

ANNALI DELLA
SCUOLA NORMALE SUPERIORE DI PISA
Classe di Scienze

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Annali della Scuola Normale Superiore di Pisa, Classe di Scienze 4^e série, tome 20, n° 3 (1993), p. 371-386

http://www.numdam.org/item?id=ASNSP_1993_4_20_3_371_0

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Vacuum Solutions of a Stationary Drift-diffusion Model

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1. - The Model

We consider a stationary drift-diffusion model for a bipolar semiconductor:

$$(1.1) \quad I_n = \nabla(nT_n) - n\nabla V, \quad \operatorname{div} I_n = 0,$$

$$(1.2) \quad I_p = -\nabla(pT_p) - p\nabla V, \quad \operatorname{div} I_p = 0, \quad x \in \Omega,$$

$$(1.3) \quad \Delta V = n - p - C(x).$$

Here n , I_n and T_n denote the electron density, the electron current density and the electron temperature respectively; p , I_p , T_p are the analogously defined quantities for the positively charged holes, namely the hole density, the hole current density and the hole temperature respectively. Obviously we require that $n \geq 0$, $p \geq 0$, $T_n \geq 0$ and $T_p \geq 0$. V denotes the electrostatic potential, $C = C(x)$ the prescribed doping profile characterizing the device under consideration and $\Omega \subseteq \mathbb{R}^m$, $m = 1, 2$ or 3 , the (bounded) semiconductor domain.

Equations (1.1)-(1.3) can be obtained as limit of the hydrodynamic model for a bipolar semiconductor as the electron and hole mean free paths tend to zero (see [1] and [2]).

We supplement the equations by the following physically motivated mixed boundary conditions (see [3]):

$$(1.4) \quad I_n \cdot \tau = I_p \cdot \tau = \nabla V \cdot \tau = 0 \quad \text{on } \Gamma_N,$$

$$(1.5) \quad n = n_D, \quad p = p_D, \quad V = V_D \quad \text{on } \Gamma_D,$$

where $\partial\Omega$ splits into the disjoint subsets Γ_N and Γ_D . τ denotes the exterior unit normal vector of $\partial\Omega$ (which is assumed to exist almost everywhere). Γ_N

models the union of insulating boundary segments (zero outflow) and Γ_D the union of Ohmic contacts, where an external potential (represented by V_D) is applied. We shall assume that the $(m - 1)$ -dimensional Lebesgue measure of Γ_D is nonzero.

Generally, the particle temperatures T_n and T_p are determined from additional equations, which are coupled to (1.1)-(1.3). In this paper we shall, however, be concerned only with the isentropic case, where T_n and T_p are given as functions of the densities n and p respectively. For the sake of simplicity, we shall assume that these functions are equal, i.e.

$$(1.6) \quad T_n = T(n), \quad T_p = T(p),$$

with $T : [0, \infty) \rightarrow [0, \infty)$. Equivalently, we may assume that the electron and hole pressures r_n and r_p , determined by the ideal-gas law:

$$(1.7) \quad r_n = nT_n, \quad r_p = pT_p,$$

are given (and equal) functions of the particle densities:

$$(1.8) \quad r_n = r(n), \quad r_p = r(p),$$

with

$$(1.9) \quad r(\rho) = \rho T(\rho).$$

Then equations (1.1) and (1.2) can be re-written as:

$$(1.10) \quad I_n = \nabla r(n) - n \nabla V, \quad \operatorname{div} I_n = 0,$$

$$(1.11) \quad I_p = -\nabla r(p) - p \nabla V, \quad \operatorname{div} I_p = 0.$$

Note that $r'(n)$ and $r'(p)$ are the (generally nonlinear) diffusion coefficients of (1.10) and (1.11) respectively. They are non-negative since (as physically reasonable) we assume $r'(\rho) > 0$ for $\rho > 0$.

In the case of a linear pressure function

$$r(\rho) = \rho$$

(i.e. constant diffusivities, isothermal model with $T_n \equiv T_p \equiv 1$), the problem (1.10), (1.11), (1.3), (1.4), (1.5) reduces to the standard drift-diffusion model based on Boltzmann statistics, which has been extensively analysed (see [2], [3] and the references therein). Moreover, the drift-diffusion model with the particular nonlinear pressure function r arising from the assumption of Fermi-Dirac equilibrium particle distributions was analysed in [4]. For both cases the existence of a solution with $n > 0$ and $p > 0$ in $\bar{\Omega}$ was shown for

all doping profiles $C \in L^\infty(\Omega)$ and all sufficiently regular boundary data with $n_D > 0$ and $p_D > 0$ on Γ_D .

It turns out that major ingredients for these existence proofs are the asymptotic values of the enthalpy function

$$(1.12) \quad h(\rho) := \int_1^\rho \frac{r'(s)}{s} ds$$

as $\rho \rightarrow 0+$ and $\rho \rightarrow \infty$. More precisely, the proofs are based on the properties $h(\rho) \rightarrow -\infty$ as $\rho \rightarrow 0+$ and $h(\rho) \rightarrow \infty$ as $\rho \rightarrow \infty$.

However, the usual thermodynamic considerations on which the isentropic hydrodynamic semiconductor model and consequently its zero-mean-free-path limit (1.10), (1.11) are based, suggest a pressure function of the form (see [5]):

$$(1.13) \quad r(\rho) = \rho^\gamma, \quad \gamma \geq 1.$$

For $\gamma > 1$ we obtain

$$(1.14) \quad h(\rho) = \frac{\gamma}{\gamma - 1} (\rho^{\gamma-1} - 1)$$

and hence

$$(1.15) \quad h(\rho) \rightarrow \frac{\gamma}{1 - \gamma} \text{ as } \rho \rightarrow 0+, \quad h(\rho) \rightarrow \infty \text{ as } \rho \rightarrow \infty.$$

The main result of this paper concerns the case excluded so far in the existing literature and represented by (1.15), namely $h(0+) > -\infty$ and $h(\infty) = \infty$. We shall extend the existence result to this case (assuming sufficient regularity on the data and $n_D > 0$, $p_D > 0$ on Γ_D); however, we demonstrate the occurrence of a vacuum for at least one particle type (i.e. the existence of a subset of Ω in which either $n = 0$ or $p = 0$) under certain assumptions on the data.

This result does not seem totally surprising, since (1.10), (1.11) contain the porous media type operator $\Delta(u^\gamma)$ when (1.13) with $\gamma > 1$ is employed.

This paper is organized as follows. In Section 2 we specify assumptions on the enthalpy h and on the data which guarantee non-vacuum solutions; Section 3 is concerned with the analysis of possible vacuum solutions in the case $h(-\infty) > -\infty$, $h(\infty) = \infty$. In this case the solutions will be obtained as limits of non vacuum solutions of approximating problems by a compactness method.

2. - Non-vacuum Solutions

We shall use the following assumptions for the subsequent analysis:

- (A1) $r \in W_{\text{loc}}^{1,\infty}[0, \infty)$ and $r(0) = 0$, $r' > 0$ a.e. in $(0, \infty)$;
- (A2) $\left\{ \begin{array}{l} \Omega \subseteq \mathbb{R}^m, \quad m = 1, 2 \text{ or } 3, \quad \Omega \text{ is bounded, } \partial\Omega \text{ is } C^{0,1}, \\ \partial\Omega = \Gamma_N \cup \Gamma_D, \quad \Gamma_N \cap \Gamma_D = \emptyset, \quad \Gamma_N \text{ is open and} \\ \Gamma_D \text{ is closed in } \partial\Omega, \quad \text{meas}_{m-1}(\Gamma_D) > 0; \end{array} \right.$
- (A3) $\left\{ \begin{array}{l} n_D, p_D, V_D \in H^{1/2}(\Gamma_D) \cap L^\infty(\Gamma_D) \\ \text{and there exists } \underline{\rho} > 0 \text{ such that} \\ \underline{\rho} \leq n_D, p_D \text{ a.e. on } \Gamma_D; \end{array} \right.$
- (A4) $C \in L^\infty(\Omega)$.

If $n > 0$ and $p > 0$ in Ω we can re-write (1.10) and (1.11) as

$$(2.1) \quad I_n = n \left(\frac{r'(n)}{n} \nabla n - \nabla V \right) = n \nabla (h(n) - V),$$

$$(2.2) \quad I_p = -p \left(\frac{r'(p)}{p} \nabla p + \nabla V \right) = -p \nabla (h(p) + V).$$

This suggests the introduction of the (so called Fermi-) potentials:

$$(2.3) \quad \psi = h(n) - V, \quad \sigma = h(p) + V.$$

From assumption (A1) we deduce that h maps the interval $(0, \infty)$ bijectively into its range (\underline{h}, \bar{h}) , where

$$(2.4) \quad \underline{h} := \lim_{\rho \rightarrow 0^+} h(\rho), \quad \bar{h} := \lim_{\rho \rightarrow \infty} h(\rho).$$

Note that $-\infty \leq \underline{h} < 0 < \bar{h} \leq \infty$. We denote the inverse function of h by g , i.e. $g : (\underline{h}, \bar{h}) \rightarrow (0, \infty)$, $g = h^{-1}$. Obviously g is strictly increasing.

Then, if $\psi + V, \sigma - V \in (\underline{h}, \bar{h})$, we can compute the densities n and p from (2.3):

$$(2.5) \quad n = g(\psi + V), \quad p = g(\sigma - V)$$

and (1.10), (1.11), (1.3) can be re-written as

$$(2.6) \quad \operatorname{div}(n \nabla \psi) = 0,$$

$$(2.7) \quad \operatorname{div}(p \nabla \sigma) = 0, \quad x \in \Omega,$$

$$(2.8) \quad \Delta V = g(\psi + V) - g(\sigma - V) - C(x),$$

subject to the boundary conditions

$$(2.9) \quad \nabla \psi \cdot \tau = \nabla \sigma \cdot \tau = \nabla V \cdot \tau = 0 \quad \text{on } \Gamma_N,$$

$$(2.10) \quad \psi = h(n_D) - V_D, \quad \sigma = h(p_D) + V_D, \quad V = V_D \quad \text{on } \Gamma_D.$$

The boundary value problem (2.5)-(2.10) must admit an equilibrium solution (for a certain yet undetermined boundary potential V_D) in order to be physically reasonable. At the thermal equilibrium $I_n \equiv I_p \equiv 0$ holds and, consequently, (2.1) and (2.2) give

$$(2.11) \quad \psi_e \equiv \text{const}, \quad \sigma_e \equiv \text{const},$$

where the index e refers to thermal equilibrium. Then (2.3) implies $h(n_e) + h(p_e) \equiv \psi_e + \sigma_e$ and evaluation at the Dirichlet boundary Γ_D gives the condition:

$$(A5) \quad \alpha := h(n_D) + h(p_D) = \text{const} \quad \text{on } \Gamma_D.$$

We remark that the Dirichlet data n_D and p_D are independent of the state of the semiconductor (see [3]), i.e. n_D and p_D are the same functions for thermal equilibrium and away from equilibrium.

Obviously, the potential V is only determined up to a constant or, equivalently, an arbitrary constant can be added to one of the Fermi-potentials. We choose

$$\psi_e = \frac{\alpha}{2}$$

and obtain from (2.10) and (2.11):

$$\sigma_e = \frac{\alpha}{2}.$$

The equilibrium potential V_e satisfies:

$$(2.12) \quad \Delta V_e = g\left(\frac{\alpha}{2} + V_e\right) - g\left(\frac{\alpha}{2} - V_e\right) - C(x), \quad x \in \Omega,$$

$$(2.13) \quad \nabla V_e \cdot \tau = 0 \quad \text{on } \Gamma_N,$$

$$(2.14) \quad V_e = h(n_D) - \frac{\alpha}{2} = \frac{\alpha}{2} - h(p_D) \quad \text{on } \Gamma_D.$$

As usual in semiconductor modeling, the boundary potential V_D for non-equilibrium situations is written as the sum of the boundary equilibrium potential and an externally applied potential $U_D \in H^{1/2}(\Gamma_D) \cap L^\infty(\Gamma_D)$:

$$(2.15)(a) \quad V_D = h(n_D) - \frac{\alpha}{2} + U_D = \frac{\alpha}{2} - h(p_D) + U_D.$$

The Dirichlet boundary Fermi-potentials then read:

$$(2.15)(b) \quad \psi_D = \frac{\alpha}{2} - U_D, \quad \sigma_D = \frac{\alpha}{2} + U_D,$$

and (2.5)-(2.9) are supplemented by the Dirichlet conditions:

$$(2.15)(c) \quad \psi = \psi_D, \quad \sigma = \sigma_D, \quad V = V_D \quad \text{on } \Gamma_D.$$

For $U_D \equiv 0$ the problem (2.5)-(2.9), (2.15) reduces (by construction) to the equilibrium problem (2.12)-(2.14). Non-equilibrium situations are described by $U_D \not\equiv 0$ on Γ_D .

For the standard drift-diffusion model with $\tau(\rho) = \rho$, condition (A5) reads

$$(2.16)(a) \quad n_D p_D = \text{const} \quad \text{on } \Gamma_D$$

(see [2] and [3]), and for $\tau(\rho) = \rho^\gamma$, $\gamma > 1$, we obtain

$$(2.16)(b) \quad n_D^{\gamma-1} + p_D^{\gamma-1} \equiv \text{const} \quad \text{on } \Gamma_D.$$

Obviously, any analysis of the system (2.5)-(2.8) has to be based on a control of $\psi + V$ and $\sigma - V$. In particular, the estimates

$$\psi + V < \bar{h}, \quad \sigma - V < \bar{h}$$

guarantee that n and p are finite and the estimates

$$\underline{h} < \psi + V, \quad \underline{h} < \sigma - V$$

imply ellipticity of (2.6) and (2.7). The existence proof to be presented in this Section is based on maximum principle estimates for (2.6)-(2.8) which allow the control of $\psi + V$ and $\sigma - V$.

For notational simplicity we write

$$i(\varphi) := \text{ess inf}_{\Gamma_D} \varphi, \quad s(\varphi) := \text{ess sup}_{\Gamma_D} \varphi, \quad \delta(\varphi) := s(\varphi) - i(\varphi)$$

for functions $\varphi \in L^\infty(\Gamma_D)$. We now denote

$$(2.17)(a) \quad \underline{\psi} := \frac{\alpha}{2} - s(U_D), \quad \bar{\psi} := \frac{\alpha}{2} - i(U_D)$$

$$(2.17)(b) \quad \underline{\sigma} := \frac{\alpha}{2} + i(U_D), \quad \bar{\sigma} := \frac{\alpha}{2} + s(U_D)$$

and define the functions

$$(2.18)(a) \quad \begin{aligned} \bar{G}(\omega) &:= g(\bar{\psi} + \omega) - g(\underline{\sigma} - \omega) - \underline{C}, \\ D(\bar{G}) &:= \{\omega \in \mathbb{R} \mid \underline{h} < \bar{\psi} + \omega, \underline{\sigma} - \omega < \bar{h}\}, \end{aligned}$$

$$(2.18)(b) \quad \begin{aligned} \underline{G}(\omega) &:= g(\underline{\psi} + \omega) - g(\bar{\sigma} - \omega) - \bar{C}, \\ D(\underline{G}) &:= \{\omega \in \mathbb{R} \mid \underline{h} < \underline{\psi} + \omega, \bar{\sigma} - \omega < \bar{h}\}, \end{aligned}$$

with

$$(2.19) \quad \underline{C} := \operatorname{ess\,inf}_{\Omega} C, \quad \bar{C} := \operatorname{ess\,sup}_{\Omega} C.$$

It is easy to check that $D(\underline{G}) \neq \emptyset$ and $D(\bar{G}) \neq \emptyset$. Obviously, (A1) implies that \underline{G} and \bar{G} are strictly increasing functions on $D(\underline{G})$ and $D(\bar{G})$ respectively.

We then have:

LEMMA 2.1. *Assume*

$$(B1) \quad \delta(U_D) < \min \left\{ \bar{h} - \frac{\alpha}{2}, \frac{\alpha}{2} - \underline{h} \right\}.$$

Then

$$(2.20) \quad [i(V_D), s(V_D)] \subseteq D(\underline{G}) \cap D(\bar{G}).$$

The proof is a straight-forward calculation.

Another simple calculation gives:

LEMMA 2.2. *If the conditions (B1) and*

$$(B2) \quad \|C\|_{L^\infty(\Omega)} < \begin{cases} +\infty & \text{if } \underline{h} = -\bar{h} = -\infty \\ g(\bar{h} - \delta(U_D)) - g(\alpha - (\bar{h} - \delta(U_D))) & \text{if } \bar{h} + \underline{h} \leq \alpha \\ g(\alpha - (\underline{h} + \delta(U_D))) - g(\underline{h} + \delta(U_D)) & \text{if } \bar{h} + \underline{h} > \alpha \end{cases}$$

hold, then there exist unique values $\omega_1, \omega_2 \in D(\bar{G}) \cap D(\underline{G})$ such that $\bar{G}(\omega_1) = \underline{G}(\omega_2) = 0$.

We now set

$$(2.21) \quad \bar{V} := \max(\omega_2, s(V_D)), \quad \underline{V} := \min(\omega_1, i(V_D))$$

and

$$(2.22) \quad \underline{n} := g(\underline{\psi} + \underline{V}), \quad \bar{n} := g(\bar{\psi} + \bar{V}),$$

$$(2.23) \quad \underline{p} := g(\underline{\sigma} - \bar{V}), \quad \bar{p} := g(\bar{\sigma} - \underline{V}).$$

Obviously, (B1) and (B2) imply

$$(2.24) \quad 0 < \underline{n} \leq \bar{n} < \infty, \quad 0 < \underline{p} \leq \bar{p} < \infty.$$

We now state the main result of this Section.

THEOREM 2.1. *Let the assumptions (A1)-(A5) and the conditions (B1) and (B2) hold. Then there exists a weak solution $(n, p, \psi, \sigma, V) \in (H^1(\Omega) \cap L^\infty(\Omega))^5$ of the problem (2.5)-(2.9), (2.15), which satisfies the estimates*

$$(2.25) \quad \underline{n} \leq n \leq \bar{n}, \quad \underline{p} \leq p \leq \bar{p}, \quad \underline{\psi} \leq \psi \leq \bar{\psi}, \quad \underline{\sigma} \leq \sigma \leq \bar{\sigma}, \quad \underline{V} \leq V \leq \bar{V}$$

a.e. in Ω .

PROOF. The proof is a modification of the (already classical) existence proof for the standard drift-diffusion problem with a linear pressure (see [2] and [3]).

We construct the fixed point operator T with domain

$$M := \{(\psi, \sigma) \in (L^\infty(\Omega))^2 \mid \underline{\psi} \leq \psi(x) \leq \bar{\psi}, \quad \underline{\sigma} \leq \sigma(x) \leq \bar{\sigma} \quad \text{a.e. in } \Omega\}$$

as follows. Given $(\psi_0, \sigma_0) \in M$, consider the Poisson equation

$$(2.26) \quad \Delta V_0 = g(\psi_0 + V_0) - g(\sigma_0 - V_0) - C(x), \quad x \in \Omega$$

$$(2.27) \quad V_0|_{\Gamma_D} = V_D|_{\Gamma_D}, \quad \frac{\partial V_0}{\partial \tau} \Big|_{\Gamma_N} = 0,$$

where V_D is given by (2.15)(a). We set

$$G_0(V, x) := g(\psi_0(x) + V) - g(\sigma_0(x) - V) - C(x).$$

Obviously, $G_0(\cdot, x)$ is monotonely increasing on $D(G_0)$. Lemma 2.1 and the definition of M imply that

$$[i(V_D), s(V_D)] \subseteq D(\underline{G}) \cap D(\bar{G}) \subseteq D(G_0).$$

Also, $\underline{G}(\omega) \leq G_0(\omega, x) \leq \bar{G}(\omega)$ for all $\omega \in D(\underline{G}) \cap D(\bar{G})$ and almost everywhere in Ω .

With ω_1 and ω_2 given by Lemma 2.2 we conclude that

$$G_0(\omega_2, x) \geq 0, \quad G_0(\omega_1, x) \leq 0 \quad \text{a.e. in } \Omega$$

and, from the monotonicity of G_0 and (2.21), that

$$G_0(\bar{V}, x) \geq 0, \quad G_0(\underline{V}, x) \leq 0 \quad \text{a.e. in } \Omega.$$

The maximum principle then implies that \bar{V} is an upper solution and \underline{V} a lower one, i.e.

$$(2.28) \quad \underline{V} \leq V_0(x) \leq \bar{V} \quad \text{a.e. in } \Omega.$$

Existence and uniqueness of a solution of (2.26), (2.27) are easily established using the a-priori bounds (2.28).

Since

$$\begin{aligned} \underline{h} < \underline{\psi} + \underline{V} \leq \psi_0 + V_0 \leq \bar{\psi} + \bar{V} < \bar{h}, \\ \underline{h} < \underline{\sigma} - \bar{V} \leq \sigma_0 + V_0 \leq \bar{\sigma} - \underline{V} < \bar{h}, \end{aligned}$$

we can define

$$n_0 = g(\psi_0 + V_0), \quad p_0 = g(\sigma_0 - V_0).$$

The bounds

$$0 < \underline{n} \leq n_0 \leq \bar{n}, \quad 0 < \underline{p} \leq p_0 \leq \bar{p}$$

clearly hold. Then, to complete the construction of the fixed point operator T , we solve

$$(2.29) \quad \operatorname{div}(n_0 \nabla \psi_1) = 0, \quad x \in \Omega$$

$$(2.30) \quad \psi_1|_{\Gamma_D} = \psi_D|_{\Gamma_D}, \quad \left. \frac{\partial \psi_1}{\partial \tau} \right|_{\Gamma_N} = 0$$

for ψ_1 and

$$(2.31) \quad \operatorname{div}(p_0 \nabla \sigma_1) = 0, \quad x \in \Omega$$

$$(2.32) \quad \sigma_1|_{\Gamma_D} = \sigma_D|_{\Gamma_D}, \quad \left. \frac{\partial \sigma_1}{\partial \tau} \right|_{\Gamma_N} = 0.$$

for σ_1 . The maximum principle and definitions (2.17)(a) and (b) imply that

$$(2.33) \quad \underline{\psi} \leq \psi_1 \leq \bar{\psi}, \quad \underline{\sigma} \leq \sigma_1 \leq \bar{\sigma} \quad \text{a.e. in } \Omega.$$

Setting $T(\psi_0, \sigma_0) = (\psi_1, \sigma_1)$ we conclude that T is well-defined and a self map of the set M .

The standard elliptic estimate gives

$$\begin{aligned}\|\nabla\psi_1\|_{L^2(\Omega)} &\leq \frac{\bar{n}}{\underline{n}} \|\nabla U_D\|_{L^2(\Omega)}, \\ \|\nabla\sigma_1\|_{L^2(\Omega)} &\leq \frac{\bar{p}}{\underline{p}} \|\nabla U_D\|_{L^2(\Omega)}\end{aligned}$$

and we conclude that $T(M)$ is precompact in $(L^2(\Omega))^2$.

It is an easy exercise to show that $T : M \rightarrow M$ is continuous when M is equipped with the $(L^2(\Omega))^2$ -topology. Thus, since M is closed and convex in $(L^2(\Omega))^2$, the Schauder fixed point theorem implies the conclusion of Theorem 2.1. \blacksquare

The assumptions (A1)-(A4) are highly natural for the drift-diffusion problem, while (B1) and (B2) restrict the set of admissible data: (B1) is obviously a smallness assumption on U_D trivially satisfied in thermal equilibrium ($U_D \equiv 0$); (B1) holds for all $U_D \in L^\infty(\Gamma_D)$, if $\underline{h} = -\bar{h} = -\infty$.

(B2) is a smallness assumption on C (depending on U_D). Only in the case $\underline{h} = -\infty = -\bar{h}$ no restriction on $\|C\|_{L^\infty(\Omega)}$ is required.

In particular, Theorem 2.1 asserts the existence of non-vacuum solutions of the drift-diffusion model for the nonlinear pressure function $r(s) = s^\gamma$, $\gamma > 1$, if the data satisfy

$$\delta(U_D) < \frac{\alpha}{2} - \underline{h}, \quad \|C\|_{L^\infty(\Omega)} \leq g(\alpha - (\underline{h} + \delta(U_D))) - g(\underline{h} + \delta(U_D)).$$

The necessity of imposing a smallness condition on the doping profile is easily understood by considering the equilibrium problem for $r(\rho) = \rho^2$. We have in this case:

$$g(u) = \frac{u}{2} + 1 \quad \text{and} \quad \alpha \equiv 2(n_D + p_D) - 4 \quad \text{on } \Gamma_D.$$

The equilibrium problem reads

$$(2.34) \quad \Delta V_e = V_e - C(x), \quad x \in \Omega$$

$$(2.35) \quad V_e|_{\Gamma_D} = (n_D - p_D)|_{\Gamma_D}, \quad \nabla V_e \cdot \tau|_{\Gamma_N} = 0.$$

The equilibrium densities are given by

$$(2.36) \quad n_e = \frac{V_e}{2} + \frac{\alpha}{4} + 1, \quad p_e = -\frac{V_e}{2} + \frac{\alpha}{4} + 1.$$

It is easy to construct functions C such that either n_e or p_e become negative somewhere in Ω . For these doping profiles the equilibrium problem (2.34), (2.35) has no physically acceptable solution. We shall see in the next Section that the reason for this lies in the reformulation (2.5)-(2.8), which is based on $n > 0$ and $p > 0$.

3. - Vacuum Solutions

We now assume that $r = r(s)$ satisfies (A1) and that $\underline{h} > -\infty$, $\bar{h} = +\infty$.

The subsequent analysis is based on an approximation of the pressure function. For $0 < \varepsilon < 1$ we set

$$(3.1) \quad r^\varepsilon(\rho) = \begin{cases} \frac{r(\varepsilon)}{\varepsilon} \rho & \text{if } 0 \leq \rho \leq \varepsilon \\ r(\rho) & \text{if } \rho \geq \varepsilon \end{cases}$$

and calculate the enthalpy

$$(3.2) \quad h^\varepsilon(\rho) = \int_1^\rho \frac{(r^\varepsilon)'(s)}{s} ds = \begin{cases} \frac{r(\varepsilon)}{\varepsilon} \ln \frac{\rho}{\varepsilon} + h(\varepsilon) & \text{if } 0 < \rho \leq \varepsilon \\ h(\rho) & \text{if } \rho \geq \varepsilon, \end{cases}$$

where $h = h(s)$ is the enthalpy associated with the pressure function $r = r(\rho)$. Obviously

$$(3.3) \quad \underline{h}^\varepsilon := \lim_{\rho \rightarrow \infty+} h^\varepsilon(\rho) = -\infty, \quad \bar{h}^\varepsilon := \lim_{\rho \rightarrow \infty} h^\varepsilon(\rho) = \lim_{\rho \rightarrow \infty} h(\rho) = \infty.$$

We set $g^\varepsilon := (h^\varepsilon)^{-1}$ and, as in Section 2, $g := h^{-1}$. A simple computation gives:

$$(3.4) \quad g^\varepsilon(u) = \begin{cases} \varepsilon \exp\left(\frac{\varepsilon}{r(\varepsilon)}(u - h(\varepsilon))\right) & \text{if } u \leq h(\varepsilon) \\ g(u) & \text{if } u \geq h(\varepsilon) \end{cases}$$

and we deduce that

$$(3.5) \quad g^\varepsilon \xrightarrow{\varepsilon \rightarrow 0} g^0 \text{ in } L^\infty(\mathbb{R}) \text{ strongly}$$

where g^0 is the 0-extension of g :

$$(3.6) \quad g^0(u) = \begin{cases} 0 & \text{if } u \leq \underline{h} \\ g(u) & \text{if } u \geq \underline{h}. \end{cases}$$

We now study the approximating problem:

$$\begin{aligned} (3.7)(a) \quad & \Delta V^\varepsilon = n^\varepsilon - p^\varepsilon - C(x), \\ (3.7)(b) \quad & \operatorname{div}(\nabla r^\varepsilon(u^\varepsilon) - n^\varepsilon \nabla V^\varepsilon) = 0, \quad x \in \Omega, \\ (3.7)(c) \quad & \operatorname{div}(\nabla r^\varepsilon(p^\varepsilon) + p^\varepsilon \nabla V^\varepsilon) = 0, \\ (3.7)(d) \quad & n^\varepsilon = n_D, p^\varepsilon = p_D, V^\varepsilon = V_D \quad \text{on } \Gamma_D, \\ (3.7)(e) \quad & \frac{\partial r^\varepsilon(n^\varepsilon)}{\partial \tau} = \frac{\partial r^\varepsilon(p^\varepsilon)}{\partial \tau} = \frac{\partial V^\varepsilon}{\partial \tau} = 0 \quad \text{on } \Gamma_N, \end{aligned}$$

with V_D given by (2.15)(a).

We shall show that a solution of

$$(3.8)(a) \quad \Delta V = n - p - C(x),$$

$$(3.8)(b) \quad \operatorname{div}(\nabla r(n) - n \nabla V) = 0, \quad x \in \Omega,$$

$$(3.8)(c) \quad \operatorname{div}(\nabla r(p) + p \nabla V) = 0,$$

$$(3.8)(d) \quad n = n_D, p = p_D, V = V_D \quad \left(= h(n_D) - \frac{\alpha}{2} + U_D \right) \quad \text{on } \Gamma_D,$$

$$(3.8)(e) \quad \frac{\partial r(n)}{\partial \tau} = \frac{\partial r(p)}{\partial \tau} = \frac{\partial V}{\partial \tau} = 0 \quad \text{on } \Gamma_N,$$

with $n \geq 0, p \geq 0$ can be obtained from (3.7) by the limit procedure $\varepsilon \rightarrow 0$.

THEOREM 3.1. *Let the assumptions (A1)-(A5), $h > -\infty$ and $\bar{h} = \infty$ hold. Then there exists a weak solution $(n, p, V) \in (L^\infty(\Omega))^3$ of problem (3.8) with $n \geq 0, p \geq 0$ and $(r(n), r(p), V) \in (H^1(\Omega))^3$.*

PROOF. From assumption (A3) and from (3.2) we conclude that there exists $\varepsilon_0 > 0$ such that $h^\varepsilon(n_D) = h(n_D)$ and $h^\varepsilon(p_D) = h(p_D)$ on Γ_D for all $\varepsilon \in (0, \varepsilon_0)$. Thus $\alpha := h(n_D) + h(p_D)$ is independent of $\varepsilon \in (0, \varepsilon_0)$. Since $h^\varepsilon = -\infty = -\bar{h}^\varepsilon$ Theorem 2.1 implies the existence of a solution $(n^\varepsilon, p^\varepsilon, V^\varepsilon) \in (H^1(\Omega) \cap L^\infty(\Omega))^3$ of (3.7) for all $\varepsilon \in (0, \varepsilon_0)$, $C \in L^\infty(\Omega)$ and $U_D \in H^{1/2}(\Gamma_D) \cap L^\infty(\Gamma_D)$. Also, the values $\underline{\psi}, \bar{\psi}, \underline{\sigma}$ and $\bar{\sigma}$ defined in (2.17) are independent of $\varepsilon \in (0, \varepsilon_0)$ and the values $\omega_1^\varepsilon, \omega_2^\varepsilon$ of Lemma 2.2 are now defined by

$$(3.9)(a) \quad 0 = g^\varepsilon(\bar{\psi} - \omega_1^\varepsilon) - g^\varepsilon(\underline{\sigma} - \omega_1^\varepsilon) - \underline{C},$$

$$(3.9)(b) \quad 0 = g^\varepsilon(\underline{\psi} - \omega_2^\varepsilon) - g^\varepsilon(\bar{\sigma} - \omega_2^\varepsilon) - \bar{C}.$$

Consider the functions $\bar{G}_0, \underline{G}_0 : [-\infty, +\infty] \rightarrow [-\infty, +\infty]$

$$(3.10)(a) \quad \bar{G}^0(\omega) = g^0(\bar{\psi} + \omega) - g^0(\underline{\sigma} - \omega) - \underline{C},$$

$$(3.10)(b) \quad \underline{G}^0(\omega) = g^0(\underline{\psi} + \omega) - g^0(\bar{\sigma} - \omega) - \bar{C}.$$

We have $\bar{G}^0(\infty) = \underline{G}^0(\infty) = \infty, \bar{G}^0(-\infty) = \underline{G}^0(-\infty) = -\infty$ and

$$\frac{d}{d\omega} \bar{G}^0(\omega) = \frac{d}{du} g^0(\bar{\psi} + \omega) + \frac{d}{du} g^0(\underline{\sigma} - \omega),$$

$$\frac{d}{d\omega} \underline{G}^0(\omega) = \frac{d}{du} g^0(\underline{\psi} + \omega) + \frac{d}{du} g^0(\bar{\sigma} - \omega).$$

Since $\bar{\psi} + \underline{\sigma} = \underline{\psi} + \bar{\sigma} = \alpha > 2h$, we conclude that

$$\frac{d}{d\omega} \bar{G}^0 > 0, \quad \frac{d}{d\omega} \underline{G}^0 > 0 \quad \text{on } \mathbb{R}$$

from (3.6). Thus, the equations $\overline{G}^0(\omega) = 0$ and $\underline{G}^0(\omega) = 0$ have unique solutions ω_1^0 and ω_2^0 respectively. Using (3.5) we conclude that:

$$\omega_1^\varepsilon \xrightarrow{\varepsilon \rightarrow 0} \omega_1^0, \quad \omega_2^\varepsilon \xrightarrow{\varepsilon \rightarrow 0} \omega_2^0.$$

Consequently, the upper and lower solutions for the potential V^ε , defined, as in (2.21), by

$$\overline{V}^\varepsilon := \max(\omega_2^\varepsilon, s(V_D)), \quad \underline{V}^\varepsilon := \min(\omega_1^\varepsilon, i(V_D)),$$

are bounded uniformly as $\varepsilon \rightarrow 0$ and therefore there exist numbers $N > 0$ and $P > 0$ independent of $\varepsilon \in (0, \varepsilon_0)$ such that

$$(3.11) \quad \overline{n}^\varepsilon := g^\varepsilon(\overline{\psi} + \overline{V}^\varepsilon) \leq N, \quad \overline{p}^\varepsilon := g^\varepsilon(\overline{\sigma} - \underline{V}^\varepsilon) \leq P.$$

Since \overline{n}^ε and \overline{p}^ε are the upper bounds for n^ε and p^ε defined in (2.22) and (2.23), we conclude that

$$(3.12) \quad V_m \leq V^\varepsilon(x) \leq V_M, \quad 0 \leq n^\varepsilon(x) \leq N, \quad 0 \leq p^\varepsilon(x) \leq P \quad \text{a.e. in } \Omega$$

for $\varepsilon \in (0, \varepsilon_0)$ with appropriate constants $V_m < V_M$. Thus, there exist functions V^0, n^0 and p^0 satisfying the bounds (3.12) such that (possibly after extracting a subsequence):

$$(3.13) \quad V^\varepsilon \xrightarrow{\varepsilon \rightarrow 0} V^0, \quad n^\varepsilon \xrightarrow{\varepsilon \rightarrow 0} n^0, \quad p^\varepsilon \xrightarrow{\varepsilon \rightarrow 0} p^0 \quad \text{in } L^\infty(\Omega) \quad \text{weak } \star.$$

From (3.7)(a), (d) and (e) we conclude immediately that

$$\|\nabla V^\varepsilon\|_{L^2(\Omega)} \leq K$$

(where from now on K denotes not necessarily equal constants, which are independent of ε). Thus

$$(3.14) \quad V^\varepsilon \xrightarrow{\varepsilon \rightarrow 0} V^0 \text{ in } H^1(\Omega) \quad \text{weakly}$$

and, since V_D is independent of $\varepsilon \in (0, \varepsilon_0)$, we conclude that V^0 is a H^1 -weak solution of

$$(3.14)(a) \quad \Delta V^0 = n^0 - p^0 - C(x), \quad x \in \Omega,$$

$$(3.14)(b) \quad V^0|_{\Gamma_D} = V_D|_{\Gamma_D}, \quad \left. \frac{\partial V^0}{\partial \tau} \right|_{\Gamma_N} = 0.$$

The standard localization argument for the Poisson equation then gives the estimate

$$(3.15) \quad \|V^\varepsilon\|_{H^2(\Omega_0)} \leq K(\Omega_0)$$

for every subdomain Ω_0 compactly contained in Ω . Thus (possibly after extracting another subsequence)

$$(3.16) \quad \nabla V^\varepsilon \xrightarrow{\varepsilon \rightarrow 0} \nabla V^0 \quad \text{in } L^2(\Omega_0) \quad \text{strongly.}$$

On the other hand, the functions $n^\varepsilon \nabla V^\varepsilon$ are bounded uniformly in $L^2(\Omega)$ and thus

$$n^\varepsilon \nabla V^\varepsilon \xrightarrow{\varepsilon \rightarrow 0} f \quad \text{in } L^2(\Omega) \quad \text{weakly}$$

(after extracting a subsequence). From (3.13) and (3.16) we conclude that

$$n^\varepsilon \nabla V^\varepsilon \xrightarrow{\varepsilon \rightarrow 0} n^0 \nabla V^0 \quad \text{in } L^2(\Omega_0) \quad \text{weakly}$$

and since $\Omega_0 \subset\subset \Omega$ is arbitrary, we have $f = n^0 \nabla V^0$. Thus

$$(3.17) \quad n^\varepsilon \nabla V^\varepsilon \xrightarrow{\varepsilon \rightarrow 0} n^0 \nabla V^0 \quad \text{in } L^2(\Omega) \quad \text{weakly.}$$

We now set $u^\varepsilon := r^\varepsilon(n^\varepsilon)$ and $v^\varepsilon := u^\varepsilon r(\tilde{n}_D)$, where $\tilde{n}_D \in L^\infty(\Omega)$ is a positive $H^1(\Omega)$ -extension of n_D . Then v^ε is the weak solution of the problem

$$\begin{aligned} \Delta v^\varepsilon &= \operatorname{div}(n^\varepsilon \nabla V^\varepsilon) - \Delta r(\tilde{n}_D), & x \in \Omega, \\ v^\varepsilon|_{\Gamma_D} &= 0, \quad \frac{\partial v^\varepsilon}{\partial r} \Big|_{\Gamma_N} = - \frac{\partial r(\tilde{n}_D)}{\partial \tau} \Big|_{\Gamma_N}, \end{aligned}$$

i.e. it solves:

$$(3.18) \quad \int_{\Omega} \nabla v^\varepsilon \cdot \nabla \varphi \, dx = \int_{\Omega} n^\varepsilon \nabla V^\varepsilon \cdot \nabla \varphi \, dx - \int_{\Omega} \nabla r(\tilde{n}_D) \cdot \nabla \varphi \, dx, \quad \forall \varphi \in H_0^1(\Omega \cup \Gamma_N).$$

Since $n^\varepsilon \nabla V^\varepsilon$ is bounded uniformly in $L^2(\Omega)$ and since $\nabla r(\tilde{n}_D) = r'(\tilde{n}_D) \nabla \tilde{n}_D \in L^2(\Omega)$ we conclude that v^ε is bounded uniformly in $H_0^1(\Omega \cup \Gamma_N)$ and therefore

$$(3.19) \quad \begin{aligned} u^\varepsilon &\xrightarrow{\varepsilon \rightarrow 0} u^0 \quad \text{in } H^1(\Omega) \quad \text{weakly,} \\ v^\varepsilon &\xrightarrow{\varepsilon \rightarrow 0} u^0 - r(\tilde{n}_D) \quad \text{in } H_0^1(\Omega \cup \Gamma_N) \quad \text{weakly} \end{aligned}$$

(after extracting another subsequence). Taking the limit as $\varepsilon \rightarrow 0$ in (3.17) proves that u^0 is the weak solution of the problem:

$$(3.18)(a) \quad \Delta u^0 = \operatorname{div}(n^0 \nabla V^0), \quad x \in \Omega,$$

$$(3.19)(b) \quad u^0|_{\Gamma_D} = r(n_D), \quad \frac{\partial u^0}{\partial \tau} \Big|_{\Gamma_N} = 0.$$

We still have to show that $u^0 = r(n^0)$.

For $1 \leq m \leq 3$ we have $H^1(\Omega) \hookrightarrow L^S(\Omega)$, $1 \leq S < 6$, compactly. Thus $u^\varepsilon = r^\varepsilon(n^\varepsilon) \xrightarrow{\varepsilon \rightarrow 0} u^0$ in $L^1(\Omega)$ strongly (after extracting a subsequence). Since $r^\varepsilon(\rho) = r(\rho)$ for $\rho \geq \varepsilon$, we have

$$\int_{\Omega} |r^\varepsilon(n^\varepsilon) - r(n^\varepsilon)| \, dx = \int_{\Omega \cap \{n^\varepsilon \leq \varepsilon\}} |r^\varepsilon(n^\varepsilon) - r(n^\varepsilon)| \, dx \leq K r(\varepsilon) \xrightarrow{\varepsilon \rightarrow 0} 0.$$

Hence $r(n^\varepsilon) \xrightarrow{\varepsilon \rightarrow 0} u^0$ in $L^1(\Omega)$ strongly. Now let q be the inverse function of r i.e. $q = r^{-1}$, $q : [0, \infty) \rightarrow [0, \infty)$. Since the functions n^ε are uniformly bounded in $L^\infty(\Omega)$, the same holds for $r(n^\varepsilon)$. The continuity of q implies $n^\varepsilon = q(r(n^\varepsilon)) \xrightarrow{\varepsilon \rightarrow 0} q(u^0)$ strongly in $L^1(\Omega)$, and $n^0 = q(u^0)$, $u^0 = r(n^0)$ follows. Clearly $n^0 \in L^\infty(\Omega)$ holds.

The assertion of the Theorem follows by proceeding analogously with the p -equation. ■

REMARK. Theorem 3.1 requires no restrictions on $\|C\|_{L^\infty(\Omega)}$ or $\|U_D\|_{L^\infty(\Gamma_D)}$, because the converging sequence $(n^\varepsilon, p^\varepsilon, V^\varepsilon)$ solves the approximating problem when h is replaced by h^ε and $\underline{h}^\varepsilon = -\infty = -\bar{h}^\varepsilon$.

It is crucial for the proof that g^ε is defined on \mathbb{R} and that $\|g^\varepsilon - g^0\|_{L^\infty(\mathbb{R})} \rightarrow 0$ as $\varepsilon \rightarrow 0$. An analogue construction of g^ε is impossible if $\bar{h} < +\infty$, since then $\lim_{s \rightarrow \bar{h}^-} g^0(s) = +\infty$. No sequence $\{g^\varepsilon\}$ defined on \mathbb{R} for all $\varepsilon \in (0, \varepsilon_0)$ can tend to g^0 uniformly on (\underline{h}, \bar{h}) . In this case, restrictions on C and U_D are required to prove existence of vacuum solutions.

Consider now the equilibrium problem:

$$(3.20) \quad \Delta V_e^\varepsilon = g^\varepsilon \left(\frac{\alpha}{2} + V_e^\varepsilon \right) - g^\varepsilon \left(\frac{\alpha}{2} - V_e^\varepsilon \right) - C(x), \quad x \in \Omega,$$

$$(3.21) \quad \nabla V_e^\varepsilon \cdot \tau = 0 \quad \text{on } \Gamma_N, \quad V_e^\varepsilon = h^\varepsilon(n_D) - \frac{\alpha}{2} \quad \text{on } \Gamma_D$$

as directly obtained from (2.12)-(2.14).

Since $\|V_e^\varepsilon\|_{L^\infty(\Omega)} \leq K$ and since

$$V_e^\varepsilon \xrightarrow{\varepsilon \rightarrow 0} V_e^0 \text{ in } L^2(\Omega) \text{ strongly}$$

(after extracting a subsequence, see (3.14)) we conclude (using (3.5)) that V_e^0 solves:

$$(3.22) \quad \Delta V_e^0 = g^0 \left(\frac{\alpha}{2} + V_e^0 \right) - g^0 \left(\frac{\alpha}{2} - V_e^0 \right) - C(x), \quad x \in \Omega,$$

$$(3.23) \quad \nabla V_e^0 \cdot \tau = 0 \quad \text{on } \Gamma_N, \quad V_e^0 = h(n_D) - \frac{\alpha}{2} \quad \text{on } \Gamma_D$$

with the equilibrium densities

$$(3.24) \quad n_e^0 = g^0 \left(\frac{\alpha}{2} + V_e^0 \right), \quad p_e^0 = g^0 \left(\frac{\alpha}{2} - V_e^0 \right).$$

Since $\alpha/2 + V_e^0 \leq \underline{h}$ implies $\alpha/2 - V_e^0 > \underline{h}$ and $\alpha/2 - V_e^0 \leq \underline{h}$ implies $\alpha/2 + V_e^0 > \underline{h}$, the right-hand side of (3.22) is a strictly increasing function of V_e^0 . Thus (3.22), (3.23) has a unique weak solution $V_e^0 \in H^1(\Omega) \cap L^\infty(\Omega)$ for every $C \in L^\infty(\Omega)$, if $n_D \in H^{1/2}(\Gamma_D) \cap L^\infty(\Gamma_D)$, $n_D \geq \underline{\rho} > 0$ on Γ_D . For the same reason we have, for arbitrary $x_0 \in \Omega$:

$$(3.25) \quad n_e(x_0) = 0 \Rightarrow p_e(x_0) > 0, \quad p_e(x_0) = 0 \Rightarrow n_e(x_0) > 0,$$

i.e. n_e and p_e cannot have a vacuum at the same points.

In case $r(\rho) = \rho^2$ existence of a solution of (3.22), (3.23) with a vacuum in (at least one of) the particle densities n_e^0 and p_e^0 , for appropriately chosen doping profiles C , follows from the non-existence of a solution of (2.34), (2.35) with positive densities n_e and p_e .

Acknowledgement

The first author is grateful for support from the Istituto di Analisi Numerica del C.N.R., Pavia, where part of this research was carried out.

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