ENTROPY APPROXIMATION FOR THE SYSTEM OF MOMENT EQUATIONS DESCRIBING CHARGE TRANSPORT IN SEMICONDUCTORS

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The question of possibility to build additional entropy conservation law for the system of moment equations, which appear in mathematical modelling of the charge transport in semiconductors, is discussed.

Introduction.

It is well known that so called *hydrodynamic models* are widely used nowadays in mathematical modelling of the physical phenomena related to charge transport in semiconductors. Last years, a lot of new mathematical models of hydrodynamic type were proposed for describing similar phenomena. Notice, however, that mathematical basis for most models of this type is not ideal.

One of the last models of hydrodynamic type was proposed recently in the papers [1], [8]. This model is a quasilinear system of equations written in the form of *the conservation laws*. These conservation laws were obtained from the system of moment equations for *Boltzmann transport equation* by the use of a certain *closing procedure*.

However, *additional entropy conservation law* was not found for the equations system obtained in [1], [8]. In this work, we propose so called *entropy*

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approximation for this mathematical model. We discuss here one of the methods of such approximation application — construction of calculation models for finding of approximate solutions to the conservation laws system from [1], [8].

1. Preliminary information.

Remind that in [1], [8] the system of moment equations describing charge transport in semiconductors was proposed. That system was obtained from the *Boltzmann transport equation* with use of *entropy maximum principle*. Application of this principle is, in essence, closing procedure (just diversity of closing procedures defines a large number of various mathematical models, which are used to describe charge transport in semiconductor devices).

Following [3], write down a quasilinear nonstationary system of mentioned above moment equations for *two-dimensional case* and in the *dimensionless form* (the process of obtaining dimensionless form is described in detail in [3]):

(1.1)
$$\begin{cases} R_{\tau} + \operatorname{div} \mathbf{J} = 0, \\ \mathbf{J}_{\tau} + \nabla(R+P) = R\mathbf{Q} + c_{11}\mathbf{J} + c_{22}\theta, \\ \frac{3}{2}P_{\tau} + \operatorname{div}(\mathbf{J}+\theta) = (\mathbf{J}, \mathbf{Q}) + cP, \\ \frac{2}{5}\theta_{\tau} + \nabla\left(P + \frac{P^{2}}{R}\right) = P\mathbf{Q} + c_{12}\mathbf{J} + c_{22}\theta. \end{cases}$$

Here R is an electron density;

 $\mathbf{J} = (J^{(x)}, J^{(y)})$ is a electron flow vector with components $J^{(x)}, J^{(y)}$ (Cartesian coordinates (x, y) are taken as a base);

$$P = R\left(\frac{2}{3}E - 1\right);$$

E is electron energy;
 $\theta = (\theta^{(x)}, \theta^{(y)})$ is a electron energy flow vector;
 $\mathbf{Q} = \nabla \varphi; \varphi = \varphi(\tau, x, y))$ is an electric potential, satisfying Poisson equation:

(1.2)
$$\epsilon^2 \Delta \varphi = R - \rho, \quad \epsilon^2 = \frac{1}{\beta};$$

coefficients $c, c_{11}, \ldots, c_{22}$ in (1.1) are smooth functions of E (exact form of them is presented in [1], [3], [8]);

 $\rho = \rho(x, y)$ is an doping density; $\beta > 0$ is some constant (see [3]). It was shown in works [3], [7] that *hyperbolicity* condition of the system (1.1) is formulated as:

E>0.

This inequality is physically defensible.

Remind again that system of moment equations (1.1) (see. [3]), written in the form of conservation laws, was obtained in [1, 8] with use of entropy maximum principle. However, *additional entropy conservation law*

(1.3)
$$\eta_{\tau} + \operatorname{div} \mathbf{\Phi} = G,$$

where $\eta = \eta(\mathbf{U})$, $\mathbf{\Phi} = (\Phi^{(x)}, \Phi^{(y)})$, $\Phi^{(x),(y)} = \Phi^{(x),(y)}(\mathbf{U})$, $G = G(\mathbf{U}, \mathbf{Q})$, and which would be consequence of all equations of the system (1.1) and fulfilled on any its smooth solution, was not obtained in works mentioned above. Here η is entropy function;

 Φ is entropy flow vector;

 Ψ is entropy now vector,

G is entropy production; $\langle R \rangle$

$$\mathbf{U} = \begin{pmatrix} \mathbf{X} \\ \mathbf{J} \\ P \\ \theta \end{pmatrix}.$$

We failed to obtain additional entropy conservation law for conservation laws system (1.1) as well. Therefore, in this work, we propose to consider the following system instead of the system (1.1):

(1.4)
$$\begin{cases} R_{\tau} + \operatorname{div} \mathbf{J} = 0, \\ \mathbf{J}_{\tau} + \nabla(R + P) = R\mathbf{Q} + c_{11}\mathbf{J} + c_{22}\theta, \\ \frac{3}{2}P_{\tau} + \operatorname{div}(\mathbf{J} + \theta) = (\mathbf{J}, \mathbf{Q}) + cP, \\ \frac{2}{5}\theta_{\tau} + \nabla(P + F'(D, x, y)) = P\mathbf{Q} + c_{12}\mathbf{J} + c_{22}\theta, \end{cases}$$

where

$$D = \frac{3}{2}P - R + D_0(x, y),$$

 $F(D, x, y), D_0(x, y)$ are some functions,

$$F'(D, x, y) = \frac{\partial F}{\partial D}.$$

We call this system *entropy approximation* of initial system (1.1).

Remark 1.1. With use of simple but bulky computations, it could be shown that hyperbolic condition of the system (1.4) is formulated as:

(1.5)
$$F'' = \frac{\partial^2 F}{\partial D^2}(D, x, y) > -\frac{2}{5}.$$

2. Obtaining of additional entropy conservation law for the system (1.4).

Rewrite the system (1.4) as:

(1.4)
$$\mathscr{P}_{\tau} + \mathbf{M}_{x} + \mathbf{N}_{y} = \mathscr{F}.$$

Here

$$\mathcal{P} = \begin{pmatrix} R \\ \mathbf{J} \\ \frac{3}{2}P \\ \frac{2}{5}\theta \end{pmatrix}, \qquad \mathbf{M} = \begin{pmatrix} J^{(x)} \\ R+P \\ 0 \\ J^{(x)}+\theta^{(x)} \\ P+F' \\ 0 \end{pmatrix}, \qquad \mathbf{N} = \begin{pmatrix} J^{(y)} \\ 0 \\ R+P \\ J^{(y)}+\theta^{(y)} \\ 0 \\ P+F' \end{pmatrix},$$
$$\mathcal{F} = \begin{pmatrix} 0 \\ R\mathbf{Q}+c_{11}\mathbf{J}+c_{12}\theta \\ (\mathbf{J},\mathbf{Q})+cP \\ P\mathbf{Q}+c_{12}\mathbf{J}+c_{22}\theta \end{pmatrix}.$$

Multiply now the system (1.4) by the vector 2U scalar. We obtain as a result:

(2.1)
$$\left\{ R^{2} + |\mathbf{J}|^{2} + \frac{3}{2}P^{2} + \frac{2}{5}|\theta|^{2} \right\}_{\tau} + \operatorname{div}\{2(R+P)\mathbf{J} + 2P\theta\} + 2(\theta, \nabla F') = \left[(2R\mathbf{J} + 2P\mathbf{J} + 2P\theta], \mathbf{Q}) + 2cP^{2} + 2\{c_{11}|\mathbf{J}|^{2} + \mu_{12}(\mathbf{J},\theta) + c_{22}|\theta|^{2} \}, \\ \mu_{12} = c_{12} + c_{21}. \right]$$

Extracting the first equation of the system (1.4) from the fourth one, we obtain:

(2.2)
$$\operatorname{div}\theta = (\mathbf{J}, \mathbf{Q}) + cP - D_{\tau}.$$

Since

(2.3)
$$(\theta, \nabla F') = \operatorname{div}(F'\theta) - F'\operatorname{div}\theta,$$

then in view of (2.2), (2.3) we rewrite (2.1) in the form (1.3) with the following expressions for η , Φ , *G*:

(2.4)
$$\begin{cases} \eta = R^2 + |\mathbf{J}|^2 + \frac{3}{2}P^2 + \frac{2}{5}|\theta|^2 + 2F, \\ \mathbf{\Phi} = 2(R+P)\mathbf{J} + 2(P+F')\theta, \\ G = ([2(R+P+F')\mathbf{J} + 2P\theta], \mathbf{Q}) + 2(P+F')cP + \\ + 2\{c_{11}|\mathbf{J}|^2 + \mu_{12}(\mathbf{J},\theta) + c_{22}|\theta|^2\}. \end{cases}$$

3. Symmetrization of the system (1.4).

It is known (see [4], [5]), that existence of additional conservation law (1.3) allows rewriting the system (1.4) in the form of *symmetric t-hyperbolic* (by Friedrichs) system. Symmetrization formalism is described in detail in [4], [5], and we present here just some essential remarks. Let's define components of the vector **q**:

$$\mathbf{q} = \begin{pmatrix} q_1 \\ q_2 \\ q_3 \\ q_4 \\ q_5 \\ q_6 \end{pmatrix},$$

such as

$$(\mathbf{q}, \mathcal{P}_{\tau} + \mathbf{M}_{x} + \mathbf{N}_{y} - \mathcal{F}) = \eta_{\tau} + \operatorname{div} \mathbf{\Phi} - G = 0.$$

To gain this we present differential $d\eta$ in the following form (see (2.4)):

$$d\eta = 2(R - F')dR + 2(\mathbf{J}, d\mathbf{J}) + 2(P + F')d\left(\frac{3}{2}P\right) + 2\left(\theta, d\left(\frac{2}{5}\theta\right)\right) = (\mathbf{q}, d\mathcal{P}).$$

Consequently, components of the vector \mathbf{q} (so caleed *canonic variables*) could be defined as:

(3.1)
$$q_1 = 2(R - F'), \quad q_2 = 2J^{(x)}, \quad q_3 = 2J^{(y)}, \\ q_4 = 2(P + F'), \quad q_5 = 2\theta^{(x)}, \quad q_6 = 2\theta^{(y)}.$$

Now define so called *generating functions* \mathcal{L} , \mathcal{M} , \mathcal{N} :

(3.2)
$$\begin{cases} \mathcal{L} = (\mathbf{q}, \mathcal{P}) - \eta, \\ \mathcal{M} = (\mathbf{q}, \mathbf{M}) - \Phi^{(x)}, \\ \mathcal{N} = (\mathbf{q}, \mathbf{N}) - \Phi^{(y)}. \end{cases}$$

Then, in view of (3.2), we obtain:

(3.3)
$$\mathcal{L}_q = \begin{pmatrix} \mathcal{L}_{q_1} \\ \vdots \\ \mathcal{L}_{q_6} \end{pmatrix} = \mathcal{P}, \quad \mathcal{M}_q = \mathbf{M}, \quad \mathcal{N}_q = \mathbf{N}.$$

Taking into account (3.3), we rewrite the system (1.4) as:

$$(\mathcal{L}_q)_{\tau} + (\mathcal{M}_q)_x + (\mathcal{N}_q)_y = \mathcal{F},$$

and then in the following form:

(3.4)
$$\mathcal{A}\mathbf{q}_{\tau} + \mathcal{B}\mathbf{q}_{x} + \mathcal{C}\mathbf{q}_{y} = \mathcal{F},$$

where $\mathcal{A} = (\mathcal{L}_{q_iq_j}), \mathcal{B} = (\mathcal{M}_{q_iq_j}), \mathcal{C} = (\mathcal{N}_{q_iq_j}), i, j = \overline{1, 6}$ are symmetric matrices.

Let's obtain matrices A, B, C. For this, we use the method described in [4], [5]. We find at first matrices I, I_0 , $I^{(x)}$, $I^{(y)}$, such as:

$$d\mathbf{q} = \begin{pmatrix} dq_1 \\ \vdots \\ dq_6 \end{pmatrix} = Id\mathbf{U} \quad (\text{see } (3.1)),$$
$$d\mathcal{L}_q = \begin{pmatrix} d\mathcal{L}_{q_1} \\ \vdots \\ d\mathcal{L}_{q_6} \end{pmatrix} = I_0 d\mathbf{U},$$
$$d\mathcal{M}_q = I^{(x)} d\mathbf{U},$$
$$d\mathcal{N}_q = I^{(y)} d\mathbf{U}.$$

Then

$$\mathcal{A} = I_0 I^{-1} = \frac{1}{2} \begin{pmatrix} \frac{2+3F''}{2+5F''} & 0 & 0 & \frac{3F''}{2+5F''} & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 \\ \frac{3F''}{2+5F''} & 0 & 0 & \frac{3(1+F'')}{2+5F''} & 0 & 0 \\ 0 & 0 & 0 & 0 & \frac{2}{5} & 0 \\ 0 & 0 & 0 & 0 & 0 & \frac{2}{5} \end{pmatrix},$$

Notice, that matrix A > 0 when hyperbolicity condition (1.5) is fulfilled (it could be verified directly). Hence, the system (3.4) is symmetric *t*-hyperbolic (by Friedrichs).

4. Another form of the system (1.4) when function F specially selected.

Symmetric system (3.4) is one of the forms of the system (1.4). One can easy find with simple calculations that:

(4.1)
$$\begin{aligned} &\mathcal{A}\mathbf{q} = \mathcal{P} + \mathbf{\Lambda}, \\ &\mathcal{B}\mathbf{q} = \mathbf{M}, \\ &\mathcal{C}\mathbf{q} = \mathbf{N}, \end{aligned}$$

where

$$\mathbf{\Lambda} = \begin{pmatrix} \frac{2[F''(D-D_0)-F']}{2+5F''} \\ 0 \\ -\frac{0}{2[F''(D-D_0)-F']} \\ \frac{2[F''(D-D_0)-F']}{2+5F''} \\ 0 \\ 0 \end{pmatrix}.$$

Let

(4.2)
$$\frac{F''(D-D_0)-F'}{2+5F''} = \frac{1}{5}D_1.$$

Here $D_1 = D_1(x, y)$ is a certain function.

Considering (4.2) as equation to find function F, we take such its solution:

(4.3)
$$F(D, x, y) = -\frac{2D_1}{5(D_0 + D_1)} \cdot \frac{D^2}{2}$$

i.e.

$$F' = -\frac{2D_1}{5(D_0 + D_1)}D, \quad F'' = -\frac{2D_1}{5(D_0 + D_1)}$$

Introduce into consideration functions $R^*(x, y) > 0$, $E^*(x, y) > 0$ and $P^*(x, y) = R^*(x, y) \left(\frac{2}{3}E^*(x, y) - 1\right)$. Assume that $P(\tau^*, x, y) = P^*(x, y)$, $R(\tau^*, x, y) = R^*(x, y)$ are valid for solution to the system (1.1) under certain $\tau = \tau^*$.

Choose functions D_0 , D_1 such as:

(4.4)
$$-\frac{2D_1}{5(D_0+D_1)}\left(\frac{3}{2}P^*-R^*+D_0\right)=\frac{(P^*)^2}{R^*}.$$

If $D_1 = -P^*$, $D_0 = R^* + P^*$, then equality (4.4) is fulfilled. Hence, if function F' in the system (1.4) is selected as:

(4.5)
$$F' = \frac{2}{5} \frac{P^*}{R^*} \left(\frac{3}{2}P - R + R^* + P^*\right),$$

then this aggregate is linear approximation of the function P^2/R in neighbor of $\tau = \tau^*$ (see (4.4)). We call system (1.4) entropy approximation of the system (1.1) by this reason namely. Notice, that $F'' = \frac{2}{5}\frac{P^*}{R^*} = -\frac{2}{5}\left(1 - \frac{2}{3}E^*\right) > -\frac{2}{5}$ in this case in view of natural physical restriction: $E^* > 0$.

So, let aggregate F' in the system (1.4) is found with use the formula (4.5). Then, in view of (4.1), (4.2), the system (1.4) can be rewritten as follows:

(4.6)
$$(\mathbf{A}\mathbf{q})_{\tau} + (\mathbf{B}\mathbf{q})_{x} + (\mathbf{C}\mathbf{q})_{y} = \mathcal{F}.$$

System (4.6) is another form of the system (1.4) (when function F' is specially selected).

5. Predictor-corrector type difference scheme for the system (1.1).

The fact that the system (1.4) can be written in the form (4.6), suggests an idea to use this fact when constructing *finite-difference schemes* to initial system (1.1). Let's describe, for example, possible construction of the finitedifference scheme of the *predictor-corrector* type for the system (1.1). We plot difference grid with steps $\Delta = \Delta \tau$, $h_x = \Delta x$, $h_y = \Delta y$ in the domain $R^3_+ = \{\tau > 0, (x, y) \in R^2\}$. Introduce new designations:

$$\mathbf{U}_{ii}^n = \mathbf{U}(n\Delta, ih_x, jh_y) = \mathbf{U}^n,$$

 $\Psi_x, \Psi_y, \Psi_x^{-1}, \Psi_y^{-1}$ are shift operators:

$$\Psi_x^{\pm 1}\mathbf{U}^n = \mathbf{U}_{i\pm 1,j}^n, \quad \Psi_y^{\pm 1}\mathbf{U}^n = \mathbf{U}_{i,j\pm 1}^n;$$

 $\xi_x, \overline{\xi}_x, \xi_y, \overline{\xi}_y, L_x, L_y, \xi_0, \eta_0$ are difference operators:

$$\begin{split} \xi_x &= \Psi_x - 1, \quad \overline{\xi}_x = 1 - \Psi_x^{-1}, \quad \xi_y = \Psi_y - 1, \quad \overline{\xi}_y = 1 - \Psi_y^{-1}, \\ L_x &= \frac{\Psi_x + \Psi_x^{-1}}{2}, \quad L_y = \frac{\Psi_y + \Psi_y^{-1}}{2}, \\ \xi_0 &= \frac{\Psi_x - \Psi_x^{-1}}{2}, \quad \eta_0 = \frac{\Psi_y - \Psi_y^{-1}}{2}, \\ r_x &= \frac{\Delta}{h_x}, \quad r_y = \frac{\Delta}{h_y}. \end{split}$$

Besides, we assume, that

$$(5.1) \qquad \qquad \mathcal{B} = \mathcal{B}_+ - \mathcal{B}_-, \quad \mathcal{C} = \mathcal{C}_+ - \mathcal{C}_-,$$

where \mathcal{B}_{\pm} , \mathcal{C}_{\pm} are symmetric positive-definite matrices. It is known, that expansion (5.1) for arbitrary symmetric matrix is always fulfilled.

We can take

$$\mathcal{B}_{\pm} = \frac{1}{2} \begin{pmatrix} 1 & \pm 1/2 & 0 & 0 & 0 & 0 \\ \pm 1/2 & 1 & 0 & \pm 1/2 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & \pm 1/2 & 0 & 1 & \pm 1/2 & 0 \\ 0 & 0 & 0 & \pm 1/2 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 \end{pmatrix}$$

$$\mathcal{C}_{\pm} = \frac{1}{2} \begin{pmatrix} 1 & 0 & \pm 1/2 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 \\ \pm 1/2 & 0 & 1 & \pm 1/2 & 0 & 0 \\ 0 & 0 & \pm 1/2 & 1 & 0 & \pm 1/2 \\ 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & \pm 1/2 & 0 & 1 \end{pmatrix}.$$

for matrices \mathcal{B} , \mathcal{C} . Notice, that $\mathcal{B}_+ + \mathcal{B}_- = I_6$, $\mathcal{C}_+ + \mathcal{C}_- = I_6$, where I_6 is unitary matrix of the order 6. Eigen values of matrices \mathcal{B}_{\pm} , \mathcal{C}_{\pm} can be easy found:

$$l_k(\mathcal{B}_{\pm}, \mathcal{C}_{\pm}) = \frac{1}{2}(1 - \cos(kl)), \quad l = \frac{\pi}{5}, \ k = \overline{1, 4};$$

 $l_{5,6}(\mathcal{B}_{\pm}, \mathcal{C}_{\pm}) = \frac{1}{2}.$

Calculational model, which we will use to find approximate solution to initial system (1.1), is build as follows. At the predictor stage we use the system (1.4), written in the form (4.6). Using difference scheme from the work [6] (see also [2]), we find auxiliary quantities $q_{1,\ldots,6}^*$:

$$\mathcal{A}\mathbf{q}^* - \mathcal{A}\mathbf{q}^n + r_x^* \overline{\xi}_x \{\mathcal{B}_+ \mathbf{q}^n\} + r_y^* \overline{\xi}_y \{\mathcal{C}_+ \mathbf{q}^n\} - r_x^* \xi_x \{\mathcal{B}_- \mathbf{q}^n\} - r_y^* \overline{\xi}_y \{\mathcal{C}_- \mathbf{q}^n\} = \Delta^* \mathcal{F}_{ij}^n$$

or

(5.2)
$$\mathcal{A}\mathbf{q}^{*} = (\mathcal{A} - (r_{x}^{*} + r_{y}^{*})I_{6})\mathbf{q}^{n} + r_{x}^{*}(\mathcal{B}_{+}\mathbf{q}_{i-1,j}^{n} + \mathcal{B}_{-}\mathbf{q}_{i+1,j}^{n}) + r_{y}^{*}(\mathcal{C}_{+}\mathbf{q}_{i,j-1}^{n} + \mathcal{C}_{-}\mathbf{q}_{i,j+1}^{n}) + \Delta^{*}\mathcal{F}_{ij}^{n}.$$

Here (see sec. 3 and sec. 4):

$$\mathcal{A} = \mathcal{A}(F''), \quad F'' = \frac{2}{5} \frac{P_{ij}^n}{R_{ij}^n}$$

$$\mathbf{q}^* = \begin{pmatrix} q_1^* \\ \vdots \\ q_6^* \end{pmatrix} \text{ is the vector of auxiliary quantites,}$$
$$0 < \Delta^* \le \Delta, \quad r_x^* = \Delta^* h_x, \quad r_y^* = \Delta^* h_y.$$

Using formulae (3.1), we find components of auxiliary vector \mathbf{U}^* by components of the vector \mathbf{q}^* , and as F' we take the following expression:

$$F' = \frac{2}{5} \frac{P_{ij}^n}{R_{ij}^n} \left(\frac{3}{2} P_{ij}^* - R_{ij}^* + R_{ij}^n + P_{ij}^n\right).$$

At the corrector stage we use initial system (1.1), which we rewrite as:

$$\mathbf{U}_{\tau} + \mathbf{V}_{x} + \mathbf{W}_{y} = \mathbf{Z},$$

 $\mathbf{T}(\mathbf{r})$

where

$$\mathbf{V} = \begin{pmatrix} J^{(x)} \\ 0 \\ R+P \\ \frac{2}{3}(J^{(x)} + \theta^{(x)}) \\ \frac{5}{2}\left(P + \frac{P^2}{R}\right) \\ 0 \end{pmatrix}, \quad \mathbf{W} = \begin{pmatrix} J^{(y)} \\ R+P \\ \frac{2}{3}(J^{(y)} + \theta^{(y)}) \\ \frac{5}{3}(J^{(y)} + \theta^{(y)}) \\ \frac{5}{2}\left(P + \frac{P^2}{R}\right) \\ \frac{5}{2}\left(P + \frac{P^2}{R}\right) \end{pmatrix},$$
$$\mathbf{Z} = \begin{pmatrix} 0 \\ R\mathbf{Q} + c_{11}\mathbf{J} + c_{12}\theta \\ \frac{2}{3}(\mathbf{J}, \mathbf{Q}) + \frac{2}{3}cP \\ \frac{5}{2}(P\mathbf{Q} + c_{21}\mathbf{J} + c_{22}\theta) \end{pmatrix}.$$

To find numeric solution to the system (5.3), we use, for example, modified Lax scheme (see [2]):

(5.4)
$$\mathbf{U}^{n+1} = L_x L_y \mathbf{U}^n - r_x L_y \xi_0 \mathbf{V}^* - r_y L_x \eta_0 \mathbf{W}^* + \Delta L_x L_y \mathbf{Z}^*,$$

where $\mathbf{V}^* = \mathbf{V}(\mathbf{U}^*)$, etc.

Described above difference model (5.2), (5.4) is one of the possible variants of using entropy approximation of the system (1.1) when finding its approximate solution. In the future, authors plan to make the series of computational experiments on using entropy approximation to find numeric solutions to typical problems of semiconductors physics.

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