LE MATEMATICHE
Vol. LXIV (2009) – Fasc. I, pp. 77–91

ON AN APPROACH TO THE CONSTRUCTION OF DIFFERENCE SCHEMES FOR THE MOMENT EQUATIONS OF CHARGE TRANSPORT IN SEMICONDUCTORS

A. M. BLOKHIN - S. A. BOYARSKIY - B. V. SEMISALOV

We discuss the construction of a class of difference schemes for a hydrodynamical model of charge transport in semiconductors.

Introduction

At present time *hydrodynamical models* are widely used for the description of various physical phenomena. Approximate solutions to such models are often found by *finite-difference methods*. Difference schemes for hydrodynamical models can be constructed in many ways. Some methods are given in [7] (see also [5,9]). One of them is an interesting method [7] based on the existence of different presentations for the system of gas dynamics.

In the present paper we apply the mentioned method to a mathematical model appearing in physics of semiconductors. It is known that hydrodynamical models also appear while simulating such physical phenomena as the charge transport in semiconductors. A lot of new mathematical models of hydrodynamical type was suggested during the last years. It is worthy to notice that for the most of them a mathematical ground is practically absent.

One of the latest models was recently suggested in [2,10]. This model is a *quasilinear system of conservation laws*. These conservation laws were derived

Entrato in redazione: 13 gennaio 2009

from *the systems of moment equations* for *the Boltzman transport equation* by a *truncation procedure*.

In this paper, we suggest a class of difference schemes for finding approximate solutions to the moment equations mentioned above.

1. Preliminary information

In [2,10] a system of moment equations well-reasoned from the physical point of view was proposed and used to describe the charge transport process in concrete semiconductor devices. These equations have the form of conservation laws. The system was obtained from the Boltzmann transport equation by a suitable truncation procedure (see [2,10]). Note that the existence of a great number of mathematical models for charge transport in semiconductors is caused by the variety of truncation procedures for them.

Following [3,8], the quasilinear system of the equations mentioned above in a dimensionless form and for the 2D case reads

$$\mathbf{U}_t + \mathcal{P}_x + \Omega_y = \mathbf{F}(\mathbf{Q}, \mathbf{U}), \tag{1.1}$$

$$\varepsilon \triangle_{x,y} \varphi = R - \rho. \tag{1.2}$$

Here

$$\mathbf{U} = \begin{pmatrix} R \\ \mathbf{J} \\ \sigma \\ \mathbf{I} \end{pmatrix}, \quad \mathcal{P} = \begin{pmatrix} J^{(x)} \\ \frac{2}{3}\sigma \\ 0 \\ I^{(x)} \\ æR \\ 0 \end{pmatrix}, \quad \Omega = \begin{pmatrix} J^{(y)} \\ 0 \\ \frac{2}{3}\sigma \\ I^{(y)} \\ 0 \\ æR \end{pmatrix},$$

$$\mathbf{F} = \begin{pmatrix} 0 \\ R\mathbf{Q} + c_{11}\mathbf{J} + c_{12}\mathbf{I} \\ (\mathbf{J}, \mathbf{Q}) + cP \\ \frac{5}{3}\sigma\mathbf{Q} + c_{21}\mathbf{J} + c_{22}\mathbf{I} \end{pmatrix},$$

$$\mathbf{J} = \begin{pmatrix} J^{(x)} \\ J^{(y)} \end{pmatrix} = R\mathbf{u} = R\begin{pmatrix} u^{(x)} \\ u^{(y)} \end{pmatrix}, \mathbf{I} = \begin{pmatrix} I^{(x)} \\ I^{(y)} \end{pmatrix} = R\mathbf{q} = R\begin{pmatrix} q^{(x)} \\ q^{(y)} \end{pmatrix},$$

R is the electron density,
$\mathbf{u}$ is the electron velocity,
$\mathbf{q}$ is the energy flux,

$\sigma = RE$, $\mathrm{P} = R(\frac{2}{3}E - 1)$, $\mathbf{Q} = \nabla\varphi$, $æ = \frac{10}{9}E^2$,
E is the electron energy,
φ is the electric potential,
$\rho = \rho(x, y)$ is the doping density,
$\triangle_{x,y} = \left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2}\right)$ is the Laplacian.

The coefficients $c_{11}, \ldots, c_{22}, c$ of system (1.1) are smooth functions of the energy E. The precise but rather cumbersome expressions for these functions in the parabolic band case can be found in [3,8]. The constant $\varepsilon > 0$ appearing in the *Poisson equation* (1.2) is a dimensionless dielectric constant. The doping density $\rho(x, y)$ is a given sufficiently smooth function.

On smooth solutions system (1.1) can also be rewritten in the *non-divergent form*

$$\mathbf{U}_t + \widetilde{\mathbb{B}} \cdot \mathbf{U}_x + \widetilde{\mathbb{C}} \cdot \mathbf{U}_y = \mathbf{F}, \tag{1.1$'$}$$

where

$$\widetilde{\mathbb{B}} = \mathcal{P}_{\mathbf{U}} = \begin{pmatrix} 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & \frac{2}{3} & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 \\ -æ & 0 & 0 & \frac{2æ}{E} & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \end{pmatrix}, \quad \widetilde{\mathbb{C}} = \Omega_{\mathbf{U}} = \begin{pmatrix} 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & \frac{2}{3} & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ -æ & 0 & 0 & \frac{2æ}{E} & 0 & 0 \end{pmatrix}.$$

Remark 1.1. It is easy to see that

$$\mathcal{P} = \widetilde{\mathbb{B}}\mathbf{U}, \quad \Omega = \widetilde{\mathbb{C}}\mathbf{U}.$$

Remark 1.2. In this paper we will construct numerical algorithms for system (1.1). Numerical algorithms for the Poisson equation (1.2) are detailed, for example, in [1,4,6]. By this reason, we will below consider only system (1.1) (or (1.1$'$)) assuming that the electric potential $\varphi(t, x, y)$ is a given sufficiently smooth and bounded function.

Remark 1.3. In [11,12] the *hyperbolicity condition* for system (1.1) is formulated as follows:

$$E > 0.$$

Clearly, this inequality is physically relevant.

Remark 1.4. In the stationary case system (1.1) has the form (see [1,4])

$$\left.\begin{aligned} &\mathrm{div}\mathbf{J} = 0,\\ &\mathrm{div}\mathbf{I} = (\mathbf{J},\mathbf{Q}) + cP,\\ &\nabla\left(\frac{2}{3}\sigma\right) = R\mathbf{Q} + c_{11}\mathbf{J} + c_{12}\mathbf{I},\\ &\nabla\left(\frac{4}{9}RE^2\right) = \frac{2}{5}\left\{\frac{5}{3}\sigma\mathbf{Q} + c_{21}\mathbf{J} + c_{22}\mathbf{I}\right\}. \end{aligned}\right\} \qquad (1.1'')$$

From the last two vector relations of system $(1.1'')$ we obtain that

$$\nabla E = a\cdot\mathbf{u} + b\cdot\mathbf{q}. \qquad (1.3)$$

Here

$$a = a(E) = \frac{3}{2}\left\{\frac{3}{5}\frac{c_{21}}{E} - c_{11}\right\}, \qquad b = b(E) = \frac{3}{2}\left\{\frac{3}{5}\frac{c_{22}}{E} - c_{12}\right\}.$$

2. Construction of symmetrizer for system $(1.1')$

We start with the following definition.

Definition 2.1. A real matrix $\mathbb{A} = \mathbb{A}^* = (a_{ij}),\ i,j = \overline{1,6}$, is called *symmetrizer* for the system $(1.1')$ if

$$1)\ \mathbb{A} > 0, \quad 2)\ \mathbb{B} = \mathbb{A}\cdot\widetilde{\mathbb{B}} = \mathbb{B}^*, \quad 3)\ \mathbb{C} = \mathbb{A}\cdot\widetilde{\mathbb{C}} = \mathbb{C}^*.$$

Here * means transposition.

Now we proceed to the construction of the symmetrizer $\mathbb{A}$. Multiplying $\mathbb{A}$ by $\widetilde{\mathbb{B}}$ and $\mathbb{A}$ by $\widetilde{\mathbb{C}}$ and accounting for the symmetry of the matrix $\mathbb{A}(a_{ij} = a_{ji})$, we obtain that the conditions 2) and 3) are fulfilled if

$$\left.\begin{array}{ll}
a_{11} = -æa_{25}, & 0 = -æa_{35}, \\
\frac{2}{3}(a_{12} + \frac{3æ}{E}a_{15}) = -æa_{45}, & a_{14} = -æa_{55}, \\
0 = -æa_{56}, & 0 = a_{13}, \\
\frac{2}{3}(a_{22} + \frac{3æ}{E}a_{25}) = a_{14}, & a_{24} = a_{15}, \\
0 = a_{16}, & \frac{2}{3}(a_{23} + \frac{3æ}{E}a_{35}) = 0, \\
0 = a_{34}, & a_{44} = \frac{2}{3}(a_{25} + \frac{3æ}{E}a_{55}), \\
0 = -æa_{26}, & 0 = a_{45}, \\
-æa_{36} = a_{11}, & -æa_{46} = \frac{2}{3}(a_{13} + \frac{3æ}{E}a_{16}), \\
0 = -æa_{56}, & a_{14} = -æa_{66}, \\
0 = a_{12}, & \frac{2}{3}(a_{23} + \frac{3æ}{E}a_{26}) = 0, \\
0 = a_{24}, & \frac{2}{3}(a_{33} + \frac{3æ}{E}a_{36}) = a_{14}, \\
0 = a_{15}, & a_{16} = a_{34}, \\
\frac{2}{3}(a_{35} + \frac{3æ}{E}a_{56}) = 0, & \frac{2}{3}(a_{36} + \frac{3æ}{E}a_{66}) = a_{44}.
\end{array}\right\} \quad (2.1)$$

Relations (2.1) are derived by equating entries of the matrices $\mathbb{B}$ and $\mathbb{B}^*$, $\mathbb{C}$ and $\mathbb{C}^*$.

Analysis of relations (2.1) shows that the desired matrix $\mathbb{A}$ and the matrices $\mathbb{B}, \mathbb{C}$ have the following form

$$\mathbb{A} = a_{55}\begin{pmatrix} æ\omega & 0 & 0 & -æ & 0 & 0 \\ 0 & \frac{10E}{3}(\omega - \frac{E}{2}) & 0 & 0 & -\omega & 0 \\ 0 & 0 & \frac{10E}{3}(\omega - \frac{E}{2}) & 0 & 0 & -\omega \\ -æ & 0 & 0 & d & 0 & 0 \\ 0 & -\omega & 0 & 0 & 1 & 0 \\ 0 & 0 & -\omega & 0 & 0 & 1 \end{pmatrix},$$

$$\mathbb{B} = a_{55}\begin{pmatrix} 0 & æ\omega & 0 & 0 & -æ & 0 \\ æ\omega & 0 & 0 & -æ & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & -æ & 0 & 0 & d & 0 \\ -æ & 0 & 0 & d & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \end{pmatrix},$$

$$\mathbb{C} = a_{55}\begin{pmatrix} 0 & 0 & æ\omega & 0 & 0 & -æ \\ 0 & 0 & 0 & 0 & 0 & 0 \\ æ\omega & 0 & 0 & -æ & 0 & 0 \\ 0 & 0 & -æ & 0 & 0 & d \\ 0 & 0 & 0 & 0 & 0 & 0 \\ -æ & 0 & 0 & d & 0 & 0 \end{pmatrix},$$

where

$$\omega = \frac{a_{11}}{æ a_{55}}, \quad d = \frac{2}{3}\left(\frac{3æ}{E} - \omega\right).$$

The matrix $\mathbb{A}$ is positive definite if

$$\frac{5}{3}E\left\{1 - \sqrt{\frac{2}{5}}\right\} < \omega < \frac{5}{3}E\left\{1 + \sqrt{\frac{2}{5}}\right\}, \quad a_{55} > 0. \tag{2.2}$$

In what follows we assume that $\omega = \frac{5}{3}E = \frac{3æ}{2E}$. Then $d = \frac{10}{9}E = \frac{æ}{E}$. Multiplying system $(1.1')$ from the left by the matrix $\mathbb{A}$ and omitting the common multiplier a_{55} in the matrices $\mathbb{A}$, $\mathbb{B}$, and $\mathbb{C}$, we finally obtain the *symmetric hyperbolic system*

$$\mathbb{A}\cdot\mathbf{U}_t + \mathbb{B}\cdot\mathbf{U}_x + \mathbb{C}\cdot\mathbf{U}_y = \mathbb{A}\mathbf{F}. \tag{2.3}$$

Taking into account the structure of the vector $\mathbf{F}$, we present the vector $\mathbb{A}\mathbf{F}$ as follows:

$$\mathbb{A}\mathbf{F} = \mathbb{D}\mathbf{U} + \mathfrak{F}. \tag{2.4}$$

Here $\mathbb{D} = \mathbb{A}D$,

$$D = \begin{pmatrix} 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & c_{11} & 0 & 0 & c_{12} & 0 \\ 0 & 0 & c_{11} & 0 & 0 & c_{12} \\ -c & 0 & 0 & \frac{2}{3}c & 0 & 0 \\ 0 & c_{21} & 0 & 0 & c_{22} & 0 \\ 0 & 0 & c_{21} & 0 & 0 & c_{22} \end{pmatrix}, \quad \mathfrak{F} = æ\begin{pmatrix} -(\mathbf{J},\mathbf{Q}) \\ R\mathbf{Q} \\ \frac{1}{E}(\mathbf{J},\mathbf{Q}) \\ 0 \\ 0 \end{pmatrix}.$$

3. Another form of system (2.3)

The aim of our work is to construct a numerical algorithm for finding stationary solutions to the original system (1.1) by the *stabilization method* when stationary solutions to (1.1) are sought as a limit of nonstationary ones as $t \to +\infty$. While doing so we assume that stationary and nonstationary solutions to (1.1) coincide for large t.

System (2.3) can be also represented as follows:

$$(\mathbb{A}\mathbf{U})_t + (\mathbb{B}\mathbf{U})_x + (\mathbb{C}\mathbf{U})_y = \mathbb{A}\mathbf{F} + \{\underset{\sim\sim\sim}{\mathbb{A}' \cdot E_t} + \mathbb{B}' \cdot \underline{E_x} + \mathbb{C}' \cdot \underline{E_y}\}\mathbf{U}. \tag{3.1}$$

Here $\mathbb{A}' = \dfrac{d\mathbb{A}}{dE}$, etc.

In view of the aforesaid, in system (3.1) we omit the summand underlined with a wavy line and replace the underlined derivatives E_x, E_y by their expressions for the stationary case using formula (1.3). The resulting system is

$$(\mathbb{A}\mathbf{U})_t + (\mathbb{B}\mathbf{U})_x + (\mathbb{C}\mathbf{U}_y) = \widetilde{\mathbb{D}}\mathbf{U} + \mathfrak{F}, \tag{3.2}$$

where $\widetilde{\mathbb{D}} = \mathbb{D} + \mathbb{L}$, $\mathbb{L} = (\mathbb{B}'u^{(x)} + \mathbb{C}'u^{(y)})a + (\mathbb{B}'q^{(x)} + \mathbb{C}'q^{(y)})b$,

$$\mathbb{B}' = \begin{pmatrix} 0 & 5æ & 0 & 0 & -2d & 0 \\ 5æ & 0 & 0 & -2d & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & -2d & 0 & 0 & \frac{10}{9} & 0 \\ -2d & 0 & 0 & \frac{10}{9} & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \end{pmatrix},$$

$$\mathbb{C}' = \begin{pmatrix} 0 & 0 & 5æ & 0 & 0 & -2d \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 5æ & 0 & 0 & -2d & 0 & 0 \\ 0 & 0 & -2d & 0 & 0 & \frac{10}{9} \\ 0 & 0 & 0 & 0 & 0 & 0 \\ -2d & 0 & 0 & \frac{10}{9} & 0 & 0 \end{pmatrix}.$$

Remark 3.1. In the stationary case systems (2.3) and (3.2) are equivalent on smooth solutions of system (1.1).

Remark 3.2. Strictly speaking, smooth bounded solutions to system (1.1) do not satisfy system (3.2). Nevertheless, following the reasons from above we assume that for large t the solutions to system (1.1) are solutions to system (3.2) as well. So, in what follows we assume that systems (2.3) and (3.2) are two equivalent forms of (1.1) on its smooth bounded solutions. With this assumption we are able to derive an *a priori estimate* for smooth bounded solutions of (1.1). Indeed, let $\mathbf{U}(t,x,y)$ be a bounded smooth solution to (1.1) in the domain

$$\Pi = \{(t,x,y) | T_0 \le t \le T < \infty, (x,y) \in R^2\}$$

with a sufficiently large $T_0 > 0$ satisfying the condition

$$(\mathbf{U},\mathbf{U}) = |\mathbf{U}|^2 \to 0 \text{ as } \sqrt{x^2+y^2} \to \infty. \tag{3.3}$$

Multiplying (2.3) and (3.2) by $\mathbf{U}$ and summing up the results, we have

$$(\mathbf{U},\mathbb{A}\mathbf{U})_t+(\mathbf{U},\mathbb{B}\mathbf{U})_x+(\mathbf{U},\mathbb{C}\mathbf{U})_y=(\mathbf{U},\Lambda\mathbf{U})+2(\mathbf{U},\mathfrak{F}). \tag{3.4}$$

Here $\quad \Lambda=\mathbb{D}+\mathbb{D}^*+\frac{\mathbb{L}+\mathbb{L}^*}{2}, \quad (\mathbf{U},\mathfrak{F})=æR(\mathbf{J},\mathbf{Q})$.

Next, we assume that in the domain Π the norms of the matrices $\mathbb{B}$ and $\mathbb{C}$ are bounded, the matrix $\mathbb{A}>0$, the functions $R\geq 0, E>0$. Besides, we assume that the electric potential φ is a given smooth bounded function in the domain Π. Integrating (3.4) over R^2 and accounting for (3.3) and the inequalities

$$\nu_0|\mathbf{U}|^2\leq(\mathbf{U},\mathbb{A}\mathbf{U}),$$

$$(\mathbf{U},\Lambda\mathbf{U})\leq\mu_0|\mathbf{U}|^2\leq\widetilde{\mu}_0(\mathbf{U},\mathbb{A}\mathbf{U}),$$

$$2æR|(\mathbf{J},\mathbf{Q})|\leq 2æR|\mathbf{J}||\mathbf{Q}|\leq 2\mu_1|\mathbf{J}|R\leq\mu_1|\mathbf{U}|^2\leq\widetilde{\mu}_1(\mathbf{U},\mathbb{A}\mathbf{U}),$$

where

$$\nu_0=\inf_{(t,x,y)\in\Pi}\lambda_{min}(\mathbb{A})>0,\quad \mu_0=\sup_{(t,x,y)\in\Pi}\lambda_{max}(\Lambda),\quad \widetilde{\mu}_0=\frac{\mu_0}{\nu_0},$$

$$\mu_1=\sup_{(t,x,y)\in\Pi}(æ|\mathbf{Q}|),\quad \widetilde{\mu}_1=\frac{\mu_1}{\nu_0},$$

$\lambda_{min}(\mathbb{A})$ is the minimal eigenvalue of $\mathbb{A}$,
$\lambda_{max}(\Lambda)$, the maximal eigenvalue of Λ,
we finally obtain the inequality

$$\frac{dI(t)}{dt}\leq\widetilde{\mu}I(t)$$

or

$$I(t)\leq I(T_0)exp\{\widetilde{\mu}(t-T_0)\},\quad T_0<t\leq T<\infty. \tag{3.5}$$

Here $\widetilde{\mu}=\widetilde{\mu}_0+\widetilde{\mu}_1$,

$$I(t)=\int_{R^2}(\mathbf{U},\mathbb{A}\mathbf{U})dxdy.$$

Inequality (3.5) is the desired a priori estimate.

The original system of the momentum equations (1.1) can be represented as (2.3) or (3.2) (for large t). This gives us an idea to use this fact while constructing finite-difference schemes for (1.1) in order to derive a finite difference analog of the a priori estimate (3.5) for approximate solutions. In terms of [7] this means the *adequacy* of the mathematical and numerical models. In the next section we describe a class of difference schemes for which we employ the mentioned idea (another examples can be found in [5,9]).

4. A class of "stable" difference schemes for system (1.1)

Now we formulate a *numerical model* for the original mathematical model (1.1). In the domain Π we construct a difference scheme with the steps $\Delta = \Delta t$, $h_x = \Delta x$, $h_y = \Delta y$. We introduce the notations:

$$\mathbf{U}^n_\alpha = \mathbf{U}(n\Delta, \alpha \cdot \mathbf{h}) = \mathbf{U}^n_{\alpha_x \alpha_y} = \mathbf{U}_\alpha = \mathbf{U}_{\alpha_x} = \mathbf{U}_{\alpha_y} = \mathbf{U}$$

is a grid vector-function,
$\alpha = (\alpha_x, \alpha_y)$ is a multiindex,
$\mathbf{h} = (h_x, h_y),\ \alpha \cdot \mathbf{h} = (\alpha_x h_x, \alpha_y h_y)$,
$|\alpha_x|,\ |\alpha_y| = 0, 1, \dots;\ n = N_0, \dots, N;\ T_0 = \Delta N_0,\ T = \Delta N$,
$\chi, \Psi_x, \Psi_y, \Psi_x^{-1}, \Psi_y^{-1}$ are translation operators:
$\chi \mathbf{U} = \mathbf{U}^{n+1}_\alpha = \widehat{\mathbf{U}}$,
$\Psi_x^{\pm 1} \mathbf{U} = \mathbf{U}^n_{\alpha_x \pm 1},\ \Psi_y^{\pm 1} \mathbf{U} = \mathbf{U}^n_{\alpha_y \pm 1} (\Psi_x^{+1} = \Psi_x,\ \Psi_y^{+1} = \Psi_y)$;
$\tau,\ \xi_x,\ \xi_y,\ \overline{\xi}_x,\ \overline{\xi}_y$ are difference operators:
$\tau = \chi - 1,\ \xi_x = \Psi_x - 1,\ \xi_y = \Psi_y - 1$,
$\overline{\xi}_x = 1 - \Psi_x^{-1},\ \overline{\xi}_y = 1 - \Psi_y^{-1}$.

As is known, the symmetric matrices $\mathbb{B}$, $\mathbb{C}$ can be represented as follows:

$$\mathbb{B} = \mathbb{B}_+ - \mathbb{B}_-, \quad \mathbb{C} = \mathbb{C}_+ - \mathbb{C}_-, \tag{4.1}$$

where $\mathbb{B}_+, \mathbb{B}_-, \mathbb{C}_+, \mathbb{C}_- \geq 0$ are symmetric matrices. Validity of (4.1) is easily checked if the matrices $\mathbb{B}_+, \mathbb{B}_-, \mathbb{C}_+, \mathbb{C}_-$ are the following

$$\mathbb{B}_+ = \frac{1}{2} R_x^* (\Lambda_x + |\Lambda_x|) R_x, \quad \mathbb{B}_- = \frac{1}{2} R_x^* (-\Lambda_x + |\Lambda_x|) R_x,$$

$$\mathbb{C}_+ = \frac{1}{2} R_y^* (\Lambda_y + |\Lambda_y|) R_y, \quad \mathbb{C}_- = \frac{1}{2} R_y^* (-\Lambda_y + |\Lambda_y|) R_y.$$

The matrices R_x, R_y are orthogonal matrices reducing the matrices $\mathbb{B}$ and $\mathbb{C}$ to the diagonal form:
$\mathbb{B} = R_x^* \Lambda_x R_x$,
$\mathbb{C} = R_y^* \Lambda_y R_y$,
$\Lambda_x = diag(\lambda_1^{(x)}, \dots, \lambda_6^{(x)})$,
$\Lambda_y = diag(\lambda_1^{(y)}, \dots, \lambda_6^{(y)})$,
$\lambda_i^{(x)}, \lambda_i^{(y)}$ are the eigenvalues of the matrices $\mathbb{B}, \mathbb{C}$, $i = \overline{1, 6}$,
$|\Lambda_x| = diag(|\lambda_1^{(x)}|, \dots, |\lambda_6^{(x)}|)$,
$|\Lambda_y| = diag(|\lambda_1^{(y)}|, \dots, |\lambda_6^{(y)}|)$.

Remark 4.1. Instead of the theoretical method from above we can propose a constructive method for finding $\mathbb{B}_+$, $\mathbb{B}_-$, $\mathbb{C}_+$, and $\mathbb{C}_-$. Namely, these matrices can be taken in the form:

$$\mathbb{B}_+ = d_x(E)\mathbb{A} + \frac{1}{2}\mathbb{B}, \quad \mathbb{B}_- = d_x(E)\mathbb{A} - \frac{1}{2}\mathbb{B},$$

$$\mathbb{C}_+ = d_y(E)\mathbb{A} + \frac{1}{2}\mathbb{C}, \quad \mathbb{C}_- = d_y(E)\mathbb{A} - \frac{1}{2}\mathbb{C},$$

where the functions $d_x(E)$, $d_y(E) > 0$ are chosen so that they guarantee the fulfillment of the inequalities

$$\mathbb{B}_+, \mathbb{B}_-, \mathbb{C}_+, \mathbb{C}_- \geq 0.$$

Let

$$d_x(E) = d_y(E) = \widetilde{d}(E) = æ\widehat{d}(E), \quad \epsilon = \frac{1}{2\widehat{d}(E)}.$$

Then

$$\mathbb{B}_\pm = \widetilde{d}(E)(\mathbb{A} \pm \frac{\epsilon}{æ}\mathbb{B}) = \widetilde{d}(E)\begin{pmatrix} æ\omega & \pm\epsilon\omega & 0 & -æ & \mp\epsilon & 0 \\ \pm\epsilon\omega & \frac{7}{2}æ & 0 & \mp\epsilon & -\omega & 0 \\ 0 & 0 & \frac{7}{2}æ & 0 & 0 & -\omega \\ -æ & \mp\epsilon & 0 & \frac{æ}{E} & \pm\frac{\epsilon}{E} & 0 \\ \mp\epsilon & -\omega & 0 & \pm\frac{\epsilon}{E} & 1 & 0 \\ 0 & 0 & -\omega & 0 & 0 & 1 \end{pmatrix},$$

$$\mathbb{C}_\pm = \widetilde{d}(E)(\mathbb{A} \pm \frac{\epsilon}{æ}\mathbb{C}) = \widetilde{d}(E)\begin{pmatrix} æ\omega & 0 & \pm\epsilon\omega & -æ & 0 & \mp\epsilon \\ 0 & \frac{7}{2}æ & 0 & 0 & -\omega & 0 \\ \pm\epsilon\omega & 0 & \frac{7}{2}æ & \mp\epsilon & 0 & -\omega \\ -æ & 0 & \mp\epsilon & \frac{æ}{E} & 0 & \pm\frac{\epsilon}{E} \\ 0 & -\omega & 0 & 0 & 1 & 0 \\ \mp\epsilon & 0 & -\omega & \pm\frac{\epsilon}{E} & 0 & 1 \end{pmatrix}.$$

The matrices $\mathbb{B}_\pm$, $\mathbb{C}_\pm \geq 0$ if

$$0 < \epsilon \leq \sqrt{\frac{3}{2}æ^2\frac{1-\sqrt{\frac{2}{5}}}{E}}, \quad \text{i.e. } \widetilde{d}(E) \geq \sqrt{\frac{E}{6(1-\sqrt{\frac{2}{5}})}}.$$

Now we propose the following finite difference scheme for finding numerical solutions to the original mathematical model (1.1):

$$\widehat{K}\widehat{\mathbb{A}} \cdot \tau\mathbf{U} + K \cdot \tau(\mathbb{A}\mathbf{U}) +$$
$$+ r_x\{\widehat{K}\mathbb{B}_+(E^{(x)}) \cdot \overline{\xi}_x\widehat{\mathbf{U}} + \widehat{K}_{\alpha_x-1} \cdot \overline{\xi}_x(\mathbb{B}_+(E^{(x)})\widehat{\mathbf{U}}) -$$
$$- \widehat{K}\mathbb{B}_-(\mathscr{E}^{(x)}) \cdot \xi_x\widehat{\mathbf{U}} - \widehat{K}_{\alpha_x+1} \cdot \xi_x(\mathbb{B}_-(\mathscr{E}^{(x)})\widehat{\mathbf{U}})\} +$$
$$+ r_y\{\widehat{K}\mathbb{C}_+(E^{(y)}) \cdot \overline{\xi}_y\widehat{\mathbf{U}} + \widehat{K}_{\alpha_y-1} \cdot \overline{\xi}_y(\mathbb{C}_+(E^{(y)})\widehat{\mathbf{U}}) -$$
$$- \widehat{K}\mathbb{C}_-(\mathscr{E}^{(y)}) \cdot \xi_y\widehat{\mathbf{U}} - \widehat{K}_{\alpha_y+1} \cdot \xi_y(\mathbb{C}_-(\mathscr{E}^{(y)})\widehat{\mathbf{U}})\} =$$
$$= \Delta\widehat{K}(2\mathbb{D} + \mathbb{L})\widehat{\mathbf{U}} + 2\Delta\widehat{K}\widehat{\mathfrak{F}}. \tag{4.2}$$

Here $\mathbb{A} = \mathbb{A}(E)$, $\widehat{\mathbb{A}} = \mathbb{A}(\widehat{E})$,

$K = diag\{R, J^{(x)}, J^{(y)}, \sigma, I^{(x)}, I^{(y)}\}$,

$\widehat{K} = diag\{\widehat{R}, \widehat{J}^{(x)}, \widehat{J}^{(y)}, \widehat{\sigma}, \widehat{I}^{(x)}, \widehat{I}^{(y)}\}$,

$\widehat{K}_{\alpha_x\pm1} = \Psi_x^{\pm1}\widehat{K}, \widehat{K}_{\alpha_y\pm1} = \Psi_y^{\pm1}\widehat{K}$,

$r_x = \dfrac{\Delta}{h_x}, r_y = \dfrac{\Delta}{h_y}$,

$E^{(x)}$, $\mathscr{E}^{(x)}$, $E^{(y)}$, $\mathscr{E}^{(y)}$ – "intermediate" values of E,

$$\widehat{\mathfrak{F}} = \widehat{æ}\begin{pmatrix} -(\widehat{\mathbf{J}}, \widehat{\mathbf{Q}}) \\ \widehat{R}\widehat{\mathbf{Q}} \\ \frac{1}{\widehat{E}}(\widehat{\mathbf{J}}, \widehat{\mathbf{Q}}) \\ 0 \\ 0 \end{pmatrix}.$$

Remark 4.2. The difference scheme (4.2) approximates a consequence of system $(1.1')$ following from (2.3) and (3.2) rather than this system itself:

$$\mathbb{A}\mathbf{U}_t + (\mathbb{A}\mathbf{U})_t + \mathbb{B}\mathbf{U}_x + (\mathbb{B}\mathbf{U})_x + \mathbb{C}\mathbf{U}_y + (\mathbb{C}\mathbf{U})_y = (2\mathbb{D} + \mathbb{L})\mathbf{U} + 2\mathfrak{F}. \tag{4.3}$$

Remark 4.3. Below we assume that the following conditions are fulfilled for the finite-difference scheme (4.2):

1) $|\mathbf{U}_\alpha^n|^2 \to 0$ as $(\alpha_x^2 + \alpha_y^2) \to \infty, n = N_0, ..., N;$ (4.4)

2) the matrix norms $\mathbb{B}_+(E^{(x)}), \mathbb{B}_-(\mathscr{E}^{(x)}), \mathbb{C}_+(E^{(y)}), \mathbb{C}_-(\mathscr{E}^{(y)})$ are bounded;

3) $\mathbb{A}(E_\alpha^n) > 0, E_\alpha^n > 0, R_\alpha^n \geq 0, |\alpha_x|, |\alpha_y| = 0, 1, ..., n = N_0, ..., N.$

Remark 4.4. The proposed difference scheme (4.2) is implicit and can be probably realized by nonlinear iterations.

Remark 4.5. We do not detail formulas for $E^{(x)}, \mathscr{E}^{(x)}, E^{(y)}, \mathscr{E}^{(y)}$ because a wide variety of choices is possible that is very useful for the numerical resolution of our problems. For example we can choose $E^{(x)}, \mathscr{E}^{(x)}, E^{(y)}, \mathscr{E}^{(y)}$ so: $E^{(x)} = \mathscr{E}^{(x)} = E^{(y)} = \mathscr{E}^{(y)} = \widehat{E}$.

Now we deduce a finite-difference analog of the a priori estimate (3.5). We multiply (4.2) by $\mathbf{V} = (1,1,1,1,1,1)^*$. As far as
$\widehat{K}\mathbf{V} = \widehat{\mathbf{U}}$, $K\mathbf{V} = \mathbf{U}$, $\Psi_x^{\pm 1}\widehat{K}\cdot\mathbf{V} = \Psi_x^{\pm}\widehat{\mathbf{U}}$, $\Psi_y^{\pm 1}\widehat{K}\cdot\mathbf{V} = \Psi_y^{\pm}\widehat{\mathbf{U}}$
we obtain

$$
\begin{aligned}
&(\widehat{\mathbf{U}}, \widehat{\mathbb{A}}\cdot\tau\mathbf{U}) + (\mathbf{U}, \tau(\mathbb{A}\mathbf{U})) + \\
&+r_x\{(\widehat{\mathbf{U}}, \mathbb{B}_+(E^{(x)})\cdot\overline{\xi}_x\widehat{\mathbf{U}}) + (\Psi_x^{-1}\widehat{\mathbf{U}}, \overline{\xi}_x(\mathbb{B}_+(E^{(x)})\widehat{\mathbf{U}})) - \\
&-(\widehat{\mathbf{U}}, \mathbb{B}_-(\mathscr{E}^{(x)})\cdot\xi_x\widehat{\mathbf{U}}) - (\Psi_x\widehat{\mathbf{U}}, \xi_x(\mathbb{B}_-(\mathscr{E}^{(x)})\widehat{\mathbf{U}}))\} + \\
&+r_y\{(\widehat{\mathbf{U}}, \mathbb{C}_+(E^{(y)})\cdot\overline{\xi}_y\widehat{\mathbf{U}}) + (\Psi_y^{-1}\widehat{\mathbf{U}}, \overline{\xi}_y(\mathbb{C}_+(E^{(y)})\widehat{\mathbf{U}})) - \\
&-(\widehat{\mathbf{U}}, \mathbb{C}_-(\mathscr{E}^{(y)})\cdot\xi_y\widehat{\mathbf{U}}) - (\Psi_y\widehat{\mathbf{U}}, \xi_y(\mathbb{C}_-(\mathscr{E}^{(y)})\widehat{\mathbf{U}}))\} = \\
&= \Delta(\widehat{\mathbf{U}}, \Lambda\widehat{\mathbf{U}}) + 2\Delta\widehat{æ}\widehat{R}(\widehat{\mathbf{J}}, \widehat{\mathbf{Q}}). \qquad (4.5)
\end{aligned}
$$

We have following relations:

1) $(\widehat{\mathbf{U}}, \widehat{\mathbb{A}}\cdot\tau\mathbf{U}) + (\mathbf{U}, \tau(\mathbb{A}\cdot\mathbf{U})) = \tau((\mathbf{U}, \mathbb{A}\mathbf{U}))$,

2) $(\widehat{\mathbf{U}}, \mathbb{B}_+(E^{(x)})\cdot\overline{\xi}_x\widehat{\mathbf{U}}) + (\Psi_x^{-1}\widehat{\mathbf{U}}, \overline{\xi}_x(\mathbb{B}_+(E^{(x)})\widehat{\mathbf{U}})) = \overline{\xi}_x(\widehat{\mathbf{U}}, \mathbb{B}_+(E^{(x)})\widehat{\mathbf{U}})$,

3) $(\widehat{\mathbf{U}}, \mathbb{B}_-(\mathscr{E}^{(x)})\cdot\xi_x\widehat{\mathbf{U}}) + (\Psi_x\widehat{\mathbf{U}}, \xi_x(\mathbb{B}_-(\mathscr{E}^{(x)})\widehat{\mathbf{U}})) = \xi_x(\widehat{\mathbf{U}}, \mathbb{B}_-(\mathscr{E}^{(x)})\widehat{\mathbf{U}})$,

4) $(\widehat{\mathbf{U}}, \mathbb{C}_+(E^{(y)})\cdot\overline{\xi}_y\widehat{\mathbf{U}}) + (\Psi_y^{-1}\widehat{\mathbf{U}}, \overline{\xi}_y(\mathbb{C}_+(E^{(y)})\widehat{\mathbf{U}})) = \overline{\xi}_y(\widehat{\mathbf{U}}, \mathbb{C}_+(E^{(y)})\widehat{\mathbf{U}})$,

5) $(\widehat{\mathbf{U}}, \mathbb{C}_-(\mathscr{E}^{(y)})\cdot\xi_y\widehat{\mathbf{U}}) + (\Psi_y\widehat{\mathbf{U}}, \xi_y(\mathbb{C}_-(\mathscr{E}^{(y)})\widehat{\mathbf{U}})) = \xi_y(\widehat{\mathbf{U}}, \mathbb{C}_-(\mathscr{E}^{(y)})\widehat{\mathbf{U}})$.

In view of 1)–5), equality (4.5) has the form

$$
\begin{aligned}
&\tau(\mathbf{U}, \mathbb{A}\mathbf{U}) + r_x\{\overline{\xi}_x(\widehat{\mathbf{U}}, \mathbb{B}_+(E^{(x)})\widehat{\mathbf{U}}) - \xi_x(\widehat{\mathbf{U}}, \mathbb{B}_-(\mathscr{E}^{(x)})\widehat{\mathbf{U}})\} + \\
&+r_y\{\overline{\xi}_y(\widehat{\mathbf{U}}, \mathbb{C}_+(E^{(y)})\widehat{\mathbf{U}}) - \xi_y(\widehat{\mathbf{U}}, \mathbb{C}_-(\mathscr{E}^{(y)})\widehat{\mathbf{U}})\} = \\
&= \Delta(\widehat{\mathbf{U}}, \Lambda\widehat{\mathbf{U}}) + 2\Delta\widehat{æ}\widehat{R}(\widehat{\mathbf{J}}, \widehat{\mathbf{Q}}). \qquad (4.5')
\end{aligned}
$$

The relation $(4.5')$ is a difference analog of (3.4).

Multiplying $(4.5')$ by $\overline{h} = h_x\cdot h_y$ and summing up the result with α_x, α_y from $+\infty$ to $-\infty$, in a view of (4.4), we finally have:

$$
\tau I_n \leq \Delta\widetilde{\mu} I_{n+1}, \quad I_n = \overline{h}\sum_{\alpha_x=-\infty}^{\infty}\sum_{\alpha_y=-\infty}^{\infty}(\mathbf{U}_\alpha^n, \mathbb{A}(E_\alpha^n)\mathbf{U}_\alpha^n) \qquad (4.6)
$$

or

$$
I_{n+1} \leq \frac{1}{1-\Delta\cdot\widetilde{\mu}} T_n, \qquad (4.6')
$$

where

$$\widetilde{\mu} = \widetilde{\mu}_0 + \widetilde{\mu}_1,\ \widetilde{\mu}_0 = \frac{\mu_0}{\nu_0},\ \widetilde{\mu}_1 = \frac{\mu_1}{\nu_0},$$

$$\nu_0 = \inf_{n,\alpha_x,\alpha_y} \lambda_{min}(\mathbb{A}),$$

$$\mu_0 = \sup_{n,\alpha_x,\alpha_y} \lambda_{max}(\Lambda),$$

$$\mu_1 = \sup_{n,\alpha_x,\alpha_y} (æ|\mathbf{Q}|).$$

From (4.6$'$) for small Δ we derive a finite-differential analog of the a priori estimate (3.5):

$$I_n \leq \left(\frac{1}{1-\Delta\widetilde{\mu}}\right)^{n-N_0} I_{N_0}, \quad n = N_0+1,\ldots,N \tag{4.7}$$

Relation (4.7) also implies the “stability” of the difference scheme (4.2) in the energy norm $\sqrt{I_n}$.

Remark 4.6. We put the word stability into quotation marks because, strictly speaking, it is necessary to prove that the conditions listed in Remark 4.3 are fulfilled on solutions to the finite-difference numerical model (4.2)

Remark 4.7. While deducing (4.6) we also used the relation (see Remark 4.3)

$$\sum_{\alpha_x=-\infty}^{\infty} \overline{\xi}_x(\widehat{\mathbf{U}}, \mathbb{B}_+(E^{(x)})\widehat{\mathbf{U}}) = \lim_{M\to\infty} \sum_{\alpha_x=-M+1}^{M} \overline{\xi}_x(\widehat{\mathbf{U}}, \mathbb{B}_+(E^{(x)})\widehat{\mathbf{U}}) =$$

$$= \lim_{M\to\infty} \{(\widehat{\mathbf{U}}, \mathbb{B}_+(E^{(x)})\widehat{\mathbf{U}})|_{\alpha_x=+M} - (\widehat{\mathbf{U}}, \mathbb{B}_+(E^{(x)})\widehat{\mathbf{U}})|_{\alpha_x=-M}\} = 0$$

5. Conclusions

We have described a class of difference schemes for the system of momentum equations of charge transport in semiconductors. Construction of such schemes is based on the possibility to represent the original system in different ways. The authors plans to carry out numerical simulations in order to check the efficiency of the proposed difference schemes.

6. Ackowledgements

We are grateful to E.V.Mishchenko and Yu.L.Trakhinin for efficient cooperation.
This work was supported by Russian Foundation for Basic Research (grant 07-01-00585), the Interdisciplinary Integration Project No. 91 (2009) for Basic Research of the Siberian Branch of the Russian Academy of Sciences, and Russian Federal Agency of Education, Russian Ministry of Education and Science ("Progress of science potential of the university education (2009-2010)", grant No. 2.1.1/4591).

REFERENCES

[1] R. D. Alaev - A. M. Blokhin - M. U. Hudojberganov, *On an aprroach to construction of a class of difference schemes for hyperbolic systems*, Submitted to Comp. Technologies.

[2] A. M. Anile - V. Romano, *Non parabolic band transport in semiconductors: closure of the moment equations*, Cont. Mech. Thermodyn. **11** (1999), 307–325.

[3] A. M. Blokhin - R. D. Alaev, *Energy integrals and thier application to study of stability of difference schemes (in Russian)*, Novosibirsk State University Publishing House, 1993.

[4] A. M. Blokhin - R. S. Bushmanov - V. Romano, *Nonlinear asymptotic stability of the equilibrium state for the MEP model of charge transport in semiconductors*, Nonlinear Analysis **65** (2006), 2169–2191.

[5] A. M. Blokhin - R. S. Bushmanov - A. S. Rudometova - V. Romano, *Linear asymptotic stability of the equilibrium state for the 2D MEP hydrodynamical model of charge transport in semiconductors*, Nonlinear Analysis **65** (2006), 1018–1038.

[6] A. M. Blokhin - A. S. Ibragimova, *Numerical method for 2D Simulation of a Silicon MESFET with a Hydrodynamical Model Based on the Maximum Entropy Principle*, SIAM Journal on Scientific Computing (accepted for publication).

[7] A. M. Blokhin - A. S. Ibragimova - N. Yu. Krasnikov, *On a variant of method of lines for the Poisson equation (in Russian)*, Comp. Technologies **12(2)** (2007), 33–42.

[8] A. M. Blokhin - A. S. Ibragimova - B. V. Semisalov, *Construction of numerical algorithm for moment equation system of charge transport in semiconductors*, Mathematical modelling (accepted for publication).

[9] A. M. Blokhin - I. G. Sokovikov, *On an approach to construction of difference schemes for quasilinear gas dynamics equations*, Sib. Math. J. **40** (1999), 1236–1243.

[10] V. Romano, *Non parabolic band transport in semiconductors: closure of the production terms in the moment equations*, Cont. Mech. Thermodyn. **12** (2000), 31–51.

[11] V. Romano, *Nonparabolic band hydrodynamical model of silicon semiconductors and simulation of electron devices*, Math. Meth. Appl. Sci. **24** (2001), 439–471.

[12] V. Romano, *2D simulation of a silicon MESFET with a non-parabolic hydrodynamical model based on the maximum entropy principle*, J. Comp. Phys. **176** (2002), 70–92.

A. M. BLOKHIN
Sobolev Institute of Mathematics
Novosibirsk State University
Novosibirsk, 630090, Russia
e-mail: blokhin@math.nsc.ru

S. A. BOYARSKIY
Novosibirsk State University
Novosibirsk, 630090, Russia
e-mail: stanvs@gmail.com

B. V. SEMISALOV
Novosibirsk State University
Novosibirsk, 630090, Russia
e-mail: vibis@ngs.ru