, (P, N) \mapsto a(P, N) \equiv (\alpha_1, \alpha_2) \) is injective.

In Section 3, the variational formulation is applied to the hydrodynamic semiconductor device equations. These equations in general possess more than one thermal equilibrium solution, but only the (unique) solution of the corresponding variational problem minimizes the total energy. If the analysis of the semiconductor device equations is restricted to the solution minimizing the total energy, then it is equivalent

- to prescribe boundary data \( (V^D_P, P_D, n_D) \) satisfying the usual compatibility relations,
- to prescribe \( (V^e, P, N) \) for the variational problem where \( V^e \) solves
\[
-\Delta V^e = C, \quad V^e = V^D_p \text{ on } \Gamma_p, \quad \nabla V^e \cdot \nu = 0 \text{ on } \Gamma_N
\]
and \( (P, N) = a^{-1}(\alpha_1, \alpha_2) \).

For the proofs of the results of Section 2 see [1].

2. THE VARIATIONAL PROBLEM

The following assumptions shall hold:

(A1) \( r \in W^{1,\infty}_{\text{loc}}([0, +\infty)), r' > 0 \) a.e. on \( (0, \infty) \).

(A2) \( \Omega \subset \mathbb{R}^m, m \in \{1, 2, 3\}; \Omega \) is a bounded domain; \( \partial \Omega \in C^{0,1}; \partial \Omega = \Gamma_N \cup \Gamma_D, \Gamma_N \cap \Gamma_D = \emptyset; \Gamma_N \) is open and \( \Gamma_D \) is closed in \( \partial \Omega \); \( \text{meas}_{m-1} \Gamma_D > 0 \); the outer unit normal vector \( \nu \) exists a.e. on \( \Gamma_N \).

(A3) \( V^e \in H^1(\Omega) \cap L^\infty(\Omega) \) satisfies \(-\Delta V^e = C = L^\infty(\Omega), \nabla V^e \cdot \nu = 0 \) on \( \Gamma_N \).

(A4) \( P > 0, N > 0 \).

Thanks to (A1), the enthalpy function \( h : (0, \infty) \to \mathbb{R}, \rho \mapsto h(\rho) \equiv \int_1^\rho (r'(\tau)/\tau) \, d\tau \) is continuous, strictly monotone increasing and belongs to \( W^{1,\infty}_{\text{loc}}((0, +\infty)) \cap L^1_{\text{loc}}((0, +\infty)) \).

Let \( \bar{h} \equiv \lim_{\rho \to +\infty} h(\rho) \in (0, \infty], \underline{h} \equiv \lim_{\rho \to 0} h(\rho) \in [0, 0). \) Since \( h \) is injective, it is possible to define \( g : [-\infty, +\infty] \to [0, +\infty] \) via
\[
t \mapsto g(t) \equiv \begin{cases} 0, & -\infty \leq t \leq \underline{h}, \\ h^{-1}(t), & \underline{h} < t < \bar{h}, \\ +\infty, & \bar{h} < t < +\infty. \end{cases} \tag{1}
\]

It is easy to see that \( g \) is continuous and monotone increasing on \([-\infty, +\infty]\) and strictly monotone increasing on \((\underline{h}, \bar{h})\). The regularity of \( h \) also implies that \( H : [0, \infty) \to \mathbb{R}, \rho \mapsto \int_1^\rho h(\tau) \, d\tau \) belongs to \( C([0, \infty)) \cap C^1((0, \infty)) \), is strictly convex and nonnegative on \([0, \infty)\). Let
\[
C \equiv \left\{(p, n) \in L^2(\Omega) \times L^2(\Omega) : p, n \geq 0, \int_\Omega p = P, \int_\Omega n = N \right\}, \tag{2}
\]
where $P, N > 0$ are the constants given in (A4). Recalling that
\[
\mathcal{E}(p, n) = \int_\Omega H(p) + \int_\Omega H(n) + \int_\Omega (p - n) V^e + \frac{1}{2} \int_\Omega |\nabla V_0 [p - n]|^2,
\]
it is easy to see that $\mathcal{E} : \mathcal{C} \to (-\infty, +\infty]$ is well defined, bounded from below and strictly convex.

The variational problem introduced in Section 1 reads:
\[
\text{Find } (p^*, n^*) \in \mathcal{C} \text{ such that } \mathcal{E}(p^*, n^*) = \inf_{(p, n) \in \mathcal{C}} \mathcal{E}(p, n). \tag{VAR}
\]

The main result is:

**Theorem 2.1.** Assume that (A1)-(A4) hold. Then:

(a) (VAR) has a unique solution $(p^*, n^*) \in \mathcal{C}$.

(b) There exist unique $\alpha_1, \alpha_2 \in \mathbb{R}$ such that
\[
(p^*, n^*) = (\alpha_1 V^e - V_0^*, \alpha_2 + V^e + V_0^*)
\]
where $V_0^* = V_0[p^* - n^*] \in L^\infty(\Omega)$ is the unique $H^1$-solution of
\[
\Delta V_0^* = g(\alpha_2 + V^e + V_0^*) - g(\alpha_1 - V^e - V_0^*)
\]
\[
V_0^* = 0 \text{ on } \Gamma_D, \quad \nabla V_0^* \cdot \nu = 0 \text{ on } \Gamma_N.
\]

(c) $p^*, n^* \in C(\Omega) \cap L^\infty(\Omega)$.

(d) If $h = -\infty$, then $p^*, n^* \geq \rho_{\min} > 0$ a.e. on $\Omega$.

**Remark 2.2.**

(a) In Theorem 2.1, no growth condition on $H(\rho)$ for $\rho \to \infty$ is employed. $\mathcal{E}(\ldots)$ is in general not coercive on
\[
\mathcal{C}^p = \left\{ (p, n) \in L^p(\Omega) \times L^p(\Omega) : p, n \geq 0, \int_\Omega p - P, \int_\Omega n - N \right\}
\]
for any $p \in [1, \infty)$. As a consequence, minimizing sequence of $\mathcal{E}$ have a priori no subsequences converging weakly in $L^p(\Omega) \times L^p(\Omega)$ for any $p \in [1, \infty)$.

(b) The parameters $\alpha_1, \alpha_2$ are the Lagrange multipliers associated to the constraints
\[
\int_\Omega p = P, \quad \int_\Omega n = N, \quad p, n \geq 0. \tag{5}
\]

**Remark 2.3.** If
\[
r(\rho) = \rho^{1+\gamma}, \quad \gamma \geq 0
\]
(see Section 3) equations of the regularity result of Theorem 2.1(c) can be strengthened as follows:

(a) If $0 \leq \gamma < 1$, then $g \in C^{1,1}_\text{loc}(\mathbb{R})$ and
\[
p^*, n^* \in C^{1,\theta}_\text{loc}(\Omega), \quad \text{ for all } \theta \in (0, 1).
\]

(b) If $1 \leq \gamma$, then $g \in C^{0,1/\gamma}_\text{loc}(\mathbb{R})$ and
\[
p^*, n^* \in C^{1,\theta}_\text{loc}(\Omega), \quad \text{ for all } \theta \in \left(0, \frac{1}{\gamma}\right).
\]

If $p^* > 0$ on $\Omega' \subset \Omega$, $n^* > 0$ on $\Omega'' \subset \Omega$, then
\[
p^* \in C^{1,\theta}_\text{loc}(\Omega'), n^* \in C^{1,\theta}_\text{loc}(\Omega''), \quad \text{ for all } \theta \in (0, 1).
\]

**Lemma 2.4.** Assume that (A1)-(A3) hold. Then the map
\[
a : (0, \infty) \times (0, \infty) \to \mathbb{R}^2
\]
\[
(P, N) \mapsto a(P, N) = (\alpha_1, \alpha_2),
\]
where $\alpha_1, \alpha_2$ are the Lagrange multipliers associated to the constraints (5), is injective.

**Remark 2.5.** Thanks to Theorem 2.1(b), the function $a : ((0, \infty))^2 \to \mathbb{R}^2$ is well-defined.
3. THE HYDRODYNAMIC MODEL

The hydrodynamic bipolar semiconductor model equations read in the case of thermal equilibrium (see [2])

\[ \nabla r(n) - n \nabla V = 0, \quad \nabla r(p) + p \nabla V = 0, \]

\[ \Delta V = n - p - C. \]  

(7)

Here \( V = V(x) \) denotes the electrostatic potential and \( C = C(x) \) is the prescribed doping profile characterizing the device under consideration. The spatial variable \( x \) ranges over \( \Omega \), the (bounded) semiconductor domain. \( p = p(x) \geq 0 \) and \( n = n(x) \geq 0 \) denote the hole and electron density, respectively. \( r = r(p) \) is the pressure function. As in Section 1, it is assumed that the respective pressures of electrons and holes are determined by the same constitutive law.

Equations (7) are usually supplemented with physically motivated boundary conditions [2]:

\[ n = n_D, \quad p = p_D, \quad V = V_D^e \text{ on } \Gamma_D, \quad \nabla V \cdot \nu = 0 \text{ on } \Gamma_N. \]  

(8)

Here \( \partial \Omega \) splits into two disjoint subsets \( \Gamma_D \) and \( \Gamma_N \). The Dirichlet boundary \( \Gamma_D \) models the union of Ohmic contacts, and the Neumann boundary \( \Gamma_N \) models the union of insulating boundary segments (zero outflow). On \( \Gamma_D \) a thermal equilibrium potential \( V_D^e \) is prescribed.

Equations (7),(8) have recently been investigated in some detail (see [3-5]) where the following assumptions were employed:

\text{(HD1)} \quad r \in \mathcal{W}^{1,\infty}_{\text{loc}}([0, +\infty)), \quad r' > 0 \text{ a.e. on } (0, \infty).

\text{(HD2)} \quad \Omega \subset \mathbb{R}^m, \quad m \in \{1, 2, 3\}; \quad \Omega \text{ is a bounded domain}; \quad \partial \Omega \in \mathcal{C}^{0,1}; \quad \partial \Omega = \Gamma_N \cup \Gamma_D, \quad \Gamma_N \cap \Gamma_D = \emptyset; \quad \Gamma_N \text{ is open and } \Gamma_D \text{ is closed in } \partial \Omega; \quad \text{meas}_{m-1}(\Gamma_D) > 0; \quad \text{the outer unit normal vector } \nu \text{ exists a.e. on } \Gamma_N.

\text{(HD3)} \quad V_D^e \in H^{1/2}(\Gamma_D) \cap L^\infty(\Omega), \quad C \in L^\infty(\Omega);

\text{(HD4)} \quad n_D, p_D \in L^\infty(\Gamma_D), n_D, p_D \geq \rho_{\text{min}} > 0; \quad \exists \alpha \in \mathbb{R}: h(p_D) + V_D^e = h(n_D) - V_D^e = \alpha.

\text{(HD5)} \quad \tilde{h} = +\infty.

For physical reasons, the (thermal equilibrium) solution of (7),(8) should be unique. In general this is, however, not the case for pressure functions \( r(p) = p^{1+\gamma}, \gamma > 0 \), see [1]. The lack of uniqueness corresponds to the fact that in thermal equilibrium the system should be in a state of minimal total energy—but the total energy is not taken into account in the model equations (7),(8).

Interpreting holes and electrons as charged gases one may try to apply the variational approach of Section 2 to describe the thermal equilibrium state of the semiconductor device. But then a problem occurs:

Assume that \( \alpha \) and \( V_D^e \) (see (HD4)) are given. How shall one choose the parameters \( P, N, V^e \) for the variational problem?

The answer to this question can be given as follows:

- Assumptions (HD1)-(HD3) allow us to define \( V^e \in H^1(\Omega) \cap L^\infty(\Omega) \) uniquely via

\[ -\Delta V^e = C, \quad V^e = V_D^e \text{ on } \Gamma_D, \quad \nabla V^e \cdot \nu = 0 \text{ on } \Gamma_N. \]  

(9)

- According to Markowich and Unterreiter [3], problem (7),(8) has a solution \( (p^+, n^+, V^+) \) with

\[ p^+ = g(\alpha + V^e + V^+), \quad n^+ = g(\alpha - V^e - V^+), \]

\[ \Delta V^+ = n^+ - p^+ - C, \quad V^+ = V_D^e \text{ on } \Gamma_D, \quad \nabla V^+ \cdot \nu = 0 \text{ on } \Gamma_N \]  

(10)

with \( g \) defined as in (1). Furthermore, \( p^+, n^+ \in L^\infty(\Omega) \subset L^1(\Omega) \), and hence

\[ P \equiv \int_{\Omega} p^+, \quad N \equiv \int_{\Omega} n^+ \]  

(11)

are well-defined.
Now consider the energy functional
\[
\mathcal{E}(p, n) \equiv \int_{\Omega} H(p) + \int_{\Omega} H(n) + \int_{\Omega} (p - n) V^e + \frac{1}{2} \int_{\Omega} |V V_0 [p - n]|^2
\]
over the set
\[
\mathcal{C} \equiv \{(p, n) \in L^2(\Omega) \times L^2(\Omega) : p, n \geq 0, \int_{\Omega} p = P, \int_{\Omega} n = N\}
\]
with \(V^e\) as in (9) and \(P, N\) as in (11). It is easy to see that assumptions (A1)-(A4) are satisfied so Theorem 2.1 applies: \(\mathcal{E}\) has a unique minimizer \((p^*, n^*) \in \mathcal{C}\) with
\[
p^* = g(\alpha_1 + V^e + V_0), \quad n^* = g(\alpha_2 - V^e - V_0),
\]
\[-\Delta V_0^* = g(\alpha_1 + V^e + V_0) - g(\alpha_2 - V^e - V_0^*), \quad V_0^* = 0 \text{ on } \Gamma_D, \quad \nabla V_0^* \cdot \nu = 0 \text{ on } \Gamma_N,
\]
and \(\alpha_1, \alpha_2 \in \mathbb{R}\). On the other hand, \((p^+, n^+) \in \mathcal{C}\). Following Unterreiter [1], it is easy to see that \((p^+, n^+) - (p^*, n^*)\) and \(\alpha \equiv \alpha_1 \equiv \alpha_2\). In other words: \((p^+, n^+)\) is the unique minimizer of the total energy and one has no problems accepting \((p^+, n^+)\) as physically relevant solution of (7),(8).

Begin conversely with the variational problem and assume that \(V^e, P, N\) are prescribed and (A1)-(A4) do hold. Then it is easy to see that the uniquely determined minimizer \((p^*, n^*)\) of \(\mathcal{E}\) in \(\mathcal{C}\) satisfies
\[
h(p^*) + V^* \begin{cases} = \alpha & \{x \in \Omega : p^*(x) > 0\}, \\ \geq \alpha & \{x \in \Omega : p^*(x) = 0\}, \end{cases}
\]
\[
h(n^*) - V^* \begin{cases} = \alpha & \{x \in \Omega : n^*(x) > 0\}, \\ \geq \alpha & \{x \in \Omega : n^*(x) = 0\}. \end{cases}
\]
\[
\Delta V^* = g(\alpha + V^*) - g(\alpha - V^*) - C, \\
V^* = V^e + \frac{\alpha_1 + \alpha_2}{2} \text{ on } \Gamma_D, \quad \nabla V^* \cdot \nu \text{ on } \Gamma_N,
\]
where \(\alpha_1, \alpha_2 \in \mathbb{R}\) are the Lagrange multipliers associated to the constraints (3). The triple \((p^*, n^*, V^*)\) is actually a solution of (7) (see [3]). If additionally \(p^*, n^*\) are regular enough and \(p^*, n^* \geq p_{\text{min}} > 0\) does hold, one gets the compatibility relation (HD4)
\[
h(p_D) - V_D^* = \alpha = h(p_D) + V_D^*.
\]
where
\[
p_D \equiv p^*|_{\Gamma_D}, \quad n_D \equiv n^*|_{\Gamma_D}.
\]

**Remark 3.1.** If \(V_D^*\) is prescribed and (HD4) does hold, then the parameter \(\alpha\) can be considered an intrinsic particle density. The variational approach shows that prescribing \((\alpha, V_D^*)\) is equivalent to prescribing the total mass of holes and electrons, respectively. A measurement of \(V_D^*, n_D, p_D\) allows us to determine the total masses of holes and electrons as long as the model equations (7),(8) perform an acceptable physical model for the semiconductor device.

**Remark 3.2.** As there are no additional conditions—like the compatibility relation of (HD4) and \(\bar{h} = +\infty\) (see (HD5))—imposed, the variational approach can be viewed as extension of the work of Markowich and Unterreiter [3].

**REFERENCES**