**SOME APPLICATIONS OF ASYMPTOTIC METHODS
IN SEMICONDUCTOR DEVICE MODELING**

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This short survey of results concerning the applications of perturbation analysis in semiconductor device modeling is devoted mostly to problems that were solved using the method of composite asymptotic expansions or the, so-called, boundary function method. Thorough description of this approach can be found in Vasil'eva and Butuzov [17], [18], [19] and in O'Malley [13], [14]. The main ideas of the method are illustrated below on the example of the singularly perturbed problem for the Gunn diode. Here the construction of the leading order terms of the asymptotic solution is discussed. This gives the opportunity to obtain the main characteristics of the device to the zeroth order. More detailed analysis of the asymptotic approximation for the solution of the Gunn diode problem, including the construction of higher order terms, will be published later. To make the presentation more compact some cumbersome details of the solution algorithm have been omitted.

§1. The statement of the problem for the Gunn diode

For the Gunn diode, consisting of a homogeneously doped piece of semiconductor (typically, gallium arsenide (GaAs)), we consider a spatially one-dimensional model for which the nondimensionalized system of equations can be written in a form:

$$(1.1) \quad \frac{\partial E}{\partial x} = n - 1 \quad (\text{Poisson equation}),$$

$$(1.2) \quad \frac{\partial n}{\partial t} = -\frac{\partial}{\partial x} J_n \quad (\text{continuity equation}),$$

$$(1.3) \quad J = J_n + \frac{\partial E}{\partial t} \quad (\text{total current density}),$$

$$(1.4) \quad J_n = nv(E) - \epsilon \frac{\partial n}{\partial x} \quad (\text{electron current density}).$$

Here $v(E)$, the charge carriers velocity, is represented in Figure 1; E_{cr} , a critical value of the field, is such that for $E > E_{cr}$, the bulk differential conductivity of the device becomes

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negative; the saturation velocity v_{sat} and E_{min} are defined so that $v_{\text{sat}} = v(\infty) = v(E_{\text{min}})$, v is scaled by v_{sat} ; the electric field density E , the charge carriers density n and the currents J and J_n are scaled by E_{cr} , constant donor concentration n_0 and $v_{\text{sat}} \cdot n_0$ respectively; the characteristic time is given by ℓ/v_{sat} , where ℓ is a characteristic length.

The following additional conditions are imposed:

$$(1.5) \quad n(0) = n(1) = 1 \quad (\text{ohmic contacts}) ,$$

$$(1.6) \quad \int_0^1 E(x) dx = U \quad (\text{bias voltage}) .$$

The applied voltage U is scaled by $E_{\text{cr}} \cdot \ell$.

There are two characteristic parameters in the problem:

$$\lambda = \sqrt{\frac{\epsilon_s E_{\text{cr}}}{qn_0 \ell}} \quad (\text{the scaled Debye length}) ,$$

and

$$\gamma = \frac{D}{v_{\text{sat}} \cdot \ell} ,$$

where ϵ_s is the permittivity of the semiconductor, q is the charge of electron, and D is a diffusivity. The case when both parameters λ and γ are small is considered in Markowich et al. [12], while discussion of the case where the diffusion term is omitted can be found in Shaw et al. [15]. We consider only the case when $\lambda \sim 0(1)$, $0 < \gamma \ll 1$. Without loss of generality we assume that $\lambda = 1$, and $\gamma = \epsilon$, where $0 < \epsilon \ll 1$ is a small parameter.

It is known that for applied voltages exceeding some threshold value, two working regimes with different currents exist for the Gunn diode, with the regime corresponding to the larger current being unstable (see, e.g. Shaw et al. [15], Szmolyan [16]). The so-called, *trivial* solution of the problem (1.1)-(1.6) corresponding to this unstable regime can be easily written out as

$$n = 1, \quad E_{\text{triv}} = U = \text{const},$$

$$J_n = n \cdot v(E_{\text{triv}}) = v(U),$$

$$J = J_n.$$

The other (stable) solution is known to have a pulse-line form (see Figure 2), with the pulses for E (and n) moving with velocity v . We will construct the asymptotic approximation for this solution when the pulse lies entirely within the domain $x \in (0, 1)$ (we will not here discuss the transition processes of formation or disappearance of such pulses).

Let us introduce the new independent variable z associated with the moving structure:

$$(1.7) \quad z = x - ct,$$

where c is unknown velocity of the structure. We seek functions E and n depending on variable z :

$$(1.8) \quad E = E(z), \quad n = n(z).$$

Taking into account (1.7), (1.8), the system (1.1)-(1.4) can be rewritten in a form:

$$(1.8) \quad c \frac{\partial n}{\partial z} = \frac{\partial}{\partial z} (nv(E) - \epsilon \frac{\partial n}{\partial z}),$$

$$(1.9) \quad J = nv(E) - \epsilon \frac{\partial n}{\partial z} - c \frac{\partial E}{\partial z},$$

$$(1.10) \quad \frac{\partial E}{\partial z} = n - 1.$$

Condition (1.6) changes very little; on the moving boundaries $z = z'(t)$ and $z = z''(t)$ (in the new coordinates) we have conditions for n similar to (1.5):

$$(1.11) \quad n(z') = n(z'') = 1,$$

$$(1.12) \quad \int_{z'}^{z''} E(x) dx = U,$$

where $z' = z'(t)$, $z'' = z''(t)$, $z'' - z' = 1$.

§2. Asymptotic algorithm

For any fixed instant of time (when the pulse is entirely within the domain), we subdivide the interval $z \in [z', z'']$ into three subintervals $[z', 0]$, $[0, \Delta z]$, $[\Delta z, z'']$ (without loss of generality, we associate $z = 0$ with the point where the maximal value of E is observed) and seek a uniform asymptotic approximation for the solution of the problem (1.8)-(1.12) in the form (cf. the notations for E -functions in Figure 3; similar for n -functions):

$$(2.1) \quad E(z) = \begin{cases} \overline{E}^1(z) + \Pi^* E(\xi), & z \in [z', 0], \xi \leq 0; \\ \overline{E}^2(z) + \Pi E(\xi) + Q^* E(\eta), & z \in [0, \Delta z], \xi \geq 0, \eta \leq 0; \\ \overline{E}^3(z) + Q E(\eta), & z \in [\Delta z, z''], \eta \geq 0; \end{cases}$$

$$(2.2) \quad n(z) = \begin{cases} \overline{n}^1(z) + \frac{1}{\epsilon} \Pi^* n(\xi), & z \in [z', 0], \xi \leq 0; \\ \overline{n}^2(z) + \frac{1}{\epsilon} \Pi n(\xi) + Q^* n(\eta), & z \in [0, \Delta z], \xi \geq 0, \eta \leq 0; \\ \overline{n}^3(z) + Q n(\eta), & z \in [\Delta z, z''], \eta \geq 0. \end{cases}$$

$$(2.3) \quad J = J_0 + \sqrt{\epsilon} J_1 + \epsilon J_2 + \dots,$$

$$(2.4) \quad c = c_0 + \sqrt{\epsilon} c_1 + \epsilon c_2 + \dots$$

Here $\xi = z/\epsilon$ and $\eta = (z - \Delta z)/\epsilon$ are stretched variables; $\overline{E}^i$, $\overline{n}^i$ ($i = 1, 2, 3$) are regular functions; boundary functions Π^* , Π and Q^* , Q depend on the variables ξ and η respectively. Each term in the sums (2.1), (2.2) is, in turn, a power series expansion in powers of $\sqrt{\epsilon}$ (the appearance of such an asymptotic sequence is connected with the construction of higher order terms of the asymptotic solution in the vicinity of the point $z = \Delta z$); for example

$$\overline{E}^1(z, \epsilon) = \sum_{i=0}^{\infty} (\sqrt{\epsilon})^i \overline{E}_i^1(z), \quad \Pi^* E(\xi, \epsilon) = \sum_{i=0}^{\infty} (\sqrt{\epsilon})^i \Pi_i^* E(\xi), \text{ etc.}$$

We require that boundary functions decay when corresponding stretched variables tend to $+\infty$ or $-\infty$; for example

$$\Pi_i^* E(-\infty) = 0, \quad \Pi_i E(+\infty) = 0, \text{ etc.}$$

The expansion (2.3) for J does not contain any boundary terms or any dependence on z . This simply reflects the fact that for a one-dimensional device without internal sources and drains the current is constant. For a nonlinear function $v(E)$ we must use an asymptotic representation similar to (2.1), (2.2):

$$(2.5) \quad v(E) = \begin{cases} \bar{v}^1(\bar{E}^1) + \Pi^* v(\xi), & z \in [z'_1 0], \xi \leq 0; \\ \bar{v}^2(\bar{E}^2) + \Pi v(\xi) + Q^* v(\eta), & z \in [0, \Delta z], \xi \geq 0, \eta \leq 0; \\ \bar{v}^3(\bar{E}^3) + Q v(\eta), & z \in [\Delta z, z''], \eta \geq 0; \end{cases}$$

where

$$\Pi^* v(\xi) = v(\bar{E}^1(\epsilon \xi) + \Pi^* E(\xi)) - v(\bar{E}^1(\epsilon \xi)), \xi \leq 0;$$

$$\Pi v(\xi) = v(\bar{E}^2(\epsilon \xi) + \Pi E(\xi)) - v(\bar{E}^2(\epsilon \xi)), \xi \geq 0;$$

and analogous expressions hold for $Q^* v(\eta)$, $Q v(\eta)$. It can be easily shown that for exponentially decaying $\Pi_i^* E$ -functions the functions $\Pi_i^* v(\xi)$ will also be exponentially decaying.

Substituting (2.1)-(2.5) into (1.8)-(1.12) we can determine the terms of the asymptotic approximation by a standard procedure (note that Δz must be determined along with the construction of the asymptotic solution).

In the present discussion, the most important aspect is the construction of the zeroth order terms for the function E , because they define at the zeroth order the main characteristics of the Gunn diode: the velocity of the structure and therefore the current, the amplitude of the pulse, etc. In the following we will take into account that the density of electrons satisfies $n \geq 0$, and that for applied voltages satisfying $U \geq 1$, the difference between $E = U$ and E_0 (see Figure 2) is of the order $0(1)$.

The determination of the regular functions to the zeroth order can be easily obtained by putting $\epsilon = 0$ in the original system (1.8)-(1.10). For the solutions on the subintervals $[z', 0]$ and $[\Delta z, z'']$ (the boundary conditions for $\bar{n}_0^i$ are $\bar{n}_0^1(z') = 1$, $\bar{n}_0^3(z'') = 1$) we write ($i = 1, 3$):

$$\bar{n}_0^i = 1, \frac{\partial \bar{E}_0^i}{\partial z} = \bar{n}_0^i - 1 = 0 \quad \text{and hence } \bar{E}_0^i = \text{const},$$

$$(2.6) \quad J_0 = \bar{n}_0^i \cdot v(\bar{E}_0^i) - c_0 \frac{\partial \bar{E}_0^i}{\partial z} = v(\bar{E}_0^i) = \text{const}.$$

By virtue of (2.6) and (1.12)

$$(2.7) \quad \overline{E}_0^1 = \overline{E}_0^3 \equiv E_0,$$

where E_0 is some unknown constant (see Figure 2). (the discussion of equality (2.7) can be also found in Markowich et al. [12].)

For the subinterval $[0, \Delta z]$ the only other solution of the degenerate system that will make it possible to satisfy the integral condition (1.12) is

$$\overline{n}_0^2 = 0,$$

$$\frac{\partial \overline{E}_0^2}{\partial z} = \overline{n}_0^2 - 1 = -1 \text{ and hence } \overline{E}_0^2 = -z + K,$$

$$(2.8) \quad J_0 = \overline{n}_0^2 \cdot v(\overline{E}_0^2) - c_0 \frac{\partial \overline{E}_0^2}{\partial z} = c_0,$$

(here, K is some unknown constant).

From (2.6), (2.7), (2.8) (with $J_0 = \text{const}$ throughout the device) it follows that

$$(2.9) \quad c_0 = v(E_0).$$

It can be easily shown that the boundary functions $\Pi_0 E, Q_0^* E, Q_0 E \equiv 0$. In the subinterval $[z', 0]$ we must construct the boundary function $\Pi_0^* E$ to give us the transition from $E_{\max} = \max_{[0, \Delta z]} \overline{E}_0^2$ to the solution $\overline{E}_0^1 = E_0$ (see Figure 4). The equations for $\Pi_0^* E, \Pi_0^* n$ can be written out as follows ($\xi \leq 0$):

$$(2.10) \quad 0 = \Pi_0^* n \cdot v(E_0 + \Pi_0^* E) - \frac{\partial \Pi_0^* n}{\partial \xi} - c_0 \frac{\partial \Pi_0^* E}{\partial \xi},$$

$$(2.11) \quad \frac{\partial \Pi_0^* E}{\partial \xi} = \Pi_0^* n.$$

Eliminating $\Pi_0^* n$ from (2.10) and adding the decay conditions at $-\infty$, we obtain

$$(2.12) \quad \frac{\partial^2 \Pi_0^* E}{\partial \xi^2} = [v(E_0 + \Pi_0^* E) - v(E_0)] \frac{\partial \Pi_0^* E}{\partial \xi},$$

$$(2.13) \quad \Pi_0^* E(-\infty) = \frac{\partial \Pi_0^* E}{\partial \xi}(-\infty) = 0.$$

Taking into account (2.13) we can integrate (2.12) once to obtain

$$(2.14) \quad \frac{\partial \Pi_0^* E}{\partial \xi} = \int_0^{\Pi_0^* E} [v(E_0 + s) - v(E_0)] ds.$$

The value $\Pi_0^* E_{\max} = \max_{\xi \leq 0}(\Pi_0^* E)$ is then defined by the well-known "equal area rule" (see Markowich et al. [12], etc.) following (2.14) (Figure 5):

$$(2.15) \quad 0 = \int_0^{\Pi_0^* E_{\max}} [v(E_0 + s) - v(E_0)] ds, \quad \Pi_0^* E_{\max} \neq 0.$$

this relation gives the implicit function $\Pi_0^* E_{\max}(E_0)$.

At the point $z = 0$ equality takes place (see Figure 4):

$$(2.16) \quad \max(\overline{E}_0^2) = E_0 + \Pi_0^* E_{\max}(E_0)$$

As soon as $\Pi_0^* E_{\max}$ is known (it depends on the still unknown constant E_0) the expression for the implicit function $\Pi_0^* E(\xi)$ can be easily written out:

$$(2.17) \quad \int_{\Pi_0^* E_{\max}}^{\Pi_0^* E} \frac{dz}{[\int_0^z (v(E_0 + s) - v(E_0)) ds]} = -\xi.$$

It follows from (2.11) that the expression for $\Pi_0^* n$ is given by (2.14). It can be easily shown that $\Pi_0^* E(\xi)$ and $\Pi_0^* n(\xi)$ decay exponentially as $\xi \rightarrow -\infty$.

To find E_0 and therefore all the other characteristics of the device to the zeroth order, we need to obtain one more relation between $\Pi_0^* E_{\max}$ and E_0 in addition to (2.15). Let us consider the integral condition (1.12). We can rewrite it (to the zeroth order) in the form:

$$(2.18) \quad U = \int_{z'}^{z''} \overline{E}_0 dz = \int_{z'}^0 E_0 dz + \int_0^{\Delta z} \overline{E}_0^2(z) dz + \int_{\Delta z}^{z''} E_0 dz.$$

The boundary function $\Pi_0^* E$ does not enter (2.18) because its impact to the integral is of the order $0(\epsilon)$. From (2.16) and the relation $\overline{E}_0^2 = -z + K$, the following expressions can be easily derived:

$$K = E_0 + \Pi_0^* E_{\max}(E_0), \quad \Delta z = \Pi_0^* E_{\max}(E_0).$$

Substituting $\overline{E}_0^2$, K and Δz into (2.18) we get

$$(2.19) \quad \Pi_0^* E_{\max}(E_0) = +\sqrt{2(U - E_0)}.$$

Substituting (2.19) into (2.15) we obtain

$$(2.20) \quad \int_0^{\sqrt{2(U-E_0)}} (v(E_0 + s) - v(E_0)) ds = 0.$$

The solution E_0 of the equation (2.20) can be found numerically. For known E_0 the values $J_0 = v(E_0)$, $c_0 = v(E_0)$, $\Pi_0^* E_{\max}(E_0)$, $\Pi_0^* E(\xi)$, $\Pi_0^* n(\xi)$, $\Delta z(E_0)$ will also be known.

Let us consider different possibilities that might occur for the solution of (2.20). The trivial solution $E_0 = U$ always exists, it corresponds to the trivial solution of the whole problem that is stable for $U < 1$ and unstable for $U > 1$. For $U > 1$ the nontrivial solution E'_0 corresponds to the point A in the Figure 6 where the curves F and G intersect ($F = \Pi_0^* E_{\max}(E_0)$ is defined implicitly by (2.14) and $G = \Pi_0^* E_{\max}(E_0)$ is defined by (2.19)). This solution is known to be stable. For $U < \alpha < 1$, where $\alpha \sim 0(1)$ is a constant that can be found, no nontrivial solution exists (Figure 7). For $\alpha < U \lesssim 1$ the situation shown in Figure 8 is possible (we take into account that $\frac{\partial F}{\partial E_0}(1) = -1$, $\frac{\partial G}{\partial E_0}(U) = -\infty$): two nontrivial solutions E'_0 and E''_0 of (2.20) exist corresponding to the intersection points A and B respectively. The trivial solution of the original problem with $U \lesssim 1$ is stable (Szmolyan [16]), the solution of the problem with $E_0 = E'_0$ is expected to be stable and the solution with $E_0 = E''_0$ to be unstable. The fact that three solutions exist (including the trivial one) can be used to explain the hysteresis effects that were experimentally observed for the Gunn diode: for increasing and decreasing applied bias voltages, different paths of voltage-current characteristics were obtained (Shaw et al. [15]). Other terms of the asymptotic solution (including higher order terms) can be constructed likewise.

§3. Other problems

In this section some other applications of the asymptotic analysis to semiconductor device modeling will be briefly discussed.

1. The most widespread model that is now used for numerical simulations of the processes in the semiconductor devices is still a drift-diffusion model. When Gummel-type

iteration schemes are applied to solve the drift-diffusion equations numerically the speed of convergence and sometimes the convergence itself depend crucially on the successfully chosen initial iterate. In Kalachev and Obukhov [9] the singularly perturbed Poisson equation (one of the drift-diffusion equations) was considered (in dimensionless form) as:

$$(3.1) \quad \alpha^2 \Delta \Psi = n - p - N,$$

$$(3.2) \quad n = \exp(\Psi - \varphi_n), p = (\varphi_p - \Psi).$$

Here $\alpha = L_0/L$, where L_0 is the Debye length, L is characteristic length; the electrostatic potential Ψ and the Fermi quasilevels φ_n, φ_p are measured in units of kT/q (k is Boltzmann's constant, T is the absolute temperature, q is the charge of the electron); n, p and N are the concentrations of electrons, holes, and the dopant concentration in units of intrinsic concentration n_i . The small parameter $\epsilon = \alpha/\sqrt{m}$, for $m = \max |N|$, enters the equation (3.1) making the problem for the Poisson equation singularly perturbed. For contemporary semiconductor devices, $\epsilon \sim 10^{-1} - 10^{-4}$. This problem has to be solved by successive approximations at each step of the iterative Gummel-type process of obtaining the solution for the full drift-diffusion model. In [9] the boundary function method was used to construct the initial iterate to solve the Poisson equation in a rectangular domain modeling the two-dimensional semiconductor structure when some voltages were applied to the contacts. Some segments of the boundary modeled the ohmic contacts, while on the rest of the boundary the homogeneous Neumann conditions were prescribed.

The solution of (3.1), (3.2) is conveniently sought in the form

$$\Psi = \Psi_0 + \varphi,$$

where Ψ_0 is the solution of the quasineutrality equation

$$n - p - N = 0$$

satisfying the boundary conditions at the ohmic contacts. Then we have the singularly perturbed boundary value problem for the potential φ :

$$(3.3) \quad \epsilon^2 \Delta \varphi = A(x, z) \sinh \varphi + B(x, z)(\cosh \varphi - 1) - g(x, z, \epsilon),$$

$$(3.4) \quad \varphi|_{\Gamma_i} = 0 \quad (\text{ohmic contacts}),$$

$$(3.5) \quad \frac{\partial \varphi}{\partial \nu}|_{\gamma_i} = -\frac{\partial \Psi_0}{\partial \nu}|_{\gamma_i} \sim 0(1) \quad (\text{rest of the boundary}).$$

Here x, z are spatial coordinates; $A(x, z)$, $B(x, z)$, $g(x, z, \epsilon)$ are known, sufficiently smooth functions; $A > B$ for all (x, z) ; and $\partial/\partial \nu$ is the outward normal derivative.

Under certain conditions the full asymptotic approximation for the solution of (3.3)-(3.5) is constructed. It happens that the boundary functions appear only to the order $O(\epsilon)$ and the explicit expressions for them can be easily obtained. This fact simplifies the use of the asymptotic solution in a numerical algorithm. Numerical computations have shown that, when the asymptotic solution is used as the initial iterate, the convergence of the numerical process for the drift-diffusion model is speeded up by a factor of 5-10. In Kalachev et al. [8] the case of a gate contact is considered and the estimation of the asymptotic remainder is presented. Problems for the singularly perturbed Poisson equation in a three-dimensional semiconductor structure and in the case of large outer electric field are solved in [10], [11] respectively.

2. The boundary function method was used to construct asymptotic solutions of the full drift-diffusion models for one-dimensional devices by Belyanin [1], [2], [3], etc., in these papers the ratio of Debye length to the length of the device was considered as small parameter. In [1] the asymptotic approximation is constructed for the solution of the system modeling a diode in a nonstationary case. The nonlinear parabolic equation for the electron concentration $\bar{n}_0$ (a regular function to zeroth order) is solved numerically, hole concentration $\bar{p}_0$ and electric field $\bar{E}_0$ are expressed algebraically through $\bar{n}_0$, and the formulae for the boundary functions and higher order terms are written out explicitly. In [2] the stationary problems for the diode in the cases of moderate and large applied currents are considered. In [3] the stationary problem is solved for a one-dimensional device containing an arbitrary number of $p-n$ junctions and bias contacts; and a theorem on estimating of the remainder is proved.

It is worthwhile to mention the paper by Vasil'eva et al. [6], where the one dimensional problem for the diode (thyristor structure) is posed as the optimal control problem. For

given voltage-current characteristics, the synthesis of the device with such characteristics is discussed, when a doping level N ($-1 \leq N \leq 1$) is considered to be the control function.

3. Some other asymptotic problems of the semiconductor device modeling concerning the asymptotic solution of the stationary drift-diffusion model in the case of large generation-recombination terms in a two-dimensional domain, the internal transition layers in a thin semiconductor films, the asymptotic derivation of the ambipolar diffusion equation for the intrinsic semiconductors with the discussion of the correct boundary conditions for this equation, are presented in [4], [5], [7].

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Figure 1. Dependence $v = v(E)$ for GaAs.

Figure 2. The structure of the solution.

Figure 3. Notations for E -functions.

Figure 4. The structure of the zeroth order approximation for function E .

Figure 5. Equal area rule.

Figure 6. Unique solution exists for $U > 1$.

Figure 7. No solutions for $U < \alpha < 1$

Figure 8. The case when $\alpha < U \lesssim 1$.

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