THE DERIVATION OF ANALYTIC DEVICE MODELS BY ASYMPTOTIC METHODS

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Abstract. In circuit simulation, device models should be as simple as possible. On the other hand, physically sound models for the electrical behaviour of semiconductor devices involve nonlinear systems of partial differential equations posed on domains with complicated geometries. Therefore simplifications have to be introduced corresponding to certain idealizing assumptions. By the use of asymptotic methods the simplification procedure can be carried out in a mathematically justifiable way.

This paper presents an overview of recent results on steady state voltage-current characteristics of multi-dimensional bipolar devices [11], [21] as well as on a new approach to the modelling of the transient behaviour of pn-diodes via integral equations [23], [24]. These ideas are extended to more general bipolar devices.

1. Introduction. The starting point of our analysis is the classical drift-diffusion model for the flow of negatively charged electrons (density $n(\mathbf{x},t)$) and positively charged holes (density $p(\mathbf{x},t)$) in a semiconductor. In scaled form it consists of the continuity equations

$$\nabla \cdot \mathbf{J}_n - \frac{1}{\delta^4}\frac{\partial n}{\partial t} = R\,, \qquad -\nabla \cdot \mathbf{J}_p - \frac{1}{\delta^4}\frac{\partial p}{\partial t} = R\,, \tag{1.1a}$$

the current relations

$$\delta^4 \mathbf{J}_n = \mu_n(\nabla n - n\nabla V)\,, \qquad \delta^4 \mathbf{J}_p = -\mu_p(\nabla p + p\nabla V)\,, \tag{1.1b}$$

and the Poisson equation

$$\lambda^2 \Delta V = n - p - C \tag{1.1c}$$

for the electrostatic potential $V(\mathbf{x},t)$. The mobilities $\mu_n, \mu_p > 0$ and the doping profile C are assumed to be given functions of position $\mathbf{x} \in \Omega$, where the bounded domain $\Omega \subset \mathbb{R}^k$, $k = 1, 2$ or 3, represents the semiconductor part of the device. We assume the recombination-generation rate to be of the form

$$R = Q(n,p,\mathbf{x})(np/\delta^4 - 1)\,, \qquad Q \geq 0\,,$$

including the standard models for band-to-band processes and recombination-generation via traps in the forbidden band. Since this work is restricted to low injection situations, our model certainly describes the relevant physical phenomena [11].

The equations (1.1) are in dimensionless form. The reference quantity for the particle densities n, p, C is the maximal doping concentration C_{max}, i.e. $\max_\Omega |C| = 1$ holds. The potential has been scaled by the thermal voltage $U_T = kT/q$ where k, T and q denote the Boltzmann constant, the lattice temperature and the elementary charge, respectively. The reference length L is the diameter of the device and, thus, $\mathrm{diam}(\Omega) = 1$. The mobilities are scaled by a characteristic value $\widetilde{\mu}$ and the reference time is given by the diffusion time $L^2/(\widetilde{\mu} U_T)$. Finally, the reference value

$$\frac{q\widetilde{\mu}U_T}{L}\frac{n_i^2}{C_{max}} \tag{1.2}$$

for the electron and hole current densities $\mathbf{J}_n$ and $\mathbf{J}_p$, respectively, contains the intrinsic density n_i. In low injection situations the factor n_i^2/C_{max} is a typical minority carrier density. Thus, the value (1.2) is

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a characteristic value for current densities in low injection. For further details on the scaling of the drift-diffusion equations we refer to [8] and [11].

The equations (1.1) contain the dimensionless parameters

$$\lambda = \frac{1}{L}\sqrt{\frac{\varepsilon U_T}{qC_{max}}}\,, \qquad \delta^2 = \frac{n_i}{C_{max}}\,,$$

which can be interpreted as scaled versions of the minimal Debye length and of the intrinsic number, respectively.

Subregions of Ω where the doping profile C is positive are called n-regions because the positively charged impurity ions attract electrons. On the other hand, in p-regions the doping profile is negative. The $(k-1)$-dimensional boundaries between n- and p-regions are called pn-junctions. We assume abrupt junctions, i.e. the doping profile has jumps across these junctions and is bounded away from zero within the n- and p-regions.

We restrict our attention to bipolar devices. Therefore, the boundary $\partial\Omega$ of the device is the disjoint union of Ohmic contacts $C_1, \cdots, C_m$ and artificial or insulating boundary segments $\partial\Omega_N$. At Ohmic contacts we assume zero space charge and thermal equilibrium:

$$n - p - C = 0\,, \quad np = \delta^4\,, \qquad \text{at } C_1, \cdots, C_m\,,$$

which translates to Dirichlet boundary conditions for the charge carrier densities:

$$n = \frac{1}{2}\left(C + \sqrt{C^2 + 4\delta^4}\right)\,, \quad p = \frac{1}{2}\left(-C + \sqrt{C^2 + 4\delta^4}\right)\,, \qquad \text{at } C_1, \cdots, C_m \tag{1.3a}$$

For the potential, we have the boundary conditions

$$V = V_{bi} - U_j(t)\,, \qquad \text{at } C_j,\ j = 1, \cdots, m\,, \tag{1.3b}$$

where $U_i(t) - U_j(t)$ is the external voltage between the contacts C_i and C_j, and the built-in potential is given by

$$V_{bi} = \ln \frac{C + \sqrt{C^2 + 4\delta^4}}{2\delta^2}\,. \tag{1.3c}$$

Along the artificial and insulating boundary segments, we assume that the normal components of the electric field and of the electron and hole current densities vanish. This amounts to homogeneous Neumann conditions for V, n and p:

$$\frac{\partial V}{\partial \boldsymbol{\nu}} = \frac{\partial n}{\partial \boldsymbol{\nu}} = \frac{\partial p}{\partial \boldsymbol{\nu}} = 0\,, \qquad \text{at } \partial\Omega_N\,, \tag{1.3d}$$

where $\boldsymbol{\nu}$ denotes the unit outward normal.

The formulation of an initial-boundary value problem is completed by prescribing initial conditions for the carrier densities:

$$n(\mathbf{x}, 0) = n_0(\mathbf{x})\,, \qquad p(\mathbf{x}, 0) = p_0(\mathbf{x}) \tag{1.4}$$

We shall assume that the initial data n_0 and p_0 correspond to steady state solutions of (1.1), (1.3).

Important quantities are the currents through the Ohmic contacts. The current $I_j(t)$ leaving the device through the contact C_j is given by

$$I_j = \int_{C_j} \mathbf{J}_{tot} \cdot \boldsymbol{\nu}\, ds$$

in terms of the total current density

$$\mathbf{J}_{tot} = \mathbf{J}_n + \mathbf{J}_p - \frac{\lambda^2}{\delta^4}\nabla\frac{\partial V}{\partial t}\,,$$

which is the sum of the particle current densities and the density of the displacement current.

The specific properties of a device are determined by the number and location of the n- and p-regions as well as of the Ohmic contacts. We consider devices meeting the following requirements: There is a finite number of open connected n-regions whose union is denoted by Ω_+. In the same way, the number of p-regions is finite and their union is denoted by Ω_-. Each n- or p-region has at most one contact and each contact is adjacent to only one n- or p-region. The union of the pn-junctions is denoted by $\Gamma = \overline{\Omega}_+ \cap \overline{\Omega}_-$. Note that these assumptions do not rule out so called floating regions without any contacts. In Figure 1 two-dimensional cross sections of three typical devices are depicted. The pn-diode consists of one n- and one p-region, each with a contact. The bipolar transistor has three differently doped regions with contacts. Finally, the thyristor is a $pnpn$-structure. Figure 1 shows the so called Shockley diode where the two middle layers are floating regions.

In this paper we both discuss the stationary problem corresponding to (1.1), (1.3) as well as the transient case. Our objective in both cases is to find simple representations of the steady state and transient voltage-current characteristics, i.e. the dependence of the currents through the contacts on the $m-1$ contact voltages $U_j - U_1$, $j = 2, \cdots, m$. Obviously, the choice of U_1 does not influence the result. Note that we only need to compute $m-1$ currents, since the total current density is divergence free, implying $I_1 + \cdots + I_m = 0$.

The dimensionless parameters λ and δ^2 are small compared to 1 in practical applications. Our approach is an asymptotic analysis where we let these parameters tend to zero consecutively.

The limit $\lambda \to 0$ corresponds to the physical assumption of zero space charge. Essentially, it amounts to replacing the left hand side of the Poisson equation (1.1c) by zero. However, since the problem is singularly perturbed in terms of λ, layer behaviour has to be expected. In particular, the jump discontinuities of the doping profile cause the limiting potential and the carrier densities to have jumps across pn-junctions. Also, an initial jump has to be expected for the time dependent problem. The nature of these jumps can be analyzed by introducing slow variables which are continuous in the limit. The construction of formal asymptotic expansions — including layer corrections at the pn-junctions and initial layers in the transient case — and their use for explaining device behaviour has received a considerable amount of attention in the literature (see [4], [7], [8], [9], [10], [11], [12], [22], [27], [33] for the stationary problem and [16], [17], [30], [31] for the time dependent case).

A rigorous theory justifying the limiting procedure is incomplete. To the authors' knowledge, no results are available for the transient case. For one-dimensional steady state problems the approximations can be justified [10], [12] by general results for singularly perturbed two-point boundary value problems [25]. In higher dimensions, a justification for steady states close to thermal equilibrium, i.e. for small enough applied voltages, can be found in [7]. A weaker convergence result for arbitrary biases and a simplified problem with constant mobilities and vanishing recombination-generation rate has been derived in [4]. A generalization of this result, proven in [21], is stated in section 2 of this work.

In terms of the exponentials of the quasi Fermi levels, which are a convenient choice of variables for the steady state problem, the limiting stationary problem is a system of two nonlinearly coupled elliptic equations. The time dependent problem becomes a parabolic-algebraic system in the limit. In the language of the theory of differential-algebraic equations [3], it is an index 2 problem [1]. This means that the initial conditions have to satisfy certain compatibility relations which is guaranteed by the assumption that the initial data originate from steady state solutions. In other words this assumption implies the absence of initial jumps [16].

A further simplification of the problem is introduced by letting δ^2 tend to zero. Keeping the applied voltages fixed as the built-in potential tends to infinity (as $\delta^2 \to 0$, see (1.3b), (1.3c)) can be interpreted as a low injection condition.

For steady state problems this limit has been formally carried out in [11] and rigorously justified in [21]. However, the zero space charge and low injection assumptions have already been used for one-dimensional model problems in the early physical literature on semiconductor devices [26]. In particular, the famous Shockley equation for the voltage-current characteristic of a pn-diode and the qualitative behaviour of bipolar transistors are derived in this way (see also [29]). Thus, the results presented in section 2 can be seen as an extension of this early work. In sections 3 and 4 we demonstrate for multi-dimensional models of a pn-diode and a bipolar transistor, respectively, that the voltage-current characteristic close to thermal equilibrium can be determined explicitly in terms of the solutions of simple elliptic reference problems. In [21], the same methods have been applied for the computation of the forward and reverse bias blocking branches of the voltage-current characteristics of Shockley diodes. As in [27] for one-dimensional models, a device dependent parameter is identified whose sign determines whether a given $pnpn$-structure is a thyristor or behaves like a pin-diode.

For the transient behaviour of pn-diodes the limit $\delta^2 \to 0$ in the zero space charge problem has been carried out in [23] and [24]. In section 5 we extend this procedure to general bipolar devices. The limiting problem consists of linear parabolic equations in the n- and p-regions coupled by interface conditions at the pn-junctions. For the pn-diode and the bipolar transistor we show in sections 6 and 7, respectively, that these problems are equivalent to systems of integral equations describing the evolution of the currents in terms of the evolution of the applied voltages. Similarly to the steady state case, the kernels of the integral equations are determined by solving simple reference problems.

The question arises if the limit problems depend on the order of the limiting procedures $\lambda \to 0$ and $\delta^2 \to 0$. In [11] it has been shown that for the thermal equilibrium problem (consisting only of a nonlinear Poisson equation) the limits commute. No proof is available, however, that the limits commute also in the general case. The limit $\delta^2 \to 0$ leads to a free boundary problem [20] having practical importance in VLSI applications, since for very small devices λ can be considerably large whereas $\delta^2 \ll 1$ is always a safe assumption. It should be mentioned in this context that the distinguished limit $\lambda = \delta \to 0$ has been considered in [15]. This amounts to the assumption that the reference length in the scaling is equal to the intrinsic Debye length.

Finally we want to discuss the limitations of our approach. They originate from keeping the applied voltages fixed in the course of the limiting procedures. It has already been pointed out that the assumption of smallness of the applied voltages compared to the built-in potential means low injection. Therefore high injection effects are neglected. A second source of error is the zero space charge assumption. We neglect the depletion regions in the neighbourhoods of the pn-junctions. This is justified, because the width of these regions is of the order of the Debye length which has been assumed to be small compared to other characteristic length scales in the device. It is well known, however, that the width grows with the potential jump across the junction. Effects involving large applied biases and, therefore, widening depletion regions have to be accounted for by an asymptotic analysis of a rescaled problem (see [2], [14], [18], [19], [28] for the stationary problem and [13] for the time dependent case). Unfortunately, in this case the most appealing feature of the close-to-thermal-eqilibrium results of this work is lost, namely the fact that the voltage-current characteristics can be given explicitely in terms of the solutions of reference problems independent of the biasing situation.

2. Steady state problems. The analysis of the stationary problem is greatly facilitated by introducing the exponentials u and v of the quasi Fermi levels as new variables instead of the carrier densities:

$$n = \delta^2 e^V u\,, \qquad p = \delta^2 e^{-V} v$$

This symmetrizing transformation for the continuity equations changes the steady state version of (1.1), (1.3) to the differential equations

$$\begin{aligned} &\nabla \cdot \left(\mu_n \delta^2 e^V \nabla u\right) = \delta^4 R\,, \\ &\nabla \cdot \left(\mu_p \delta^2 e^{-V} \nabla v\right) = \delta^4 R\,, \\ &\lambda^2 \Delta V = \delta^2 e^V u - \delta^2 e^{-V} v - C\,, \end{aligned} \tag{2.1}$$

subject to the boundary conditions

$$\begin{aligned} u = e^{U_j}\,, \quad v = e^{-U_j}\,, \quad V = V_{bi} - U_j\,, &\qquad \text{at } C_j\,,\ j = 1, \cdots, m\,, \\ \frac{\partial V}{\partial \boldsymbol{\nu}} = \frac{\partial u}{\partial \boldsymbol{\nu}} = \frac{\partial v}{\partial \boldsymbol{\nu}} = 0\,, &\qquad \text{at } \partial\Omega_N\,. \end{aligned} \tag{2.2}$$

Now the recombination-generation rate is given by

$$R = Q(\delta^2 e^V u, \delta^2 e^{-V} v, \mathbf{x})(uv - 1)\,.$$

Note that the differential operators in the continuity equations are formally self-adjoint. Also we expect the derivatives of u and v to be bounded uniformly with respect to λ. This makes them slow variables in the language of singular perturbation theory. Before we can state the convergence result for $\lambda \to 0$, a few regularity assumptions for the data are needed: The domain Ω is Lipschitz and the $(k-1)$-dimensional Lebesgue measure of the union of the contacts is positive. The Dirichlet boundary data for V, u and v at the contacts can be extended to Ω as functions in $H^1(\Omega)$. The nonnegative reaction rate Q in the recombination-generation term is a smooth function of the carrier densities as well as a bounded function of position. The doping profile and the mobilities satisfy

$$C \in L^\infty(\Omega) \cap W^{2,1}(\Omega_0)\,, \qquad \mu_n, \mu_p \in L^\infty(\Omega) \cap H^1(\Omega_0)\,,$$

where $\Omega_0 = \Omega \setminus \Gamma$ denotes the semiconductor domain without the pn-junctions. Additionally we assume the mobilities to be bounded away from zero.

Theorem 2.1. *a) ([8]) Under the above assumptions the problem (2.1), (2.2) has a solution* $(V, u, v) \in \left(H^1(\Omega) \cap L^\infty(\Omega)\right)^3$.
b) ([21]) For every sequence $\lambda_k \to 0+$ *there exists a subsequence (again denoted by* λ_k*) such that corresponding solutions* (V_k, u_k, v_k) *of (2.1), (2.2) satisfy*

$$\begin{aligned} V_k &\to V_0\,, \quad \text{in } L^2(\Omega)\,, \\ u_k &\to u_0\,, \quad \text{weakly in } H^1(\Omega)\,, \\ v_k &\to v_0\,, \quad \text{weakly in } H^1(\Omega)\,, \end{aligned}$$

where (V_0, u_0, v_0) *is a solution of (2.1), (2.2) with* λ *replaced by zero.*

Remark. Note that the limiting potential would not satisfy general Dirichlet boundary conditions since it is determined from an algebraic equation (the reduced Poisson equation). However, the assumption of zero space charge at the Ohmic contacts is compatible with the limiting problem, and therefore the limiting solution satisfies the complete set of Dirichlet conditions.

After elimination of the potential the zero space charge equations can be written as

$$\begin{aligned} &\delta^4 \mathbf{J}_n = \mu_n \frac{C + \sqrt{C^2 + 4\delta^4 uv}}{2u} \nabla u\,, \qquad \delta^4 \mathbf{J}_p = -\mu_p \frac{-C + \sqrt{C^2 + 4\delta^4 uv}}{2v} \nabla v\,, \\ &\nabla \cdot \mathbf{J}_n = -\nabla \cdot \mathbf{J}_p = R\,. \end{aligned} \tag{2.3}$$

The carrier densities are given in terms of u and v by

$$n = \frac{1}{2}\left(C + \sqrt{C^2 + 4\delta^4 uv}\right)\,, \qquad p = \frac{1}{2}\left(-C + \sqrt{C^2 + 4\delta^4 uv}\right)\,.$$

This shows that

$$\begin{aligned} n &= C + O(\delta^4)\,, \quad p = O(\delta^4)\,, \qquad \text{in } \Omega_+\,, \\ p &= -C + O(\delta^4)\,, \quad n = O(\delta^4)\,, \qquad \text{in } \Omega_-\,. \end{aligned}$$

The statement that the density of the majority carriers (electrons in n-regions, holes in p-regions) is close to the modulus of the doping profile and the density of the minority carriers is small compared to that, is usually called a low injection condition.

Performing the formal limit $\delta^2 \to 0$ in (2.3) implies

$$\nabla u = 0 \quad \text{in } \Omega_+\,, \qquad \nabla v = 0 \quad \text{in } \Omega_-\,. \tag{2.4a}$$

In other words, in each n- or p-region the quasi Fermi level corresponding to the majority carriers is constant. The current relations for the minority carriers are divided by δ^4 before passing to the limit. We obtain

$$\begin{aligned} \nabla \cdot \left(\frac{\mu_n}{|C|} \nabla u\right) &= Q(0, |C|)(u - v^{-1})\,, \qquad \text{in } \Omega_-\,, \\ \nabla \cdot \left(\frac{\mu_p}{C} \nabla v\right) &= Q(C, 0)(v - u^{-1})\,, \qquad \text{in } \Omega_+\,. \end{aligned} \tag{2.4b}$$

For the limiting minority carrier current densities we have

$$\mathbf{J}_n = \frac{\mu_n v}{|C|} \nabla u \quad \text{in } \Omega_-\,, \qquad \mathbf{J}_p = -\frac{\mu_p u}{C} \nabla v \quad \text{in } \Omega_+\,.$$

Concerning the limit $\delta^2 \to 0$ the following result holds:

Theorem 2.2. *For every sequence $\delta_k^2 \to 0+$ there exists a subsequence (again denoted by δ_k^2) such that corresponding solutions (u_k, v_k) of (2.2), (2.3) satisfy*

$$u_k \to u_0\,, \quad \text{weakly in } H^1(\Omega)\,,$$
$$v_k \to v_0\,, \quad \text{weakly in } H^1(\Omega)\,,$$

where the limit (u_0, v_0) satisfies (2.2), (2.4).

Assuming the constant values of u in the n-regions and of v in the p-regions to be known, the problem has been reduced to the solution of the linear elliptic equations (2.4b). At first glance, it seems disturbing, however, that only the minority carrier current densities are determined by the limiting problem. This means that the total current density is known only at pn-junctions. On the other hand, by current continuity it is sufficient to know the currents through the pn-junctions for computing the currents through the contacts. In the following two sections we shall demonstrate that the voltage-current characteristics can be determined explicitely in terms of a number of device dependent parameters from the simplified problem (2.2), (2.4).

3. The Shockley equation for the pn-diode. We denote the n-region of a pn-diode by Ω_n, the p-region by Ω_p, the adjacent Ohmic contacts by Γ_n and Γ_p, respectively, and the pn-junction by Γ (see Figure 2).

From a simple one-dimensional model problem Shockley (1949, [26]) computed the approximation

$$I = I_s(e^U - 1) \tag{3.1}$$

for the steady state voltage-current characteristic which is now known as the Shockley equation. In (3.1), I denotes the current through the device and U the contact voltage. The reverse bias saturation current I_s has been determined by Shockley as a function of the doping levels in the n- and p-regions, the mobilities and recombination parameters. An application of the results of the preceding section will show that the Shockley equation remains valid in the multi-dimensional case with an appropriately chosen value of I_s.

In terms of the contact voltage U, the variables u and v satisfy the boundary conditions

$$u = v = 1\,, \quad \text{at } \Gamma_p\,, \qquad u = e^U\,,\ v = e^{-U}\,, \quad \text{at } \Gamma_n\,.$$

From (2.4a) we immediately obtain

$$u = e^U\,, \quad \text{in } \Omega_n\,, \qquad v = 1\,, \quad \text{in } \Omega_p\,.$$

For u in Ω_p and v in Ω_n we choose the representations

$$u = 1 + (e^U - 1)\varphi_p\,, \quad \text{in } \Omega_p\,, \qquad v = e^{-U} + (1 - e^{-U})\varphi_n\,, \quad \text{in } \Omega_n\,,$$

in terms of the reference functions φ_p and φ_n, respectively, solving the problem

$$\nabla \cdot \left(\frac{\mu_n}{|C|} \nabla \varphi_p \right) = Q(0, |C|)\varphi_p\,, \qquad \text{in } \Omega_p\,, \tag{3.2a}$$

$$\nabla \cdot \left(\frac{\mu_p}{C} \nabla \varphi_n \right) = Q(C, 0)\varphi_n\,, \qquad \text{in } \Omega_n\,, \tag{3.2b}$$

$$\varphi_n = \varphi_p = 1\,, \quad \text{at } \Gamma\,, \qquad \varphi_n = 0\,, \quad \text{at } \Gamma_n\,, \qquad \varphi_p = 0\,, \quad \text{at } \Gamma_p\,. \tag{3.2c}$$

Important is the fact that φ_n and φ_p only depend on the device but not on the biasing situation. With the formulas for the current densities from the preceding section we obtain the Shockley equation (3.1) from an integration along the pn-junction Γ. The saturation current is given by

$$I_s = \int_\Gamma \left(\frac{\mu_n}{|C_p|} \nabla \varphi_p - \frac{\mu_p}{C_n} \nabla \varphi_n \right) \cdot \boldsymbol{\nu}\, ds\,,$$

where $\boldsymbol{\nu}$ is the unit normal vector along Γ pointing into Ω_n, and C_n (C_p) is the doping profile evaluated at the n-(p-)side of the junction. It is easy to see that both terms which sum up to the integrand are positive. If a one-dimensional model with constant mobilities and a piecewise constant doping profile is considered, the differential equations for φ_n and φ_p are linear homogeneous ODEs with constant coefficients. In this case, I_s can be computed explicitely, recovering Shockley's formulas.

4. The current gain of the bipolar transistor. A bipolar transistor consists of three differently doped regions each having a contact. Among the two possibilities of *npn*- and *pnp*-configurations we choose to consider the latter. The arguments of this section carry over to *npn*-transistors with the obvious changes.

Note that three contacts cannot be incorporated into a one-dimensional model. Therefore we have to assume $k = 2$ or 3 for the space dimension in this section. Below we shall see that multi-dimensional effects are indeed important for the performance of bipolar transistors.

The outer (p-)regions are called emitter (Ω_E) and collector (Ω_C), the sandwiched n-region is the base (Ω_B). The corresponding contacts are denoted by Γ_E, Γ_C and Γ_B, respectively, the emitter junction by Γ_{EB} and the collector junction by Γ_{BC} (see Figure 3). Contact voltages are measured with respect to the emitter: U_{BE} is the base-emitter voltage and U_{CE} the collector-emitter voltage. The Dirichlet conditions for u and v are then given by

$$u = v = 1\,, \quad \text{at } \Gamma_E\,, \qquad u = e^{U_{CE}}\,,\ v = e^{-U_{CE}}\,, \quad \text{at } \Gamma_C\,,$$
$$u = e^{U_{BE}}\,,\ v = e^{-U_{BE}}\,, \quad \text{at } \Gamma_B\,.$$

Considering (2.4a) we have

$$v = 1\,, \quad \text{in } \Omega_E\,, \qquad u = e^{U_{BE}}\,, \quad \text{in } \Omega_B\,, \qquad v = e^{-U_{CE}}\,, \quad \text{in } \Omega_C\,.$$

For the computation of the flow of minority carriers we again use a representation in terms of reference functions:

$$\begin{aligned} u &= 1 + (e^{U_{BE}} - 1)\varphi_1\,, && \text{in } \Omega_E\,,\\ v &= e^{-U_{BE}} + (1 - e^{-U_{BE}})\varphi_2 + (e^{-U_{CE}} - e^{-U_{BE}})\varphi_3\,, && \text{in } \Omega_B\,,\\ u &= e^{U_{CE}} + (e^{U_{BE}} - e^{U_{CE}})\varphi_4\,, && \text{in } \Omega_C\,, \end{aligned}$$

where φ_1 and φ_4 satisfy the differential equations (3.2a), φ_2 and φ_3 satisfy (3.2b) and the boundary conditions for $\varphi_1, \cdots, \varphi_4$ are indicated in Figure 3.

The currents I_E, entering the device through the emitter, and I_C, leaving the device through the collector, can be computed by integrations along the emitter and collector junctions. Then the base current is given by $I_B = I_E - I_C$. The bipolar transistor serves as an amplifier in the following way: A certain collector-emitter voltage is applied and the base current is used for triggering the collector current. Thus, we are interested in the dependence of I_C on I_B and U_{CE}. This is achieved by computing U_{BE} from the formula for I_B and substituting the result into the equation for I_C. Straightforward algebra gives

$$I_C = (I_B + a_3 + a_4)\frac{a_1 - a_2 e^{-U_{CE}}}{a_3 + a_4 e^{-U_{CE}}} - a_1 + a_2$$

where the parameters $a_1, \cdots, a_4$ can be given in terms of the reference functions $\varphi_1, \cdots, \varphi_4$, and, in particular,

$$a_1 = -\int_{\Gamma_{BC}} \frac{\mu_p}{C_B}\nabla\varphi_2 \cdot \boldsymbol{\nu}\, ds\,,$$
$$a_3 = \int_{\Gamma_{EB}} \frac{\mu_n}{|C_E|}\nabla\varphi_1 \cdot \boldsymbol{\nu}\, ds - \int_{\Gamma_B} \frac{\mu_p}{C_B}\nabla\varphi_2 \cdot \boldsymbol{\nu}\, ds\,,$$

holds. Here C_B denotes the doping profile evaluated at the base side of the junctions, with similar definitions for C_E and C_C.

A measure for the device performance is the common-emitter current gain

$$\beta = \frac{\partial I_C}{\partial I_B} = \frac{a_1 - a_2 e^{-U_{CE}}}{a_3 + a_4 e^{-U_{CE}}}\,.$$

For collector-emitter voltages significantly larger than the thermal voltage, β can be approximated by a_1/a_3 which is large iff both terms summing up to a_3 are small compared to a_1. Usually the doping in the emitter region is much higher than that in the base region implying that the ratio between a_1 and the first term in a_3 is large. However, we also require

$$-\int_{\Gamma_B} \frac{\mu_p}{C_B} \nabla\varphi_2 \cdot \boldsymbol{\nu}\, ds \ll -\int_{\Gamma_{BC}} \frac{\mu_p}{C_B} \nabla\varphi_2 \cdot \boldsymbol{\nu}\, ds \tag{4.1}$$

which refers only to the base region. The reference function φ_2 describes a situation where the potential at the emitter junction is raised. The hole current entering through the emitter junction is split into two parts leaving through the base contact and the collector junction, respectively. The above inequality means that the current through the base contact is much smaller than that through the collector junction, i.e. essentially all the holes injected into the base reach the collector. Consider a simplified model with constant hole mobility, constant doping in the base region and neglecting recombination-generation effects. Then φ_2 solves the Laplace equation and the validity of (4.1) only depends on the geometry of the base region.

The classical analysis of bipolar transistors (see e.g. [29]) uses a one-dimensional model. As pointed out above, this means that there is no obvious way of incorporating the base contact into the model. A priori assumptions on the flow in the base region have to be made. For the classical model it is assumed that the left hand side of (6.1) vanishes, i.e. there is no minority carrier current through the base contact. However, situations where in a_3 the second term dominates can be easily imagined. Then it is necessary to use the more general theory presented here.

5. Time dependent problems. Mathematically, the biggest difference between this section and section 2 is that only formal limiting procedures are considered for the transient problem whereas these limits have been rigorously justified for the steady state case.

The limit of the equations (1.1) as $\lambda \to 0$ constitutes a differential-algebraic system in time. If the algebraic solution component V (no time derivatives of V appear in the equations) could be determined from the algebraic equation

$$0 = n - p - C\,, \tag{5.1}$$

the system would be of index 1 [3]. Since this is not the case we are confronted with a system of higher index. As usual in the analysis of differential algebraic equations, we differentiate (5.1) with respect to time and obtain from (1.1a)

$$\nabla \cdot (\mathbf{J}_n + \mathbf{J}_p) = 0\,. \tag{5.2}$$

Since this can be interpreted as an elliptic equation for V, we obtain an index 1 system replacing (5.1) by (5.2). Therefore the original system is of index 2 in the language of the theory of differential algebraic equations, as has been pointed out by Ascher [1]. Initial data for the problem have to be compatible with both (5.1) and (5.2). It has already been observed [16], [30] that initial layers of rapid variation occur if the initial data do not satisfy (5.1), (5.2). For the steady state solutions used as initial conditions in this work, these conditions are certainly true and, thus, no initial layers are present.

For the further analysis of the transient problem it is convenient to introduce the new variables w and $\widetilde{V}$ by

$$np = \delta^4 w\,, \qquad \widetilde{V} = V - \widetilde{V}_{bi}\,,$$

where

$$\widetilde{V}_{bi} = \begin{cases} \ln(C/\delta^2)\,, & \text{in } \Omega_+; \\ -\ln(|C|/\delta^2)\,, & \text{in } \Omega_- \end{cases}$$

is an approximation for the built-in potential for small δ^2: $V_{bi} = \widetilde{V}_{bi} + O(\delta^4)$

The limiting equations for $\lambda \to 0$ in terms of w and $\widetilde{V}$ can be written as

$$\begin{aligned} &\nabla \cdot \mathbf{J}_n = -\nabla \cdot \mathbf{J}_p = \frac{1}{\sqrt{C^2 + 4\delta^4 w}} \frac{\partial w}{\partial t} + Q(n,p,\mathbf{x})(w-1)\,, \\ &\nabla w = p\mathbf{J}_n/\mu_n - n\mathbf{J}_p/\mu_p\,, \\ &(n+p)\nabla\widetilde{V} = \nabla C \left(1 - \frac{n+p}{|C|}\right) - \delta^4(\mathbf{J}_n/\mu_n + \mathbf{J}_p/\mu_p) \end{aligned} \tag{5.3}$$

with the carrier densities given by

$$n = \frac{1}{2}\left(C + \sqrt{C^2 + 4\delta^4 w}\right), \qquad p = \frac{1}{2}\left(-C + \sqrt{C^2 + 4\delta^4 w}\right). \tag{5.4}$$

The boundary conditions at the Ohmic contacts for the new variables read

$$w = 1\,, \quad \widetilde{V} = -U_j(t) + O(\delta^4)\,, \qquad \text{at } C_j\,,\ j = 1, \cdots, m\,.$$

As in the steady state case, jump conditions at the pn-junctions have to be considered. The jump conditions are the same as for the steady state problem [16]. The variables u and v introduced in section 2 — and therefore also $w = uv$ — as well as the normal components of the current densities are continuous across the junctions. From these conditions the equation

$$w = \frac{1}{4} e^{\widetilde{V}_- - \widetilde{V}_+}\left(1 + \sqrt{1 + 4\delta^4 w / C_+^2}\right)\left(1 + \sqrt{1 + 4\delta^4 w / C_-^2}\right), \qquad \text{on } \Gamma\,,$$

can be deduced, where the subscripts "+" and "−" refer to one-sided limits from the Ω_+- and the Ω_--sides, respectively.

Now we perform the limit $\delta^2 \to 0$. As in the steady state case we obtain from (5.4)

$$n = \max(0, C)\,, \qquad p = \max(0, -C)$$

and, in particular, $n + p = |C|$ in the limit. Therefore the last equation in (5.3) implies that $\widetilde{V}$ is independent of position in each n- and p-region. The limiting w satisfies

$$\frac{\partial w}{\partial t} = \begin{cases} C\left(\nabla \cdot \left(\frac{\mu_p}{C} \nabla w\right) - Q(C, 0, \mathbf{x})(w - 1)\right), & \text{in } \Omega_+, \\ |C|\left(\nabla \cdot \left(\frac{\mu_n}{|C|} \nabla w\right) - Q(0, -C, \mathbf{x})(w - 1)\right), & \text{in } \Omega_-. \end{cases} \tag{5.5}$$

The equation at the pn-junctions reduces to

$$w = e^{\widetilde{V}_- - \widetilde{V}_+}\,, \qquad \text{on } \Gamma\,. \tag{5.6}$$

The initial datum $w_0(\mathbf{x})$ for w is the solution of a stationary version of (5.5), (5.6) with the initial values of $\widetilde{V}$ denoted by $\widetilde{V}(\mathbf{x}, 0) = \widetilde{V}^0(\mathbf{x})$ (constant in each n- and p-region). The new variable

$$z = w - w_0$$

solves the equations

$$\frac{\partial z}{\partial t} = \begin{cases} C\left(\nabla \cdot \left(\frac{\mu_p}{C} \nabla z\right) - Q(C, 0, \mathbf{x}) z\right), & \text{in } \Omega_+, \\ |C|\left(\nabla \cdot \left(\frac{\mu_n}{|C|} \nabla z\right) - Q(0, -C, \mathbf{x}) z\right), & \text{in } \Omega_-, \end{cases} \tag{5.7}$$

subject to the auxiliary conditions

$$\begin{aligned} &z = 0\,, \quad \text{on } C_1, \cdots, C_m\,, \qquad z(\mathbf{x}, 0) = 0\,, \\ &z = e^{\widetilde{V}_- - \widetilde{V}_+} - e^{\widetilde{V}_-^0 - \widetilde{V}_+^0}\,, \quad \text{on } \Gamma\,, \end{aligned} \tag{5.8}$$

and homogeneous Neumann conditions along $\partial\Omega_N$. Note that the values of z on Γ are the only inhomogeneities in (5.7), (5.8).

Similar comments as in the steady state case are also relevant here. Assuming the (spatially constant) values of $\widetilde{V}$ in each n- and p-region to be given, the flow of the minority carriers can be obtained by solving the linear problem (5.7), (5.8). The currents through the contacts are computed from the currents through pn-junctions.

6. Switching of the pn-diode. In this section we present the derivation of an equation relating the evolution of the contact voltage and the current through a pn-diode as well as the analysis of a model for a simple switching application in the form of a Volterra integral equation [23], [24].

With the notation of section 3 the last condition in (5.8) reads for the pn-diode

$$z = e^{U(t)} - e^{U_0}, \qquad \text{on } \Gamma, \tag{6.1}$$

where $U(t)$ denotes the contact voltage with the initial value U_0. The current through the diode is given by $I(t) = I[w_0] + I[z](t)$ where the functional $I[\cdot]$ is defined by

$$I[z] = \int_\Gamma \left[\left(\frac{\mu_n}{|C|} \nabla z \right)_- - \left(\frac{\mu_p}{C} \nabla z \right)_+ \right] \cdot \boldsymbol{\nu}\, ds .$$

We consider the linear operator $\mathcal{A}\colon D(\mathcal{A}) \to L^2(\Omega_0)$ with domain

$$D(\mathcal{A}) = \Big\{ z \in H^2(\Omega_0) \mid z = 0 \text{ on } \Gamma_n \cup \Gamma_p,\ \frac{\partial z}{\partial \boldsymbol{\nu}} = 0 \text{ on } \partial\Omega_N, \\ z = \text{const on } \Gamma,\ I[z] = 0 \Big\},$$

whose action on a function $z \in D(\mathcal{A})$ is defined by the right hand side of (5.7). It is easy to see that $\mathcal{A}$ is symmetric with respect to the $L^2(\Omega_0)$-inner product

$$\langle z_1, z_2 \rangle = \int_{\Omega_+} \frac{z_1 z_2}{C} d\mathbf{x} + \int_{\Omega_-} \frac{z_1 z_2}{|C|} d\mathbf{x} .$$

It can be shown [23] that there exists an orthonormal basis of $L^2(\Omega_0)$ consisting of eigenfunctions φ_k, $k = 1, 2, \cdots$, of a self-adjoint extension of $\mathcal{A}$. The corresponding eigenvalues λ_k, $k = 1, 2, \cdots$, are negative and have $-\infty$ as their only accumulation point.

The Fourier coefficients in the representation

$$z(\mathbf{x}, t) = \sum_{k=1}^\infty z_k(t) \varphi_k(\mathbf{x}) \tag{6.2}$$

of the solution of (5.7), (5.8) satisfy the initial value problems

$$\dot z_k = \lambda_k z_k + \Phi_k I[z](t), \quad z_k(0) = 0, \qquad k = 1, 2, \cdots,$$

where Φ_k denotes the constant value of φ_k on Γ. With (6.1), evaluation of (6.2) on Γ gives

$$e^{U(t)} - e^{U_0} = \int_0^t \widetilde K(t-s) I[z](s)\, ds, \qquad \widetilde K(t) = \sum_{k=1}^\infty \Phi_k^2 e^{\lambda_k t}. \tag{6.3}$$

The kernel $\widetilde K$ is integrable and we introduce the normalized version

$$K(t) = I_s \widetilde K(t), \qquad \text{with } \frac{1}{I_s} = \int_0^\infty \widetilde K(t) dt = \sum_{k=1}^\infty \frac{\Phi_k^2}{-\lambda_k} .$$

The choice of the symbol I_s for the normalization constant is justified. It is equal to the saturation current computed in section 3. For the initial current the Shockley equation can be used, and we have

$$I(t) = I[z](t) + I_s (e^{U_0} - 1) .$$

Substitution of this relation into (6.3) gives

$$\int_0^t K(t-s)I(s)\,ds = I_s(e^{U(t)}-1) - I_s(e^{U_0}-1)\int_t^\infty K(s)\,ds\,. \tag{6.4}$$

Equation (6.4) is the main result of this section. It provides the desired relation between the evolution of the current $I(t)$ and the contact voltage $U(t)$. The integral term on the left hand side accounts for the influence of the history of the evolution, i.e. in particular for charge-storage effects. The exponentially decaying kernel $K(t)$ has an integrable singularity at $t=0$ ($K(t) = O(t^{-1/2})$ for a one-dimensional model problem [24]).

Instead of solving the eigenvalue problem for the operator $\mathcal{A}$, the kernel can also be determined from a Green's function[1] Z solving a modified version of problem (5.7), (5.8) where the last condition in (5.8) is replaced by

a) Z is independent from the position along Γ and

b) $I[Z](t) = \delta(t)$.

The kernel is then given in terms of the values of Z on Γ:

$$K(t) = I_s Z|_\Gamma$$

As in the stationary case, the voltage-current relation can be determined completely in terms of the solution of a device dependent reference problem.

As expected, (6.4) has the property that $I(t)$ converges as $t\to\infty$ if and only if $U(t)$ also converges. It is easy to see that in this case the limiting values satisfy the Shockley equation.

For given contact voltage, (6.4) is a Volterra integral equation of the first kind for $I(t)$. It is well known that this problem is mathematically ill posed. Jumps in the voltage, for example, correspond to singularities in the current. Also the purely voltage controlled problem is not very sensible from a physical point of view. The effect of a serial resistance always has to be taken into account.

The simple switching circuit depicted in Figure 4 has been considered in [23] and [24]. For $t<0$ we assume a steady state with the contact voltage $U=U_0$ and the corresponding current $I = I_s(e^{U_0}-1)$. At time $t=0$ the switch S is suddenly thrown to the right. For positive t the relation

$$V = U(t) + R\,I(t)$$

holds. If this is substituted in (6.4), a nonlinear Volterra integral equation of the second kind for $I(t)$ results:

$$\int_0^t K(t-s)I(s)\,ds = I_s(e^{V-RI(t)}-1) - I_s(e^{U_0}-1)\int_t^\infty K(s)\,ds\,. \tag{6.5}$$

For this equation the following result can be proven:

Theorem 6.1. *([23]) Equation (6.5) has a unique solution $I\in C[0,\infty)\cap C^\infty(0,\infty)$ converging as $t\to\infty$ to the unique solution I_∞ of*

$$I_\infty = I_s(e^{V-RI_\infty}-1)\,.$$

Finally we wish to demonstrate the capability of the model (6.5) to describe charge-storage effects by discussing the example of switching a pn-diode from a forward conduction to a reverse blocking state. In this case $U_0>0$ and $V<0$ holds. We rescale the current by the modulus of its initial value $I(0) = (V-U_0)/R$:

$$I = \frac{U_0 - V}{R}y$$

Equation (6.5) in terms of the new variable y reads

$$e^{(V-U_0)(y(t)+1)} = 1 - \int_0^t K(t-s)\left(1 - e^{-U_0} - \frac{U_0-V}{RI_se^{U_0}}y(s)\right)ds\,. \tag{6.6}$$

[1] We are indebted to Pierre Degond for pointing out this fact.

We wish to discuss a situation where the involved voltages have absolute values large compared to the thermal voltage, i.e. $U_0, -V \gg 1$. The factor

$$\alpha = \frac{U_0 - V}{RI_s e^{U_0}}$$

in (6.6) is an approximation for the ratio of the initial reverse current immediately after the switching and the forward current before the switching. We consider the limits $U_0 \to \infty$ and $V \to -\infty$ keeping the value of α fixed. As a convenient small parameter we choose

$$\varepsilon = \frac{1}{U_0 - V}.$$

With the new parameters we write (6.6) as

$$e^{-(y(t)+1)/\varepsilon} = 1 - \int_0^t K(t-s)[1 - \varepsilon\alpha RI_s - \alpha y(s)]ds. \tag{6.7}$$

The limit $\varepsilon \to 0$ in (6.7) has been carried out and justified for a simple model problem with explicitely known kernel in [24]. The limiting behaviour can be described as follows: Initially, a so called 'constant current phase' appears:

$$y(t) = -1, \qquad \text{for } 0 \le t \le t_0,$$

whose length t_0 is the solution of the equation

$$0 = 1 - (1+\alpha)\int_0^{t_0} K(s)ds. \tag{6.8}$$

The constant current phase is a time period where the resistivity of the diode is dominated by the serial resistance. Its occurrence is a charge-storage effect. When a sufficient amount of excess charges has been removed the current starts decaying to its steady state value. In this decay phase the exponential in (6.7) can be neglected, and the approximate solution $y(t)$ is determined from the Volterra equation of the first kind

$$0 = 1 - \int_0^t K(s)ds - \alpha\int_0^{t_0} K(t-s)ds + \alpha\int_{t_0}^t K(t-s)y(s)ds, \qquad \text{for } t > t_0.$$

The approximate current is continuous, but its derivative in general has a singularity at $t = t_0+$ [24].

For the model problem treated in [24] (infinitely long one-dimensional diode) the length of the constant current phase and the solution in the decay phase have already been computed by Kingston (1954, [5]) and Lax and Neustadter (1954, [6]). As in the steady state case our analysis leads to an extension of classical results.

7. The transient behaviour of the bipolar transistor. In this section we show that the currents through a bipolar transistor and the contact voltages are related by a system of two integral equations.

We recall the transistor geometry considered in section 4 (Figure 3). Then the last condition in (5.8) can be written as

$$z = e^{U_{BE}(t)} - e^{U_{BE}^0}, \quad \text{on } \Gamma_{EB}, \qquad z = e^{U_{BC}(t)} - e^{U_{BC}^0}, \quad \text{on } \Gamma_{BC}.$$

Here U_{BE} and U_{BC} denote the base-emitter voltage and the base-collector voltage, respectively; U_{BE}^0 and U_{BC}^0 are their values at $t = 0$.

Similarly to the preceding section we define the current functionals $I_E[\cdot]$ by

$$I_E[z] = \int_{\Gamma_{EB}} \left[\left(\frac{\mu_n}{|C|}\nabla z\right)_- - \left(\frac{\mu_p}{C}\nabla z\right)_+\right] \cdot \boldsymbol{\nu}\, ds,$$

and $I_C[\cdot]$ analogously by an integral over Γ_{BC}. We procede as for the pn-diode by considering the operator $\mathcal{A}$. Functions in the domain of $\mathcal{A}$ are now required to be constant along the junctions Γ_{EB} and Γ_{BC} with $I_E[z] = I_C[z] = 0$ for $z \in D(\mathcal{A})$. We again derive a Fourier series expansion of the solution z of (5.7), (5.8) in terms of eigenfunctions of $\mathcal{A}$. Evaluation of this representation on the pn-junctions leads to the system

$$
\begin{aligned}
e^{U_{BE}(t)} - e^{U_{BE}^0} &= \int_0^t \left[K_E(t-s)(I_E(s) - I_E^0) + K_{EC}(t-s)(I_C(s) - I_C^0)\right] ds\,, \\
e^{U_{BC}(t)} - e^{U_{BC}^0} &= \int_0^t \left[K_{EC}(t-s)(I_E(s) - I_E^0) + K_C(t-s)(I_C(s) - I_C^0)\right] ds\,.
\end{aligned}
\tag{7.1}
$$

These integral equations are the equivalent of equation (6.4) for the pn-diode. They relate the contact voltages to the emitter and collector currents $I_E(t)$ and $I_C(t)$, respectively, whose initial values are denoted by I_E^0 and I_C^0. The kernel functions are given by

$$
K_E(t) = \sum_{k=1}^{\infty} \Phi_{Ek}^2 e^{\lambda_k t}\,, \qquad K_C(t) = \sum_{k=1}^{\infty} \Phi_{Ck}^2 e^{\lambda_k t}\,,
$$
$$
K_{EC}(t) = \sum_{k=1}^{\infty} \Phi_{Ek}\Phi_{Ck} e^{\lambda_k t}\,,
$$

where Φ_{Ek} and Φ_{Ck} are the values of the k-th eigenfunction of $\mathcal{A}$ at Γ_{EB} and Γ_{BC}, respectively. An application of the Cauchy-Schwarz inequality shows that the kernel matrix of the two-dimensional system (7.1) is symmetric positive definite.

The kernel functions can again be computed by solving parabolic reference problems. We consider a function Z_E solving a version of (5.7), (5.8) with

$$
I_E[Z_E](t) = \delta(t)\,, \qquad I_C[Z_E](t) = 0\,,
$$

as well as a function Z_C satisfying

$$
I_E[Z_C](t) = 0\,, \qquad I_C[Z_C](t) = \delta(t)\,.
$$

Then the kernel functions are given by evaluation of these Green's functions at the pn-junctions:

$$
K_E(t) = Z_E|_{\Gamma_{EB}}\,, \qquad K_C(t) = Z_C|_{\Gamma_{BC}}\,, \qquad K_{EC}(t) = Z_E|_{\Gamma_{BC}} = Z_C|_{\Gamma_{EB}}
$$

8. Conclusions. Asymptotic methods have been used to reduce the computation of voltage-current characteristics of multidimensional bipolar semiconductor devices to the solution of simple, bias-point independent reference problems.

For the transient behaviour a new type of models in the form of integral equations has been presented. These models are well suited for an analysis of switching processes. Furthermore, they are simple enough to be used in circuit simulation programs as an alternative for equivalent circuit models. Preliminary numerical experiments [32] indicate that an efficient implementation is possible.

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