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MATHEMATICAL ASPECTS OF HYDRODYNAMIC MODELS FOR SEMICONDUCTORS DEVICE SIMULATION

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Two hydrodynamic models of a semiconductor device are considered. The first one takes into account thermal and collisional effects, while neglecting viscous terms, which are included in the second. A qualitative analysis of stationary one-dimensional solutions is performed and some numerical results are presented.

1. Introduction.

In recent years hydrodynamic models describing carrier flow in semiconductor devices have attracted considerable interest. The role of simulation has become more and more relevant in designing and analyzing new electronic devices. A fully kinetic treatment of carrier dynamics gives a complete description of the physical system, but realistic applications require complicated and very expensive numerical calculations. The *drift-diffusion* model has been widely used in the past, when it provided a good description of the relevant physical mechanisms. In modern devices, whose size is in the submicron range, ballistic and inertial effects play an important role and are not adequately modeled by the previous approach. In fact the *drift-diffusion* scheme does not take into account thermal and inertial

effects and collisions are roughly described by the mobility. Recently, hydrodynamic models have been introduced [1, 2], which have been derived from kinetic equations. The should adequately treat the aforesaid phenomena, without the high cost of kinetic simulation. The model we consider has been proposed by Baccarani and Wordeman [1]. The evolution of an electron gas in a semiconductor is described by the balance equations for electric charge, momentum and energy. Collisions of the electrons with the lattice are taken into account via suitable relaxation terms on the right hand side of the equations. Energy exchange between the electrons is modeled by the Fourier law. In the scheme they propose, viscous effects are considered negligible. As a consequence of this approximation, a "characteristic velocity" appears, which is different from the usual sound speed [3]. This velocity discriminates between "subsonic" and "supersonic" flow, in a way analogous to what happens in classical gas dynamics.

2. Field equations.

The physical system under consideration is a gas of electrons that interact with the lattice. The electron gas is treated as a perfect, monatomic classical gas, defined by a density, temperature and velocity. The effect of the holes is neglected. This scheme seems suitable for n-doped device simulation.

The balance equations are given by

$$\frac{\partial n}{\partial t} + \nabla \cdot (n\mathbf{v}) = Q_n \tag{2.1}$$

$$\frac{\partial}{\partial t}(mn\mathbf{v}) + \nabla \cdot (mn\mathbf{v} \otimes \mathbf{v}) + \nabla \cdot \mathcal{P} + en\mathbf{E} = m\mathbf{Q}_v \tag{2.2}$$

$$\frac{\partial W}{\partial t} + \nabla \cdot (W\mathbf{v} + \mathcal{P} \cdot \mathbf{v} + \mathbf{q}) + en\mathbf{E} \cdot \mathbf{v} = Q_\varepsilon \tag{2.3}$$

where n is the particle density (per unit mass), $\mathbf{v}$ is the mean velocity, e is the negative of the electron charge ($e > 0$), and m represents the effective electron mass. The electric field is denoted by $\mathbf{E}$, and the stress tensor by $\mathcal{P} = (\mathcal{P}_{ij})$; $\mathbf{q}$ represents the heat flux, and W the electron energy. These equations constitute the usual balance equations for charge, momentum and energy. The terms Q_n, $\mathbf{Q}_v$

and Q_ε derive from the contribution of the collisional operator that describes the interactions between the electrons and the lattice. The electric field is related to the potential V and the density of donors N_D and acceptors N_A, via the Poisson equation

$$\nabla \cdot (\varepsilon \mathbf{E}) = e\,(N_D - N_A - n) \tag{2.4}$$

$$\mathbf{E} = -\nabla V \tag{2.5}$$

where ε denotes the dielectric constant. The equation of state of the electron gas is

$$W = \frac{3}{2} n k_B T + \frac{1}{2} m n \mathbf{v} \cdot \mathbf{v} \tag{2.6}$$

where k_B is the Boltzmann constant and T the electron temperature. Assuming the usual linear constitutive relations, the heat flux and the stress tensor are given by

$$\mathbf{q} = -k \nabla T \tag{2.7}$$

$$\mathcal{P}_{ij} = n k_B T \delta_{ij} - \mu \left(\frac{\partial v_i}{\partial x_j} + \frac{\partial v_j}{\partial x_i} \right) + \frac{2}{3} \mu \sum_{k=1}^{3} \frac{\partial v_k}{\partial x_k} \delta_{ij} \tag{2.8}$$

where k and μ are thermal conductivity and kinematic viscosity, respectively. In the model treated in [1] and [3] the viscous terms are neglected ($\mu = 0$). Following [2] we assume that thermal conductivity and kinematic viscosity are given by

$$k = \frac{3 \mu_{n0}}{2e} T_0 \, k_B^2 \, n, \qquad \mu = \bar{\mu} \frac{m}{k_B} k,$$

where μ_{n0} is the low field mobility, T_0 the lattice bulk temperature, which is supposed to be constant, and $\bar{\mu}$ is a nondimensional constant (which is zero in the inviscid model). An appropriate value of the viscosity parameter $\bar{\mu}$ could be derived by determining the transport coefficients from the kinetic equation. However the qualitative results that we present do not depend on the particular value of $\bar{\mu}$; therefore we avoided this derivation and used some reasonable value for $\bar{\mu}$, in accordance with the Prandtl relation between thermal conductivity and viscosity.

Plane one dimensional flow.

In the sequel we shall not consider creation and recombination effects and therefore we take $Q_n \equiv 0$. We are interested in one dimensional solutions of the system (2.1-2.8), which have the form

$$n = n(x,t),\ \mathbf{v} = (v(x,t),0,0),\ T = T(x,t),\ \mathbf{E} = (E(x,t),0,0),$$

$$\mathbf{q} = (q(x,t),0,0),\ (\mathcal{P})_{11} = nk_BT + \tilde{p}(x,t)\ ,\ \mathbf{Q}_v = (Q_v,0,0)\,.$$

In this case system (2.1-2.8) reduces to

$$\text{(3.1)}\qquad \begin{cases} n_t + (nv)_x = 0 \\ (mnv)_t + \left(mnv^2 + nk_BT + \tilde{p}\right)_x + enE = mQ_v \\ \left(\frac{1}{2}mnv^2 + \frac{3}{2}nk_BT\right)_t + \left[\frac{1}{2}n\left(5k_BT + mv^2\right)v + \tilde{p}v + q\right]_x \\ \qquad\qquad + enEv = Q_\varepsilon \\ \varepsilon E_x = e\left(N_D - N_A - n\right) \\ E = -V_x \\ q = -kT_x \\ \tilde{p} = -\frac{4}{3}\mu v_x \end{cases}$$

where $(\cdot)_x \equiv \dfrac{\partial}{\partial x}$, $\quad (\cdot)_t \equiv \dfrac{\partial}{\partial t}$.

If $\mu \neq 0$ and $k \neq 0$ then there are seven field variables, n, v, T, E, V, q and $\tilde{p}$. By introducing the vector field

$$\mathbf{U} = (n, v, T, E, V, q, \tilde{p})^T,$$

equations (3.1) can be written in the form

$$\mathcal{A}^0\frac{\partial \mathbf{U}}{\partial t} + \mathcal{A}^1\frac{\partial \mathbf{U}}{\partial x} = \mathbf{B}.$$

The characteristic speeds are the solutions of the equation

$$\text{(3.2)}\qquad \det(\mathcal{A}^1 - \lambda\mathcal{A}^0) = 0.$$

A simple calculation shows that

$$|\det(\mathcal{A}^1 - \lambda\mathcal{A}^0)| = \frac{4}{3}k\varepsilon\mu|v - \lambda|$$

therefore the only characteristic speed is $\lambda = v$.

In the case $\mu = 0$ the number of unknowns reduces to six, because $\tilde{p} \equiv 0$ and therefore $\mathcal{A}^0$ and $\mathcal{A}^1$ are 6×6 matrices. The solutions of the characteristic equation are

$$\lambda_1 = v, \quad \lambda_{2,3} = v \pm c^*,$$

where $c^* = \sqrt{k_B T/m}$.

In the case $k = 0$ and $\mu = 0$ it is $q = 0$, $\mathcal{A}^0$ and $\mathcal{A}^1$ are 5×5 matrices and the eigenvalues are

$$\lambda_1 = v, \quad \lambda_{2,3} = v \pm c_s,$$

where $c_s = \sqrt{(5/3)k_B T/m}$ is the usual sound speed for a polytropic gas with $\gamma = 5/3$.

The results of the analysis of the last two cases are also mentioned in Ref. [3]. Whereas the sound speed c_s has a precise and well known physical meaning, the role of the velocity c^* is obscure. As we shall see, the time independent equations become singular when v approaches c^*, in the case $k \neq 0$, $\mu = 0$. This singularity is unphysical and it disappears when $\mu \neq 0$, or μ and k are both zero. This result is general because the eigenvalues do not depend on $\mathbf{B}$ and therefore they are the same for any choice of the collisional term Q_ε, Q_v.

4. Non-dimensional equations.

It is useful to introduce non dimensional variables, through the following scale transformations

$$x = \bar{L}X, \quad n = \bar{n}\nu, \quad v = \sqrt{\frac{k_B}{m}T_0}\, w, \quad T = T_0\,\theta, \quad E = \frac{k_B T_0}{e\bar{L}}\,\eta,$$

$$V = \frac{k_B T_0}{e}\,\phi, \quad q = \sqrt{\frac{k_B}{m}T_0}\, k_B T_0 \bar{n}\,\zeta, \quad \tilde{p} = \bar{n}\, k_B T_0\,\psi,$$

where $\bar{L}$ is a characteristic length and $\bar{n}$ a characteristic electron density in the device.

We are interested in time independent solutions. In the new variables the stationary equations (3.1) become

$$
\text{(4.1)}\qquad \begin{cases} (\nu w)' = 0 \\ \\ \left(\nu w^2 + \nu\theta + \psi\right)' + \nu\eta = C_v \\ \\ \left[\dfrac{1}{2}\nu\left(5\theta + w^2\right)w + \psi w + \zeta\right]' + \nu w\eta = C_\varepsilon \\ \\ \eta' = c_1\left(\nu_0 - \nu\right) \\ \\ \eta = -\phi' \\ \\ \zeta = -k_0\,\nu\,\theta' \\ \\ \psi = -\mu_0\,\nu\,w' \end{cases}
$$

where

$$
c_1 = \frac{e^2\bar{L}^2\bar{n}}{\varepsilon k_B T_0},\quad k_0 = \frac{3\mu_{n0}}{2e\bar{L}}\sqrt{m k_B T_0},\quad \mu_0 = \frac{4}{3}k_0\bar{\mu},
$$

$$
\nu_0 = \nu_0(x) = \frac{1}{\bar{n}}\left(N_D - N_A\right),\quad Q_v = \frac{\bar{n}k_B T_0}{\bar{L}m}\,C_v,
$$

$$
Q_\varepsilon = \frac{\bar{n}k_B T_0}{\bar{L}}\sqrt{\frac{k_B}{m}T_0}\,C_\varepsilon,\quad {}' = \frac{d}{dX}.
$$

We do not specify here the form of the collisional terms, but we assume only that C_v and C_ε are some given continuous function of w and θ. The first equation is integrated immediately, giving

$$
\text{(4.2)}\qquad w\nu = J,
$$

J being a constant determined by the initial or boundary conditions. We assume that $J > 0$ so that w is always strictly positive. System (4.1) can be written as a set of three equations of second order, by eliminating the variables ζ, η, ψ

$$
\text{(4.3)}\qquad \begin{cases} \mu_0 w'' = ww' + \theta' - \dfrac{\theta}{w}w' + \dfrac{\mu_0}{w}(w')^2 - \phi' + K(w,\theta) \\ \\ k_0\theta'' = \dfrac{3}{2}w\theta' + \dfrac{k_0}{w}w'\theta' + \theta w' - \mu_0(w')^2 + H(w,\theta) \\ \\ \phi'' = -c_1\left(\nu_0 - \dfrac{J}{w}\right) \end{cases}
$$

where $K(w,\theta) = -wC_v/J$, $H(w,\theta) = (w^2C_v - wC_\varepsilon)/J$. For $\mu_0 = 0$ the first equation reduces to a first order equation and system (4.3) becomes

$$(4.4)\qquad \begin{cases} \left(\dfrac{\theta}{w} - w\right) w' = \theta' - \phi' + K(w,\theta) \\ k_0\theta'' = \dfrac{3}{2}w\theta' + \dfrac{k_0}{w}w'\theta' + \theta w' + H(w,\theta) \\ \phi'' = -c_1\left(\nu_0 - \dfrac{J}{w}\right) \end{cases}$$

When $w^2 = \theta$, the coefficient of w' in the first equation vanishes and the system becomes singular. In the physical variables this condition corresponds to $v = c^*$.

A qualitative analysis of systems (4.3) and (4.4) near the surface $\theta = w^2$ was performed by the authors (see Ref. [4]).

5. The Baccarani-Wordeman model.

We apply our results to the model described in Ref. [1]. The expressions for the collisional terms are

$$\mathbf{Q}_v = -\frac{eT}{m\mu_{n0}T_0}n\mathbf{v},$$

$$Q_\varepsilon = -\left(W - \frac{3}{2}nk_B T_0\right)\left(\frac{m}{2}\frac{\mu_{n0}}{e}\frac{T_0}{T} + \frac{3}{2}\frac{\mu_{n0}}{ev_s^2}k_B\frac{TT_0}{T+T_0}\right)^{-1}$$

From the non-dimensional form of the collisional terms we obtain

$$K(w,\theta) = \frac{3}{2k_0}\theta w, \quad H(w,\theta) = \frac{9\theta}{2k_0}\frac{w_s^2(\theta^2-1) - (\theta w)^2}{w_s^2(\theta+1) + 3\theta^2}.$$

We used the following numerical values of the parameters: silicon effective mass, $m = 0.26m_e$, where m_e is the electron rest mass; silicon dielectric constant: $\varepsilon_r = 11.7$; mobility $\mu_{n0} = 1400\text{cm}^2/(\text{s}\cdot\text{V})$, saturation velocity $v_s = 10^7\text{cm/s}$ (see [1]), lattice temperature $T_0 = 300°K$, characteristic electron density $\bar{n} = 2\times 10^{15}\text{cm}^{-3}$, characteristic length $\bar{L} = 0.1\mu\text{m}$.

An explicit solution of system (4.1), for constant ν_0, is obtained by assuming that all quantities but ϕ are constant. One exact solution is the following

$$\zeta_* = \psi_* = 0\ ,\ \nu_* = \nu_0.$$

The other equations become

$$\nu_* w_* = J,$$

$$\nu_* \eta_* = -\frac{3J}{2k_0}\theta_*,$$

$$\frac{3J}{2k_0}\theta_* w_* = \frac{3}{2k_0}\nu_*\theta_*(\theta_*+1)w_s^2\frac{3\theta_* - 3 + w_*^2}{w_s^2(\theta_*+1)+3\theta_*^2}.$$

From these equations we obtain

$$\theta_*^2(w_s^2 - w_*^2) = w_s^2, \quad \eta_* = -\frac{3}{2k_0}w_*\theta_*.$$

If $w_s > w_*$, i.e. if the velocity is smaller than the saturation speed, we obtain

$$\begin{aligned}
\theta_* &= \frac{w_s}{\sqrt{w_s^2 - w_*^2}}, \\
\eta_* &= -\frac{3w_*}{2k_0}\frac{w_s}{\sqrt{w_s^2 - w_*^2}}, \\
\phi_* &= \frac{3w_*}{2k_0}\frac{w_s}{\sqrt{w_s^2 - w_*^2}}X + \text{costante}.
\end{aligned} \tag{5.1}$$

Such a solution has a precise physical meaning. It corresponds to the following boundary conditions: assign values of the electric potential, set the electron density equal to the doping density and impose zero heat flux.

Let us consider this solution as a solution of an initial value problem. If we perturb the initial data, then the perturbation will be amplified by a factor that depends exponentially on the product of the device length and the eigenvalues of the matrix that defines the linearised system. The error amplification factor depends on the real part of the eigenvalues λ_i and is given by $\exp(\max_i \Re\lambda_i L)$, where L is the interval of integration. Let us linearise system (4.3) around the solution (5.1). The characteristic equation becomes

(5.2)

$$\begin{vmatrix}
\mu_0\lambda^2 - w_*\lambda + \dfrac{\theta_*}{w_*}\lambda - \dfrac{3}{2k_0}\theta_* & -\lambda - \dfrac{3}{2k_0}w_* & \lambda \\
-\lambda\theta_* + \dfrac{9}{k_0}\dfrac{\theta_*^3 w_*}{w_s^2(\theta_*+1)+3\theta_*^2} & k_0\lambda^2 - \dfrac{3}{2}w_*\lambda - \dfrac{9}{k_0}\dfrac{w_s^2}{w_s^2(\theta_*+1)+3\theta_*^2} & 0 \\
c_1\dfrac{\nu_*}{w_*} & 0 & \lambda^2
\end{vmatrix} = 0$$

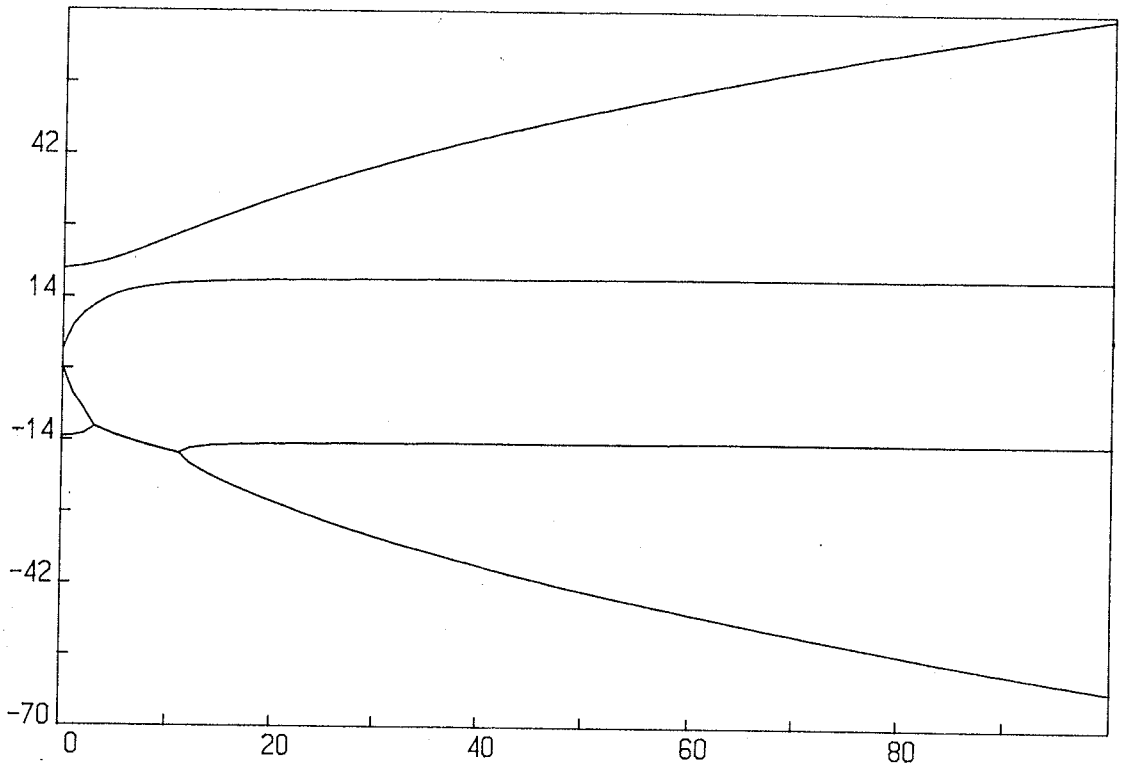

Fig. 1 - Dispersion relation for the linear problem. Real part of λL versus doping density (in units $2 \times 10^{15}\text{cm}^{-3}$). Inviscid model. Applied potential: $\Delta V = 0.1V$.

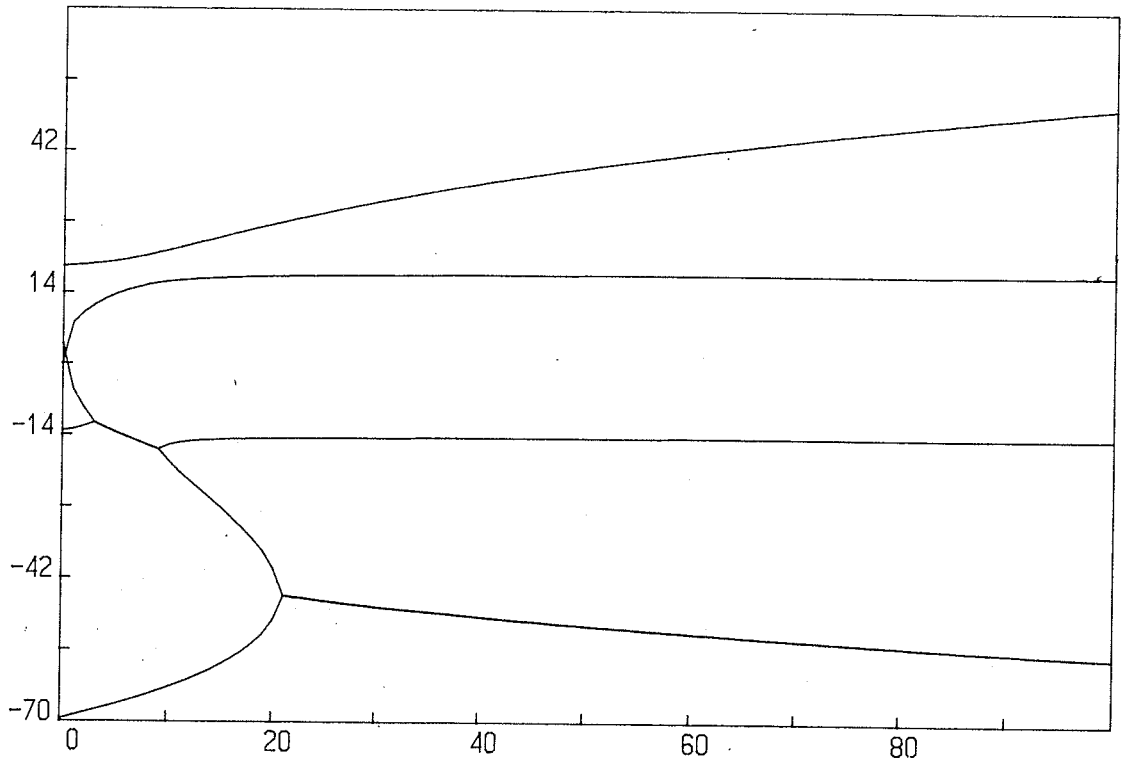

Fig. 2 - Dispersion relation for the linear problem. Real part of λL versus doping density (in units $2 \times 10^{15}\text{cm}^{-3}$). Viscous model with viscosity parameter $\bar{\mu} = 1$. Applied potential: $\Delta V = 0.1V$.

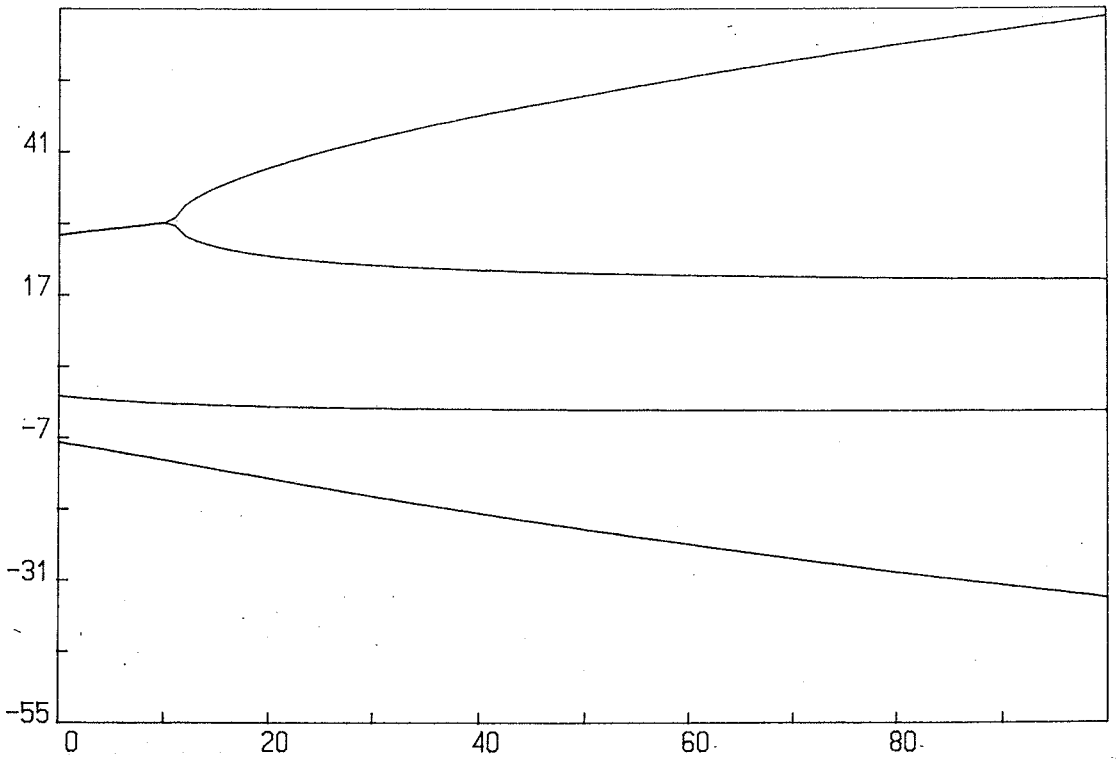

Fig. 3 - Dispersion relation for the linear problem. Real part of λL versus doping density (in units $2 \times 10^{15}\text{cm}^{-3}$). Inviscid model. Applied potential: $\Delta V = 1V$.

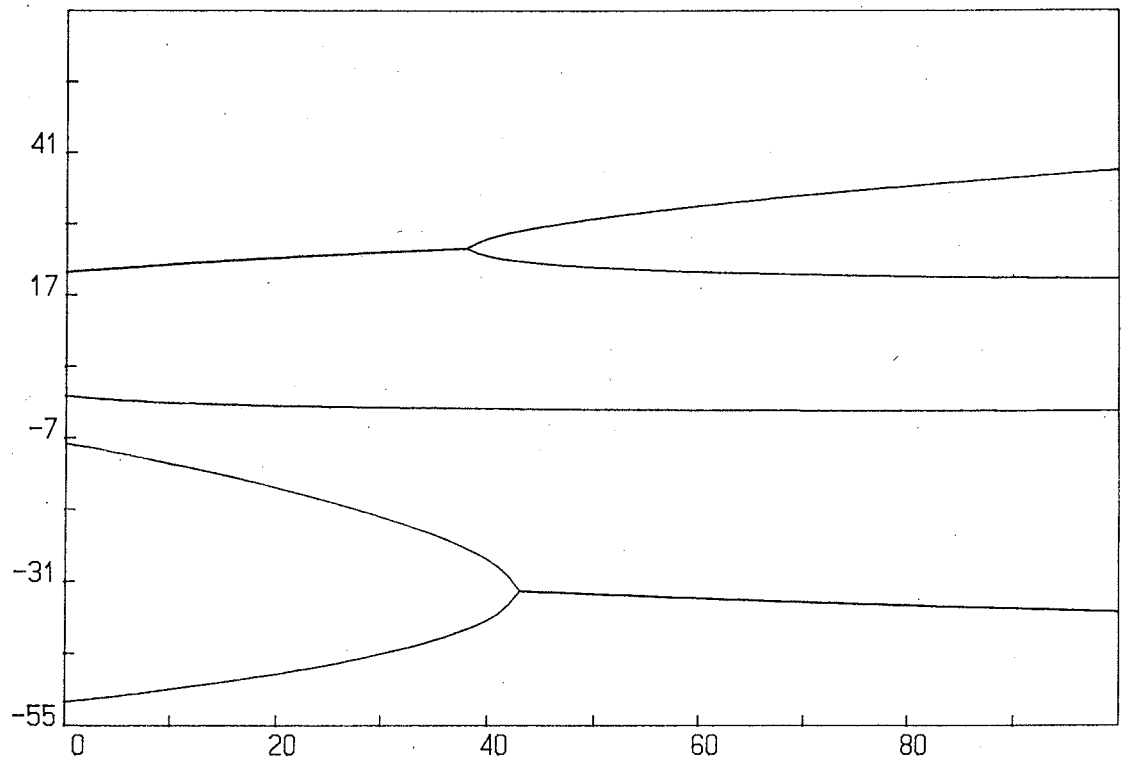

Fig. 4 - Dispersion relation for the linear problem. Real part of λL versus doping density (in units $2 \times 10^{15}\text{cm}^{-3}$). Viscous model with viscosity parameter $\bar{\mu} = 1$. Applied potential: $\Delta V = 1V$.

The characteristic equation corresponding to system (4.4) is obtained from (5.2) simply by setting $\mu_0 = 0$. Let us study the dependence of the real part of the solutions of the characteristic equations on the doping density, for typical values of the parameters. Figure 1 shows the real part λ_R of λ multiplies by L as a function of the doping density $N_D - N_A$. The device length is 0.6μm and the applied potential is $0.1V$.

In Figure 1 we plot the solutions for system (4.4), and in Figure 2 we give the real parts of the eigenvalues corresponding to system (4.3). In the first case there are 4 non zero eigenvalues (the fifth eigenvalue is zero, because the electric potential does not appear directly in the equations, but only through the electric field), while in the second case there are 5 non zero eigenvalues. Note how two branches collapse into one when the eigenvalues become complex. The conditioning of the problem depends critically on the doping. For small values of ν_0 the real parts of the eigenvalues are rather small, and the initial value problem is rather well-conditioned. In inviscid case an eigenvalue appears with negative real part and large absolute value. This makes the numerical integration problem moderately stiff. For high doping the real parts become large in absolute value, and with both positive and negative sign. This makes the initial value problem ill-conditioned, when integrating in both directions.

In Figure 2 and 3 we report the behavior of the eigenvalues for an applied potential of $1V$. The conditioning of the problem is still bad for high doping. Such large eigenvalues make the numerical treatment of the models very difficult, especially for high doping [3].

Acknowledgments.

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REFERENCES

[1] Baccarani G., Wordeman M. R., *An investigation of steady state velocity overshoot effects in Si and GaAs devices*, Solid State Electron. **ED-29** (1982), 970-977.

[2] Blotekjaer K., *Transport equations for electrons in two-valley semiconductors*, IEEE Trans. Electron Devices **ED-17** (1970), 38-47.

[3] Gardner C. L., Jerome J. W., Rose D. J., *Numerical Methods for the Hydrodynamic Device Model: Subsonic Flow*, IEEE Transactions on Computer Aided Design (5) **8** (1989), 501-507.

[4] Majorana A., Russo G., *Stationary solutions of hydrodynamic models for semiconductor device simulation* (1991), preprint.

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