


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A DETERMINISTIC PARTICLE METHOD
FOR THE SIMULATION OF THE BOLTZMANN
TRANSPORT EQUATION OF SEMICONDUCTORS

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Abstract

We present a deterministic simulation scheme for the Boltzmann Semiconductor Equation. The convergence of the method is shown for a simplified space homogeneous case. Numerical experiments, which are very promising, are also given in this situation. The extension for the application to the space inhomogeneous equation with a self consistent electric field is quoted. Theoretical considerations in that case are in preparation.

1. Introduction

In this paper we present a new deterministic particle method for the numerical solution of a one-dimensional space-homogeneous transport equation, which describes the carrier transport in semiconductors.

Most of the numerical studies in semiconductor-modelling are based upon the drift-diffusion equations. But as turned out in the last few years, these equations are not an adequate tool to describe the transport-phenomena appearing in semiconductors with very small structures, like the new submicron chips.

A more suitable description of such devices is given by the following kinetic equation

$$\begin{aligned} \frac{\partial f(t, \mathbf{x}, \mathbf{k})}{\partial t} + \mathbf{v} \cdot \nabla_{\mathbf{x}} f(t, \mathbf{x}, \mathbf{k}) + E(t, \mathbf{x}) \cdot \nabla_{\mathbf{k}} f(t, \mathbf{x}, \mathbf{k}) &= I[f](\mathbf{x}, \mathbf{k}) \\ I[f](\mathbf{x}, \mathbf{k}) &= \int Q(\mathbf{k}, \mathbf{k}') \cdot (f(t, \mathbf{x}, \mathbf{k}') - f(t, \mathbf{x}, \mathbf{k})) d\mathbf{k}', \\ \mathbf{v} &= \mathbf{g}(\mathbf{k}), \\ \operatorname{div} E(t, \mathbf{x}) &= \int f(t, \mathbf{x}, \mathbf{k}) d\mathbf{k} - n(t, \mathbf{x}). \end{aligned} \tag{1}$$

Our aim is to find a numerical method to compute the distribution function $f(t, \mathbf{x}, \mathbf{k})$. Since this is quite difficult, we restrict our considerations to a simplified case.

We will investigate the following, one-dimensional, homogeneous transport equation with a time-dependent electric field:

$$\begin{aligned} \frac{\partial f(t, k)}{\partial t} + E(t) \frac{\partial f(t, k)}{\partial k} &= I[f](k) \\ I[f](k) &= \int P(k, k') f(t, k') dk' - f(t, k) \int Q(k, k') dk'. \end{aligned} \tag{2}$$

In order to solve this equation, we use a generalized version of the deterministic particle method introduced in [6].

This paper is organized as follows:

In chapter 2 we explain the physical background of our problem. Afterwards the numerical method is introduced. In chapter 4 it is applied to two physically relevant problems, the so-called relaxation time models [1]. In the last chapter we will give some comments on the extension of our method to the general case of solving the kinetic equation (1).

2. The Transport-Equation

In order to understand the physical background of our equation we use the following model. For a detailed presentation we refer to [4],[8],[9]. We describe the electron distribution in a semiconductor by the density - function $f(t, \mathbf{x}, \mathbf{k})$, $t \in \mathbb{R}$, $\mathbf{x} \in \mathbb{R}^3$, $\mathbf{k} \in \mathbb{R}^3$, where t denotes the time, \mathbf{x} the space coordinate and \mathbf{k} the wavevector. The probability of finding at time t an electron with wavevector \mathbf{k} in the interval $[\mathbf{x}, \mathbf{x} + \Delta \mathbf{x}]$ is equal to $f(t, \mathbf{x}, \mathbf{k}) d\mathbf{x}$. The time dependence of f is caused by diffusion effects, external fields and collisions.

First we consider the influence of the diffusion effects. If $v(\mathbf{k})$ denotes the velocity of an electron with wavevector \mathbf{k} , then the carriers in this state move in the time t a distance $t \cdot v(\mathbf{k})$. Thus, according to Liouville's theorem on the invariance of volume in the phase space, the number of carriers in the neighbourhood of \mathbf{x} at time t is equal to the number of carriers in the neighbourhood of $\mathbf{x} - t \cdot v(\mathbf{k})$ at time 0.

$$\Rightarrow f(t, \mathbf{x}, \mathbf{k}) = f(0, \mathbf{x} - t \cdot v(\mathbf{k}), \mathbf{k}).$$

This means, that the change of density $f(t, \mathbf{x}, \mathbf{k})$ caused by diffusion is

$$(3) \quad \left. \frac{\partial f(t, \mathbf{x}, \mathbf{k})}{\partial t} \right|_{\text{Diff}} = -v(\mathbf{k}) \cdot \nabla_{\mathbf{x}} f(t, \mathbf{x}, \mathbf{k}).$$

In consequence of an electric field one obtains for the \mathbf{k} -vector

$$\dot{\mathbf{k}} = E(t, \mathbf{x}).$$

$$\Rightarrow f(t, \mathbf{x}, \mathbf{k}) = f(0, \mathbf{x}, \mathbf{k} - \dot{\mathbf{k}} \cdot t) \Rightarrow$$

$$(4) \quad \left. \frac{\partial f(t, \mathbf{x}, \mathbf{k})}{\partial t} \right|_{\text{el. Field}} = -E(t, \mathbf{x}) \cdot \nabla_{\mathbf{k}} f(t, \mathbf{x}, \mathbf{k}).$$

The distribution changes because of elastic scattering at the rate

$$(5) \quad \left. \frac{\partial f(t, \mathbf{x}, \mathbf{k})}{\partial t} \right|_{\text{Scatt}} = \int (P(\mathbf{k}, \mathbf{k}') \cdot (f(t, \mathbf{x}, \mathbf{k}') \cdot (1 - f(t, \mathbf{x}, \mathbf{k}))) - Q(\mathbf{k}, \mathbf{k}') \cdot (f(t, \mathbf{x}, \mathbf{k}) \cdot (1 - f(t, \mathbf{x}, \mathbf{k}'))) d\mathbf{k}.$$

$Q(\mathbf{k}, \mathbf{k}')$ is the transition probability from \mathbf{k} to \mathbf{k}' , whereas $P(\mathbf{k}, \mathbf{k}') = Q(\mathbf{k}', \mathbf{k})$ denotes the probability for a transition from \mathbf{k}' to \mathbf{k} .

For the total change in time of the distribution - function $f(t, \mathbf{x}, \mathbf{k})$ we have

$$\frac{\partial f(t, \mathbf{x}, \mathbf{k})}{\partial t} = \left. \frac{\partial f(t, \mathbf{x}, \mathbf{k})}{\partial t} \right|_{\text{Diff}} + \left. \frac{\partial f(t, \mathbf{x}, \mathbf{k})}{\partial t} \right|_{\text{el. Field}} + \left. \frac{\partial f(t, \mathbf{x}, \mathbf{k})}{\partial t} \right|_{\text{Scatt}}$$

Together with (3), (4) and (5) we get the following transport - equation

$$\frac{\partial f(t, \mathbf{x}, \mathbf{k})}{\partial t} + v(\mathbf{k}) \nabla_{\mathbf{x}} f(t, \mathbf{x}, \mathbf{k}) + E(t, \mathbf{x}) \nabla_{\mathbf{k}} f(t, \mathbf{x}, \mathbf{k}) = I[f](\mathbf{x}, \mathbf{k}),$$

$$(6) \quad I[f](\mathbf{x}, \mathbf{k}) = \int \left(P(\mathbf{k}, \mathbf{k}') \cdot (f(t, \mathbf{x}, \mathbf{k}') \cdot (1 - f(t, \mathbf{x}, \mathbf{k}))) \right. \\ \left. - Q(\mathbf{k}, \mathbf{k}') \cdot (f(t, \mathbf{x}, \mathbf{k}) \cdot (1 - f(t, \mathbf{x}, \mathbf{k}'))) \right) d\mathbf{k}'.$$

For weakly doped semiconductors we may assume, that $f(t, \mathbf{x}, \mathbf{k})$ is small compared with one, so that we can approximate $1 - f(t, \mathbf{x}, \mathbf{k})$ by 1. With this simplification we receive the linearized form of the collision - term

$$\frac{\partial f(t, \mathbf{x}, \mathbf{k})}{\partial t} + v(\mathbf{k}) \nabla_{\mathbf{x}} f(t, \mathbf{x}, \mathbf{k}) + E \nabla_{\mathbf{k}} f(t, \mathbf{x}, \mathbf{k}) = I[f](\mathbf{x}, \mathbf{k}),$$

$$(7) \quad I[f](\mathbf{x}, \mathbf{k}) = \int (P(\mathbf{k}, \mathbf{k}') f(t, \mathbf{x}, \mathbf{k}') - Q(\mathbf{k}, \mathbf{k}') f(t, \mathbf{x}, \mathbf{k})) d\mathbf{k}'.$$

In this paper we will restrict our investigations to the easier, one - dimensional, space - homogeneous case. We consider the following problem

$$\frac{\partial f(t, k)}{\partial t} + E(t) \frac{\partial f(t, k)}{\partial k} = I[f](k)$$

$$(8) \quad I[f](k) = \int P(k, k') f(t, k') dk' - f(t, k) \int Q(k, k') dk'.$$

P and Q are uniform Lipschitz - continuous functions with

$$\int P(k, k') dk' - \int Q(k, k') dk'.$$

f is the integrable solution of (8) with the initial condition

$$f_0(k) = f(0, k)$$

and the normalization

$$\int_{\eta} f_0(k) dk = 1.$$

E is also a uniform Lipschitz - continuous function.

3. The Method

Based on the particle method used in [6] for the calculation of the transport equation

$$\frac{\partial f(t, k)}{\partial t} = \int P(k, k') f(t, k') dk' - f(t, k) \int Q(k, k') dk'$$

we develop a numerical procedure for the simulation of (8).

In that case, two effects are responsible for a change of the wavevector k of a particle: the external electric field $E(t)$ and the collision term $I[f]$. The simultaneous numerical handling of those effects is not very practicable. Therefore we distinguish between the collision and the drift phase.

The drift, which is the change of the wavevector k at time t coming from the electric field, is given by

$$(9) \quad T_{\tau t} k := k + \int_t^{\tau} E(\rho) d\rho.$$

At first we approximate the differential operator

$$D := \frac{\partial}{\partial t} + E(t) \frac{\partial}{\partial k}$$

by

$$\frac{1}{\Delta t} [f(t_{n+1}, T_{t_n, t_{n+1}}(k)) - f(t_n, k)].$$

With $f^n(\cdot) := f(t_n, \cdot)$ and $G(k) := \int Q(k, k') dk'$ we get the following scheme:

$$(10) \quad \begin{aligned} f^{n+1}(T_{t_n, t_{n+1}}(k)) &= f^n(k) + \Delta t I[f^n](k) \\ &= (1 - \Delta t G(k)) f^n(k) + \Delta t \int_{\mathbb{R}^3} P(k, k') f^n(k') dk'. \end{aligned}$$

If $1 - \Delta t G(k) \geq 0$, the non-negativity of f^0 is preserved.

As above mentioned, we divide one timestep into two parts

a) Computation of the collision

$$(11) \quad \hat{f}^{n+1}(k) = f^n(k) + \Delta t I[f^n](k).$$

b) Calculation of the drift

$$(12) \quad f^{n+1}(k) = \hat{f}^{n+1}(T_{t_n, t_{n+1}}(k)).$$

Because of the non-negativity and the conservation-property $\int f^n(k) dk = 1$, we can interpret f^n as the density function of an absolutely continuous probability measure μ^n , which can be approximated by a discrete measure μ_N^n of the form

$$(13) \quad \mu_N^n := \frac{1}{N} \sum_{i=1}^N \delta(k - k_i^n).$$

To obtain from k_i^n the values \hat{k}_i^{n+1} , which take into account the effect of the collision term, we replace in the Euler-scheme (10) the function f^n by the measure μ_N^n . This yields to the measure

$$(14) \quad v_N^n = (1 - \Delta t G(k)) \mu_N^n + \Delta t \int_{\mathbb{T}} P(k, k') \mu_N^n(dk'),$$

which consists of a discrete and a continuous part.

To evaluate now a discrete approximation of v_N^n , we use the technique of [6]. At first we determine \hat{k}_i by

$$(15) \quad \frac{i}{N} = \int_{\hat{k}_0}^{\hat{k}_i} dv_N^n, \quad i = 1(1)N$$

and then we compute \hat{k}_i^{n+1} from

$$(16) \quad \hat{k}_i^{n+1} = N \int_{\hat{k}_{i-1}}^{\hat{k}_i} k dv_N^n(dk), \quad i = 1(1)N.$$

So the \hat{k}_i^{n+1} are the mean values of the intervals $[\hat{k}_{i-1}, \hat{k}_i]$.

It remains to consider the influence of the external electric field $E(t)$. Therefore we approximate the drift $T_{\tau t_n} k$ by

$$\bar{T}_{\tau t_n} k = k + (\tau - t_n) E(t_n)$$

and calculate the k_i^{n+1} by

$$(17) \quad k_i^{n+1} = \hat{k}_i^{n+1} + \Delta t E(t_n).$$

This results in the measure

$$(18) \quad \mu_N^{n+1} = \frac{1}{N} \sum_{i=1}^N \delta(k - k_i^{n+1}).$$

This is an approximation of μ^{n+1} and therefore of f^{n+1} .

The convergence of the numerical method presented above, in the case of a periodic geometry, was shown in [3] by proving the following

Theorem.

Let $f : [0, \hat{t}] \times T_1 \rightarrow \mathbb{R}^+$, $\hat{t} > 0$ be the integrable solution of the equation

$$\frac{\partial f(t, k)}{\partial t} + E(t) \frac{\partial f(t, k)}{\partial k} = \int_{T_1} P(k, k') f(t, k') dk' - f(t, k) \int_{T_1} Q(k, k') dk',$$

$T_j \sim [0, 1]^j$, j - dimensional Torus,

$P, Q : T_2 \rightarrow \mathbb{R}^+$ uniformly Lipschitz - continuous functions with

$$\int_{T_1} P(k, k') dk = \int_{T_1} Q(k', k) dk,$$

$Q(k, k') = Q(k+z, k'+z')$, $P(k, k') = P(k+z, k'+z')$, $z, z' \in \mathbb{Z}$,

$$\int_{T_1} f_0(k) dk = 1, \quad f(t, k) = f(t, k+z), \quad z \in \mathbb{Z},$$

$E : [0, \hat{t}] \rightarrow \mathbb{R}$ uniformly Lipschitz - continuous.

Then the sequence of discrete probability measures μ_N^n , defined by (15), (16), (17) and (18), converges to the measure μ , where

$$\mu(dk) = f(t, k) dk$$

for any finite time interval, if $\Delta t \rightarrow 0$, N and $N \Delta t \rightarrow \infty$, provided that $\lim \mu_N^0 = \mu^0$.

Remark.

Under certain assumptions, the convergence for the case of an unbounded domain can be obtained using a transformation from the unbounded region to the torus (see [3],[6]). Otherwise we only get weak convergence in any finite interval of the unbounded domain. But for physically relevant models we assume, that the $f(t, \cdot)$ are the density functions of a tight class of measures, so that it is enough to consider a compact interval.

4. Numerical Results

In this section we present some applications of our procedure. To show, that our scheme is able to produce accurate results, we investigate two models, which were already used in [2] to test a deterministic particle method (for a detailed description of the models we refer to [1],[2]). The advantage of this models is, that one can obtain analytical solutions, which can be compared with the numerical computations.

The first test case is the simplest relaxation time model, which is described by the following equation

$$(19) \quad \frac{\partial f(t,k)}{\partial t} - \frac{q}{h} E \frac{\partial f(t,k)}{\partial k} = \frac{1}{\tau} \int_{\mathbb{R}} (M_T(k) f(t,k') - M_T(k') f(t,k)) dk'$$

Here is

$$M_T(k) = \frac{h}{\sqrt{2\pi m^* k_B T}} e^{-\frac{\epsilon(k)}{k_B T}}$$

the Maxwell - distribution to the temperature $T (= 77 \text{ K})$.

The constants in (19) are

$\epsilon(k) := \frac{h k^2}{2m^*}$	the kinetic energy of the state k ,
$h = \frac{h}{2\pi}$	the reduced Planck constant,
$m^* = 0.067 m_0$	the effective electron mass,
$k_B = 1.38062 \cdot 10^{-23} \frac{\text{J}}{\text{K}}$	the Boltzmann constant,
$q = 1.602192 \cdot 10^{-19} \text{ As}$	the electron charge,
$\tau \in [10 \text{ fs}, 1 \text{ ns}]$	the relaxation time.

For the computation we have chosen the following inputs :

$$E = 10^6 \frac{\text{V}}{\text{m}},$$

$$\tau = 10^{-13} \text{ s},$$

$$\Delta t = 10^{-15} \text{ s},$$

$$N = 255.$$

In figures 1.1 up to 1.5 ($t = 0, 0.5 \cdot 10^{-13} \text{ s}, 10^{-13} \text{ s}, 2 \cdot 10^{-13} \text{ s}, 3 \cdot 10^{-13} \text{ s}$) the numerical results (dots) are compared with the exact solution (lines).

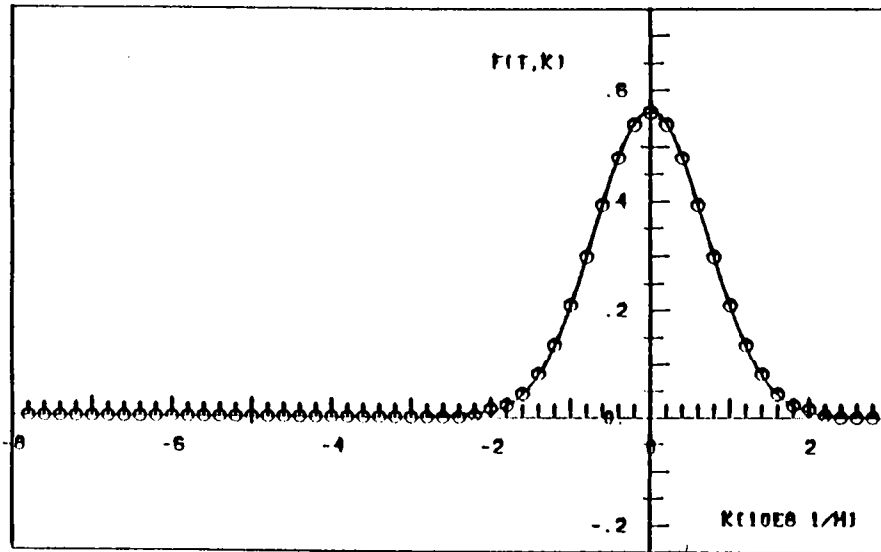


Fig. 1.1

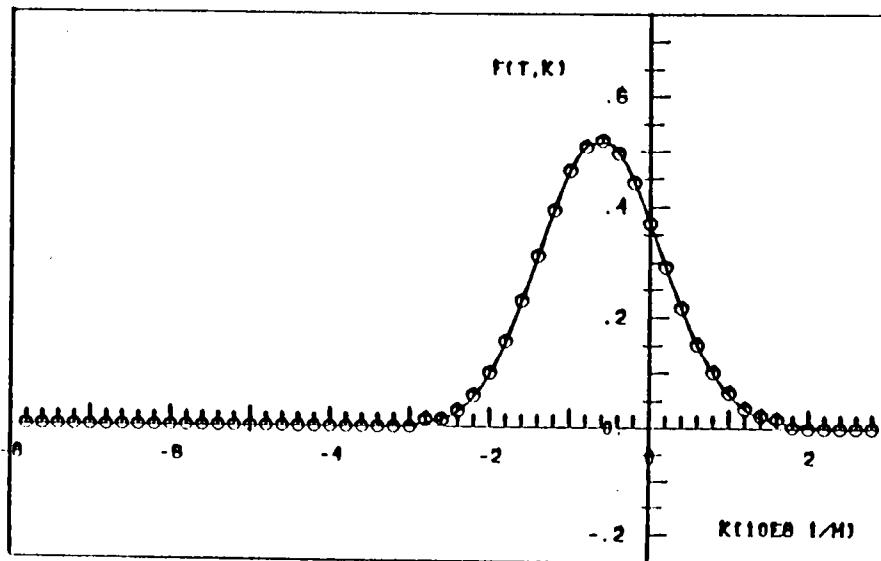


Fig. 1.2

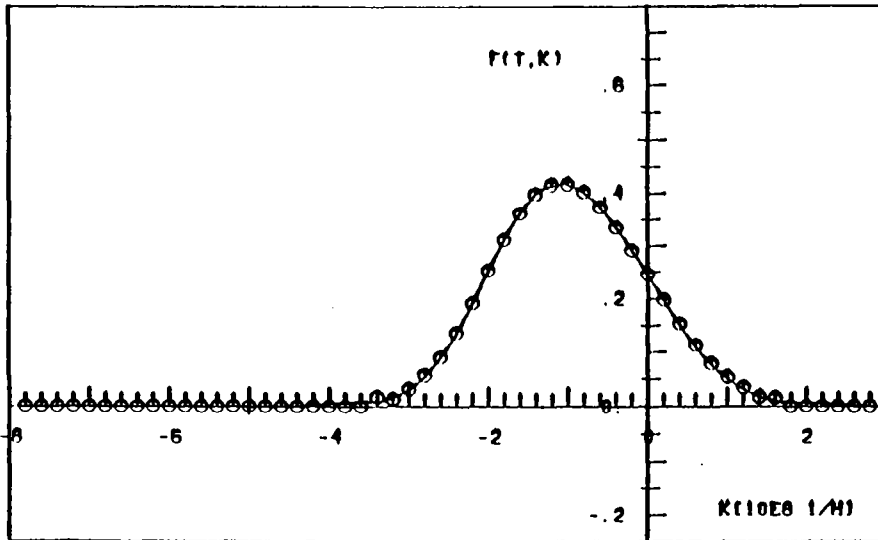


Fig. 1.3

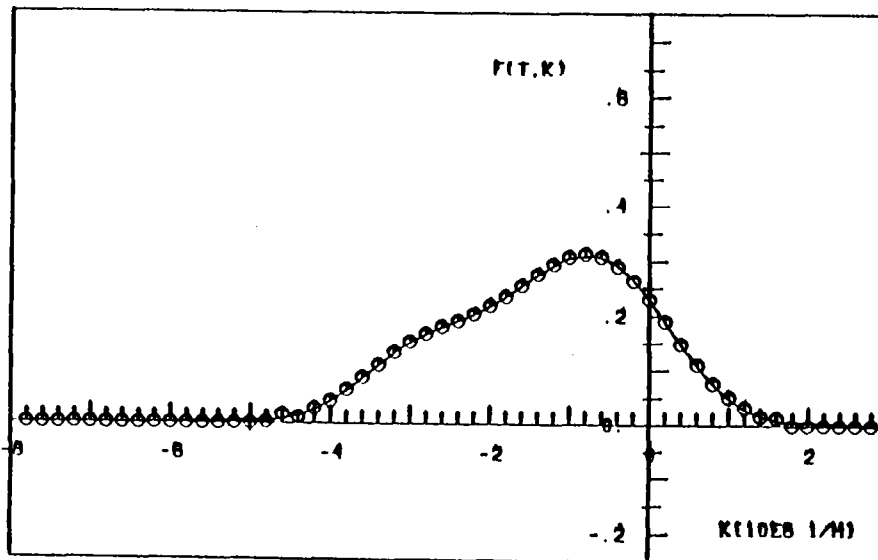


Fig. 1.4

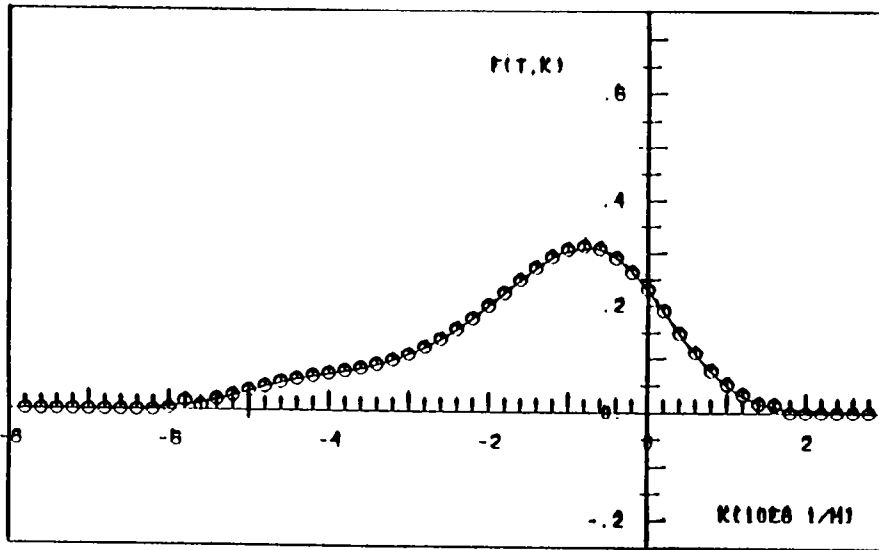


Fig. 1.5

For a second test, we apply the scheme to a relaxation time model for a polar optical scattering, given by

$$\frac{\partial f(t, k)}{\partial t} - \frac{q}{\hbar} E \frac{\partial f(t, k)}{\partial k} = \int_{\mathbb{R}} P(k, k') f(t, k') dk' - f(t, k) \int_{\mathbb{R}} Q(k, k') dk',$$

$$(20) \quad P(k, k') = \frac{M_T(k)}{\tau(k) \tau(k') \int_{\mathbb{R}} \frac{M_T(k)}{\tau(k)} dk},$$

$$Q(k, k') = \frac{M_T(k')}{\tau(k) \tau(k') \int_{\mathbb{R}} \frac{M_T(k)}{\tau(k)} dk}.$$

The relaxation time with a threshold is described by

$$\tau(k) = \begin{cases} \tau_1 & \text{if } \epsilon(k) \leq \epsilon_t \\ \tau_2 & \text{if } \epsilon(k) > \epsilon_t \end{cases}$$

The calculations, which yield to the figures 2.1 up to 2.5 were performed with the following parameters :

$$N = 255,$$

$$\epsilon_t = \hbar \omega_0 = 0.035 \text{ eV},$$

$$T = 77 \text{ K},$$

$$m^* = 0.067 m_0,$$

$$E = 10^5 \frac{\text{V}}{\text{m}},$$

$$\tau_1 = 10^{-11} \text{ s},$$

$$\tau_2 = 10^{-12} \text{ s}$$

and correspond to the times $t = 0, 5 \cdot 10^{-13} \text{ s}, 15 \cdot 10^{-13} \text{ s}, 30 \cdot 10^{-13} \text{ s}, 75 \cdot 10^{-13} \text{ s}.$

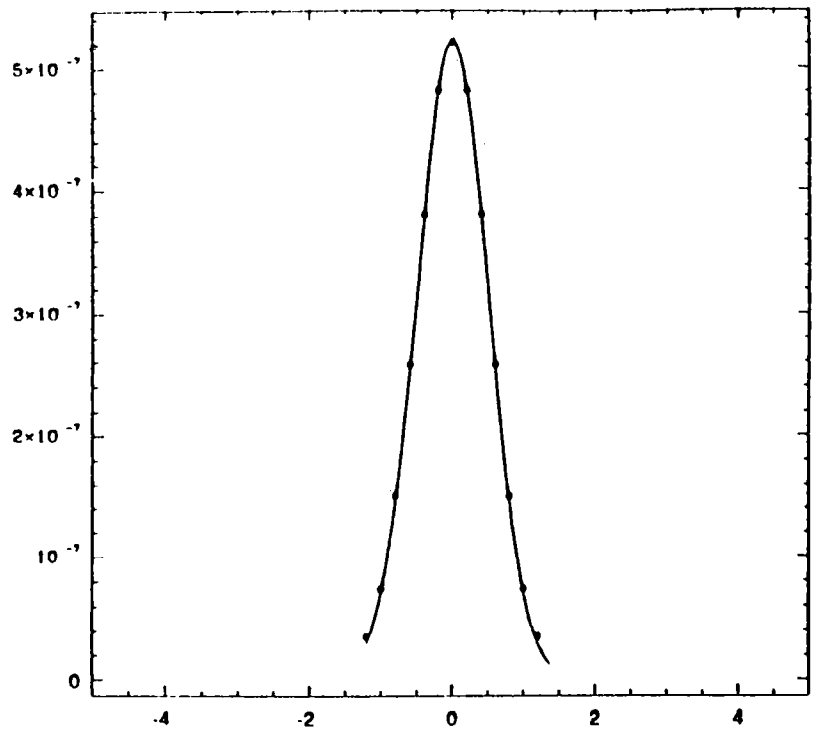


Fig 2.1

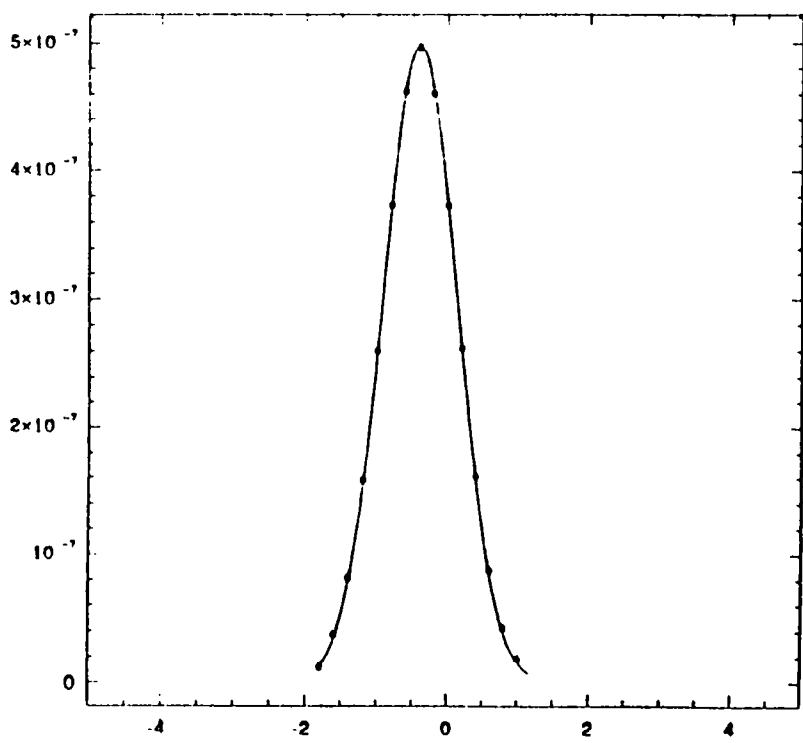


Fig. 2.2

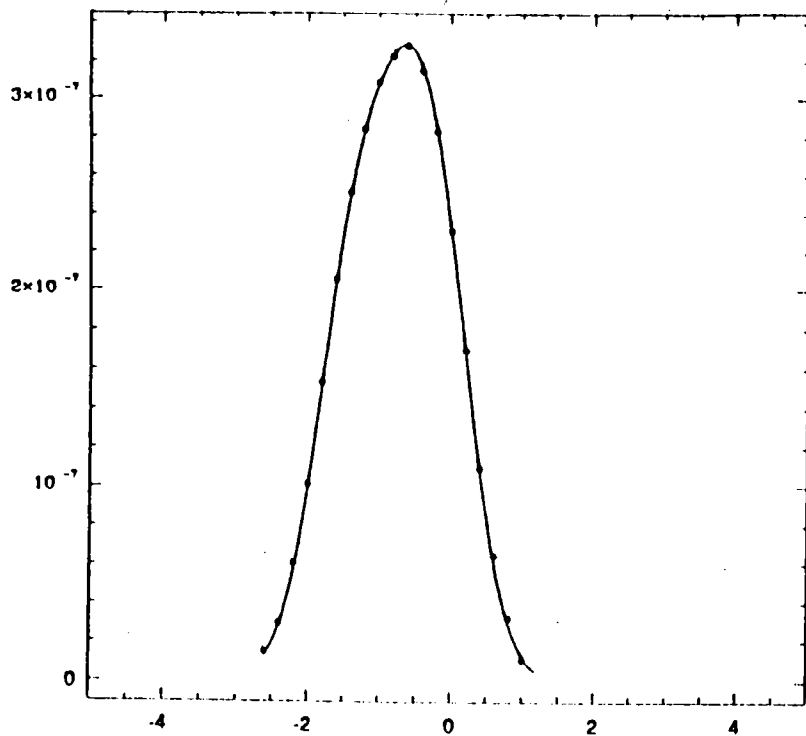


Fig. 2.3

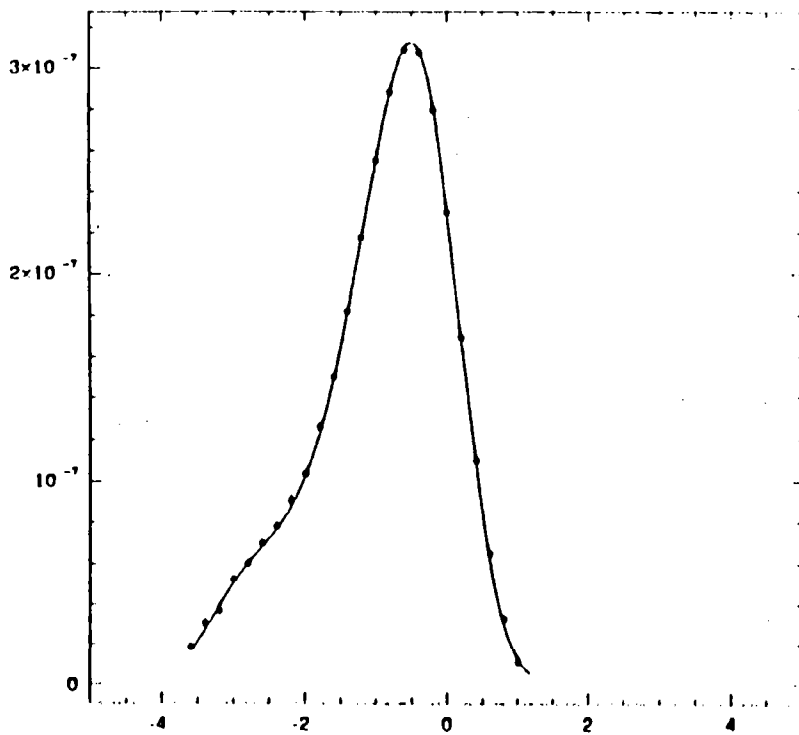


Fig. 2.4

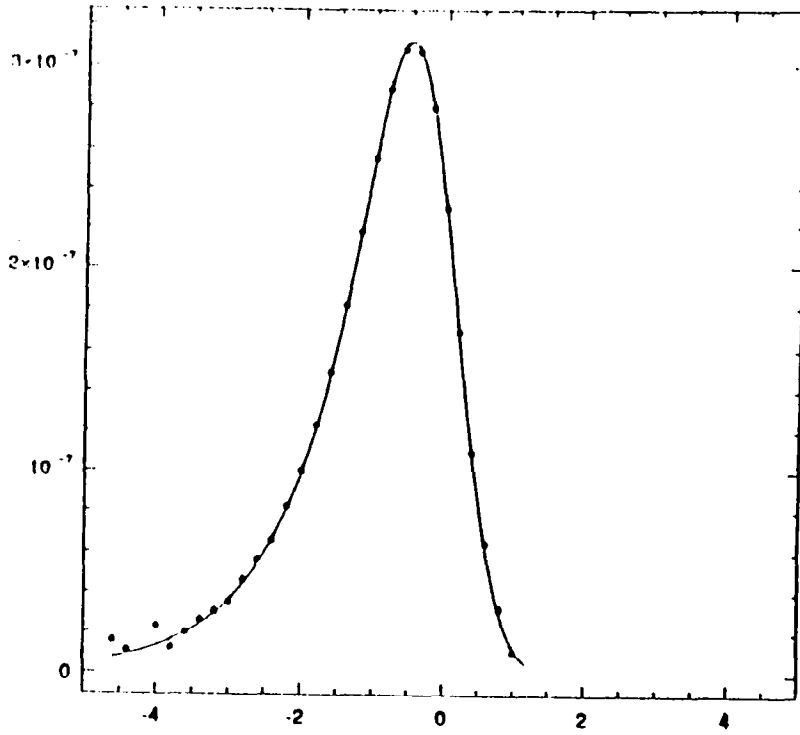


Fig. 2.5

5. Extension to the inhomogeneous case

In chapter 3 and 4 we dealt with a numerical procedure for the homogeneous field case, a simplified but physically relevant model. Our aim is to handle the full semiconductor equation (1) with a selfconsistent electric field. Therefore it is necessary to extend the method defined by (15), (16), (17) to the inhomogeneous case.

In [5] the numerical handling of a space - inhomogeneous linear transport equation without an electric field is presented. Now we will combine the schemes of [5] and chapter 3 to find a way to solve the full equation. Additionally, we have to take a look on how to compute the selfconsistent electric field $E(t, x)$. But since (1), neglecting the collision term $I[f]$, has a strong resemblance to the Vlasov equation from plasma physics, we can apply to it the same particle - in - cell methods.

As in chapter 3 we approximate the differential operator

$$D := \frac{\partial}{\partial t} + g(k) \nabla_x + E(t, x) \nabla_k$$

by

$$\frac{1}{\Delta t} [f(t_{n+1}, T_{t_n, t_{n+1}}(x, k)) - f(t_n, x, k)],$$

where T_{t_0} is the solution of the following system of ODE's :

$$\dot{x}(t) = g(k(t)),$$

$$\dot{k}(t) = E(t, x).$$

We get again for the collision and the drift phase

$$\hat{f}^{n+1}(x, k) = f^n(x, k) + \Delta t I[f^n](x, k),$$

$$f^{n+1}(x, k) = \hat{f}^{n+1}(T_{t_n, t_{n+1}}(x, k)).$$

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Interpretation of $f^n(\cdot)$ as the density function of a probability measure μ^n and approximation of μ^n by a discrete measure

$$\mu_N^n = \frac{1}{N} \sum_{i=1}^N \delta(x - x_i^n) \delta(k - k_i^n)$$

yields to the following numerical scheme :

- Approximation of the initial distribution f^0 by

$$\mu_N^0 = \frac{1}{N} \sum_{i=1}^N \delta(x - x_i^0) \delta(k - k_i^0).$$

For every time step

- 1) Splitting of the spatial range in intervals of equal size.
- 2) Space - homogeneous computation of the new k - values.
Replacing f^n in (20) by the discrete measure μ_N^n .
Rediscretization of the resulting measure ν_N^n with a discrete and a continuous part.
- 3) Calculation of the electric field using a particle - in - cell method.
- 4) Determination of the new particle position and velocity by

$$k_i^{n+1} = \tilde{k}_i^{n+1} + \Delta t E(t_n, x_i^n),$$

$$x_i^{n+1} = x_i^n + g(k_i^{n+1}).$$

The convergence proof of this method should result from the convergence proof of the homogeneous case with an electric field [3], the non-homogeneous case without an electric field [5] and on simultaneous consideration of the error occurring from the computation of $E(t,x)$. For a detailed proof and first numerical experiments we refer to [6].

6. Conclusions

We presented a deterministic particle method for the simulation of the Boltzmann transport equation of semiconductors. In the space-homogeneous case, the convergence is proved and the computer implementation gives accurate results for a small number of particles ($N = 255$). The extension to the space-inhomogeneous case including a selfconsistent electric field was quoted. A convergence proof and numerical experiments for this case are in preparation.

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