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Reduced kinetic equations for 1D carrier flow in semiconductor devices (**)

1 - Introduction

The movement of electrons in crystal is governed by complex physical laws, so that fine models are required to achieve correct results. The drift-diffusion model has been widely used in the past, when it provided a good description of relevant physical mechanisms. In the modern device, whose size is in the submicron range, thermal and intertial effects play an important role and are not adequately modeled by the previous approach.

A fully kinetic treatment of carrier dynamics guarantees accurate results but requires very expensive numerical procedures in order to solve realistic problems. To reduce the complexity of the use of the full Boltzmann equation, many authors [1], [4] (see also [6] and references therein) have introduced more simple models, assuming particular forms of the distribution function. For example Legendre or harmonic expansions with respect to the molecular velocity were often applied.

In this paper we consider the Boltzmann equation, which describes the evolution of an electron gas in a semiconductor [7], [11]. The collision operator takes into account the interactions between electrons and molecules of the lattice. This is assumed to be in thermal equilibrium. Our approach is restricted to one-dimensional flow, so the distribution function f depends only on one spatial coordinate.

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The paper is organized as follows. In Section 2 we introduce the Boltzmann equation and deduce some integrals arising from the collision operator. In Section 3 we present the main results concerning the two methods, which allow us to derive sets of new equations, where the unknowns depend on the molecular velocity only through the molecular energy. For this reason they are still kinetic equations. In the last section we show, in a simple case, these equations and draw some conclusions.

Throughout the paper, boldface and lightface symbols denote vectors and scalar quantities respectively.

2 - Basic equations and preliminary results

We consider an electron gas, which moves in a lattice, subjects to an external electric field $\boldsymbol{E}$. This can be applied or related, by Poisson equation, to the density of the gas. We assume that the motion of the gas can be described by a distribution function f, satisfying the *Boltzmann equation*

$$\frac{\partial f}{\partial t} + \boldsymbol{v} \cdot \nabla f - \frac{e}{m^*} \boldsymbol{E} \cdot \nabla_v f = Q(f) \tag{1}$$

where $\boldsymbol{v}$, $-e$ and m^* are the velocity, the charge and the effective mass respectively of an electron. The velocity $\boldsymbol{v}$ is related to the wave vector $\boldsymbol{k}$ of the particle by the relation $\boldsymbol{v} = \frac{1}{\hbar} \nabla_k \varepsilon$, where $\hbar$ is the Planck constant divided by 2π and ε is the energy of the particle. The symbol ∇_k means gradient with respect to $\boldsymbol{k}$ and ∇_v the gradient with respect to $\boldsymbol{v}$. The integral operator $Q(f)$ describes the collisions between electrons and molecules of the lattice. The principal characteristics of this operator have been established by the author in [8]-[10], both in the linear and non-linear case. Here we assume that the low-density approximation holds, so that Q is linear in f.

If $S(\boldsymbol{v}, \boldsymbol{v}_*)$ is the sum of the scattering kernels, which describe the nature of the collisions (for example, electron-acoustic phonons, electron-polar optical phonons, electron-impurities and so on), then the collision operator is

$$Q(f) = \int_{\mathrm{R}^3} S(\boldsymbol{v}, \boldsymbol{v}_*)\, \delta(\varepsilon_* - \varepsilon - \hbar\omega)[(\boldsymbol{n}_q + 1) f_* - \boldsymbol{n}_q f]\, \mathrm{d}\boldsymbol{v}_*$$

$$+ \int_{\mathrm{R}^3} S(\boldsymbol{v}_*, \boldsymbol{v})\, \delta(\varepsilon_* - \varepsilon + \hbar\omega)[\boldsymbol{n}_q f_* - (\boldsymbol{n}_q + 1) f]\, \mathrm{d}\boldsymbol{v}_* .$$

The constant quantity n_q represents the thermal-equilibrium numbers of phonons and is given by

$$n_q = \frac{1}{\exp\left(\frac{\hbar\omega}{k_B T_L}\right) - 1}$$

where k_B is the Boltzmann constant, T_L is the lattice temperature and ω is the constant phonon frequency.

The single-particle energy ε of the electron is in general a function of the wave vector or of the velocity $\boldsymbol{v}$. We consider the parabolic case, so that $\varepsilon = \frac{1}{2} m^* v^2$, where v denotes the magnitude of $\boldsymbol{v}$. Since the interactions cause an electron to scatter from one Bloch state $\frac{m^*}{\hbar}\boldsymbol{v}$ to another $\frac{m^*}{\hbar}\boldsymbol{v}_*$ inelastically by absorbing or emitting a phonon, so that the particle energy satisfies the relation $\varepsilon_* = \varepsilon \pm \hbar\omega$, only one delta-function appears in the collision operator.

As usually, due to the isotropy of the phase-space, the kernel $S(\boldsymbol{v}, \boldsymbol{v}_*)$ is symmetric with respect to the two velocities $\boldsymbol{v}$ and $\boldsymbol{v}_*$. Moreover, since the kernel is a scalar, it depends on $\boldsymbol{v}$ and $\boldsymbol{v}_*$ only through the scalar quantities v, v_* and $\boldsymbol{v}\cdot\boldsymbol{v}_*$.

It is useful to introduce the unit vectors $\boldsymbol{q}$ and $\boldsymbol{q}_*$ defined by the equations $\boldsymbol{v} = v\boldsymbol{q}$ and $\boldsymbol{v}_* = v_*\boldsymbol{q}_*$. Taking into account the definition of ε, then S can be considered as function of ε, ε_* and $\boldsymbol{q}\cdot\boldsymbol{q}_*$, so that, we can write $S(\boldsymbol{v}, \boldsymbol{v}_*) = \sigma(\varepsilon, \varepsilon_*, \boldsymbol{q}\cdot\boldsymbol{q}_*)$.

We are interested to study the case when f depends only on one spatial coordinate, say z. Let us denote with $\boldsymbol{u}$ the unit vector of z-axis. Since any rotation around this axis does not change the value of f, then it depends on $\boldsymbol{v}$ by means of the scalar quantities ε (i.e. v^2) and $\boldsymbol{v}\cdot\boldsymbol{u}$ or $\gamma = \boldsymbol{q}\cdot\boldsymbol{u}$. Therefore

$$f(t, z, \boldsymbol{v}) = F(t, z, \varepsilon, \gamma). \tag{2}$$

We use the above four variables as independent, so that v becomes a function of ε. Often in the following, we shall continue to use the symbol v, as function of ε, to avoid the cumbersome expression $\sqrt{2\varepsilon/m^*}$. It is also evident that solutions of the Boltzmann equation of this type, require that $\boldsymbol{E} = E\boldsymbol{u}$. Under these hypotheses, we can transform equation (1) into

$$\frac{\partial F}{\partial t} + \gamma v \frac{\partial F}{\partial z} - \frac{e}{m^*} E\left[m^* \gamma v \frac{\partial F}{\partial \varepsilon} + \frac{1}{v}(1 - \gamma^2)\frac{\partial F}{\partial \gamma}\right] = Q(F). \tag{3}$$

We note only that, of course, the new coordinates introduce a singularity at $v = 0$, which in this step can be eliminated, assuming $\boldsymbol{v} \neq \boldsymbol{0}$. The collision operator Q does not simplify significantly, replacing F instead of f.

Now, we derive some formulas, which will be used in the following, Let's consider

$$A_n(\varepsilon, \gamma) = \int_{R^3} S(\boldsymbol{v}, \boldsymbol{v}_*)\, \delta(\varepsilon_* - \varepsilon + \hbar\omega)(\boldsymbol{v}_* \cdot \boldsymbol{u})^n \, d\boldsymbol{v}_* \tag{4}$$

$$B_n(\varepsilon, \gamma) = \int_{R^3} S(\boldsymbol{v}, \boldsymbol{v}_*)\, \delta(\varepsilon_* - \varepsilon - \hbar\omega)(\boldsymbol{v}_* \cdot \boldsymbol{u})^n \, d\boldsymbol{v}_* \,. \tag{5}$$

We show that it is possible to reduce the order of the above integrals. The functions $A_n(\varepsilon, \gamma)$ and $B_n(\varepsilon, \gamma)$ depend only on γ and ε, because they are scalar. We assume that $S(\boldsymbol{v}, \boldsymbol{v}_*)$ is a continuous function in the open set $\mathcal{A}$ defined by $\mathcal{A} = \{\boldsymbol{v} \in \boldsymbol{R}^3,\ \boldsymbol{v}_* \in \boldsymbol{R}^3 : \boldsymbol{v} \neq \boldsymbol{v}_*\}$. This is always verified for the physical kernels.

Proposition 1. *If* $S(\boldsymbol{v}, \boldsymbol{v}_*) = \sigma(\varepsilon, \varepsilon_*, \boldsymbol{q} \cdot \boldsymbol{q}_*)$ *is a continuous function in* $\mathcal{A}$, *then for any positive integer* n *we have*

$$A_n(\varepsilon, \gamma) = 0 \qquad \text{if } \varepsilon \leqslant \hbar\omega \tag{6}$$

$$A_n(\varepsilon, \gamma) = \sqrt{\left(\frac{\varepsilon - \hbar\omega}{\varepsilon}\right)^{n+1}} B_n(\varepsilon - \hbar\omega, \gamma) \qquad \text{if } \varepsilon > \hbar\omega \,. \tag{7}$$

Proof. Equation (6) is simply a consequence of the delta function appearing inside the integral and of the non-negativity of ε. Moreover, for every $\varepsilon > \hbar\omega$, since $\boldsymbol{q}_* = (\sin\varphi_* \cos\vartheta_*, \sin\varphi_* \sin\vartheta_*, \cos\varphi_*)$, $(\varphi_*, \sigma_*$ spherical coordinates), we obtain

$$A_n(\varepsilon, \gamma) = \int_0^{+\infty} d\varepsilon_* \int_{\Omega_*} d\omega_*\, \sigma(\varepsilon, \varepsilon_*, \boldsymbol{q} \cdot \boldsymbol{q}_*)\, \delta(\varepsilon_* - \varepsilon + \hbar\omega)(\boldsymbol{q}_* \cdot \boldsymbol{u})^n$$

$$\cdot \left(\frac{2}{m^*}\varepsilon_*\right)^{\frac{n+2}{2}} \sqrt{\frac{2}{m^*}} \frac{1}{2\sqrt{\varepsilon_*}} \sin\varphi_*$$

$$= \frac{1}{m^*}\left(2\frac{\varepsilon - \hbar\omega}{m^*}\right)^{\frac{n+1}{2}} \int_{\Omega_*} d\omega_*\, \sigma(\varepsilon, \varepsilon - \hbar\omega, \boldsymbol{q} \cdot \boldsymbol{q}_*)(\boldsymbol{q}_* \cdot \boldsymbol{u})^n \sin\varphi_*$$

where $$\int_{\Omega_*} d\omega_* = \int_0^{2\pi} d\vartheta_* \int_0^{\pi} d\varphi_* .$$

Analogously, for every ε positive,

$$B_n(\varepsilon, \gamma) = \frac{1}{m^*}\left(2\frac{\varepsilon+\hbar\omega}{m^*}\right)^{\frac{n+1}{2}} \int_{\Omega_*} d\omega_* \, \sigma(\varepsilon, \varepsilon+\hbar\omega, \boldsymbol{q}\cdot\boldsymbol{q}_*)(\boldsymbol{q}_*\cdot\boldsymbol{u})^n \sin\varphi_* .$$

A comparison between the two formulas and the use of the identity $\sigma(\varepsilon, \varepsilon_*, \boldsymbol{q}\cdot\boldsymbol{q}_*) = \sigma(\varepsilon_*, \varepsilon, \boldsymbol{q}\cdot\boldsymbol{q}_*)$, allows us to deduce the relation (7). Therefore it is sufficient to know $B_n(\varepsilon, \gamma)$, to evaluate $A_n(\varepsilon, \gamma)$.

Proposition 2. *If $S(\boldsymbol{v}, \boldsymbol{v}_*) = \sigma(\varepsilon, \varepsilon_*, \boldsymbol{q}\cdot\boldsymbol{q}_*)$ is a continuous function in $\mathcal{A}$ and $S_0(\varepsilon_*) = S(0, \boldsymbol{v}_*)$, then for every positive integer n we have*

$$B_n(0, \gamma) = \frac{2\pi}{m^*}\,\frac{(-1)^n+1}{n+1}\left(2\frac{\hbar\omega}{m^*}\right)^{\frac{n+1}{2}} S_0(\hbar\omega) \tag{8}$$

and for $\varepsilon > 0$

$$B_n(\varepsilon, \gamma) = \frac{1}{m^*}\left[\left(2\frac{\varepsilon+\hbar\omega}{m^*}\right)^{\frac{n+1}{2}}\right] \sum_{j=0}^{[\frac{n}{2}]} \beta_{jn}(\varepsilon)\gamma^{n-2j} \tag{9}$$

where $s_0 = 2\pi$, $$s_h = \int_0^{2\pi} \sin^h \vartheta_* \, d\vartheta_* = \begin{cases} 0 & \textit{if } h > 0 \textit{ is odd} \\ 2\pi\dfrac{(h-1)!!}{h!!} & \textit{if } h > 0 \textit{ is even} \end{cases}$$

$[m]$ means the greatest integer less or equal to m and

$$\beta_{jn}(\varepsilon) = \sum_{k=j}^{[\frac{n}{2}]} \binom{n}{2k}\binom{k}{j}(-1)^{k-j} s_{2k} \int_{-1}^{1} \sigma(\varepsilon, \varepsilon+\hbar\omega, s)(1-s^2)^k s^{n-2k} ds .$$

Proof. When we consider $B_n(\varepsilon, \gamma)$, ε can be zero. This case must be treated separately.

By the definition of $B_n(\varepsilon, \gamma)$, we obtain

$$\int_{R^3} S(0, \boldsymbol{v}_*)\delta(\varepsilon - \hbar\omega)(\boldsymbol{v}_*\cdot\boldsymbol{u})^n d\boldsymbol{v}_* = S_0(\hbar\omega)\int_{R^3} \delta(\varepsilon - \hbar\omega)(\boldsymbol{v}_*\cdot\boldsymbol{u})^n d\boldsymbol{v}_* .$$

Since the integral is a scalar, it can be evaluated in a convenient reference frame, where $\boldsymbol{u} \to (0, 0, 1)$. Then we obtain

$$B_n(0, \gamma) = \frac{1}{m^*}\left(2\,\frac{\hbar\omega}{m^*}\right)^{\frac{n+1}{2}} S_0(\hbar\omega) \int_{\Omega_*} \mathrm{d}\omega_* (\cos\varphi_*)^n \sin\varphi_*$$

$$= \frac{2\pi}{m^*}\,\frac{(-1)^n + 1}{n+1}\left(2\,\frac{\hbar\omega}{m^*}\right)^{\frac{n+1}{2}} S_0(\hbar\omega)$$

that is equation (8).

As ε is positive, we again choose a particular reference frame, in order to simplify the integral. Since $\boldsymbol{q}\cdot\boldsymbol{u} = \gamma$, if $\boldsymbol{q} \to (0, 0, 1)$ and $\boldsymbol{u} \to (0, \sqrt{1-\gamma^2}, \gamma)$, we have

$$\int_{\Omega_*} \mathrm{d}\omega_* \sigma(\varepsilon, \varepsilon + \hbar\omega, \boldsymbol{q}\cdot\boldsymbol{q}_*)(\boldsymbol{q}_*\cdot\boldsymbol{u})^n \sin\varphi_*$$

$$= \int_{\Omega_*} \mathrm{d}\omega_* \sigma(\varepsilon, \varepsilon + \hbar\omega, \cos\varphi_*)[\sin\varphi_* \sin\vartheta_* \sqrt{1-\gamma^2} + \gamma\cos\varphi_*]^n \sin\varphi_*$$

$$= \sum_{h=0}^{n} \binom{n}{h} (1-\gamma^2)^{\frac{h}{2}} \gamma^{n-h} s_h \int_0^{\pi} \sigma(\varepsilon, \varepsilon+\hbar\omega, \cos\varphi_*)(\sin\varphi_*)^{h+1}(\cos\varphi_*)^{n-h}\,\mathrm{d}\varphi_*$$

$$= \sum_{h=0}^{n} \binom{n}{h} (1-\gamma^2)^{\frac{h}{2}} \gamma^{n-h} s_h \int_{-1}^{1} \sigma(\varepsilon, \varepsilon+\hbar\omega, s)\sqrt{(1-s^2)^h} s^{n-h}\,\mathrm{d}s\,.$$

We note that the integrals

$$\int_{-1}^{1} \sigma(\varepsilon, \varepsilon+\hbar\omega, s)\sqrt{(1-s^2)^h} s^{n-h}\,\mathrm{d}s$$

are scalar depending only the variable ε. Moreover, since $s_h = 0$ if h is odd, we have

$$\int_{\Omega_*} \mathrm{d}\omega_* \sigma(\varepsilon, \varepsilon + \hbar\omega, \boldsymbol{q}\cdot\boldsymbol{q}_*)(\boldsymbol{q}_*\cdot\boldsymbol{u})^n \sin\varphi_*$$

$$= \sum_{k=0}^{[\frac{n}{2}]} \binom{n}{2k} (1-\gamma^2)^k \gamma^{n-2k} s_{2k} \int_{-1}^{1} \sigma(\varepsilon, \varepsilon+\hbar\omega, s)(1-s^2)^k s^{n-2k}\,\mathrm{d}s$$

$$= \sum_{k=0}^{[\frac{n}{2}]} \binom{n}{2k} \sum_{j=0}^{k} \binom{k}{j} (-1)^{k-j} \gamma^{n-2j} s_{2k} \int_{-1}^{1} \sigma(\varepsilon, \varepsilon+\hbar\omega, s)(1-s^2)^k s^{n-2k}\,\mathrm{d}s$$

$$= \sum_{j=0}^{[\frac{n}{2}]} \beta_{jn}(\varepsilon)\,\gamma^{n-2j}\,.$$

As a consequence of the above formula, it is clear that $B_n(\varepsilon, \gamma)$ is a polynomial in the variable γ of degree less or equal to n and can be written as

$$B_n(\varepsilon, \gamma) = \frac{1}{m^*}[(2\frac{\varepsilon + \hbar\omega}{m^*})^{\frac{n+1}{2}}]\sum_{j=0}^{[\frac{n}{2}]} \beta_{jn}(\varepsilon)\gamma^{n-2j}.$$

Analogously we can prove that

$$A_n(\varepsilon, \gamma) = \frac{1}{m^*}[(2\frac{\varepsilon - \hbar\omega}{m^*})^{\frac{n+1}{2}}]\sum_{j=0}^{[\frac{n}{2}]} \alpha_{jn}(\varepsilon)\gamma^{n-2j} \qquad \varepsilon > \hbar\omega \tag{10}$$

with $\alpha_{jn}(\varepsilon) = \sum_{k=j}^{[\frac{n}{2}]} \binom{n}{2k}\binom{k}{j}(-1)^{k-j} s_{2k} \int_{-1}^{1} \sigma(\varepsilon, \varepsilon - \hbar\omega, s)(1-s^2)^k s^{n-2k} ds$.

Therefore, for every $\varepsilon > \hbar\omega$, we have

$$\alpha_{jn}(\varepsilon) = \beta_{jn}(\varepsilon - \hbar\omega). \tag{11}$$

3 - Derived kinetic equations

We have performed some integrals, which show as the variable ε plays a particular role. This derives by the physical laws of the collisions, where only the energy is involved. The other variable γ appears as a power, independently on the type of the scattering. Therefore many authors have proposed simple forms for the distribution function F, based on the assumption that it can be approximated by a polynomial in γ (usually of low degree). We prove that, in general, one can obtain a set of kinetic equations for any arbitrary order.

Let us assume that

$$F(t, z, \varepsilon, \gamma) = \sum_{n=0}^{p} (\gamma v)^n f_n(t, z, \varepsilon) + R_p(t, z, \varepsilon, \gamma) \tag{12}$$

where p is a non-negative integer and $R_p(t, z, \varepsilon, \gamma)$ indicates the remainder. We have introduced the factor γv instead of γ to avoid the singularity at $v = 0$ into the free streaming operator. In fact, neglecting the remainder, we obtain

$$\frac{\partial F}{\partial t} + \gamma v \frac{\partial F}{\partial z} - \frac{e}{m^*} E[m^* \gamma v \frac{\partial F}{\partial \varepsilon} + \frac{1}{v}(1-\gamma^2)\frac{\partial F}{\partial \gamma}]$$

$$\simeq \sum_{n=0}^{p} [(\gamma v)^n \frac{\partial}{\partial t} f_n(t, z, \varepsilon) + (\gamma v)^{n+1} \frac{\partial}{\partial z} f_n(t, z, \varepsilon)$$

$$-eE(\gamma v)^{n+1} \frac{\partial}{\partial \varepsilon} f_n(t, z, \varepsilon) - \frac{e}{m^*} n(\gamma v)^{n-1} E f_n(t, z, \varepsilon)]$$

and therefore

$$\sum_{n=0}^{p} [\frac{\partial}{\partial t} f_n(t, z, \varepsilon) + \frac{\partial}{\partial z} f_{n-1}(t, z, \varepsilon) - eE \frac{\partial}{\partial \varepsilon} f_{n-1}(t, z, \varepsilon) - \frac{e}{m^*}(n+1) E f_{n+1}(t, z, \varepsilon)](\gamma v)^n = Q(F) \quad (13)$$

defining $f_{-1}(t, z, \varepsilon) = 0$ and putting $f_{p+1}(t, z, \varepsilon) = 0$. To calculate the collision operator, we note that

$$\int_{\mathrm{R}^3} S(\boldsymbol{v}, \boldsymbol{v}_*)\, \delta(\varepsilon_* - \varepsilon - \hbar\omega) F_* \, \mathrm{d}\boldsymbol{v}_*$$

$$\simeq \sum_{n=0}^{p} f_n(t, z, \varepsilon + \hbar\omega) \int_{\mathrm{R}^3} S(\boldsymbol{v}, \boldsymbol{v}_*)\, \delta(\varepsilon_* - \varepsilon - \hbar\omega)(\boldsymbol{v}_* \cdot \boldsymbol{u})^n \, \mathrm{d}\boldsymbol{v}_* .$$

Then

$$Q(F) \simeq \sum_{n=0}^{p} [(\boldsymbol{n}_q + 1) B_n(\varepsilon, \gamma) f_n(t, z, \varepsilon + \hbar\omega)$$

$$+\boldsymbol{n}_q A_n(\varepsilon, \gamma) f_n(t, z, \varepsilon - \hbar\omega) - \nu(\varepsilon)(\gamma v)^n f_n(t, z, \varepsilon)]$$

where

$$\nu(\varepsilon) = \boldsymbol{n}_q B_0(\varepsilon, \gamma) + (\boldsymbol{n}_q + 1) A_0(\varepsilon, \gamma).$$

Since, for $n = 0, 1, \ldots, p$, the functions $A_n(\varepsilon, \gamma)$ and $B_n(\varepsilon, \gamma)$ are polynomials in γ of degree less or equal to p, then the Boltzmann equation, in this approximation, is equivalent to $p + 1$ equations in the unknowns $f_n(t, z, \varepsilon)$ $(n = 0, 1, \ldots, p)$. The set of equations is closed, because we have *eliminated* the remainder $R_p(t, z, \varepsilon, \gamma)$. The case $p = 1$ is explicitly shown in the next section.

We think useful at this point, to make some considerations. This technique allows us to derive a finite closed set of kinetic equations, where the dimension of the domain of the velocity quantities is reduced. Unfortunately the assumption given by (12) is valid only as F is *approximately* near to a polynomial in γ; otherwise $R_p(t, z, \varepsilon, \gamma)$ becomes large. Moreover it is hard to estimate the remainder also in simple norm of the uniform convergence.

Another difficulty arises, when one is interested in evaluating hydrodynamical quantities. If we have solved the equations and, therefore, we know $f_n(t, z, \varepsilon)$ $(n = 0, 1, \dots, p)$, then, for example, we may obtain only an approximate value of the density of the gas, because we do not know the remainder $R_p(t, z, \varepsilon, \gamma)$.

To overcome these difficulties, we introduce a new method, to derive kinetic equations. The new unknowns are defined as follows

$$\phi_n(t, z, \varepsilon) = \int_\Omega \mathrm{d}\omega \, F(t, z, \varepsilon, \gamma)(\boldsymbol{v}\cdot\boldsymbol{u})^n v \sin\varphi = v^{n+1}\int_\Omega \mathrm{d}\omega \, F(t, z, \varepsilon, \gamma)\gamma^n \sin\varphi \tag{14}$$

where n is a non-negative integer. The form of $\phi_n(t, z, \varepsilon)$ recalls the definition of moment of the distribution function. In fact a further integration with respect to ε gives, apart a constant multiplicative factor, a classical moment; hence we call $\phi_n(t, z, \varepsilon)$ a *quasi-moment*. The factor v appearing in (14) serves to avoid the singularity at $v = 0$ in the differential operator.

Since $\boldsymbol{u} = (0, 0, 1)$, we have $\gamma = \cos\varphi$ and

$$\phi_n(t, z, \varepsilon) = 2\pi v^{n+1}\int_{-1}^{1} F(t, z, \varepsilon, \gamma)\gamma^n \, \mathrm{d}\gamma \, . \tag{15}$$

From the Boltzmann equation (1), by multiplying for $(\boldsymbol{v}_*\cdot\boldsymbol{u})^n v \sin\varphi$ and integrating with respect to ϑ and φ, we obtain (for any n) a new kinetic equation. To calculate the term arising from the free streaming operator, we first show that

$$\int_\Omega \mathrm{d}\omega \left[m^*\gamma v \frac{\partial F}{\partial \varepsilon} + \frac{1}{v}(1-\gamma^2)\frac{\partial F}{\partial \gamma}\right](\boldsymbol{v}\cdot\boldsymbol{u})^n v \sin\varphi$$

$$= v^{n+1}\int_\Omega \mathrm{d}\omega \left[m^*\gamma v \frac{\partial F}{\partial \varepsilon} + \frac{1}{v}(1-\gamma^2)\frac{\partial F}{\partial \gamma}\right](\cos\varphi)^n \sin\varphi$$

$$= 2\pi v^{n+1}\int_{-1}^{1}\left[m^*\gamma v \frac{\partial F}{\partial \varepsilon} + \frac{1}{v}(1-\gamma^2)\frac{\partial F}{\partial \gamma}\right]\gamma^n \mathrm{d}\gamma$$

$$= 2\pi m^* v^{n+2}\int_{-1}^{1}\gamma^{n+1}\frac{\partial F}{\partial \varepsilon}\,\mathrm{d}\gamma + 2\pi v^n \int_{-1}^{1}[(n+2)\gamma^2 - n]\gamma^{n-1}F\,\mathrm{d}\gamma \, .$$

Since

$$\frac{\partial}{\partial \varepsilon}\phi_n(t, z, \varepsilon) = 2\pi v^{n-1}\left[\frac{n+1}{m^*}\int_{-1}^{1}F(t, z, \varepsilon, \gamma)\gamma^n \mathrm{d}\gamma + v^2\int_{-1}^{1}\frac{\partial}{\partial \varepsilon}F(t, z, \varepsilon, \gamma)\gamma^n \mathrm{d}\gamma\right]$$

we obtain

$$\int_{\Omega} d\omega \left\{ \frac{\partial F}{\partial t} + \gamma v \frac{\partial F}{\partial z} - \frac{e}{m^*} E \left[m^* \gamma v \frac{\partial F}{\partial \varepsilon} + \frac{1}{v}(1-\gamma^2)\frac{\partial F}{\partial \gamma} \right] \right\} (\boldsymbol{v}\cdot\boldsymbol{u})^n v \sin\varphi$$

$$= \frac{\partial}{\partial t}\phi_n(t,z,\varepsilon) + \frac{\partial}{\partial z}\phi_{n+1}(t,z,\varepsilon) - eE\frac{\partial}{\partial \varepsilon}\phi_{n+1}(t,z,\varepsilon) - n\frac{e}{m^*}E\phi_{n-1}(t,z,\varepsilon).$$

The collision operator gives

$$\int_{\Omega} d\omega\, Q(F)(\boldsymbol{v}\cdot\boldsymbol{u})^n v \sin\varphi$$

$$= (\boldsymbol{n}_q + 1)\int_{\Omega} d\omega\, v^{n+1}\gamma^n \sin\varphi \int_{\mathrm{R}^3} S(\boldsymbol{v},\boldsymbol{v}_*)\,\delta(\varepsilon_* - \varepsilon - \hbar\omega)F_*\, d\boldsymbol{v}_*$$

$$+\boldsymbol{n}_q\int_{\Omega} d\omega\, v^{n+1}\gamma^n \sin\varphi \int_{\mathrm{R}^3} S(\boldsymbol{v},\boldsymbol{v}_*)\,\delta(\varepsilon_* - \varepsilon + \hbar\omega)F_*\, d\boldsymbol{v}_*$$

$$-\nu(\varepsilon)\int_{\Omega} d\omega\, v^{n+1}\gamma^n F(t,z,\varepsilon,\gamma)\sin\varphi.$$

Now

$$\int_{\Omega} d\omega\, v^{n+1}\gamma^n \sin\varphi \int_0^{+\infty} d\varepsilon_* \int_{\Omega_*} d\omega_*\, \sigma(\varepsilon,\varepsilon_*,\boldsymbol{q}\cdot\boldsymbol{q}_*)$$

$$\cdot\,\delta(\varepsilon_* - \varepsilon - \hbar\omega)F(t,z,\varepsilon_*,\gamma_*)\frac{\sqrt{2\varepsilon_*}}{(m^*)^{\frac{3}{2}}}\sin\varphi_*$$

$$= \int_{\Omega} d\omega\, v^{n+1}\gamma^n \sin\varphi \int_{\Omega_*} d\omega_*\, \sigma(\varepsilon,\varepsilon+\hbar\omega,\boldsymbol{q}\cdot\boldsymbol{q}_*)F(t,z,\varepsilon+\hbar\omega,\gamma_*)$$

$$\cdot\,\frac{\sqrt{2}}{(m^*)^{\frac{3}{2}}}\sqrt{\varepsilon+\hbar\omega}\,\sin\varphi_*$$

$$= \int_{\Omega_*} d\omega_* \left[\int_{\Omega} d\omega\, \sigma(\varepsilon,\varepsilon+\hbar\omega,\boldsymbol{q}\cdot\boldsymbol{q}_*)(\boldsymbol{q}\cdot\boldsymbol{u})^n \sin\varphi\right] v^{n+1}$$

$$\cdot\,F(t,z,\varepsilon+\hbar\omega,\gamma_*)\frac{\sqrt{2}}{(m^*)^{\frac{3}{2}}}\sqrt{\varepsilon+\hbar\omega}\,\sin\varphi_*$$

$$= \int_{\Omega_*} d\omega_* \left[\sum_{j=0}^{[\frac{n}{2}]} \beta_{jn}(\varepsilon)\gamma_*^{n-2j}\right] v^{n+1} F(t, z, \varepsilon + \hbar\omega, \gamma_*) \frac{\sqrt{2(\varepsilon + \hbar\omega)}}{(m^*)^{\frac{3}{2}}} \sin\varphi_*$$

$$= \frac{\sqrt{2}}{(m^*)^{\frac{3}{2}}} \sqrt{\varepsilon + \hbar\omega}\, v^{n+1} \sum_{j=0}^{[\frac{n}{2}]} \beta_{jn}(\varepsilon) \int_{\Omega_*} d\omega_* \gamma_*^{n-2j} F(t, z, \varepsilon + \hbar\omega, \gamma_*) \sin\varphi_*$$

$$= \frac{\sqrt{2}}{(m^*)^{\frac{3}{2}}} \sqrt{\varepsilon + \hbar\omega} \sum_{j=0}^{[\frac{n}{2}]} \beta_{jn}(\varepsilon) v^{2j} \phi_{n-2j}(t, z, \varepsilon + \hbar\omega).$$

Then

$$\int_{\Omega} d\omega\, Q(F)(\boldsymbol{v}\cdot\boldsymbol{u})^n v \sin\varphi$$

$$= (\boldsymbol{n}_q + 1) \frac{\sqrt{2}}{(m^*)^{\frac{3}{2}}} \sqrt{\varepsilon + \hbar\omega} \sum_{j=0}^{[\frac{n}{2}]} \beta_{jn}(\varepsilon) v^{2j} \phi_{n-2j}(t, z, \varepsilon + \hbar\omega)$$

$$+ \boldsymbol{n}_q \frac{\sqrt{2}}{(m^*)^{\frac{3}{2}}} \sqrt{\varepsilon - \hbar\omega} \sum_{j=0}^{[\frac{n}{2}]} \alpha_{jn}(\varepsilon) v^{2j} \phi_{n-2j}(t, z, \varepsilon - \hbar\omega) - \nu(\varepsilon)\phi_n(t, z, \varepsilon).$$

Therefore from the Boltzmann equation, we obtain the equation

$$\frac{\partial}{\partial t}\phi_n(t, z, \varepsilon) + \frac{\partial}{\partial z}\phi_{n+1}(t, z, \varepsilon) - eE\frac{\partial}{\partial\varepsilon}\phi_{n+1}(t, z, \varepsilon) - n\frac{e}{m^*}E\phi_{n-1}(t, z, \varepsilon)$$

$$= (\boldsymbol{n}_q + 1) \frac{\sqrt{2}}{(m^*)^{\frac{3}{2}}} \sqrt{\varepsilon + \hbar\omega} \sum_{j=0}^{[\frac{n}{2}]} \beta_{jn}(\varepsilon) v^{2j} \phi_{n-2j}(t, z, \varepsilon + \hbar\omega)$$

$$+ \boldsymbol{n}_q \frac{\sqrt{2}}{(m^*)^{\frac{3}{2}}} \sqrt{\varepsilon - \hbar\omega} \sum_{j=0}^{[\frac{n}{2}]} \alpha_{jn}(\varepsilon) v^{2j} \phi_{n-2j}(t, z, \varepsilon - \hbar\omega) - \nu(\varepsilon)\phi_n(t, z, \varepsilon).$$

These equations derive rigorously by the Boltzmann equation under reasonable simple assumptions. As in the moment methods, the equations, in general, contain more unknowns then the number of the involved equations. However, the right-hand side contains $\phi_k(t, z, \varepsilon)$ only for $k \leqslant n$.

For example, if we consider the set of $N+1$ equations, obtained for $n=0, 1, \dots, N$, then we have $N+2$ variables $\phi_n(t, z, \varepsilon)$ $(n=0, 1, \dots, N, N+1)$. Therefore, in order to obtain a closed set of equations, it is necessary to assume another further relation, which contains $\phi_{N+1}(t, z, \varepsilon)$.

This can be suggested by the physical characteristic of the studied phenomena, or by the expression given in (15). For example, a pure mathematical relation can be derived, replacing the quantity γ^{N+1} appearing in $\phi_{N+1}(t, z, \varepsilon)$ by a polynomial of N-degree in γ. In this way $\phi_{N+1}(t, z, \varepsilon)$ is approximated by a linear combination of $\phi_k(t, z, \varepsilon)$ for $(k=0, 1, \dots, N)$. Since $\gamma \in [-1, 1]$, the Chebyshev polynomials arise naturally in order to apply the well known theorem of best approximation.

There is a particular, but not trivial, case, when this set of equations is closed. It happens when F does not depend on z and $E=0$. If, for example, we consider only the first equations, then there follows

$$\begin{aligned} \frac{\partial}{\partial t}\phi_0(t, \varepsilon) &= (\boldsymbol{n}_q + 1)\frac{\sqrt{2(\varepsilon + \hbar\omega)}}{(m^*)^{\frac{3}{2}}}\beta_{00}(\varepsilon)\phi_0(t, \varepsilon + \hbar\omega) \\ &+\boldsymbol{n}_q \frac{\sqrt{2(\varepsilon - \hbar\omega)}}{(m^*)^{\frac{3}{2}}}\alpha_{00}(\varepsilon)\phi_0(t, \varepsilon - \hbar\omega) - \nu(\varepsilon)\phi_0(t, \varepsilon). \end{aligned} \tag{16}$$

A similar equation was founds also in [9]. A solution of this equation allows to obtain a tiny information on $F(t, \varepsilon, \gamma)$, but sufficient to determine, for example, the density and the temperature of the gas. If we want to known the hydrodynamical velocity, then it is sufficient to consider also the equation given by $n=1$.

Analytical and numerical studies on equation (16) are in progress.

4 - Examples and conclusions

We examine a simple set of equations, obtained applying the two different methods. Let

$$\beta_{00}(\varepsilon) = 2\pi\int_{-1}^{1}\sigma(\varepsilon, \varepsilon+\hbar\omega, s)\,ds \qquad \beta_{01}(\varepsilon) = 2\pi\int_{-1}^{1}\sigma(\varepsilon, \varepsilon+\hbar\omega, s)\,s\,ds$$

then

$$B_0(\varepsilon, \gamma) = \frac{1}{m^*}\sqrt{\frac{2}{m^*}}\sqrt{\varepsilon + \hbar\omega}\,\beta_{00}(e) = b_0(\varepsilon)$$

$$A_0(\varepsilon, \gamma) = \frac{1}{m^*}\sqrt{\frac{2}{m^*}}\sqrt{\varepsilon - \hbar\omega}\,\beta_{00}(e - \hbar\omega) = a_0(\varepsilon) \qquad \varepsilon > \hbar\omega$$

$$B_1(\varepsilon, \gamma) = \frac{2}{(m^*)^2}(\varepsilon + \hbar\omega)\beta_{01}(\varepsilon)\gamma = \gamma v\, b_1(\varepsilon) \qquad v \neq 0$$

$$A_1(\varepsilon, \gamma) = \frac{2}{(m^*)^2}(\varepsilon - \hbar\omega)\beta_{01}(\varepsilon - \hbar\omega)\gamma = \gamma v\, a_1(\varepsilon) \qquad \varepsilon > \hbar\omega.$$

Using the first method, we obtain the following *system of equations*

$$\frac{\partial}{\partial t} f_0(t, z, \varepsilon) - \frac{e}{m^*} E f_1(t, z, \varepsilon)$$

$$= (\boldsymbol{n}_q + 1)\, b_0(\varepsilon) f_0(t, z, \varepsilon + \hbar\omega) + \boldsymbol{n}_q a_0(\varepsilon) f_0(t, z, \varepsilon - \hbar\omega) - \nu(\varepsilon) f_0(t, z, \varepsilon)$$

$$\frac{\partial}{\partial t} f_1(t, z, \varepsilon) + \frac{\partial}{\partial z} f_0(t, z, \varepsilon) - eE\frac{\partial}{\partial \varepsilon} f_0(t, z, \varepsilon)$$

$$= (\boldsymbol{n}_q + 1)\, b_1(\varepsilon) f_1(t, z, \varepsilon + \hbar\omega) + \boldsymbol{n}_q a_1(\varepsilon) f_1(t, z, \varepsilon - \hbar\omega) - \nu(\varepsilon) f_1(t, z, \varepsilon)$$

where now $\nu(\varepsilon) = \boldsymbol{n}_q b_0(\varepsilon) + (\boldsymbol{n}_q + 1)\, a_0(\varepsilon)$.

In the other case, we have the set

$$\frac{\partial}{\partial t}\phi_0(t, z, \varepsilon) + \frac{\partial}{\partial z}\phi_1(t, z, \varepsilon) - eE\frac{\partial}{\partial \varepsilon}\phi_1(t, z, \varepsilon)$$

$$= (\boldsymbol{n}_q + 1)\, b_0(\varepsilon)\phi_0(t, z, \varepsilon + \hbar\omega) + \boldsymbol{n}_q a_0(\varepsilon)\phi_0(t, z, \varepsilon - \hbar\omega) - \nu(\varepsilon)\phi_0(t, z, \varepsilon)$$

$$\frac{\partial}{\partial t}\phi_1(t, z, \varepsilon) + \frac{\partial}{\partial z}\phi_2(t, z, \varepsilon) - eE\frac{\partial}{\partial \varepsilon}\phi_2(t, z, \varepsilon) - \frac{e}{m^*}E\phi_0(t, z, \varepsilon)$$

$$= (\boldsymbol{n}_q + 1)\frac{\sqrt{2}}{(m^*)^{\frac{3}{2}}}\sqrt{\varepsilon + \hbar\omega}\,\beta_{01}(\varepsilon)\phi_1(t, z, \varepsilon + \hbar\omega)$$

$$+\boldsymbol{n}_q\frac{\sqrt{2}}{(m^*)^{\frac{3}{2}}}\sqrt{\varepsilon - \hbar\omega}\,\alpha_{01}(\varepsilon)\phi_1(t, z, \varepsilon - \hbar\omega) - \nu(\varepsilon)\phi_1(t, z, \varepsilon).$$

The two systems of equations are very similar, but apart the differences concerning the number of involved unknowns, they present peculiar different characteristics. The choice of these variables avoids the singularity ($v = 0$) in the differential operator, but, as it is evident, for example in the definitions of $b_1(\varepsilon)$, the coefficients at the right side of the first system are not defined for $\varepsilon = 0$ and in general could not be bounded as $\varepsilon \to 0^+$.

In the more common physical kernels the singularity can be eliminated in $b_1(\varepsilon)$ (due to the presence of the factor v^2 in the Jacobian of the spherical transformation), but not in general in $\beta_{ij}(\varepsilon)$ for $j > 1$. The second set of equations does not present this trouble for any n.

The main difficulty of the above equations is the presence of shifted arguments in the collision terms. Unfortunately forward and backward terms appear simultaneously. Then analytical treatment of initial or boundary value problems is not immediate. From a numerical point of view, a difference scheme seems to arise naturally [5], because it models in a simple way the shifted arguments. Researches concerning both aspects are in project.

It is clear that both techniques can be used also in the case, when an elastic scattering, which contains the $\delta(\varepsilon_* - \varepsilon)$ instead of the $\delta(\varepsilon_* - \varepsilon \pm \hbar\omega)$, is included in the collision operator. The corresponding equations can be easily derived.

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Sommario

In questo lavoro si considera l'equazione di Boltzmann che descrive l'evoluzione di un gas di elettroni in un semiconduttore. Si suppone che la funzione di distribuzione degli elettroni dipenda dal tempo t, dalla velocità molecolare tridimensionale, ma dipenda da una sola coordinata spaziale. Per questo flusso planare sono proposti e analizzati due diversi metodi di approssimazione della funzione incognita. In entrambi i casi l'equazione di Boltzmann viene sostituita con un sistema di equazioni, nelle quali le incognite dipendono dall'energia delle particelle invece che dalle tre componenti della velocità molecolare. Si ritiene che questo approccio possa essere utile in ricerche di tipo analitico o numerico.

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