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SPHERICAL-HARMONIC TYPE EXPANSION FOR THE BOLTZMANN EQUATION IN SEMICONDUCTOR DEVICES

ARMANDO MAJORANA

The Boltzmann equation for an electron gas in a semiconductor is considered. The electron energy is assumed to have a very general form, so that, for instance, parabolic or non parabolic band approximations can be treated. A technique, which recalls the classical moment method due to Grad, to deduce an approximate quasi-hydrodynamical model is shown and compared with the spherical harmonic expansion. Some characteristics of the model, as entropy inequality, are explicitly presented.

1. Introduction.

The Boltzmann equation represents a well-defined model to describe the motion of a rarefied gas, when microscopic effects must be considered. This is the case of an electron flow in a modern submicron device. The problem of solving the full Boltzmann equation for realistic semiconductors seems to be so hard, that alternative approaches as Monte Carlo simulations are often preferred. In order to avoid the high cost of the Monte Carlo methods, many authors [3], [4], [14], have proposed an analytical and numerical approach, which briefly we recall.

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The unknown of the Boltzmann equation is the distribution function $f(t, \boldsymbol{x}, \boldsymbol{k})$; here t is the time, $\boldsymbol{x}$ the spatial coordinates and $\boldsymbol{k}$ the wave vector of the electron. If we assume an approximation of f of the type

$$f(t, \boldsymbol{x}, \boldsymbol{k}) \approx f_0(t, \mathbf{x}, \varepsilon) + \boldsymbol{k} \cdot \boldsymbol{f}_1(t, \boldsymbol{x}, \varepsilon). \tag{1}$$

where $\varepsilon = \varepsilon(\boldsymbol{k})$ is the electron kinetic energy, it is clear that, via Galerkin's method, a set of two equations are obtained. Now, the unknowns $f_0(t, \boldsymbol{x}, \varepsilon)$ and the vector $\boldsymbol{f}_1(t, \boldsymbol{x}, \varepsilon)$ depend on fewer variables than f. This advantage makes attractive the approximation (1). Obviously, one may consider more terms in (1) and then more equations are obtained.

In this article we propose a technique, which is similar to the moment method of Grad [5]. A new set of unknowns and equations are derived; they are in some cases equivalent to those obtained by using (1). Nevertheless, also in these cases new features come to light. The principal characteristic of this new technique is the possibility of treating in an intrinsic way any functional form for electron energy $\varepsilon(\boldsymbol{k})$. Also it allows to make comparisons, with respect to exact solutions of the Boltzmann equation.

2. Basic equations.

We consider an electron gas, which interacts with a bath of phonons assumed to be in thermal equilibrium. In this case the Boltzmann equation writes [6], [11]

$$\frac{\partial f}{\partial t} + \frac{1}{\hbar}\nabla_{\boldsymbol{k}}\varepsilon \cdot \nabla_{\boldsymbol{x}} f - \frac{e}{\hbar}\boldsymbol{E} \cdot \nabla_{\boldsymbol{k}} f = Q(f), \tag{2}$$

where the parameters $\hbar$ and e are the Planck constant divided by 2π and the positive electric charge, respectively. The symbol $\nabla_{\boldsymbol{k}}$ stands for the gradient with respect to the variables $\boldsymbol{k}$ and $\nabla_{\boldsymbol{x}}$ that with respect to the space coordinates $\boldsymbol{x}$. The particle energy ε is an assigned nonnegative function defined on $\mathbb{R}^3$. In (2) the external force represents the electric field $(t, \boldsymbol{x}) \to \boldsymbol{E}(t, \boldsymbol{x})$, which satisfies a suitable Poisson equation. Since our analysis does not involve this equation, we do not write it explicitly. The spatial coordinates $\boldsymbol{x}$ belong to a subset of $\mathbb{R}^3$. The wave vector $\boldsymbol{k} \in \mathbb{R}^3$. The group velocity of the electron, depending on $\boldsymbol{k}$ through the function $\varepsilon(\boldsymbol{k})$, is given by

$$\boldsymbol{v}(\boldsymbol{k}) := \frac{1}{\hbar}\nabla_{\boldsymbol{k}}\varepsilon. \tag{3}$$

We follow a semi-classical approach for the collision term $Q(f)$, so that, in the low density regime, it is

$$Q(f)(t, \boldsymbol{x}, \boldsymbol{k}) = \int_{\mathbb{R}^3} \Big[S(\boldsymbol{k}', \boldsymbol{k}) f(t, \boldsymbol{x}, \boldsymbol{k}') - S(\boldsymbol{k}, \boldsymbol{k}') f(t, \boldsymbol{x}, \boldsymbol{k}) \Big] d\boldsymbol{k}'. \tag{4}$$

The kernel S, which takes into account the scattering processes between electrons and phonons, is defined by

$$\begin{aligned} S(\boldsymbol{k}, \boldsymbol{k}') &= K_0(\boldsymbol{k}, \boldsymbol{k}')\delta(\varepsilon(\boldsymbol{k}') - \varepsilon(\boldsymbol{k})) + K(\boldsymbol{k}, \boldsymbol{k}') \\ &\quad \times \Big[(\boldsymbol{n}_q + 1)\delta(\varepsilon(\boldsymbol{k}') - \varepsilon(\boldsymbol{k}) + \hbar\omega) + \boldsymbol{n}_q \delta(\varepsilon(\boldsymbol{k}') - \varepsilon(\boldsymbol{k}) - \hbar\omega) \Big]. \end{aligned} \tag{5}$$

The constant $\mathbf{n}_q$ is the occupation number of phonons and is given by

$$\boldsymbol{n}_q = \Big[\exp\Big(\frac{\hbar\omega}{k_B T_L} \Big) - 1 \Big]^{-1},$$

where ω is the constant phonon frequency, k_B is the Boltzmann constant and T_L the lattice temperature. The symbol δ indicates the usual Dirac distribution. This is composed with the function $\varepsilon(\boldsymbol{k})$. The following assumptions on ε will be needed throughout the paper.

($\mathbb{A}$1) $\varepsilon : \mathbb{R}^3 \to \mathbb{R}_0^+$ *belongs to* $C^1(\mathbb{R}^3)$.

($\mathbb{A}$2) *Let* $\boldsymbol{n} = (\sin\varphi\cos\vartheta, \sin\varphi\sin\vartheta, \cos\varphi)$ *and* $R = [0, 2\pi] \times [0, \pi]$. *There exists* $\boldsymbol{k}_0 \in \mathbb{R}^3$ *such that, if* $\hat{\varepsilon}(\rho, \vartheta, \varphi) := \varepsilon(\boldsymbol{k}_0 + \rho\boldsymbol{n})$ *for* $\rho \geq 0$ *and* $(\vartheta, \varphi) \in R$, *then*

($\mathbb{A}$2a) *the function* $\hat{\varepsilon}(\rho, \vartheta, \varphi)$ *admits a continuous and positive partial derivative with respect to* ρ *for every* $(\rho, \vartheta, \varphi) \in (0, +\infty) \times R$;

($\mathbb{A}$2b) $\lim_{\rho \to 0^+} \rho^2 \Big[\frac{\partial\hat{\varepsilon}}{\partial\rho}(\rho, \vartheta, \varphi) \Big]^{-1} = 0$ *uniformly in* $(\theta, \varphi) \in R$;

($\mathbb{A}$2c) *there exist two constants* $c_1 > 0$ *and* $\rho_1 \geq 0$, *such that*

$$\frac{\partial\hat{\varepsilon}}{\partial\rho}(\rho, \vartheta, \varphi) \geq c_1, \quad \text{for every } \rho \geq \rho_1 \text{ and } \quad (\vartheta, \varphi) \in R.$$

$\mathbb{R}_0^+$ is the set of nonnegative real numbers, and $C^m(\mathbb{R}^3)$ $(m = 0, 1, 2, \ldots)$ is the usual space of all functions defined on $\mathbb{R}^3$, having continuous partial derivatives up to order m. We denote by $u_0 = \varepsilon(\boldsymbol{k}_0)$ the minimum of the function ε.
Assumption ($\mathbb{A}$2) allows, for example, to evaluate integrals in (4) by means of a change of variables. This is equivalent to the use of the spherical coordinate transformation in the case of the parabolic band approximation [6].

The kernels K and K_0 satisfy the symmetric conditions $K(\boldsymbol{k}'\boldsymbol{k}) = K(\boldsymbol{k}, \boldsymbol{k}')$ and $K_0(\boldsymbol{k}', \boldsymbol{k}) = K_0(\boldsymbol{k}, \boldsymbol{k}')$. Moreover, they are certainly defined and continuous in the open set $\{(\boldsymbol{k}, \boldsymbol{k}') \in \mathbb{R}^3 \times \mathbb{R}^3 : \|\boldsymbol{k} - \boldsymbol{k}'\| > 0\}$, where $\|\cdot\|$ is the standard Euclidean norm in $\mathbb{R}^3$. It is possible ([9]) to prove the existence of a suitable continuous extensions of the kernels over the whole $\mathbb{R}^3$, such that $Q(f)$ does not change for any admissible function. Therefore, we consider these continuous extensions, in order to avoid useless troubles. The previous hypotheses on the kernels and on $\varepsilon(\boldsymbol{k})$ guarantee ([9]) that the operator $Q(f)$ maps continuous functions into continuous functions.

3. The energy-depending equations.

Let be $\mathscr{P}(\boldsymbol{k})$ a function belonging to $C^1(\mathbb{R}^3)$ and u a real parameter. At variance with the usual moment method, we multiply both sides of Eq. (2) for $\mathscr{P}(\boldsymbol{k})\delta(\varepsilon(\boldsymbol{k}) - u)$ and then we integrate with respect to $\boldsymbol{k}$ over $\mathbb{R}^3$. We also note that the function $\mathscr{P}(\boldsymbol{k})$ is unnecessarily restricted to be of polynomial form. The presence of the composition between the δ distribution function and the function $\varepsilon(\boldsymbol{k})$ requires some care in performing the change of order of differential and integral operators. We are interested to study classical solutions of Eq. (2), so that the previous operations, that are well-known in the distribution sense, here need some new auxiliary results. In Appendix A, we give the mathematical tools, which allow us to write the following energy-depending equation

$$
\begin{aligned}
(6) \qquad & \frac{\partial}{\partial t}\int_{\mathbb{R}^3} f(t, \boldsymbol{x}, \boldsymbol{k})\mathscr{P}(\boldsymbol{k})\delta(\varepsilon(\boldsymbol{k}) - u)\, d\boldsymbol{k} \\
& \quad + \nabla_{\boldsymbol{x}}\int_{\mathbb{R}^3} \boldsymbol{v}(\boldsymbol{k}) f(t, \boldsymbol{x}, \boldsymbol{k})\mathscr{P}(\boldsymbol{k})\delta(\varepsilon(\boldsymbol{k}) - u)\, d\boldsymbol{k} \\
& + e\boldsymbol{E}\cdot\Big\{\frac{1}{\hbar}\int_{\mathbb{R}^3} f(t, \boldsymbol{x}, \boldsymbol{k})\Big[\nabla_{\boldsymbol{k}}\mathscr{P}(\boldsymbol{k})\Big]\delta(\varepsilon(\boldsymbol{k}) - u)\, d\boldsymbol{k} \\
& \quad - \frac{\partial}{\partial u}\int_{\mathbb{R}^3} f(t, \boldsymbol{x}, \boldsymbol{k})\mathscr{P}(\boldsymbol{k})\boldsymbol{v}(\boldsymbol{k})\delta(\varepsilon(\boldsymbol{k}) - u)\, d\boldsymbol{k}\Big\} \\
& \qquad = \int_{\mathbb{R}^3} Q(f)(t, \boldsymbol{x}, \boldsymbol{k})\mathscr{P}(\boldsymbol{k})\delta(\varepsilon(\boldsymbol{k}) - u)\, d\boldsymbol{k}.
\end{aligned}
$$

If, for fixed $(t, \boldsymbol{x})$, the function $\boldsymbol{k} \to f(t, \boldsymbol{x}, \boldsymbol{k})$ is continuous in $\mathbb{R}^3$, then all integrals in Eq. (6) exist. Now, in (6) the *independent variables* are only u (the value of the electron energy), $\boldsymbol{x}$ and t. Since, for every $\phi \in C^0(\mathbb{R}^3)$, we have

$$
\int_{\mathbb{R}^3} \phi(\boldsymbol{k})\delta(\varepsilon(\boldsymbol{k}) - u)\, d\boldsymbol{k} = 0 \qquad \text{for every} \quad u \le u_0,
$$

then Eq. (6) is meaningful only for $u > u_0$. Therefore, in the following we shall intend that the value of any function of u vanishies, if $u \leq u_0$. This makes simple some formulas.

For every choice of the function $\mathscr{P}(\boldsymbol{k})$ a new equation is obtained. As it happens for the moment method, each equation contains, except for particular cases [8], [10] at least two unknown functions. For example, if we choose $\mathscr{P}(\boldsymbol{k}) \equiv 1$, then the left hand side of Eq. (6) contains in general the following unknowns

$$N(t, \boldsymbol{x}, u) := \int_{\mathbb{R}^3} f(t, \boldsymbol{x}, \boldsymbol{k}) \delta(\varepsilon(\boldsymbol{k}) - u)\, d\boldsymbol{k} \tag{7}$$

$$\boldsymbol{V}(t, \boldsymbol{x}, u) := \int_{\mathbb{R}^3} f(t, \boldsymbol{x}, \boldsymbol{k}) \boldsymbol{v}(\boldsymbol{k}) \delta(\varepsilon(\boldsymbol{k}) - u)\, d\boldsymbol{k}. \tag{8}$$

In fact, from Eq. (6) we obtain

$$\frac{\partial N}{\partial t} + \nabla_{\boldsymbol{x}} \boldsymbol{V} - \mathbb{e}\boldsymbol{E} \cdot \frac{\partial \boldsymbol{V}}{\partial u} = \int_{\mathbb{R}^3} Q(f)(t, \boldsymbol{x}, \boldsymbol{k}) \delta(\varepsilon(\boldsymbol{k}) - u)\, d\boldsymbol{k}. \tag{9}$$

The production arising from the collisional operator will be studied in the next section. This equation still belongs to the framework of transport theory both for the integral-differential form and for the presence of the kinematical variable u. Since, in general, two unknowns appear in Eq. (9), it is necessary to add at least another equation. We suggest, as the simplest choice, to consider again (6) with $\mathscr{P}(\boldsymbol{k}) = \boldsymbol{v}(\boldsymbol{k})$. Since again more unknowns are introduced, a closure problem arises. A solution of this is proposed in [7], where the two only unknowns N and $\boldsymbol{V}$ are considered.

The scalar quantity $N(t, \boldsymbol{x}, u)$ is the probability density function to find at time t and position $\boldsymbol{x}$ an electron with energy u. The function N must be nonnegative, because the probability density f is always nonnegative. If the function N is known, then we can obtain all hydrodynamical scalar quantities. For example, to find the hydrodynamical density $\rho(t, \boldsymbol{x})$, it is sufficient to integrate (see Appendix B) N with respect to all values of energy u; i.e.

$$\rho(t, \boldsymbol{x}) := \int_{\mathbb{R}^3} f(t, \boldsymbol{x}, \boldsymbol{k})\, d\boldsymbol{k} = \int_{u_0}^{+\infty} N(t, \boldsymbol{x}, u)\, du.$$

The physical meaning of the vector $\boldsymbol{V}(t, \boldsymbol{x}, u)$ can be understood following a similar argument.

4. The collisional operator.

It is proved in Appendix C, that the kernel K_0 does not give any contribution in r.h.s of Eq. (9). Let for all $\boldsymbol{k} \in \mathbb{R}^3$,

$$A(\boldsymbol{k}) := \boldsymbol{n}_q \int_{\mathbb{R}^3} K(\boldsymbol{k}', \boldsymbol{k})\delta(\varepsilon(\boldsymbol{k}') - \varepsilon(\boldsymbol{k}) + \hbar\omega)\, d\boldsymbol{k}', \tag{10}$$

$$B(\boldsymbol{k}) := \boldsymbol{n}_q \int_{\mathbb{R}^3} K(\boldsymbol{k}, \boldsymbol{k}')\delta(\varepsilon(\boldsymbol{k}') - \varepsilon(\boldsymbol{k}) - \hbar\omega)\, d\boldsymbol{k}', \tag{11}$$

$$a := \frac{\boldsymbol{n}_q + 1}{\boldsymbol{n}_q} = \exp\Big(\frac{\hbar\omega}{k_B T_L}\Big). \tag{12}$$

If the kernels and the energy $\varepsilon(\boldsymbol{k})$ are isotropic, then the functions $A(\boldsymbol{k})$ and $B(\boldsymbol{k})$ depend on $\boldsymbol{k}$ only through the function ε, so that we can write

$$A(\boldsymbol{k}) = \alpha(\varepsilon(\boldsymbol{k})) \quad \text{and} \quad B(\boldsymbol{k}) = \beta(\varepsilon(\boldsymbol{k})). \tag{13}$$

This happens in almost every physical model of kernels and energy ε. In fact, the function

$$\nu(\boldsymbol{k}) = B(\boldsymbol{k}) + aA(\boldsymbol{k})$$

is called *collisional frequency* and $1/\nu(\boldsymbol{k})$ is a relaxation time, and usually they are scalar. On the contrary, if the crystal presents some anisotropy or the ellipsoidal model is assumed for $\varepsilon(\boldsymbol{k})$, then relationship (13) might be false. Here, this last possibility is not considered, so that we assume (13), in order to obtain the next results.
In [10] we prove that, for every $(t, \boldsymbol{x}, u)$,

$$\begin{aligned}\int_{\mathbb{R}^3} Q(f)(t, \boldsymbol{x}, \boldsymbol{k})\delta(\varepsilon(\boldsymbol{k}) - u)d\boldsymbol{k} &= a\alpha(u + \hbar\omega)N(t, \boldsymbol{x}, u + \hbar\omega) \\ &+ \beta(u - \hbar\omega)N(t, \boldsymbol{x}, u - \hbar\omega) - [\beta(u) + a\alpha(u)]N(t, \boldsymbol{x}, u).\end{aligned} \tag{14}$$

Then, Eq. (9) contains exactly only the unknowns N and $\boldsymbol{V}$. We remark that the use of the distribution $\delta(\varepsilon(\boldsymbol{k}) - u)$ gives Eq. (9) without specifying the band structure. The collisional integral (14) requires only the calculation of the functions α and β, when kernels and band structure have been chosen. We want to show that the principal characteristics of the collisional operator $Q(f)$ of the Boltzmann equation, as collisional invariants, self-adjontness in suitable Hilbert space and H-theorem, can be found from Eq. (14). Let be

$$M(\varepsilon) := \exp\Big(-\frac{\varepsilon}{k_B T_L}\Big) = a^{-\frac{\varepsilon}{\hbar\omega}},$$

$$\sigma(u) := \int_{\mathbb{R}^3} \delta(\varepsilon(\boldsymbol{k}) - u)\, d\boldsymbol{k}.$$

We denote by $G(N)$ the r.h.s. of Eq. (14). Set $I_0 := \{u \in \mathbb{R} : u_0 < u \leq u_0 + \hbar\omega\}$. Let us fix t, $\boldsymbol{x}$ and $\bar{u} \in I_0$. Let h be an arbitrary function depending on $(t, \boldsymbol{x}, u)$, with $u \in \mathbb{R}$. For every $j \in \mathbb{N}_0$ (the set of nonnegative integers), we put

$$\alpha_j = \alpha(\bar{u} + j\hbar\omega), \quad \beta_j = \beta(\bar{u} + j\hbar\omega), \quad \sigma_j = \sigma(\bar{u} + j\hbar\omega),$$
$$N_j = N(t, \boldsymbol{x}, \bar{u} + j\hbar\omega), \quad h_j = h(t, \boldsymbol{x}, \bar{u} + j\hbar\omega), \quad M_j = M(\bar{u} + j\hbar\omega)$$

Then, following [10], if $n \in \mathbb{N}$, we have

$$\sum_{j=0}^{n} h_j G(N)(t, \boldsymbol{x}, \bar{u} + j\hbar\omega) = (a\alpha_{n+1}N_{n+1} - \beta_n N_n)h_n + \sum_{j=0}^{n-1}(h_j - h_{j+1})(a\alpha_{j+1}N_{j+1} - \beta_j N_j)$$
$$= (a\alpha_{n+1}N_{n+1} - \beta_n N_n)h_n + \sum_{j=0}^{n-1}(h_j - h_{j+1})\beta_j M_j \sigma_j \Big[\frac{N_{j+1}}{M_{j+1}\sigma_{j+1}} - \frac{N_j}{M_j\sigma_j}\Big]. \tag{15}$$

Using Eq. (15) in [10] we have deduced conservation laws and self-adjointness (see also [2] and [12]). Here, we show the *discrete* entropy inequality. If we choose

$$h(t, \boldsymbol{x}, u) = \log\Big[\frac{N(t, \boldsymbol{x}, u)}{M(u)\sigma(u)} + \mu_0\Big],$$

where μ_0 is a positive constant, the last sum in (15) is negative or null. Now, if $\lim_{n\to+\infty}(a\alpha_{n+1}N_{n+1} - \beta_n N_n)h_n = 0$, and, for $n \to +\infty$, the series in the r.h.s of (15) converges, then the entropy inequality is obtained.
The analogous for the Boltzmann equation, in the case of parabolic band approximation, was obtained in [8] (see also [3] and [12] and references therein). We remark that (15) and their consequences hold for every $\bar{u} \in I_0$. The global (in the sense of *for all values of the energy u)* conservation of the mass or the global entropy inequality can be obtained directly by integration from the operator $G(N)$.

5. Final remarks and conclusions.

The scope of this paper is to highlight how a new transport model can be derived from the Boltzmann equation. The principal advantages are two. The

first is the number of independent variables, which are less then the original. The second consists in recovering the most important features of the collisional operator of the Boltzmann equation from Eq. (9). This aspect seems to be important to guarantee the physical meaning of the model. Moreover, the entropy inequality often assures the stability of the solution. From a theoretical point of view, we expect that we can perform, directly and with reasonable less difficulties, analytical investigations about asymptotic or fluid limits.
A final observation concerns the number of equations to deduce from (9). The simplest choice is two: $\mathscr{P}(\boldsymbol{k}) \equiv 1$ and $\mathscr{P}(\boldsymbol{k}) = \boldsymbol{v}(\boldsymbol{k})$. This was made in the past by many authors, furnishing considerable results. Our recent investigations seem to confirm this.

6. Appendix A.

Let r be a positive real number and ω_r the function defined by setting, for any $z \in \mathbb{R}$,

$$\omega_r(z) = \begin{cases} \dfrac{\exp(1/2)}{K_1(1/2) - K_0(1/2)} \dfrac{1}{r} \exp\left(-\dfrac{r^2}{r^2 - z^2}\right) & \text{if } |z| < r \\ 0 & \text{otherwise,} \end{cases}$$

where K_0 and K_1 are modified Bessel functions ([1]). It follows that

$$\int_{\mathbb{R}} \omega_r(z)\, dz = 1 \quad \text{for every} \quad r > 0.$$

Proposition 1. *We assume that the function $\varepsilon(\boldsymbol{k})$ satisfies the hypotheses* ($\mathbb{A}1$)–($\mathbb{A}2$). *Let $\boldsymbol{k} \to A(\boldsymbol{k})$ be a function belonging to $C^1(\mathbb{R}^3)$. Then, for every $u > u_0$, we have*

$$\int_{\mathbb{R}^3} \delta(\varepsilon(\boldsymbol{k}) - u) \frac{\partial A(\boldsymbol{k})}{\partial k_i}\, d\boldsymbol{k} = \frac{\partial}{\partial u} \int_{\mathbb{R}^3} A(\boldsymbol{k}) \delta(\varepsilon(\boldsymbol{k}) - u) \frac{\partial \varepsilon}{\partial k_i}\, d\boldsymbol{k}, \tag{16}$$

where k_i is a generic but assigned component of the vector $\boldsymbol{k}$.

Proof. Let $(u_a, u_b) \subset (u_0, +\infty)$ be a bounded open interval. We define in (u_a, u_b) the function

$$F_r(u) := \int_{\mathbb{R}^3} \omega_r(\varepsilon(\boldsymbol{k}) - u) \frac{\partial A(\boldsymbol{k})}{\partial k_i}\, d\boldsymbol{k}. \tag{17}$$

The assumptions on ε guarantee ([9]) that, for every fixed u, the function $\boldsymbol{k} \to \omega_r(\varepsilon(\boldsymbol{k}) - u)$ has compact support in $\mathbb{R}^3$. Hence, (17) is a real-valued

function for every $u \in (u_a u_b)$. It is a simple matter to verify that the support of the function $(u, \boldsymbol{k}) \to \omega_r(\varepsilon(\boldsymbol{k}) - u)$ is contained in the bounded set

$$(u_a, u_b) \times \left\{\boldsymbol{k} \in \mathbb{R}^3 : u_a - r \leq \varepsilon(\boldsymbol{k}) \leq u_b + r\right\}.$$

Therefore, there exists a closed cube $S = \left\{\boldsymbol{k} \in \mathbb{R}^3 : |k_i| \leq L_S, i = 1, 2, 3\right\}$ such that, we have

$$\omega_r(\varepsilon(\boldsymbol{k}) - u) = 0, \quad \text{for every } (u, \boldsymbol{k}) \in (u_a, u_b) \times \partial S$$

and

$$F_r(u) = \int_S \omega_r(\varepsilon(\boldsymbol{k}) - u) \frac{\partial A(\boldsymbol{k})}{\partial k_i} d\boldsymbol{k}, \quad \forall\, u \in (u_a, u_b).$$

In fact, it is sufficient to choose S so that

$$\bigcup_{u_a < u < u_b} \operatorname{supp}\left\{\boldsymbol{k} \to \omega_r(\varepsilon(\boldsymbol{k}) - u)\right\} \subseteq S.$$

Now, it is trivial to carry out, for any $u \in (u_a, u_b)$, the following operations

$$\begin{aligned}\int_S \omega_r(\varepsilon(\boldsymbol{k}) - u) \frac{\partial A(\boldsymbol{k})}{\partial k_i}\, d\boldsymbol{k} &= -\int_S A(\boldsymbol{k}) \frac{\partial}{\partial k_i}[\omega_r(\varepsilon(\boldsymbol{k}) - u)]\, d\boldsymbol{k} \\ = -\int_S A(\boldsymbol{k}) \frac{\partial \omega_r(\varepsilon(\boldsymbol{k}) - u)}{\partial \varepsilon} \frac{\partial \varepsilon}{\partial k_i}\, d\boldsymbol{k} &= \int_S A(\boldsymbol{k}) \frac{\partial \omega_r(\varepsilon(\boldsymbol{k}) - u)}{\partial u} \frac{\partial \varepsilon}{\partial k_i}\, d\boldsymbol{k} \\ &= \frac{\partial}{\partial u} \int_S A(\boldsymbol{k}) \omega_r(\varepsilon(\boldsymbol{k}) - u) \frac{\partial \varepsilon}{\partial k_i}\, d\boldsymbol{k}.\end{aligned}$$

Therefore,

$$F_r(u) = \frac{\partial}{\partial u} \int_{\mathbb{R}^3} A(\boldsymbol{k}) \omega_r(\varepsilon(\boldsymbol{k}) - u) \frac{\partial \varepsilon}{\partial k_i}\, d\boldsymbol{k}.$$

Taking into account ([9]) the definition of an integral containing the term $\delta(\varepsilon(\boldsymbol{k}) - u)$, for every $u \in (u_a, u_b)$, we have

$$\lim_{r \to 0^+} F_r(u) = \int_{\mathbb{R}^3} \delta(\varepsilon(\boldsymbol{k}) - u) \frac{A(\boldsymbol{k})}{\partial k_i}\, d\boldsymbol{k}$$

and

$$\lim_{r \to 0^+} \int_{\mathbb{R}^3} A(\boldsymbol{k}) \omega_r(\varepsilon(\boldsymbol{k}) - u) \frac{\partial \varepsilon}{\partial k_i}\, d\boldsymbol{k} = \int_{\mathbb{R}^3} A(\boldsymbol{k}) \delta(\varepsilon(\boldsymbol{k}) - u) \frac{\partial \varepsilon}{\partial k_i}\, d\boldsymbol{k}.$$

Both limits are uniform on any compact subset of (u_a, u_b). Now, let be $u_* \in (u_a, u_b)$ and $h > 0$ is such that $[u_* - h, u_* + h] \subset (u_a, u_b)$. If $\{r_n\}$ is a sequence having $\lim_{n\to+\infty} r_n = 0$, then it follows

$$\lim_{n\to+\infty} \int_{\mathbb{R}^3} A(\boldsymbol{k})\omega_{r_n}(\varepsilon(\boldsymbol{k}) - u)\frac{\partial \varepsilon}{\partial k_i}\, d\boldsymbol{k} = \int_{\mathbb{R}^3} A(\boldsymbol{k})\delta(\varepsilon(\boldsymbol{k}) - u)\frac{\partial \varepsilon}{\partial k_i}\, d\boldsymbol{k}$$

and, uniformly on $[u_* - h, u_* + h]$,

$$\lim_{n\to+\infty} \frac{\partial}{\partial u}\int_{\mathbb{R}^3} A(\boldsymbol{k})\omega_{r_n}(\varepsilon(\boldsymbol{k}) - u)\frac{\partial \varepsilon}{\partial k_i}\, d\boldsymbol{k} = \int_{\mathbb{R}^3} \delta(\varepsilon(\boldsymbol{k}) - u)\frac{\partial A(\boldsymbol{k})}{\partial k_i}\, d\boldsymbol{k}.$$

This (see, for example, [13], p. 152) implies (16), for every $u \in [u_* - h, u_* + h]$. □

We apply this result to terms arising from the free streaming operator of the Boltzmann equation (2). If, for fixed $(t, \boldsymbol{x})$, the function $\boldsymbol{k} \to f(t, \boldsymbol{x}, \boldsymbol{k})$ belongs to $C^1(\mathbb{R}^3)$, by using (16), it follows

$$\begin{aligned}
&\int_{\mathbb{R}^3} \nabla_{\boldsymbol{k}} f(t, \boldsymbol{x}, \boldsymbol{k})\mathscr{P}(\boldsymbol{k})\delta(\varepsilon(\boldsymbol{k}) - u)\, d\boldsymbol{k} \\
&= \int_{\mathbb{R}^3} \{\nabla_{\boldsymbol{k}}[f(t, \boldsymbol{x}, \boldsymbol{k})\mathscr{P}(\boldsymbol{k})] - f(t, \boldsymbol{x}, \boldsymbol{k})\nabla_{\boldsymbol{k}}\mathscr{P}(\boldsymbol{k})\}\delta(\varepsilon(\boldsymbol{k}) - u)\, d\boldsymbol{k} \\
&\qquad = \hbar\frac{\partial}{\partial u}\int_{\mathbb{R}^3} f(t, \boldsymbol{x}, \boldsymbol{k})\mathscr{P}(\boldsymbol{k})\boldsymbol{v}(\boldsymbol{k})\delta(\varepsilon(\boldsymbol{k}) - u)\, d\boldsymbol{k} \\
&\qquad\qquad - \int_{\mathbb{R}^3} f(t, \boldsymbol{x}, \boldsymbol{k})[\nabla_{\boldsymbol{k}}\mathscr{P}(\boldsymbol{k})]\delta(\varepsilon(\boldsymbol{k}) - u)\, d\boldsymbol{k}.
\end{aligned}$$

The change of order between integral operator and $\nabla_{\boldsymbol{k}}$ or $\dfrac{\partial}{\partial t}$ is easily performed, by using again the sequence $\omega_{r_n}(\varepsilon(\boldsymbol{k}) - u)$.

7. Appendix B.

Let $C_0^0(\mathbb{R})$ denote the space of the continuous functions defined in $\mathbb{R}$, having compact support. If $\psi \in C_0^0(\mathbb{R})$ and $r > 0$, we define

$$w_1(r; \psi) := \sup\left\{\left|\psi(\varepsilon(\boldsymbol{k}) - \int_{\mathbb{R}} \psi(u)\omega_r(\varepsilon(\boldsymbol{k}) - u)\, du\right| : \boldsymbol{k} \in \mathbb{R}^3\right\}.$$

Lemma 1. *For any $\psi \in C_0^0(\mathbb{R})$, we have* $\lim_{r\to 0^+} w_1(r; \psi) = 0$.

Proof. By using the mean value theorem, for every fixed $\boldsymbol{k} \in \mathbb{R}^3$, we obtain

$$\Big|\psi(\varepsilon(\boldsymbol{k})) - \int_{\mathbb{R}} \psi(u)\omega_r(\varepsilon(\boldsymbol{k}) - u)\, du\Big| = \big|\psi(\varepsilon(\boldsymbol{k})) - \psi(\xi)\big|,$$

where $\xi \in \mathbb{R} : \big|\varepsilon(\boldsymbol{k}) - \xi\big| \leq r$. Then

$$w_1(r; \psi) \leq \sup\{|\psi(w) - \psi(\xi)| : w, \xi \in \mathbb{R}, |w - \xi| \leq r\}$$

and our assertion is established, due the uniform continuity of the function ψ. □

Let $h \in C^0(\mathbb{R}^3)$ and $\psi \in C_0^0(\mathbb{R})$. We define

$$w_3(r; h, \psi) := \sup\Big\{\Big|\int_{\mathbb{R}^3} h(\boldsymbol{k}) w_r(\varepsilon(\boldsymbol{k}) - u)\, d\boldsymbol{k} - \int_{\mathbb{R}^3} h(\boldsymbol{k})\delta(\varepsilon(\boldsymbol{k}) - u)\, d\boldsymbol{k}\Big| : u \in \operatorname{supp}\psi\Big\}.$$

It is an immediate consequence of Lemma B.3 in [9] the following property

$$\lim_{r \to 0^+} w_3(r, h, \psi) = 0.$$

We denote by $L^1(\mathbb{R}^3)$ the usual space of Lebesgue integrable functions defined in $\mathbb{R}^3$.

Lemma 2. *If $h \in C^0(\mathbb{R}^3) \cap L^1(\mathbb{R}^3)$ and $\psi \in C_0^0(\mathbb{R})$, then*

$$\int_R \psi(u)\Big[\int_{\mathbb{R}^3} h(\boldsymbol{k})\delta(\varepsilon(\boldsymbol{k}) - u)\, d\boldsymbol{k}\Big] du = \int_{\mathbb{R}^3} \psi(\varepsilon(\boldsymbol{k}))h(\boldsymbol{k})\, d\boldsymbol{k}.$$

Proof. From

$$\begin{aligned}
&\Big|\int_{\mathbb{R}} \psi(u)\Big[\int_{\mathbb{R}^3} h(\boldsymbol{k})\delta(\varepsilon(\boldsymbol{k}) - u)\, d\boldsymbol{k}\Big] du - \int_{\mathbb{R}^3} \psi(\varepsilon(\boldsymbol{k}))h(\boldsymbol{k})\, d\boldsymbol{k}\Big| \\
&= \Big|\int_{\mathbb{R}} \psi(u)\Big[\int_{\mathbb{R}^3} h(\boldsymbol{k})\delta(\varepsilon(\boldsymbol{k}) - u)\, d\boldsymbol{k} - \int_{\mathbb{R}^3} h(\boldsymbol{k})\omega_r(\varepsilon(\boldsymbol{k}) - u)\, d\boldsymbol{k}\Big] du \\
&\quad + \int_{\mathbb{R}} \psi(u)\Big[\int_{\mathbb{R}^3} h(\boldsymbol{k})\omega_r(\varepsilon(\boldsymbol{k}) - u)\, d\boldsymbol{k}\Big] du - \int_{\mathbb{R}^3} \psi(\varepsilon(\boldsymbol{k}))h(\boldsymbol{k})\, d\boldsymbol{k}\Big| \\
&\leq w_3(r; h, \psi) \int_{\mathbb{R}} |\psi(u)|\, du + w_1(r; \psi) \int_{\mathbb{R}^3} |h(\boldsymbol{k})|\, d\boldsymbol{k},
\end{aligned}$$

as $r \to 0^+$, it follows our claim. □

Remark. The assumption $h \in L^1(\mathbb{R}^3)$ can be relaxed. We have not made this in view of the next result.

Proposition 2. *If* $h \in C^0(\mathbb{R}^3) \cap L^1(\mathbb{R}^3)$, *then*

$$\int_{\mathbb{R}} \Big[\int_{\mathbb{R}^3} h(\boldsymbol{k}) \delta(\varepsilon(\boldsymbol{k}) - u)\, d\boldsymbol{k} \Big] du = \int_{\mathbb{R}^3} h(\boldsymbol{k})\, d\boldsymbol{k}.$$

Proof. First, we suppose that $h(\boldsymbol{k}) \geq 0\ \forall \boldsymbol{k} \in \mathbb{R}^3$. Now, let $\psi_n : \mathbb{R} \to \mathbb{R}_0^+$, $n \in \mathbb{N}$, be defined by setting, for $z \in \mathbb{R}$,

$$\psi_n(z) = \begin{cases} 1 & \text{if} \quad |z| \leq n, \\ 1 + n - |z| & \text{if} \quad n < |z| < n + 1, \\ 0 & \text{if} \quad |z| \geq n + 1. \end{cases}$$

By Lebesgue Dominated Convergence, we obtain

$$\lim_{n \to +\infty} \int_{\mathbb{R}^3} \psi_n(\varepsilon(\boldsymbol{k})) h(\boldsymbol{k})\, d\boldsymbol{k} = \int_{\mathbb{R}^3} h(\boldsymbol{k})\, d\boldsymbol{k}$$

and the assertion is reached. Now, the case when $h(\boldsymbol{k})$ changes of sign, is trivial. □

8. Appendix C.

We prove that, if for fixed $(t, \boldsymbol{x})$, the function $\boldsymbol{k} \to f(t, \boldsymbol{x}, \boldsymbol{k})$ is continuous in $\mathbb{R}^3$, then

$$\int_{\mathbb{R}^3} \Big\{ \int_{\mathbb{R}^3} K_0(\boldsymbol{k}, \boldsymbol{k}') \delta(\varepsilon(\boldsymbol{k}') - \varepsilon(\boldsymbol{k}))[f(t, \boldsymbol{x}, \boldsymbol{k}') - f(t, \boldsymbol{x}, \boldsymbol{k})]\, d\boldsymbol{k}' \Big\} \cdot \cdot \delta(\varepsilon(\boldsymbol{k}) - u)\, d\boldsymbol{k} = 0. \tag{18}$$

First, we note (see [9]) that we can separate the integrals, because both exist. Now, by using Lemma B.5 of [9] and Lemma 3 of [10], we have

$$\begin{aligned} &\int_{\mathbb{R}^3} \Big[\int_{\mathbb{R}^3} K_0(\boldsymbol{k}, \boldsymbol{k}') \delta(\varepsilon(\boldsymbol{k}') - \varepsilon(\boldsymbol{k}))\, f(t, \boldsymbol{x}, \boldsymbol{k}')\, d\boldsymbol{k}' \Big] \delta(\varepsilon(\boldsymbol{k}) - u)\, d\boldsymbol{k} \\ &= \lim_{r \to 0^+} \int_{\mathbb{R}^3} \Big[\int_{\mathbb{R}^3} K_0(\boldsymbol{k}, \boldsymbol{k}') \delta(\varepsilon(\boldsymbol{k}') - \varepsilon(\boldsymbol{k}))\, f(t, \boldsymbol{x}, \boldsymbol{k}')\, d\boldsymbol{k}' \Big] \omega_r(\varepsilon(\boldsymbol{k}) - u)\, d\boldsymbol{k} \\ &= \lim_{r \to 0^+} \int_{\mathbb{R}^3} \Big[\int_{\mathbb{R}^3} K_0(\boldsymbol{k}, \boldsymbol{k}') \delta(\varepsilon(\boldsymbol{k}') - \varepsilon(\boldsymbol{k}))\, f(t, \boldsymbol{x}, \boldsymbol{k}') \omega_r(\varepsilon(\boldsymbol{k}) - u)\, d\boldsymbol{k} \Big] d\boldsymbol{k}' \\ &= \lim_{r \to 0^+} \int_{\mathbb{R}^3} \omega_r(\varepsilon(\boldsymbol{k}') - u) \Big[\int_{\mathbb{R}^3} K_0(\boldsymbol{k}, \boldsymbol{k}') \delta(\varepsilon(\boldsymbol{k}') - \varepsilon(\boldsymbol{k}))\, f(t, \boldsymbol{x}, \boldsymbol{k}')\, d\boldsymbol{k} \Big] d\boldsymbol{k}' \\ &= \int_{\mathbb{R}^3} \delta(\varepsilon(\boldsymbol{k}') - u) \Big[\int_{\mathbb{R}^3} K_0(\boldsymbol{k}, \boldsymbol{k}') \delta(\varepsilon(\boldsymbol{k}') - \varepsilon(\boldsymbol{k}))\, f(t, \boldsymbol{x}, \boldsymbol{k}')\, d\boldsymbol{k} \Big] d\boldsymbol{k}'. \end{aligned}$$

This gives (18).

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REFERENCES

[1] M. Abramowitz - I.A. Stegun, *Handbook of Mathematical Functions with Formulas, Graphs, and Mathematical Tables,* Dover Publ., New York, 1972.

[2] J. Banasiak, *Mathematical properties of inelastic scattering models in the kinetic theory,* to appear in Math. Models Methods Appl. Sci., (1999).

[3] N. Ben Addallah - P. Degond, *On a hierarchy of macroscopic models for semiconductors,* J. Math. Phys., 37 (1996), pp. 3306-3333.

[4] W. Cox, *Boundary value problem in Boltzmann modeling of hot electron transport,* Solid-State Electronics, 30 (1987), pp. 364–367.

[5] H. Grad, *Thermodynamics of gases,* in: S. Flügge (ed.), Handbuch der Physik Vol. 12, Springer-Verlag , 1958.

[6] C. Jacoboni - P. Lugli, *The Monte Carlo Method for Semiconductor Device Simulation,* Springer-Verlag, New York, 1989.

[7] S. F. Liotta - A. Majorana, *Energy-kinetic equations modeling electron transport in semiconductors,* Preprint (1998).

[8] A. Majorana, *Conservation laws from the Boltzmann equation describing electron-phonon interaction in semiconductors,* Transport Theory Statist. Phys., 22 (1993), pp. 81–93.

[9] A. Majorana - A. Marano, *Space homogeneous solutions to the Cauchy problem for semiconductor Boltzmann equations,* SIAM J. Math. Anal., 28 (1997), pp. 1294–1308.

[10] A. Majorana, *Trend to Equilibrium of Electron Gas in a Semiconductor According to the Boltzmann Equation,* Transport Theory Statist. Phys., 27 (1998), pp. 547–571.

[11] P. A. Markowich - C. Ringhofer - C. Schmeiser, *Semiconductor Equations,* Springer-Verlag, New York, 1990.

[12] P. A. Markowich - C. Schmeiser, *The Drift-Diffusion limit for electron-phonon interaction in semiconductors,* Math. Models Methods Appl. Sci., 7 (1997), pp. 707–729.

[13] W. Rudin, *Principles of Mathematical Analysis. Third Edition,* Mc Graw-Hill, London, 1976.

[14] M.C. Vecchi - J. Mohring - M. Rudan, *An Efficient Solution Scheme for the Spherical-Harmonics Expansion of the Boltzmann Transport Equation,* IEEE Trans. Computer-Aided Design, 16 (1997), pp. 353–361.

Dipartimento di Matematica,
Università di Catania,
Viale Andrea Doria 6,
95125 Catania (ITALY)