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Time Discretization of a Nonlinear Initial Value Problem

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Time-dependent models of semiconductor devices are readily formulated as a system of three partial-differential equations in three variables. Each of the equations is linear and well posed for one of the variables; however, if the equations are solved sequentially at each step, a nonlinear instability arises from the coupling terms, unless prohibitively small time steps are used. Three methods are proposed for avoiding such an instability. Convergence and stability results are obtained for each method, and the relative merits of each method are discussed from a practical viewpoint. An example of a computation using one of these methods is included.

I. INTRODUCTION

We consider numerical methods for the system

$$u_t = \Delta u - \nabla \cdot (u \nabla \psi), \tag{1.1a}$$

$$v_t = \Delta v + \nabla \cdot (v \nabla \psi), \tag{1.1b}$$

$$\kappa \, \Delta \psi = u - v - f, \qquad (x, t) \in D \times (0, T), \tag{1.2}$$

$$B_1(\psi) = B_2(u, \psi) = B_3(v, \psi) = 0, \qquad (x, t) \in \partial D \times (0, T); \tag{1.3}$$

$u(\cdot, 0)$, $v(\cdot, 0)$ specified. In (1.1)–(1.3), u, v, ψ are dependent variables, κ is a positive constant, and f is a given function of x. D is a bounded domain in R^N. The well posedness of this problem depends on u, v being nonnegative [8], and this is assumed true of the initial data.

This problem arises in the theory of semiconductor devices; u and v are the local densities of electrons (negatively charged) and holes (positively charged), which move by diffusion and by drift in the self-consistent electric field [14]. Equations (1.1) are continuity equations for u, v. Equation (1.2) is a Poisson equation, with ψ the electrostatic potential, κ the dielectric constant of the material, and f the density of stationary charged ions. B_2, B_3 are linear boundary conditions on u, v, respectively; they may depend on ψ, however, as is the case if the normal flux of particles is specified on part of the boundary. B_1 is a linear boundary condition on ψ. In this context, a simple but interesting example of the domain and boundary conditions is for D to be a rectangle in R^2, with u, v, and ψ specified on two opposite sides and their normal derivatives required to vanish on the other two. All of our results will be consistent with a domain and boundary conditions of this form. However, as several problems of engineering interest differ only in the specifics of the boundary conditions, we shall leave the precise form of the boundary conditions unspecified, stating our specific requirements at each step.

Viewed as such a model, several simplifying assumptions have been incorporated into the system (1.1)–(1.2). In particular, we have neglected recombination (annihilation of electron-hole pairs) because this process in semiconductors is very slow compared with the time scales, which will be of interest below [11].

The discretization of (1.1)–(1.3) with respect to the space variables posses no particular problem. Either finite-difference or finite-element methods can be used, and substantial information of both experimental and analytical form exists for the associated stationary problem [5, 7, 12]. For this reason and for notational simplicity, we shall discuss semidiscrete (discrete in time but not in space) approximations below.

In the case of one-space dimension, the solution of a nonlinear discrete system at each time step is feasible, and several numerical investigations have been performed in this manner [1, 4, 6]. A stability proof for this procedure is given in [8]. For higher-space dimensions, we adopt the following philosophy, which is based on the interpretation of this system as an engineering model: First-order accuracy in the time step (h) is sufficient, but we are unwilling to solve nonlinear systems at each time step. In fact, we wish to limit the computation at each time step to the solution of three separate linear systems, each corresponding to the discretization of one of the three Eqs. (1.1a), (1.1b) and (1.2).

The trouble with this approach is that the straightforward linearization of the system (1.1)–(1.2) is unstable, unless prohibitively small time steps are used. To see this, let u_n be a function of x, $x \in D$, approximating $u(\cdot, t_n)$, $t_n = nh$, with v_n and ψ_n similarly. If the system (1.1)–(1.3) is linearized in the obvious manner and backward time differencing is used, we obtain

$$u_n - u_{n-1} = h\,\Delta u_n - h\nabla \cdot (u_n \nabla \psi_{n-1}), \tag{1.4}$$

$$v_n - v_{n-1} = h\,\Delta v_n + h\nabla \cdot (v_n \nabla \psi_{n-1}), \tag{1.5}$$

$$\kappa\,\Delta \psi_n = u_n - v_n - f. \tag{1.6}$$

From (1.6), substituting from (1.4) and (1.5), we get

$$\begin{aligned} \kappa\,\Delta\psi_n - \kappa\,\Delta\psi_{n-1} &= (u_n - u_{n-1}) - (v_n - v_{n-1}) \\ &= h\,\Delta u_n - h\nabla \cdot (u_n\,\nabla\psi_{n-1}) - h\,\Delta v_n - h\nabla \cdot (v_n\,\nabla\psi_{n-1}) \\ &= h\Delta(u_n - v_n) - h\nabla \cdot ((u_n + v_n)\,\nabla\psi_{n-1}) \\ &= h\kappa\,\Delta^2\psi_n - h\nabla \cdot ((u_n + v_n)\,\nabla\psi_{n-1}) + h\,\Delta f, \end{aligned} \tag{1.7}$$

as an evolution equation satisfied by ψ_n. From (1.7) it is apparent that unless h is of the order of the minimum value of the local "dielectric relaxation time" $\tau = \kappa/(u_n + v_n)$, instability is likely. In fact, this instability has been observed, and for a special case, we shall display the unstable modes explicitly below.

Such a limitation on the time step is considered unacceptable. In practice, for present day silicon devices we are interested in values of $T \sim 10^{-8}$–10^{-10} sec. As a physical model of such a device, the system (1.1)–(1.2) may be useful down to time scales of 10^{-12}–10^{-13} sec, at which point the acceleration time for mobile carriers becomes important [11]. The values of τ, however, easily can be as small as 10^{-16}–10^{-17} sec, depending on the particular problem.

Below, we discuss three methods, based on different treatment of the Poisson equation (1.2), for circumventing this difficulty. Each method has advantages and disadvantages with respect to the others, and the results of our analysis will require interpretation in choosing a method for a specific problem of this type. For example, asymptotic convergence results are obtained in Section 3, but may not be very important, since computations with h small compared with τ are not anticipated in general, even as test cases. Stability of the linearized problem at equilibrium is discussed in Section 4. In the special case where the equilibrium carrier densities are constants, the linearized problem can be fully characterized [10], and our discretization schemes are compared with these results in Section 5. An example of such a computation is presented in Section 6. The relative merits of the various schemes are discussed in Section 7.

II. Three Possible Computation Schemes

It is useful to replace the variables u, v, by $\zeta_u = ue^{-\psi}$, $\zeta_v = ve^{\psi}$; the continuity equations assume self-adjoint form in these variables.

Our first method is to replace ψ_{n-1} by ψ_n in the right side of (1.7), and use this relation instead of (1.2) in the original system. An additional linear boundary condition for ψ, denoted by $\tilde{B}_1$ is also required. Then, we find ψ_n, $\zeta_{u,n}$, $\zeta_{v,n}$ by successively solving

$$\kappa\,\Delta\psi_n - \kappa\,\Delta\psi_{n-1} = h\kappa\,\Delta^2\psi_n - h\nabla\cdot((\zeta_{u,n-1}e^{\psi_{n-1}} + \zeta_{n,n-1}e^{-\psi_{n-1}})\,\nabla\psi_n) + h\,\Delta f, \qquad x \in D; \quad (2.1)$$

$$B_1(\psi_n) = \tilde{B}(\psi_n) = 0, \qquad x \in \partial D;$$

$$\zeta_{u,n}e^{\psi_n} - \zeta_{u,n-1}e^{\psi_{n-1}} = h\nabla\cdot(e^{\psi_n}\,\nabla\zeta_{u,n}), \qquad x \in D; \qquad (2.2)$$

$$B_2(\zeta_{u,n}e^{\psi_n}, \psi_n) = 0, \qquad x \in \partial D;$$

$$\zeta_{v,n}e^{-\psi_n} - \zeta_{v,n-1}e^{-\psi_{n-1}} = h\nabla\cdot(e^{-\psi_n}\,\nabla\zeta_{v,n}), \qquad x \in D; \qquad (2.3)$$

$$B_3(\zeta_{v,n}e^{-\psi_n}, \psi_n) = 0, \qquad x \in \partial D.$$

In such a computation, the first step requires the solution of a fourth-order linear elliptic system, but the last two steps presumably can be reduced to a sequence of one-dimensional problems by the method of fractional steps [2].

In the second method we discuss, the Poisson equation (1.2) is retained, but a stabilizing term is added, as done by Gummel [5] for the stationary problem. We obtain the following equation for ψ_n :

$$\begin{aligned} \kappa \Delta\psi_n - (\zeta_{u,n-1}e^{\psi_{n-1}} + \zeta_{v,n-1}e^{-\psi_{n-1}})(\psi_n - \psi_{n-1}) \\ = \zeta_{u,n-1}e^{\psi_{n-1}} - \zeta_{v,n-1}e^{-\psi_{n-1}} - f, \qquad x \in D, \\ B_1(\psi_n) = 0, \qquad x \in \partial D; \end{aligned} \tag{2.4}$$

Eqs. (2.2) and (2.3) are subsequently solved for $\zeta_{u,n}$, $\zeta_{v,n}$. This procedure requires no additional boundary conditions, and also requires the solution of only one N-dimensional linear elliptic system at each time step. In this case, however, the system is second order, self-adjoint, and strongly diagonally dominant, so that very fast iterative methods are applicable [3, 13].

Our third method involves an additional approximation in the system (1.1) and (1.2), considered as a model of a semiconductor. In semiconductors it is frequently true that regions in which the carrier densities (u or v or both) are large are "charge neutral" in the sense that $\kappa \mid \Delta\psi \mid$ is very small compared with the larger of u, v. In such regions, we consider the system obtained by replacing the dielectric constant κ by zero, and dropping one of the boundary condition requirements [9]. We also assume that the original boundary conditions are consistent with charge neutrality, so that this is justified on physical grounds.

We anticipate that in practice, the region D will be divided into two regions, one in which the charge neutral approximation is physically justified, and one in which $u + v$ is sufficiently small that direct methods such as that described by (1.4)–(1.6) can be used without unreasonable restrictions on h. In the following, however, it is assumed for simplicity that the charge neutral approximation is made throughout the region D. Two schemes for implementing the charge neutral method are suggested: Drop the boundary condition B_1, solve a quadratic equation at each point for ψ_n,

$$\zeta_{u,n-1}e^{\psi_n} - \zeta_{v,n-1}e^{-\psi_n} = f, \tag{2.5}$$

and find $\zeta_{u,n}$ from (2.2) and $\zeta_{v,n}$ from (2.3); alternatively, drop one of the other boundary conditions, say B_3, find ψ_n from

$$\begin{aligned} \nabla \cdot ((\zeta_{u,n-1}e^{\psi_{n-1}} + \zeta_{v,n-1}e^{-\psi_{n-1}}) \nabla\psi_n) = \Delta f, \qquad x \in D, \\ B_1(\psi_n) = 0, \qquad x \in \partial D; \end{aligned} \tag{2.6}$$

then find $\zeta_{u,n}$ from (2.2) and $\zeta_{v,n}$ from a statement of charge neutrality,

$$\zeta_{u,n}e^{\psi_n} - \zeta_{v,n}e^{-\psi_n} - f = 0, \qquad x \in D. \tag{2.7}$$

III. Convergence as $h \to 0$

In this section, we obtain asymptotic convergence results for the three methods presented above, assuming that a sufficiently smooth solution exists in each case. We will also assume that the number of space dimensions $N \leqslant 3$, and make some assumptions about the boundary conditions consistent with those described in the introduction.

Let $(\;,\;)$ denote the L_2 scalar product over D, and $\|\cdot\|$ the L_2-norm. We will assume that for functions $g(x)$, satisfying the homogeneous form of one of the three boundary conditions, B_1, B_2, B_3,

$$\| g \|_1 = \left(\int_D | \nabla g |^2 \, dx \right)^{1/2} \qquad \text{and} \qquad \| g \|_2 = \| \Delta g \|,$$

are equivalent to the usual H^1 and H^2 norms over D; for two such functions, g, $\tilde{g}$ we further assume that $(\Delta g, \tilde{g}) = \int_D \nabla g \cdot \nabla \tilde{g} \, dx$, i.e., the associated boundary integral vanishes.

Let $t_n = nh$, $n = 0, 1, 2,\ldots$ be the discrete time points, although the use of uniform steps is not necessary for our results. We use the following notation: $u_n = \zeta_{u,n} e^{\psi_n}$, $v_n = \zeta_{v,n} e^{-\psi_n}$ are the approximate values of the carrier densities; $\eta_n = \zeta_{u,n} - \zeta_u(\cdot, t_n)$, $\rho_n = \zeta_{v,n} - \zeta_v(\cdot, t_n)$, $\xi_n = \psi_n - \psi(\cdot, t_n)$, $w_n = u_n - u(\cdot, t_n)$, $\tilde{w}_n = v_n - v(\cdot, t_n)$, are the error functions. We use c, ϵ below for large and small (positive) generic constants, respectively.

The continuity equations associated with each method can be analyzed using straightforward energy inequalities. We use the following two lemmas:

Lemma 1. *Suppose $\zeta_{u,n} \in H^1(D)$ and $\psi_n \in H^2(D)$ satisfy (2.2) weakly, then, for h sufficiently small,*

$$\| w_n \|^2 + h \| w_n \|_1^2 \leqslant [1 + ch + G(\| \xi_n \|_2)\, h \, \| \xi_n \|_2][\| w_{n-1} \|^2 + ch \| \xi_n \|_1^2 + ch^3], \tag{3.1}$$

where $G(\cdot)$ is a continuous positive generic function.

Proof. Comparing (2.2) with (1.1a), we have

$$\begin{aligned} w_n - w_{n-1} &= h\nabla \cdot (e^{\psi_n} \nabla \zeta_{u,n}) - h\nabla \cdot (e^{\psi(\cdot, t_n)} \nabla \zeta_u(\cdot, t_n)) + O(h^2) \\ &= h\nabla \cdot (e^{\psi_n} \nabla (e^{-\psi_n} w_n + e^{\psi(\cdot, t_n) - \psi_n} \zeta_u(\cdot, t_n)) \\ &\quad - h\nabla \cdot (e^{\psi(\cdot, t_n)} \nabla \zeta_u(\cdot, t_n)) + O(h^2) \\ &= h \,\Delta w_n - h \,\nabla w_n \cdot \nabla \psi_n - h w_n \,\Delta \psi_n + h\nabla \cdot (u(\cdot, t_n) \nabla \xi_n) + O(h^2). \end{aligned} \tag{3.2}$$

Taking the scalar product of (3.2) with w_n gives

$$\| w_n \|^2 - (w_n, w_{n-1}) = -h \| w_n \|_1^2 - h(w_n, \nabla w_n \cdot \nabla \psi_n) - h(w_n^2, \Delta \psi_n) - h(u(\cdot, t_n), \nabla w_n \cdot \nabla \xi_n) + O(h^2) \| w_n \|,$$

so that

$$\begin{aligned} \| w_n \|^2 &\leqslant \| w_{n-1} \|^2 - 2h \| w_n \|_1^2 + ch \| w_n \|_1 (\| \xi_n \|_1 + \| w_n \|) \\ &\quad - h(w_n, \nabla w_n \cdot \nabla \xi_n) - h(w_n^2, \Delta \xi_n) + O(h^2) \| w_n \| \\ &\leqslant \| w_{n-1} \|^2 - (2 - \epsilon) h \| w_n \|_1^2 + ch(\| \xi_n \|_1^2 + \| w_n \|^2) \\ &\quad + ch \| w_n \|_1 \| w_n \|_{L_4} \| \xi_n \|_{W_4^1} + ch \| w_n \|_{L_4}^2 \| \xi_n \|_2 + ch^2 \| w_n \| \\ &\leqslant \| w_{n-1} \|^2 - (2 - \epsilon) h \| w_n \|_1^2 + ch(\| \xi_n \|_1^2 + \| w_n \|^2) \\ &\quad + ch \| w_n \|_{L_4}^2 (\| \xi_n \|_2 + \| \xi_n \|_{W_4^1}^2) + ch^2 \| w_n \|. \end{aligned} \tag{3.3}$$

Since $N \leqslant 3$, $\| \cdot \|_{W_4^1} \leqslant c \| \cdot \|_2$ and $\| \cdot \|_{L_4} \leqslant \epsilon \| \cdot \|_1 + c(\epsilon) \| \cdot \|$; using these estimates in (3.3) gives

$$\begin{aligned} \| w_n \|^2 &\leqslant \| w_{n-1} \|^2 - (2 - \epsilon) h \| w_n \|_1^2 + ch(\| \xi_n \|_1^2 + \| w_n \|^2) \\ &\quad + G(\| \xi_n \|_2) h \| w_n \|^2 (\| \xi_n \|_2 + \| \xi_n \|_2^2) + ch^2 \| w_n \|, \end{aligned}$$

from which (3.1) follows easily, assuming h sufficiently small.

LEMMA 2. *Suppose $\zeta_{u,n} \in H^2(D)$ and $\psi_n \in H^2(D)$ satisfy* (2.2) *strongly, then, for sufficiently small h,*

$$\| w_n \|_1^2 + h \| w_n \|_2^2 \leqslant [1 + ch + G(\| \xi_n \|_2) h \| \xi_n \|_2^2][\| w_{n-1} \|_1^2 + ch \| \xi_n \|_2^2 + ch^3]. \tag{3.4}$$

The proof is similar to that of Lemma 1, except that we take the scalar product of (3.2) with Δw_n. We also use $\| \cdot \|_{L_\infty} \leqslant \epsilon \| \cdot \|_2 + c(\epsilon) \| \cdot \|_1$, which again is valid since $N \leqslant 3$.

When $\zeta_{v,n}$ is determined from (2.3), similar estimates hold for $\| \hat{w}_n \|$.

For the first method proposed, an energy inequality also can be obtained for the error in ψ.

LEMMA 3. *Suppose $\psi_n \in H^3(D)$, $u_n \in H^1(D)$, $v_n \in H^1(D)$ satisfy* (2.1). *Suppose also that $\tilde{B}(\psi(\cdot, t_n)) = 0$, and that the homogeneous form of the boundary conditions $B_1(\psi_n) = \tilde{B}(\psi_n) = 0$ is such that $\xi_n = \psi_n - \psi(\cdot, t_n)$ satisfies $-(\Delta \xi_n, \Delta^2 \xi_n) =$*

$\int_D |\nabla \Delta\xi_n|^2\,dx = \|\xi_n\|_3^2$, and $\|\xi_n\|_3$ is equivalent to the usual H^3 norm for functions satisfying such boundary conditions. Then, for h sufficiently small,

$$\begin{aligned}&\|\xi_n\|_2^2 + h\|\xi_n\|_3^2\\ &\leqslant [1 + ch + ch\|w_{n-1} + \hat{w}_{n-1}\|_1^2][\|\xi_{n-1}\|_2^2 + ch\|w_{n-1} + \hat{w}_{n-1}\|^2 + ch^3]. \qquad (3.5)\end{aligned}$$

Remark. This requirement on the boundary conditions is satisfied, for example, if ψ and $\Delta\psi$ are specified on all or part of ∂D and the normal derivatives of ψ and $\Delta\psi$ are specified on the remainder.

Proof. Comparing (2.1) with (1.1) and (1.2), we obtain

$$\begin{aligned}\kappa\,\Delta\xi_n - \kappa\,\Delta\xi_{n-1} &= h\kappa\,\Delta^2\xi_n - h\nabla\cdot((u_{n-1} + v_{n-1})\nabla\psi_n)\\ &\quad + h\nabla\cdot((u(\cdot, t_n) + v(\cdot, t_n))\nabla\psi(\cdot, t_n)) + O(h^2)\\ &= h\kappa\,\Delta^2\xi_n - h\nabla\cdot((w_{n-1} + \hat{w}_{n-1})\nabla\psi_n)\\ &\quad - h\nabla\cdot((u(\cdot, t_n) + v(\cdot, t_n))\nabla\xi_n) + O(h^2)\end{aligned} \qquad (3.6)$$

as an evolution equation satisfied by ξ. Taking the scalar product with $\Delta\xi_n$ gives

$$\begin{aligned}&\kappa\|\xi_n\|_2^2 - \kappa(\Delta\xi_n, \Delta\xi_{n-1})\\ &\quad = -h\kappa\|\xi_n\|_3^2 + h(w_{n-1} + \hat{w}_{n-1}, \nabla\psi_n\cdot\nabla\Delta\xi_n)\\ &\qquad - h(\Delta\xi_n, \nabla\cdot((u(\cdot, t_n) + v(\cdot, t_n))\nabla\xi_n) + \|\xi_n\|_2\,O(h^2);\end{aligned}$$

$$\begin{aligned}\|\xi_n\|_2^2 &\leqslant \|\xi_{n-1}\|_2^2 - (2-\epsilon)\,h\|\xi_n\|_3^2\\ &\qquad + ch\,\|(w_{n-1} + \hat{w}_{n-1})\,|\nabla\psi_n|\,\|^2 + ch\|\xi_n\|_2^2 + ch^2\|\xi_n\|\\ &\leqslant \|\xi_{n-1}\|_2^2 - (2-\epsilon)\,h\|\xi_n\|_3^2 + ch\|w_{n-1} + \hat{w}_{n-1}\|^2\\ &\qquad + ch\|w_{n-1} + \hat{w}_{n-1}\|_{L_4}^2\|\xi_n\|_{W_4^1}^2 + ch\|\xi_n\|_2^2 + ch^3\\ &\leqslant \|\xi_{n-1}\|_2^2 - h\|\xi_n\|_3^2 + ch\|w_{n-1} + \hat{w}_{n-1}\|^2\\ &\qquad + ch\|w_{n-1} + \hat{w}_{n-1}\|_1^2\|\xi_n\|_2^2 + ch\|\xi_n\| + ch^3,\end{aligned}$$

from which (3.5) follows. The convergence of the first method proposed follows from Lemmas 2 and 3.

THEOREM 1. *Suppose $\zeta_{u,n} \in H^2(D)$, $\zeta_{v,n} \in H^2(D)$, $\psi_n \in H^3(D)$ are determined from* (2.1)–(2.3), *and suppose the extra boundary condition $\tilde{B}$ satisfies the requirements* *of Lemma* 3. *Suppose further that the initial approximations satisfy* $\| w_0 \|_1 + \| \hat{w}_0 \|_1 + \| \xi_0 \|_2 = O(h)$. *Let* $t_n = nh$ *be fixed as* $h \to 0$; *then,*

$$\| u_n - u(\cdot, t_n)\|_1 + \| v_n - v(\cdot, t_n)\|_1 + \| \zeta_{u,n} - \zeta_u(\cdot, t_n)\|_1 + \| \zeta_{v,n} - \zeta_v(\cdot, t_n\|_1 + \| \psi_n - \psi(\cdot, t_n)\|_2 \leqslant ch, \tag{3.7}$$

and

$$\| u_n - u(\cdot, t_n)\|_2 + \| v_n - v(\cdot, t_n)\|_2 + \| \zeta_{u,n} - \zeta_u(\cdot, t_n)\|_2 + \| \zeta_{v,n} - \zeta_v(\cdot, t_n)\|_2 + \| \psi_n - \psi(\cdot, t_n)\|_3 \leqslant ch^{1/2}. \tag{3.8}$$

Proof. Set

$$E_n = \| w_n \|_1^2 + \| \hat{w}_n \|_1^2 + \| \xi_n \|_2^2 + h(\| w_n \|_2^2 + \| \hat{w}_n \|_2^2 + \| \xi_n \|_3^2);$$

it follows from (3.4) and (3.5) that E_n satisfies

$$E_n \leqslant (1 + ch + chE_{n-1}G(E_{n-1}))(E_{n-1} + ch^3).$$

Since $E_1 = O(h^2)$ by hypothesis and an application of (3.4) and (3.5), we have $E_n = O(h^2)$, from which (3.7) and (3.8) follows.

The asymppototic convergence of the second method depends on Lemma 1 and the following estimate for $\| \xi_n \|_2$.

LEMMA 4. *Suppose* $\psi_n \in H^2(D)$ *is determined by* (2.4), *and suppose that for each nonnegative integer* $m \leqslant n - 1$, $u_m + v_m$ *is uniformly positive and bounded in* D. *Then*

$$\| \xi_n \|_2 \leqslant G(\operatorname*{Max}_j \| u_j + v_j \|_{L_\infty}, \operatorname*{Max}_k \|(u_k + v_k)^{-1} \|_{L_\infty})[h + \operatorname*{Max}_m(\| w_m \| + \| \hat{w}_m \|)], \tag{3.9}$$

where the integers j, k, and m are between 0 *and* $n - 1$.

Proof. Comparing (2.4) with (1.2) we obtain

$$\kappa \Delta \xi_n = w_{n-1} + \hat{w}_{n-1} + (u_{n-1} + v_{n-1})(\xi_n - \xi_{n-1} + O(h)); \tag{3.10}$$

collecting the ξ_n terms, multiplying (3.10) by $(u_{n-1} + v_{n-1})^{-1/2}$ and squaring, we obtain

$$\begin{aligned} &\kappa^2((u_{n-1} + v_{n-1})^{-1}, (\Delta \xi_n)^2) + \kappa \| \xi_n \|_1^2 + (u_{n-1} + v_{n-1}, \xi_n^{\,2}) \\ &\quad = \|(u_{n-1} + v_{n-1})^{1/2} (\xi_{n-1} + O(h)) - (u_{n-1} + v_{n-1})^{-1/2} (w_{n-1} + \hat{w}_{n-1})\|^2 \\ &\quad \leqslant (1 + \epsilon)((u_{n-1} + v_{n-1}), \xi_{n-1}^2) \\ &\qquad + G(\epsilon, \| u_{n-1} + v_{n-1} \|_{L_\infty}, \|(u_{n-1} + v_{n-1})^{-1} \|_{L_\infty})(h^2 + \| w_{n-1} \|^2 + \| w_{n-1} \|^2). \end{aligned} \tag{3.11}$$

In (3.11), we choose ϵ sufficiently small, depending on $u_{n-1} + v_{n-1}$, so that the left side is $\geqslant (1 + 2\epsilon)((u_{n-1} + v_{n-1}), \xi_n^2)$; it then follows that

$$((u_{n-1} + v_{n-1}), \xi_n^2) \leqslant G(\operatorname*{Max}_j \| u_j + v_j \|_{L_\infty}, \operatorname*{Max}_k \|(u_k + v_k)^{-1}\|_{L_\infty}) \times (h^2 + \operatorname*{Max}_m(\| w_m \|^2 + \| \hat{w}_m \|^2)), \tag{3.12}$$

where the integers j, k, and $m \in [0, n-1]$. The result (3.9) then follows from (3.11) and (3.12).

THEOREM 2. *Suppose* $\zeta_{u,n}$, $\zeta_{v,n} \in H^1(D) \cap L_\infty(D)$, $\psi_n \in H^2(D)$ *satisfy* (2.2), (2.3), and (2.4), *with the extra provision that the factor* $(u_{n-1} + v_{n-1})$ *occurring in the left side of* (2.4) *is restricted to the range* $[\epsilon, c_1]$ *uniformly in D and independent of h, for some positive* ϵ. *Suppose that* $\| \xi_0 \| + \| w_0 \| + \| w_0 \| = O(h)$. *Let* $t_n = nh$ *be fixed as* $h \to 0$; *then,*

$$\| u_n - u(\cdot, t_n)\| + \| v_n - v(\cdot, t_n)\| + \| \zeta_{u,n} - \zeta_u(\cdot, t_n)\| + \| \zeta_{v,n} - \zeta_v(\cdot, t_n)\| + \| \psi_n - \psi(\cdot, t_n \|_2 \leqslant ch \tag{3.13}$$

and

$$\| u_n - u(\cdot, t_n)\| + \| v_n - v(\cdot, t_n)\|_1 \leqslant ch^{1/2}. \tag{3.14}$$

Proof. With this restriction on the stabilizing term in (2.4), (3.9) may be simplified to

$$\| \xi_n \|_2 \leqslant c(h + \operatorname*{Max}_m(\| w_m \| + \| \hat{w}_m \|)$$

and the conclusion is immediate from Lemma 1.

The use of such a restriction on the stabilizing term can be avoided if smoother approximating functions are used.

THEOREM 3. *The conclusions of Theorem* 1 *remain valid if* $\zeta_{u,n}$, $\zeta_{v,n}$, $\psi_n \in H^2(D)$ *are determined from* (2.2), (2.3), *and* (2.4), *and the inital data satisfy* $\| w_0 \|_1 + \| w_0 \|_1 + \| \xi_0 \| = O(h)$.

Proof. We use Lemmas 2 and 4; setting

$$E_n = \operatorname*{Max}_{m \leqslant n} [\| w_m \|_1^2 + \| \hat{w}_m \|_1^2 + h(\| w_m \|_2^2 + \| \hat{w}_m \|_2^2)];$$

(3.9) becomes

$$\| \xi_n \|_2 \leqslant G(E_{n-1})(h + E_{n-1}^{1/2}),$$

since $\| \cdot \|_2$ estimates $\| \cdot \|_{L_\infty}$ in three dimensions, and the results follow from (3.1).

Finally, for the charge neutral method, we have the following:

THEOREM 4. *Suppose* $\zeta_{u,n}$, ψ_n, $\zeta_{v,n} \in H^2(D)$ *are determined from* (2.2), (2.6), *and* (2.7), *respectively. Suppose a smooth charge neutral solution with* $u + v$ *uniformly positive in* $D \times [0, T]$ *exists, and that the initial data satisfies* $u_0 + f = v_0$, $u_0 + v_0 \geqslant \epsilon > 0$ *uniformly in* D *and* $\| w_0 \|_1 + h \| w_0 \|_2 = O(h)$. *If* $t_n = nh$ *is fixed as* $h \to 0$, *then* (3.7) *holds and*

$$\| u_n - u(\cdot, t_n)\|_2 + \| v_n - v(\cdot, t_n)\|_2 + \| \zeta_{u,n} - \zeta_u(\cdot, t_n)\|_2 + \| \zeta_{v,n} - \zeta_v(\cdot, t_n)\|_2 \leqslant ch^{1/2}. \tag{3.15}$$

Proof. We rewrite (2.6) in the form

$$\nabla \cdot ((2u_{n-1} + f) \nabla \psi_n) = \Delta f, \qquad x \in D, \quad B_1(\psi_n) = 0, \quad x \in \partial D, \tag{3.16}$$

using (2.7) at t_{n-1}. If a smooth charge neutral solution exists, ψ satisfies

$$\nabla \cdot ((2u(\cdot, t_n) + f) \nabla \psi(\cdot, t_n)) = \Delta f, \qquad x \in D, \quad B_1(\psi(\cdot, t_n)) = 0, \quad x \in \partial D, \tag{3.17}$$

so that $\xi_n = \psi_n - \psi(\cdot, t_n)$ satisfies

$$\nabla \cdot ((2u_{n-1} + f) \nabla \xi_n) = -2\nabla \cdot (w_{n-1} \nabla \psi(\cdot, t_n)) + O(h), \qquad x \in D, \tag{3.18}$$

and the homogeneous form of B_1. We assume $u_{n-1} + v_{n-1} = 2u_{n-1} + f$ is uniformly positive in D; then, (3.18) has a solution $\xi_n e H^2(D)$ if $w_n \in H^1(D)$, and

$$\| \xi_n \|_1 \leqslant G(\| w_{n-1} \|_{L_\infty})(\| w_{n-1} \| + h). \tag{3.19}$$

Writing the left side of (3.18) as $(2u_{n-1} + f) \Delta \xi_n + \nabla(2u_{n-1} + f) \cdot \nabla \xi_n$ and using (3.19) we obtain

$$\begin{aligned}
\| \xi_n \|_2 &\leqslant G(\| w_{n-1} \|_{L_\infty})[\| w_{n-1} \|_1 + h + \| \xi_n \|_1 + \| w_{n-1} \|_{W_4^1} \| \xi_n \|_{W_4^1}] \\
&\leqslant G(\| w_{n-1} \|_2)[\| w_{n-1} \|_1 + h + \| w_{n-1} \|_2 (\epsilon \| \xi_n \|_2 + c(\epsilon) \| \xi_n \|_1)] \\
&\leqslant G(\| w_{n-1} \|_2)[\| w_{n-1} \|_1 + h + \| w_{n-1} \|_2 \| \xi_n \|_1] \\
&\leqslant G(\| w_{n-1} \|_2)(\| w_{n-1} \|_1 + h).
\end{aligned} \tag{3.20}$$

Setting $E_n = \| w_n \|_1^2 + h \| w_n \|_2^2$, and noting that $\hat{w}_n = -w_n$ for the charge neutral problem, (3.7) and (3.15) follow from (3.20) and Lemma 2. Since the second space derivatives of u_n, v_n are converging to those of $u(\cdot, t_n)$, $v(\cdot, t_n)$, the assumption of uniformly positive $u_n + v_n$ is justified.

IV. The Linearized Problem

In this and the next section, we assume that the boundary conditions are consistent with a stationary solution of the system (1.1)–(1.3), of the form [8]

$$\begin{gathered}\zeta_u(x) = \zeta_v(x) = 1, \quad u(x, t) = a(x) = e^{\psi_e(x)}, \quad v(x, t) = b(x) = e^{-\psi_e(x)} \\ \kappa\, \Delta\psi_e = e^{\psi_e} - e^{-\psi_e} - f, \qquad x \in D, \quad B_1(\psi_e) = 0, \quad x \in \partial D.\end{gathered} \tag{4.1}$$

The eigenvalues of the system (1.1)–(1.3), linearized at the stationary solution, are known to be real and negative. In this section, we examine the discrete eigenvalues for two of our methods. We seek discrete solutions of the form $t_n = nh$,

$$u(x, t_n) = a(x)(1 + z^n(\omega(x) - \theta(x))), \tag{4.2}$$

$$v(x, t_n) = b(x)(1 + z^n(\phi(x) - \omega(x))), \tag{4.3}$$

$$\psi(x, t_n) = \psi_e(x) + z^n \omega(x), \tag{4.4}$$

where z is the discrete (complex) eigenvalue and θ, ϕ, ω are complex valued and sufficiently small that it suffices to retain only first-order terms. Hereafter, we use (,) for the complex scalar product, and introduce the additional notation

$$\| \theta \|_a^2 = (\theta, a\theta), \qquad \| \theta \|_{1,a}^2 = \int_D a(x) \mid \nabla\theta \mid^2 dx,$$

similarly for the other variables. We shall assume that the boundary conditions are such that if g is any of the three small quantities θ, ϕ, ω, then $\| g \|_1^2 = -(g, \Delta g)$, and $\| g \| \leqslant c \|g\|_1$.

The linearized form of (2.2), and (2.3) is

$$z\nabla \cdot (a\nabla\theta) = a(z - 1)(\theta - \omega)/h \tag{4.5}$$

$$z\nabla \cdot (b\, \Delta\phi) = b(z - 1)(\phi - \omega)/h; \tag{4.6}$$

we will discuss two cases: that in which ψ_n is determined from (2.4), the linearized form of which is

$$\kappa z\, \Delta\omega - (a + b)\, z\omega = -a\theta - b\phi, \tag{4.7}$$

and the charge neutral case with ψ_n determined by (2.5), which becomes

$$z(a + b)\, \omega = a\theta + b\phi. \tag{4.8}$$

THEOREM 5. *Assuming h positive, the system* (4.5), (4.6), *and* (4.7) *has nontrivial solutions only if* $| z | < 1$ *and* $\mathrm{Re}(z) > 0$.

Proof. We take the scalar products of (4.5) with θ, of (4.6) with ϕ, and of (4.7) with ω; the terms involving $(a\theta, \omega)$ and $(b\phi, \omega)$ can be eliminated, obtaining

$$\kappa\bar{z} \,\| \omega \|_1^2 + \bar{z} \,\| \omega \|_{a+b}^2 = \| \theta \|_a^2 + \| \phi \|_b^2 + (hz/(z-1))(\| \theta \|_{1,a}^2 + \| \phi \|_{1,b}^2). \quad (4.9)$$

If $\omega \equiv 0$, then $z \in (0, 1)$ is immediate from (4.9). If $\omega \not\equiv 0$, then (4.9) is a quadratic equation for z, of the form

$$\begin{aligned} Pz\bar{z} - P\bar{z} - (Q + hR)\, z + Q &= 0, \\ P &= \kappa \,\| \omega \|_1^2 + \| \omega \|_{a+b}^2, \\ Q &= \| \theta \|_a^2 + \| \phi \|_b^2, \\ R &= \| \theta \|_{1,a}^2 + \| \phi \|_{1,b}^2 . \end{aligned} \quad (4.10)$$

There are no nontrivial solutions with Q and R equal to zero. With, h, P, Q, R all positive, it follows from (4.10) that either z is real and positive, or $P = Q + hR$. If z is real, since $z = 1$ is impossible from (4.5) and (4.6), it suffices to show that $z > 1$ is impossible. Otherwise, the scalar product of (4.5) with θ can be written

$$(hz/(z-1))\, \| \theta \|_{1,a}^2 + \| \theta \|_a^2 = (a\theta, \omega) \leqslant (1/2)(\| \theta \|_a^2 + \| \omega \|_a^2)$$

and it follows that $\| \theta \|_a < \| \omega \|_a$. We get $\| \phi \|_b < \| \omega \|_b$, similarly, from (4.6), and thus, $Q < P$. But the scalar product of (4.7) with ω gives

$$\begin{aligned} zP &= (\omega, a\theta + b\phi) \\ &\leqslant \tfrac{1}{2}(\| \omega \|_a^2 + \| \theta \|_a^2 + \| \omega \|_b^2 + \| \phi \|_b^2) \\ &\leqslant \tfrac{1}{2}(P + Q), \end{aligned} \quad (4.11)$$

which implies $P < Q$ if $z > 1$.

If $P = Q + hR$ and z is complex, (4.11) may be written

$$| z | \leqslant \frac{P + Q}{2P} = \frac{Q + hR/2}{Q + hR} < 1.$$

The conclusion $\mathrm{Re}(z) > 0$ follows in this case from considering the real part of (4.10) as a quadratic equation for $\mathrm{Re}(z)$.

For the charge neutral method, we have the following:

THEOREM 6. *Assuming h positive, the system* (4.5, 4.6, 4.8) *has nontrivial solutions only if* $| z | < 1$ *and* $\mathrm{Re}(z) > 0$.

Proof. Equation (4.8) is obtained by setting $\kappa = 0$ in (4.7). The proof of Theorem 5 remains valid if we set $\kappa = 0$.

V. The Case of Constant Doping

A mathematically interesting special case occurs when f and ψ_e are constant in D. The solution of (1.1)–(1.3) can be interpreted physically in this case: First, the magnitude of the electric field, $|\nabla\psi|$, decays rapidly, in a time scale of order τ, by the drift of mobile carriers; then, the carriers diffuse toward the stationary (constant) distributions [10]. Near the stationary solution, drift and diffusion mechanisms are uncoupled, in the sense that the eigenfunctions are divided into two classes: drift modes, with $\omega \not\equiv 0$ and associated time constants of order $\tau = \kappa/(a+b)$, and diffusion modes, with $\omega \equiv 0$ and time constants independent of κ.

In this section, we compare these results for the continuous system (1.1)–(1.3) to the corresponding results for our proposed discrete methods. In this case, we are also able to display explicitly the instability associated with direct methods such as (1.4)–(1.6).

We linearize the equations as in Section 4; the continuity equations (2.2) and (2.3), or (4.5) and (4.6) become

$$z\,\Delta\theta = ((z-1)/h)(\theta-\omega), \tag{5.1}$$

$$z\,\Delta\phi = ((z-1)/h)(\phi-\omega). \tag{5.2}$$

The linearization of (2.1) gives

$$\kappa((z-1)/h)\,\Delta\omega = \kappa z\,\Delta^2\omega - (a+b)\,z\,\Delta\omega, \tag{5.3}$$

so that (5.1)–(5.3) describes our first method. For the second method, we have (5.1), (5.2), and (4.7); for the two forms of the charge neutral method we have (5.1), (5.2), and (4.8), or (5.1) or (5.2) with $\omega \equiv 0$, respectively (since the linearization of (2.6) gives $\Delta\omega = 0$). In the following, we denote by $\lambda(\theta)$ an arbitrary element of $\sigma(\Delta;\theta)$, the discrete spectrum of Δ in $H^2(D)$ with the boundary conditions for θ, which are assumed to be homogeneous and such that $\sigma(\Delta;\theta)(-\infty, 0)$. Other variables are denoted similarly.

The explicit form of (5.3) makes the analysis of the system (5.1)–(5.3) trivial, and we have the following:

Theorem 7. *Suppose that the homogeneous form of the boundary conditions is such that* $(\omega, \Delta\omega) \leqslant 0$ *and* $(\omega, \Delta^2\omega) \geqslant 0$. *Then, the nontrivial solutions of* (5.1)–(5.3) *occur only for real positive z and are of two forms: drift modes, with* $\omega \not\equiv 0$ *and* $z \leqslant (1 + h/\tau)^{-1}$; *and diffusion modes, with* $\omega \equiv 0$ *and* $z = (1 - h\lambda(\theta))^{-1}$ *or* $z = (1 - h\lambda(\phi))^{-1}$.

THEOREM 8. *Suppose that the homogeneous form of the boundary conditions is such that $\sigma(\Delta; \Delta\omega)$ is a discrete point set in $(-\infty, 0)$; then, the drift mode solutions of* (5.1)–(5.3) *correspond to* $z = (1 + h/\tau - h\lambda(\Delta\omega))^{-1}$.

For our second method, we have a somewhat weaker result:

THEOREM 9. *Suppose that the homogeneous form of the boundary conditions is such that $(\omega, \Delta\omega) \leqslant 0$ and $(\omega, \Delta^2\omega) \geqslant 0$. Then, the real values of z for which* (4.7), (5.1), (5.2) *has a nontrivial solution are as in Theorem* 7, *and the complex values satisfy* $|z| \leqslant (1 + ch)^{-1/2}$.

Proof. In view of Theorem 7, it suffices to consider the case $\omega \not\equiv 0$. We can combine (4.7), (5.1), and (5.2) into a fourth-order equation for ω, obtaining

$$h^2\kappa z^2 \Delta^2\omega - hz(h(a+b)z + \kappa(z-1))\Delta\omega + (a+b)(z-1)^2\omega = 0; \quad (5.4)$$

taking the scalar product with ω and setting $s = (z/(z-1)) = \alpha + i\beta$, we obtain

$$h^2[\kappa(\omega, \Delta^2\omega) + (a+b)\|\omega\|_1^2]\, s^2 + h\kappa\|\omega\|_1^2\, s + (a+b)\|\omega\|^2 = 0. \quad (5.5)$$

For z real, it follows from (5.4) that $h(a+b)z + \kappa(z-1) < 0$, so $z < (1 + h/\tau)^{-1}$. For z complex, solving (5.5) as a quadratic equation for s, we find $-(\tau/h) \leqslant \alpha \leqslant 0$, $\beta^2 \leqslant \|\omega\|/(h\|\omega\|_1) \leqslant c/h$. Since $z = s/(s-1)$, our results follow.

We get only diffusion modes with $z = (1 - h\lambda(\theta))^{-1}$, or $z = (1 - h\lambda(\phi))^{-1}$ for the charge neutral method (2.2), (2.6), and (2.7); this follows immediately from setting $\kappa = 0$ in (5.3). The other charge neutral method, (2.2), (2.3), and (2.5), is described by (4.8), (5.1), and (5.2), with a, b constant in this case, and we have the following:

THEOREM 10. *The real values of z for which* (4.8), (5.1), and (5.2) *has a nontrivial solution correspond to diffusion modes with* $z = (1 - h\lambda(\theta))^{-1}$ *or* $z = (1 - h\lambda(\phi))^{-1}$; *the complex values satisfy* $|z| \leqslant (1 + ch)^{-1/2}$.

Proof. Combining (4.8), (5.1), and (5.2) we obtain $hz^2\Delta\omega = (z-1)^2\omega$, which has nontrivial solutions only for $s^2 = -\|\omega\|^2/h\|\omega\|_1^2)$; the proof proceeds as for Theorem 9.

Finally, we display the unstable modes associated with a direct method; for simplicity, we consider the method obtained by dropping the stabilizing term from (2.4), and finding ψ_n from

$$\kappa\,\Delta\psi_n = \zeta_{u,n-1}e^{\psi_{n-1}} - \zeta_{v,n-1}e^{-\psi_{n-1}} - f, \qquad x \in D, \quad B_1(\psi_n) = 0, \quad x \in \partial D. \quad (5.6)$$

The linearized form of (5.6) is

$$\kappa z\,\Delta\omega - (a+b)\,\omega = -a\theta - b\phi; \quad (5.7)$$

combining (5.1), (5.2), and (5.7) we get an equation similar to (5.4) for ω,

$$z\kappa\, \Delta^2\omega - (a + b + \kappa(z - 1)/h))\, \Delta\omega = 0. \tag{5.8}$$

Thus, if the boundary conditions are such that $\sigma(\Delta; \Delta\omega)$ is not empty, for any $\lambda \in \sigma(\Delta; \Delta\omega)$, there exists a nontrivial solution of (5.1), (5.2), and (5.7) with with $z = (1 - h/\tau)/(1 - \lambda h)$, which requires $h = O(\tau)$ for $|z| \leqslant 1$.

VI. A Sample Computation

The geometry and boundary conditions adopted for a sample computation are taken from a simple model of the "insulated-gate field-effect transistor" (IGFET), as illustrated in Fig. 1. (In Fig. 1, V_0 is the "built-in" source potential, and $V_G(t)$,

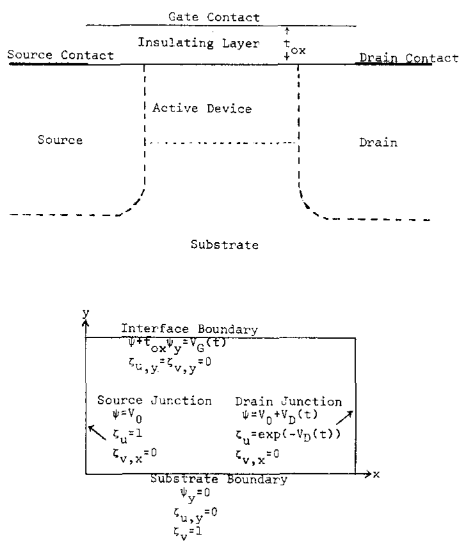

FIG. 1. Device model and boundary conditions.

$V_D(t)$ are the applied voltages between gate and source and between drain and source, respectively, as functions of time.) This device has an "ohmic contact" in each of the separated source and drain regions, which are characterized by large positive f, $u \approx f$, v negligible. The intermediate region is characterized by large negative f, and (as shown in Fig. 1) for sufficiently large negative y, by $v \approx -f$, u negligible. A third electrical contact is made to a metallic "gate," which is insulated from the semiconductor material by a thin nonconducting layer, typically of silicon dioxide. A positive voltage applied to the gate, however causes the formation of a thin "inversion layer" of electrons under the oxide interface, allowing current to flow between the source and drain, controlled by the voltages applied to the gate and drain. Although this is an important device in semiconductor engineering, its transient behavior is not well understood.

Because of the inversion layer, the charge neutral approximation is not useful in the treatment of this device. The method described by Eqs. (2.2)–(2.4) was used. A rectangular mesh was employed in the space coordinates, uniform in the x direction, with geometrically decreasing spaces with increasing y. (Nonuniform spacing is required in the y direction, in this device, to resolve the thin inversion layer under the oxide interface.) The standard five-point approximation to (2.4) was used, with the method of [3] for its approximate inversion at each time step. Equations (2.2) and (2.3) were treated by the method of fractional steps; within each half-step, a three-point discretization was used that admits interpretation and analysis as a finite-element method [7, 12].

The results of a typical calculation are shown in Fig. 2, in which the applied

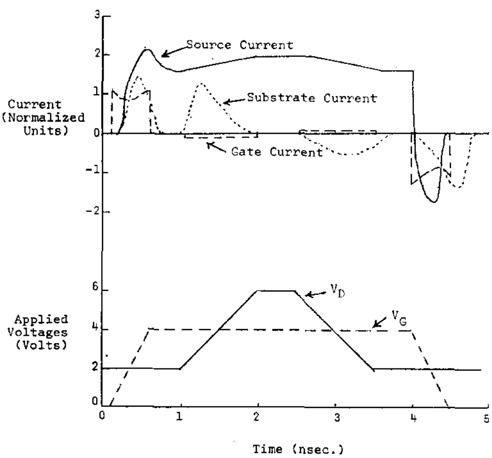

FIG. 2. Applied voltages and current flow.

gate and drain voltages are plotted together with the current flow (in normalized units) at the source, gate, and substrate contacts. The gate current is displacement current, and our results indicate that to first approximation, geometric capacitance accounts for the gate current, with the inversion layer considered as coupled to the source.

VI. Discussion and Summary

In the preceding, we have obtained some analytical results for two general methods for approximately solving the problem (1.1)–(1.3). We have also considered two forms of a charge neutral method, which correspond essentially to setting $\kappa = 0$ in the two general methods.

A general statement of which method "works best" will not be attempted here; we will simply itemize the relative merits of each method. In our discussion, the importance of the asymptotic convergence results is discounted in favor of bounds independent of h on the computed solutions. Boundedness of the computed solutions is clearly necessary, but we cannot expect h to be small compared with τ; in fact, convergence as $h \to 0$ is readily established for the direct methods, which we found unsatisfactory.

In this context, the advantage of our first method (2.1), (2.2), and (2.3) might be summarized as follows:

(1) This method admits a bound (independent of h) for the magnitude of the electric field, as may be seen by taking the scalar product of (2.1) with ψ_n.

(2) In the special case of a constant equilibrium potential, this discrete method accurately reflects spectral properties of the continuous system.

(3) Higher space derivatives of the dependent variables are controlled by this method.

(4) An energy inequality exists for the error in the electrostatic potential for this method.

Some disadvantages of this method are the following:

(1) A relatively complicated equation for the electrostatic potential has to be solved at each step.

(2) An extra boundary condition for the electrostatic potential is required.

(3) The generalization of this method to the case of unequal carrier mobilities is awkward.

(4) If the space discretization is to be effected by a finite-element method consistent with our convergence proof, relatively smooth elements are required.

For the second general method (2.2), (2.3), and (2.4) we have the following:

(1) A strong local stability result (Theorem 5) holds for this method.

(2) The residual error associated with the Poisson equation, given by $\kappa\,\Delta\psi_n - u_n + v_n + f$, is readily monitored and controlled in this method, by reducing the time step as necessary.

(3) A space discretization of this method consistent with the convergence proof could be made in such a way that the discrete form of (2.2) and (2.3) will satisfy a maximum–minimum principle, for example by using piecewise linear elements for u, v. Such a property would assure the uniform positivity of the computed carrier densities.

(4) As mentioned in Section 2, the form of the Poisson equation (2.4) is such that it is easily inverted at each step.

The two forms of the charge neutral method exhibit similar properties. In each case they allow a substantially simpler computation scheme at the expense of some of the theory. A more serious limitation on the charge neutral method, in our opinion, is that the approximation of charge neutrality is not physically justified in some problems of current engineering interest, as in the sample computation discussed in Section 6.

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