LE MATEMATICHE
Vol. LV (2000) – Fasc. I, pp. 161–168

A BGK TYPE APPROXIMATION FOR THE COLLISION OPERATOR OF THE TRANSPORT EQUATION FOR SEMICONDUCTORS

GIOVANNI MASCALI

In the attempt of obtaining macroscopic models which describe the flow of electrons through a semiconductor crystal, many authors start from the Boltzmann transport equation, often using a generalized BGK type approximation for the collision operator. In this work, by means of this approximation, we shall show that it is possible to obtain a new drift-diffusion equation valid in the high electric field regime.

1. Introduction and basic equations.

On a microscopic level, the electron transport in a semiconductor is modeled by the Boltzmann transport equation (BTE), [1], [2]

$$(1) \qquad \frac{\partial F}{\partial t} + \vec{v} \cdot \nabla_{\vec{x}} F - \frac{q}{m^*} \vec{E}(\vec{x}, t) \cdot \nabla_{\vec{v}} F = Q(F) \quad t > 0,\ \vec{x} \in \Re^3,\ \vec{v} \in \Re^3$$

where $F(t, \vec{x}, \vec{v})$ is the electron distribution function in the one-particle phase-space $(t, \vec{x}, \vec{v})$, $\vec{v} = \frac{1}{h} \nabla_{\vec{k}} \epsilon(\vec{k})$ is the electron group velocity, with $\epsilon(\vec{k})$ electron energy in the conduction band, and $\vec{k}$ the electron wave vector. We are using the

Entrato in Redazione il 21 dicembre 2000.

Key-words: Boltzmann equation, Chapman-Enskog expansion, drift-diffusion equation.

parabolic band approximation and, for the sake of simplicity, supposing that the conduction band is unique. q is the elementary charge, m^* the electron effective mass and Q the Boltzmann operator, which takes into account interactions of electrons with lattice-defects and electron-electron short-range interactions.

$\vec{E}(\vec{x}, t)$ is the electric field, sum of an external (applied to the crystal) and an internal field produced by an ion background, having density $C(\vec{x})$, and the carriers, i. e. $\vec{E} = -\nabla\Phi$ with Φ electric potential satisfying the Poisson equation

$$\nabla \cdot (\epsilon \nabla \Phi) = q\Big(\int F d^3v - C(\vec{x})\Big) \tag{2}$$

ϵ being the permittivity of the material.

The effort to solve this system directly by numerical methods seems to be a formidable task also for the present computing resources. Moreover solutions of kinetic equations contain, in many cases, a good deal of redundant information. For these reasons, many fluid dynamical models for semiconductors have been introduced in recent years.

One of the most used approaches for the derivation of these models starting from the Boltzmann equation, is based on perturbation arguments, [1], [2], which exploit the smallness of a dimensionless parameter, the scaled mean free path, appearing in an appropriately scaled version of the Boltzmann equation.

For high electric fields, a new convenient scaling seems to be that proposed by Poupaud in 1992 [3].

In this work, using this scaling and the Chapman-Enskog expansion, we will obtain an approximated drift-diffusion equation for the number density of carriers

$$\rho(\vec{x}, t) = \langle F \rangle,$$

henceforth the symbol $\langle f(\vec{v}) \rangle$ will denote the integral of any scalar or vector-valued measurable function $f = f(\vec{v})$ over the 3-dimensional Lebesgue measure d^3v, that is

$$\langle f \rangle = \int_{\Re^3} f(\vec{v})\, d^3v,$$

all functions appearing in this paper are understood to be Lebesgue measurable in all variables.

Moreover we will approximate the Boltzmann operator by means of a generalized BGK collision operator, that is by means of an operator having the form

$$Q(F) = \nu_1(\mathcal{E} - F) + (\nu_2 - \nu_1)(\mathcal{D} - F) + (\nu_3 - \nu_2)(\mathcal{F} - F) \tag{3}$$

where $\nu_i = \nu_i(\vec{x}, t)$ are strictly ordered mean relaxation rates:

$$0 < \nu_1 < \nu_2 < \nu_3.$$

Actually this is the third in a whole family of multiscale generalized BGK operators. We have maintained only the terms which give a contribution when one wants to derive a drift-diffusion equation.
In the above expression,

$$\mathcal{E} = \frac{\rho}{\sqrt{(\frac{2\pi\theta_L}{m^*})^3}} exp\Big(-\frac{m^*}{2\theta_L}v^2\Big)$$

is the lattice temperature Maxwellian, with θ_L lattice temperature and $\rho = \langle F \rangle$.

$$\mathcal{D} = \frac{\rho}{\sqrt{(\frac{2\pi\theta_L}{m^*})^3}} exp\Big(-\frac{m^*}{2\theta_L}(\vec{v}-\vec{u})^2\Big)$$

is a displaced lattice temperature Maxwellian with $\rho\vec{u} = \langle \vec{v}F \rangle$, $\vec{u}$ being the electron average velocity.
And

$$\mathcal{F} = \frac{\rho}{\sqrt{(\frac{2\pi\theta}{m^*})^3}} exp\Big(-\frac{m^*}{2\theta}(\vec{v}-\vec{u})^2\Big)$$

is a displaced Maxwellian with $\rho\frac{\theta}{m^*} = \frac{2}{3}\Big[\langle\frac{1}{2}v^2F\rangle - \frac{1}{2}\rho u^2\Big]$, θ being the electron temperature different from θ_L.
As a consequence of this choice, the following properties hold

1. $\langle \mathcal{E} - F \rangle = 0$
2. $\langle \begin{pmatrix} 1 \\ \vec{v} \end{pmatrix} (\mathcal{D} - F) \rangle = 0$
3. $\langle \begin{pmatrix} 1 \\ \vec{v} \\ v^2 \end{pmatrix} (\mathcal{F} - F) \rangle = 0$
4. $\langle Q(F) \rangle = 0$
5. $\langle \vec{v} Q(F) \rangle = -\nu_1 \langle \vec{v}\, F \rangle = -\nu_1\, \rho\, \vec{u}$

The fourth property expressing the conservation of the electron number density.

The approximation (3) for the Boltzmann operator was introduced in the framework of gas dynamics with the aim of facilitating the closure of the

hierarchies of systems of moment equations which can be obtained starting from generic classical kinetic theories (see [4] and references therein).

This approximation is motivated by the fact that some of the essential properties (of conservation, dissipation, and symmetry) of the original operator remain valid for the BGK one, using which it is also possible to recover the correct Navier-Stokes fluid dynamic approximation.
Here, we will use it to find a drift-diffusion equation for the density ρ.

2. A drift-diffusion equation in the high electric field limit.

As said, we will use the same scaling of the BTE as Poupaud.
Let us introduce the scaled variables

$$t' = \frac{t}{t_0}; \quad \vec{x'} = \frac{\vec{x}}{l_0}; \quad \vec{v'} = \frac{\vec{v}}{v_{th}}.$$

where t_0 is a reference time, l_0 a reference length and $v_{th} = \sqrt{\frac{\theta_L}{m^*}}$ the thermal velocity. Furthermore let τ_r be the characteristic relaxation time, then we can define a scaled collision term Q_s by

$$Q_s = \tau_r Q.$$

The length $l_r = v_{th}\tau_r$ is a mean free path and $\alpha = \frac{l_r}{l_0}$ a scaled version of this mean free path.
Let us also define the thermal voltage U_{th} and a scaled external field $\vec{E'}_{ex}$ by

$$U_{th} = \frac{m^* v_{th}^2}{q} \quad \vec{E'}_{ex} = \frac{\vec{E}_{ex}}{E_{ex}^0}.$$

where E_{ex}^0 is an external reference field.
Then the BTE reads

$$\frac{\tau_r}{t_0}\frac{\partial F}{\partial t'} + \frac{l_r}{l_o}\vec{v'} \cdot \nabla_{\vec{x'}} F - \frac{E_{in}^0 l_r}{U_{th}}\vec{E'}_{in} \cdot \nabla_{\vec{v'}} F - \frac{E_{ex}^0 l_r}{U_{th}}\vec{E'}_{ex} \cdot \nabla_{\vec{v'}} F = Q_s(F).$$

where E_{in}^0 is an internal reference field.
If we assume

$$t_0 = \frac{\tau_r}{\alpha} \quad E_{ex}^0 = \frac{U_{th}}{l_r} \quad \frac{E_{in}^0}{E_{ex}^0} = \alpha$$

and drop primes in order to simplify notation, we obtain the following scaled version of the BTE

$$\frac{\partial F}{\partial t} + \vec{v} \cdot \nabla_{\vec{x}} F - \vec{E}_{in} \cdot \nabla_{\vec{v}} F = \frac{1}{\alpha}[\nu_1(\mathcal{E} - F) + (\nu_2 - \nu_1)(\mathcal{D} - F) + (\nu_3 - \nu_2)(\mathcal{F} - F) + \vec{E}_{ex} \cdot \nabla_{\vec{v}} F]. \tag{4}$$

If we consider the Chapman-Enskog expansion of this equation in the mean free path parameter α, we will have

$$F = \sum_{n \geq 0} \alpha^n F^{(n)} \quad \text{with} \quad \langle F \rangle = \langle F^{(0)} \rangle \quad \text{and} \quad \langle F^{(n)} \rangle = 0 \text{ for } n \geq 1. \tag{5}$$

Our aim is to derive a first order correct drift-diffusion equation for the density ρ, so we will start from the mass conservation equation

$$\frac{\partial \langle F \rangle}{\partial t} + \nabla_{\vec{x}} \cdot \langle \vec{v} F \rangle = 0. \tag{6}$$

Substituting into it the Chapman-Enskog expansion of F, we will obtain at the first order in α

$$\frac{\partial \langle F^{(0)} \rangle}{\partial t} + \nabla_{\vec{x}} \cdot \langle \vec{v} F^{(0)} \rangle + \alpha \nabla_{\vec{x}} \cdot \langle \vec{v} F^{(1)} \rangle = 0. \tag{7}$$

Therefore we need to calculate

$$\langle \vec{v} F^{(0)} \rangle \qquad \text{and} \qquad \langle \vec{v}\, F^{(1)} \rangle.$$

Considering the leading order term in the Chapman-Enskog expansion, we have, substituting (5) into (4),

$$-\vec{E}_{ex} \cdot \nabla_{\vec{v}} F^{(0)} = Q(F^{(0)}). \tag{8}$$

from which

$$\langle \vec{v}\, Q(F^{(0)}) \rangle = -\langle \vec{v} \Big(\vec{E}_{ex} \cdot \nabla_{\vec{v}}\, F^{(0)} \Big) \rangle = \rho\, \vec{E}_{ex}.$$

Combining this last result with property 5, we find

$$\rho \vec{u}_{F^{(0)}} \equiv \langle \vec{v}\, F^{(0)} \rangle = -\rho \nu_1\, \vec{E}_{ex}. \tag{9}$$

Now, considering the first order correction to the Chapman-Enskog expansion gives us

$$\frac{\partial F^{(0)}}{\partial t} + \vec{v} \cdot \nabla_{\vec{x}}(F^{(0)}) - \vec{E}_{in} \cdot \nabla_{\vec{v}} F^{(0)} = Q^{(1)}(F) + \vec{E}_{ex} \cdot \nabla_{\vec{v}} F^{(1)}$$

where $Q^{(1)}(F)$ denotes the first order term in the expansion of Q.

Multiplicating this equation by $\vec{v}$, integrating over the $\vec{v}$-space and eliminating the time derivative of ρ from the resulting equation by using the mass conservation law at the leading order, we obtain

$$\rho \frac{\partial \vec{u}_{F^{(0)}}}{\partial t} - \vec{u}_{F^{(0)}}[\nabla_{\vec{x}} \cdot (\rho \vec{u}_{F^{(0)}})] + \nabla_{\vec{x}} \cdot \langle \vec{v} \otimes \vec{v}\, F^{(0)} \rangle + \rho \vec{E}_{in} = \langle \vec{v}\, Q^{(1)}(F) \rangle \tag{10}$$

$\otimes$ denoting the usual tensor product .
From property 5, we have

$$\langle \vec{v} Q^{(1)}(F) \rangle = -\nu_1 \langle \vec{v}\, F^{(1)} \rangle. \tag{11}$$

Then, from (10) we can derive $\langle \vec{v}\, F^{(1)} \rangle$ once we calculate

$$\langle \vec{v} \otimes \vec{v}\, F^{(0)} \rangle.$$

To begin with, we notice that the following results stem from the definitions of $\mathcal{E}$, $\mathcal{D}$ and $\mathcal{F}$:

$$\langle \vec{v} \otimes \vec{v} \Big(\mathcal{E} - F^{(0)} \Big) \rangle = \rho\, \hat{I} - \langle \vec{v} \otimes \vec{v}\, F^{(0)} \rangle$$

$$\langle \vec{v} \otimes \vec{v} \Big(\mathcal{D}^{(0)} - F^{(0)} \Big) \rangle = \rho\, \hat{I} + \rho\, (\vec{u}_{F^{(0)}} \otimes \vec{u}_{F^{(0)}}) - \langle \vec{v} \otimes \vec{v}\, F^{(0)} \rangle$$

$$\langle \vec{v} \otimes \vec{v} \Big(\mathcal{F}^{(0)} - F^{(0)} \Big) \rangle = \rho (\vec{u}_{F^{(0)}} \otimes \vec{u}_{F^{(0)}})^{TF} - \langle (\vec{v} \otimes \vec{v})^{TF}\, F^{(0)} \rangle$$

where $\hat{I}$ is the identity matrix of $\Re^3$ and TF indicates the traceless part of a symmetric tensor.
From these it immediately follows that

$$\langle \vec{v} \otimes \vec{v}\, Q(F^{(0)}) \rangle = -\nu_1 \rho (\vec{u}_{F^{(0)}} \otimes \vec{u}_{F^{(0)}}) + \nu_2\, \hat{I} \Big[\rho \Big(1 + \frac{1}{3} u^2_{F^{(0)}} \Big) - \frac{1}{3} \langle v^2\, F^{(0)} \rangle \Big] +$$

$$+ \nu_3 \big[\rho (\vec{u}_{F^{(0)}} \otimes \vec{u}_{F^{(0)}})^{TF} - \langle (\vec{v} \otimes \vec{v})^{TF}\, F^{(0)} \rangle \big]$$

On the other hand, from (8) we also have

$$\langle \vec{v} \otimes \vec{v}\, Q(F^{(0)})\rangle = -\frac{2\rho}{\nu_1}\vec{E}_{ex} \otimes \vec{E}_{ex}$$

Combining the last two expressions and using (9) we eventually find

$$\langle \vec{v} \otimes \vec{v}\, F^{(0)}\rangle = \rho\Big[\Big(\frac{1}{\nu_1^2} + \frac{1}{\nu_1\nu_3}\Big)\vec{E}_{ex} \otimes \vec{E}_{ex} + \frac{1}{3}\Big(\frac{1}{\nu_1\nu_2} - \frac{1}{\nu_1\nu_3}\Big)E_{ex}^2\hat{I} + \hat{I}\Big] \tag{12}$$

Substituting (9), (11) and (12) into (10) gives

$$\langle \vec{v}F^{(1)}\rangle = -\frac{1}{\nu_1^2}\Big[\nabla_{\vec{x}} \cdot \Big(\frac{\rho}{\nu_1}\vec{E}_{ex}\Big)\Big]\vec{E}_{ex} - \frac{1}{\nu_1}\nabla_{\vec{x}} \cdot \Big\{\rho\Big[\Big(\frac{1}{\nu_1^2} + \frac{1}{\nu_1\nu_3}\Big)\cdot \tag{13}$$

$$\cdot\vec{E}_{ex} \otimes \vec{E}_{ex} + \frac{1}{3}\Big(\frac{1}{\nu_1\nu_2} - \frac{1}{\nu_1\nu_3}\Big)E_{ex}^2\hat{I} + \hat{I}\Big]\Big\} - \frac{1}{\nu_1}\rho\vec{E}_{in} + \frac{1}{\nu_1}\rho\frac{\partial}{\partial t}\Big(\frac{1}{\nu_1}\vec{E_{ex}}\Big).$$

Now we are in condition to obtain our drift-diffusion equation.
In fact inserting (9) and (13) into (7) we have

$$\frac{\partial\rho}{\partial t} - \nabla_{\vec{x}} \cdot \Big(\frac{\rho}{\nu_1}\vec{E}_{ex}\Big) + \alpha\nabla_{\vec{x}} \cdot \Big\{ - \frac{1}{\nu_1^2}\Big[\nabla_{\vec{x}} \cdot \Big(\frac{\rho}{\nu_1}\vec{E}_{ex}\Big)\Big]\vec{E}_{ex} - \frac{1}{\nu_1}\nabla_{\vec{x}}\cdot$$

$$\Big[\rho\Big(\Big(\frac{1}{\nu_1^2} + \frac{1}{\nu_1\nu_3}\Big)\vec{E}_{ex} \otimes \vec{E}_{ex} + \frac{1}{3}\Big(\frac{1}{\nu_1\nu_2} - \frac{1}{\nu_1\nu_3}\Big)E_{ex}^2\hat{I} + \hat{I}\Big)\Big]+$$

$$-\frac{1}{\nu_1}\rho\vec{E}_{in} + \frac{1}{\nu_1}\rho\frac{\partial}{\partial t}\Big(\frac{1}{\nu_1}\vec{E_{ex}}\Big)\Big\} = 0.$$

We underline that this drift-diffusion equation has been derived without solving (8). If we consider the stationary homogeneous case, the current density will be given by

$$\vec{j} = -\big(\langle \vec{v}\ F^{(0)}\rangle + \alpha\langle \vec{v}\ F^{(1)}\rangle\big) =$$

$$\Big\{\frac{1}{\nu_1}\rho\vec{E}_{ex} + \alpha\Big[\frac{1}{\nu_1}\rho\vec{E}_{in}\Big]\Big\}.$$

which is in accordance with the more general expression

$$\vec{u} = -\frac{q}{\nu_1\ m^*}\vec{E}$$

which directly results from taking the moment of the BTE corresponding to $\vec{v}$ and from property 5. From this we notice that, as known, models derived by using the BGK approximation of the collision operator cannot predict a velocity saturation at large electric fields unless we let the coefficient ν_1 depend on $\vec{x}$ through the electric field.

Acknowledgements. The author wishes to thank Prof. A.M. Anile and Prof. C.D. Levermore for precious discussions. This work was supported by Italian Consiglio Nazionale delle Ricerche (Prog. N.97.04709.PS01), M. U. R. S. T. (Prog. Mathematical Problems of Kinetic Theories 1998) and Training and Mobility of Researchers Programme N. ERBFMRXCT970157.

REFERENCES

[1] C. Cercignani, *The Boltzmann equation and its applications,* Applied Mathematical Sciences 67, Springer-Verlag, New York, 1998.

[2] A. Markowich - C.A. Ringhofer - C. Schmeiser, *Semiconductor equations,* Springer Verlag, Wien, 1990.

[3] F. Poupaud, *Runaway phenomena and fluid approximations under high electric fields in semiconductor kinetic theory,* Zamm, 72 - 8 (1992), pp. 359-372.

[4] C.D. Levermore, *Moment Closure Hierarchies for Kinetic Theories,* J. Stat. Phys., 83 (1996), pp. 1021–1065.

Dipartimento di Matematica e Informatica,
Viale A. Doria 6,
95125 Catania (ITALY)
e-mail: mascali@dmi.unict.it