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# A NONSTANDARD FINITE DIFFERENCE SCHEME FOR THE DRIFT-DIFFUSION SYSTEM

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Abstract. We derive a nonstandard finite difference scheme for the coupled, nonlinear PDE's modeling laser generated electrons and holes in a semiconductor. Our scheme has the essential feature of giving numerical solutions for which the charge densities are non-negative. Many of the standard schemes do not have this physically required property.

1. **Introduction.** An important problem in solid state physics is to understand the interactions of electrons and holes created by the action of a laser with a semiconductor [1, 2]. The simplest model of this phenomena is given by three coupled, nonlinear PDE's in one space dimension, where the dependent variables are, respectively, the charge densities of the electrons, $n(x,t)$, and the holes, $p(x,t)$, and the electric field $E(x,t)$ [1, 2]. Physically, $n(x,t)$ and $p(x,t)$ must be non-negative, while $E(x,t)$ can be of either sign, i.e.,

$$n(x,t) \geq 0, \quad p(x,t) \geq 0, \qquad -\infty < E(x,t) < \infty. \tag{1.1}$$

In more detail, the time evolution equations are

$$\frac{\partial n}{\partial t} = \mu_n \frac{\partial (nE)}{\partial x} + D_n \frac{\partial^2 n}{\partial x^2}\,, \tag{1.2}$$

$$\frac{\partial p}{\partial t} = -\mu_p \frac{\partial (pE)}{\partial x} + D_p \frac{\partial^2 p}{\partial x^2}\,, \tag{1.3}$$

$$\frac{\partial E}{\partial x} = \left(\frac{e}{\varepsilon_r \varepsilon_0}\right)(p-n), \tag{1.4}$$

where $(\mu_n, \mu_p, D_n, D_p, e, \varepsilon_r, \varepsilon_0)$ are, for a given physical system, known parameters. These three equations are collectively known as the drift-diffusion equations.

Since, in general, exact solutions that are explicitly given in terms of the elementary functions are not known for Eqs. (1.2), (1.3), and (1.4), along with the associated boundary and/or initial conditions, it follows that numerical solutions must be calculated. However, the application of most standard finite difference numerical integration techniques [3, 4] give results that violate the positivity conditions of Eq. (1.1) [3]. The main purpose of this paper is to demonstrate, using the nonstandard finite difference scheme methodology of Mickens [6, 7], that discretizations of the drift-diffusion equations can be constructed such that the positivity

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condition for $n(x,t)$ and $p(x,t)$ holds. Since the positivity condition is required only for the $n$ and $p$ variables, we need only consider Eqs. (1.2) and (1.3).

In the work to come, the following discretization notation is used

$$x \to x_m = (\Delta x)m, \qquad t \to t_k = (\Delta t)k, \tag{1.5a}$$

$$n(x,t) \to n_m^k, \quad p(x,t) \to p_m^k, \quad E(x,t) \to E_m^k \tag{1.5b}$$

$$\beta \equiv \frac{\Delta t}{\Delta x}, \qquad R \equiv \frac{\Delta t}{(\Delta x)^2}. \tag{1.5c}$$

The space and time step-sizes are, respectively, $\Delta x$ and $\Delta t$; and, $k$ and $m$ are integers.

The paper is organized as follows: the next section presents certain preliminaries required for the understanding of the nonstandard finite difference scheme to be constructed in Section 3. The final section summarizes what has been done and gives our thoughts on the next step to be taken with regard to finite difference discretizations of the drift-diffusion PDE's. From now on, we use NSFD to stand for "nonstandard finite difference" [6, 7].

2. **Preliminaries.** Note that

$$\frac{\partial(nE)}{\partial x} = E\,\frac{\partial n}{\partial x} + n\,\frac{\partial E}{\partial x}, \tag{2.1}$$

and make the following notational changes:

$$\mu_n = \mu_1, \quad D_n = D_1, \quad \mu_p = \mu_2, \quad D_p = D_2, \quad \frac{e}{\varepsilon_r \varepsilon_0} = \mu_3. \tag{2.2}$$

Thus, Eq. (2.1) can be written as

$$\frac{\partial(nE)}{\partial x} = E\,\frac{\partial n}{\partial x} + \mu_3 n(p-n). \tag{2.3}$$

Substitution of this result into Eq. (1.2) gives

$$\frac{\partial n}{\partial t} = (\mu_1\mu_3)np - (\mu_1\mu_3)n^2 + \mu_1 E\,\frac{\partial n}{\partial x} + D_1\,\frac{\partial^2 n}{\partial x^2}. \tag{2.4}$$

Doing a similar calculation for Eq. (1.3) gives the expression

$$\frac{\partial p}{\partial t} = (\mu_2\mu_3)np - (\mu_2\mu_3)p^2 - \mu_2 E\,\frac{\partial p}{\partial x} + D_2\,\frac{\partial^2 p}{\partial x^2}. \tag{2.5}$$

It is these latter two equations that we will apply the NSFD methodology [6, 7].

Note that the right-sides of Eqs. (2.4) and (2.5) have the same structure:

(i) the first two terms correspond to reaction expressions;
(ii) the third terms correspond to nonlinear advection and the direction of the advection depends on the sign of the electric field;
(iii) the fourth terms correspond to diffusion of the charges.

Putting all this together, it is seen that these evolution equations represent a system in which reaction, advection and diffusion is taking place [8].

If we isolate the advection terms, then Eqs. (2.4) and (2.5) can be written as

$$\frac{\partial n}{\partial t} = \cdots + \mu_1 E\,\frac{\partial n}{\partial x} + \cdots, \tag{2.6}$$

$$\frac{\partial p}{\partial t} = \cdots - \mu_2 E\,\frac{\partial p}{\partial x} + \cdots, \tag{2.7}$$

where $\mu_1 E$ and $\mu_2 E$ are the respective advection velocities [8], and, for a given $E$, are of opposite signs since $\mu_1$ and $\mu_2$ are positive. Within the NSFD methodology, exact finite difference representations exist for these two situations [6]. For example, consider the two linear PDE's

$$u_t + a u_x = 0, \qquad v_t - a v_x = 0, \qquad a > 0; \tag{2.8}$$

then the corresponding exact finite difference schemes are, respectively,

$$\frac{u_m^{k+1} - u_m^k}{\Delta t} + a\left(\frac{u_m^k - u_{m-1}^k}{\Delta x}\right) = 0, \qquad \frac{v_m^{k+1} - v_m^k}{\Delta t} - a\left(\frac{v_{m+1}^k - v_m^k}{\Delta x}\right) = 0, \tag{2.9}$$

with the following condition holding between the step-sizes

$$\Delta x = a\Delta t. \tag{2.10}$$

Observe that in the first case, the discrete space-derivation is a backward-Euler, while for the second case, it is a forward-Euler representation. We will use these results in the next section to construct a positivity preserving NSFD scheme for Eqs. (2.4) and (2.5). The major result to take away from these considerations is that different discrete representations will be required for positive and negative values of $E$.

3. **A NSFD Scheme.** We now construct a NSFD scheme for the $p$ evolution equation; see Eq. (2.5). The particular discretizations for all the terms on the right-side of this equation are exactly the same except for the $(-\mu_2 E\, \partial p/\partial x)$ expression. There are two cases to consider, Case A: $E > 0$ and Case B: $E < 0$. Using the results suggested by Eq. (2.9), we have

<u>Case A: $E > 0$</u>

$$-\mu_2 E\,\frac{\partial p}{\partial x} \longrightarrow -\mu_2 E_m^k\left(\frac{p_m^k - p_{m-1}^k}{\Delta x}\right); \tag{3.1}$$

<u>Case B: $E < 0$</u>

$$-\mu_2 E\,\frac{\partial p}{\partial x} \longrightarrow \mu_2 |E_m^k|\left(\frac{p_{m+1}^k - p_m^k}{\Delta x}\right). \tag{3.2}$$

The remaining terms, for both signs of $E$, have the following discrete representations:

$$\frac{\partial p}{\partial t} \to \frac{p_m^{k+1} - p_m^k}{\Delta t}, \qquad np \to \bar{n}_m^k \bar{p}_m^k, \tag{3.3a}$$

$$-p^2 \to -\bar{p}_m^k p_m^{k+1}, \qquad \frac{\partial^2 p}{\partial x^2} \to \frac{p_{m+1}^k - 2p_m^k + p_{m-1}^k}{(\Delta x)^2}, \tag{3.3b}$$

where the barred quantities are average values; examples are any of the following expressions (illustrated by use of the $n$ variable):

$$\bar{n}_m^k = \begin{cases} n_m^k \\ \dfrac{n_{m+1}^k + 2n_m^k + n_{m-1}^k}{4} \\ \text{etc.} \end{cases} \tag{3.4}$$

For the product $np$, any one or a suitable linear combination of the following terms can be used for the discretization:

$$np \to \begin{cases} n_m^k p_m^k, \\ \dfrac{n_{m+1}^k p_{m+1}^k + 2n_m^k p_m^k + n_{m-1}^k p_{m-1}^k}{4}, \\ \text{etc.} \end{cases} \tag{3.5}$$

Putting all of this together gives a NSFD scheme for Eq. (2.5); in detail, we have

Case A: $E > 0$

$$\frac{p_m^{k+1} - p_m^k}{\Delta t} = (\mu_2\mu_3)\bar{n}_m^k \bar{p}_m^k - (\mu_2\mu_3)\bar{p}_m^k p_m^{k+1} - \mu_2 E_m^k \left(\frac{p_m^k - p_{m-1}^k}{\Delta x}\right) + D_2\left[\frac{p_{m+1}^k - 2p_m^k + p_{m-1}^k}{(\Delta x)^2}\right]; \tag{3.6}$$

Case B: $E < 0$

$$\frac{p_m^{k+1} - p_m^k}{\Delta t} = (\cdots) - (\cdots) + \mu_2 |E_m^k| \left(\frac{p_{m+1}^k - p_m^k}{\Delta x}\right) + (\cdots), \tag{3.7}$$

where $(\cdots)$ means exactly the same expression as in Eq. (3.6).

Note that in both Eqs. (3.6) and (3.7), $p_m^{k+1}$ always occurs as a linear factor in any terms for which it appears. Consequently, we can solve for $p_m^{k+1}$ to obtain, for example the case for which $E > 0$, the expression

$$\begin{aligned}[1 + (\mu_2\mu_3\Delta t)\bar{p}_m^k] p_m^{k+1} = {} & (\mu_2\mu_3\Delta t)\bar{n}_m^k \bar{p}_m^k \\ & + (\beta\mu_2 E_m^k) p_{m-1}^k + D_2 R(p_{m+1}^k + p_{m-1}^k) \\ & + (1 - \mu_2\beta E_m^k - 2D_2R) p_m^k, \end{aligned} \tag{3.8}$$

where $(\beta, R)$ are defined in Eq. (1.5c). Now positivity for $p_m^{k+1}$ is assured, given

$$n_m^k \geq 0, \qquad p_m^k \geq 0, \qquad E_m^k \geq 0, \tag{3.9}$$

provided that

$$1 - \mu_2\beta E_m^k - 2D_2R \geq 0. \tag{3.10}$$

Maintaining the physical identity of the material in which the drift-diffusion is occurring places an upper bound on the magnitude of the electric field. Thus, we have

$$|E(x,t)| \leq E^* \Rightarrow |E_m^k| \leq E^*. \tag{3.11}$$

(The existence of such a bound has been emphasized to us by Ryan Murdick [5], a physicist who carried out these types of experiments.) A special, particular form of a relationship satisfying Eq. (3.10) is

$$1 - \mu_2\beta E^* - 2D_2R = \gamma D_2 R, \qquad \gamma \geq 0, \tag{3.12}$$

where $\gamma$ is a non-negative parameter. From this expression, the following restriction can be determined between the space and time step-sizes

$$\Delta t = \frac{(\Delta x)^2}{(2+\gamma)D_2 + \mu_2 E^* \Delta x}. \tag{3.13}$$

Finally, with this result, we have for $p_m^{k+1}$, with $E > 0$, the form

$$\begin{aligned} p_m^{k+1} = {} & \big[D_2R(p_{m+1}^k + \gamma p_m^k + p_{m-1}^k) + (\beta\mu_2 E_m^k) p_{m-1}^k \\ & + (\Delta t)\mu_2\mu_3 \bar{n}_m^k \bar{p}_m^k\big] \big/ \big[1 + (\Delta t)\mu_2\mu_3 \bar{p}_m^k\big]. \end{aligned} \tag{3.14}$$

Similar expressions can also be worked out for $p_m^{k+1}$, for $E<0$; and $n_m^{k+1}$, for $E>0$ and $E<0$. They are now listed:

Case A: $E>0$

$$n_m^{k+1} = \frac{A_m^k + \mu_1 \beta E_m^k n_{m+1}^k}{1+B_m^k}\,, \tag{3.15a}$$

$$p_m^{k+1} = \frac{C_m^k + \mu_2 \beta E_m^k p_{m-1}^k}{1+D_m^k}\,; \tag{3.15b}$$

Case B: $E=-|E|<0$

$$n_m^{k+1} = \frac{A_m^k + \mu_1 \beta |E_m^k| n_{m-1}^k}{1+B_m^k}\,, \tag{3.16a}$$

$$p_m^{k+1} = \frac{C_m^k + \mu_2 \beta |E_m^k| p_{m+1}^k}{1+D_m^k}\,, \tag{3.16b}$$

where

$$A_m^k = (\Delta t)\mu_1\mu_3 \bar{n}_m^k \bar{p}_m^k + D_1 R(n_{m+1}^k + \gamma n_m^k + n_{m-1}^k), \tag{3.17a}$$

$$B_m^k = (\Delta t)\mu_1\mu_3 \bar{n}_m^k, \tag{3.17b}$$

$$C_m^k = (\Delta t)\mu_2\mu_3 \bar{n}_m^k \bar{p}_m^k + D_2 R(p_{m+1}^k + \gamma p_m^k + p_{m-1}^k), \tag{3.17c}$$

$$D_m^k = (\Delta t)\mu_2\mu_3 \bar{p}_m^k. \tag{3.17d}$$

The relationship between the step-sizes is

$$\Delta t = \mathrm{Min}((\Delta t)_1, (\Delta t)_2), \tag{3.18}$$

where

$$(\Delta t)_1 = \frac{(\Delta x)^2}{(2+\gamma)D_1 + \mu_1 E^* \Delta x}\,, \tag{3.19a}$$

$$(\Delta t)_2 = \frac{(\Delta x)^2}{(2+\gamma)D_2 + \mu_2 E^* \Delta x}\,. \tag{3.19b}$$

The implementation of this NSFD scheme for the numerical solution of the "$n$" and "$p$" evolution equations requires the following steps:

(a) select values for the physical parameters: $\mu_1$, $\mu_2$, $\mu_3$, $D_1$, $D_2$, and $E^*$;

(b) choose values for the space step-size $\Delta x$ and the parameter $\gamma$;

(c) calculate $\Delta t$, $\beta$, and $R$; see Eqs. (3.18) and (1.5c);

(d) select initial and/or boundary values for the dependent variables, i.e.,

$$N_m^0 = N(x_m, 0), \qquad p_m^0 = p(x_m, 0), \qquad E_m^0 = E(x_m, 0);$$

(e) calculate $n_m^1$, $p_m^1$, and $E_m^1$; for the $n$ and $p$ discrete variables use Eqs. (3.15) and (3.16).

(f) iterated step (e).

It should be noted that the electric field, in (e), is obtained by first solving numerically Laplace's equation for the potential and then taking the derivative, with respect to $x$, to calculate the electric field. The potential functions can be conveniently solved using a successive over-relaxation (SOR) method [5]. However, this standard numerical method for finding the electric field only gives valid results if the numerical values for $n$ and $p$ can be trusted, i.e., the numerical input for $n_m^k$ and $p_m^k$ must satisfy the positivity restriction. The primary purpose of this paper is to demonstrate that this is possible.

4. **Summary.** The main goal of this paper was achieved by the results presented in Section 3. There we explicitly demonstrated that a physically meaningful discretization could be constructed for the two charge densities appearing in the three coupled, nonlinear PDE's modeling drift-diffusion in solid state physics. In addition, a relationship between the space and time step-sizes was derived. This means that once a space step-size is selected, the time step-size has a value determined by $\Delta x$ and the other parameters appearing in the differential equations. A consequence of this result is that for small values of $\Delta x$, the $\Delta t$ is proportional to $(\Delta x)^2$. This is a general relationship that holds for parabolic PDE's [6, 7]. We also presented the steps required to implement the numerical scheme.

A future research issue is to optimize the accuracy of this finite difference scheme with regard to the best representations for $\bar{n}_m^k$ and $\bar{p}_m^k$, and the value of the parameter $\gamma$.

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