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A. M. Anile W. Allegretto
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Mathematical Problems in Semiconductor Physics

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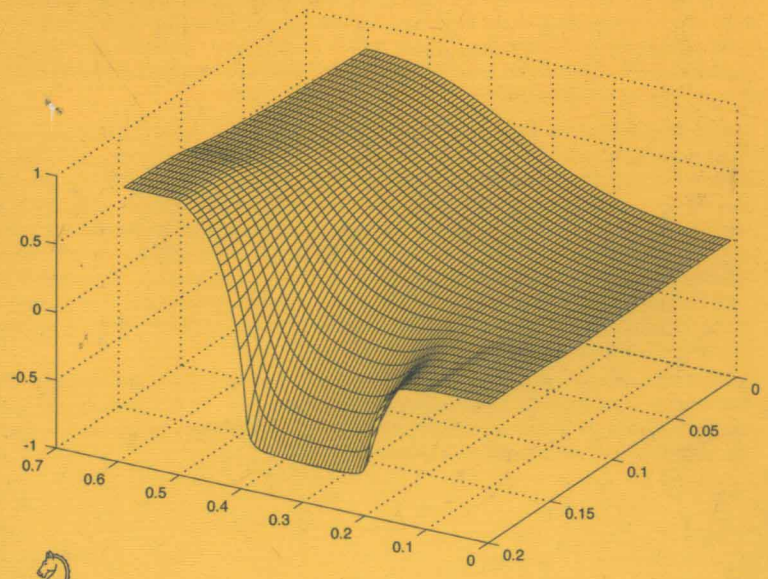

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Mathematical Problems in Semiconductor Physics

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C.I.M.E. Summer School
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With the collaboration of
G. Mascali and V. Romano

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Preface

The increasing demand on ultra miniturized electronic devices for ever improving performances has led to the necessity of a deep and detailed understanding of the mathematical theory of charge transport in semiconductors. Because of their very short dimensions of charge transport, these devices must be described in terms of the semiclassical Boltzmann equation coupled with the Poisson equation (or some phenomenological consequences of these equations) because the standard approach, which is based on the celebrated drift-diffusion equations, leads to very inaccurate results whenever the dimensions of the devices approach the carrier mean free path.
In some cases, such as for very abrupt heterojunctions in which tunneling occurs it is even necessary to resort to quantum transport models (e.g. the Wigner-Boltzmann-Poisson system or equivalent descriptions).
These sophisticated physical models require an appropriate mathematical framework for a proper understanding of their mathematical structure as well as for the correct choice of the numerical algorithms employed for computational simulations.
The resulting mathematical problems have a broad spectrum of theoretical and practical conceptually interesting aspects.
From the theoretical point of view, it is of paramount interest to investigate wellposedness problems for the semiclassical Boltzmann equation (and also for the quantum transport equation, although this is a much more difficult case). Another problem of fundamental interest is that of the hydrodynamical limit which one expects to be quite different from the Navier-Stokes-Fourier one, since the collision operator is substantially different from the one in rarefied gas case.
From the application viewpoint it is of great practical importance to study efficient numerical algorithms for the numerical solution of the semiclassical Boltzmann transport equation (e.g spherical harmonics expansions, Monte Carlo method, method of moments, etc.) because such investigations could have a great impact on the performance of industrial simulation codes for

TCAD (Technology Computer Aided Design) in the microelectronics industry.

The CIME summer course entitled **MATHEMATICAL PROBLEMS IN SEMICONDUCTOR PHYSICS** dealt with this and related questions. It was addressed to researchers (either PhD students, young post-docs or mature researchers from other areas of applied mathematics) with a strong interest in a deep involvement in the mathematical aspects of the theory of carrier transport in semiconductor devices.
The course took place in the period 15-22 July 1998 on the premises of the Grand Hotel San Michele di Cetraro (Cosenza), located at a beach of astounding beauty in the Magna Graecia part of southern Italy. The Hotel facilities were more than adequate for an optimal functioning of the course. About 50 "students", mainly from various parts of Europe, participated in the course. At the end of the course, in the period 23-24 July 1998, a related workshop of the European Union TMR (Training and Mobility of Researchers) on "Asymptotic Methods in Kinetic Theory" was held in the same place and several of the participants stayed for both meetings. Furthermore the CIME course was considered by the TMR as one of the regular training schools for the young researchers belonging to the network.
The course developed as follows:

- W. Allegretto delivered 6 lectures on analytical and numerical problems for the drift-diffusion equations and also on some recent results concerning the electrothermal model. In particular he highlighted the relationship with integrated sensor modeling and the relevant industrial applications, inducing a considerable interest in the audience.
- F. Poupaud delivered 6 lectures on the rigorous derivation of the quantum transport equation in semiconductors, utilizing recent developments on Wigner measures introduced by Gérard, in order to obtain the semiclassical limit. His lectures, in the French style of pure mathematics, were very clear, comprehensive and of advanced formal rigour.The lectures were particularly helpful to the young researchers with a strong background in Analysis because they highlighted the analytical problems arising from the rigorous treatment of the semiclassical limit.
- C. Ringhofer delivered 6 lectures which consisted of an overview of the state of the art on the models and methods developed in order to study the semiclassical Boltzmann equation for simulating semiconductor devices. He started his lectures by recalling the fundamentals of semiconductor physics then introduced the methods of asymptotic analysis in order to obtain a hierarchy of models, including: drift-diffusion equations, energy transport equations, hydrodynamical models (both classical and quantum), spherical harmonics and other kinds of expansions. His lectures provided comprehensive review of the modeling aspects of carrier transport in semiconductors.

d) D. Levermore delivered 6 lectures on the mathematical foundations and applications of the moment methods. He presented in detail and depth the concepts of exponential closures and of the principle of maximum entropy. In his lectures he gave several physical examples of great interest arising from rarefied gas dynamics, and pointed out how the method could also be applied to the semiclassical Boltzmann equation. He highlighted the relationships between the method of moments and the mathematical theory of hyperbolic systems of conservation laws.

During the course several seminars on specialized topics were given by leading specialists. Of particular interest were these of P. Markowich (co-director of the course) on the asymptotic limit for strong fieds, of P. Pietra on the numerical solution of the quantum hydrodynamical model, of A. Jungel on the entropy formulation of the energy transport model, of O. Muscato on the Monte Carlo validation of hydrodynamical models, of C. Schmeiser on extended moment methods, of A. Arnold on the Wigner-Poisson system, and of A. Marrocco on the mixed finite element discretization of the energy transport model.

A. M. Anile

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Contents

Recent Developments in Hydrodynamical Modeling of Semiconductors

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Summary. We present a review of recent developments in hydrodynamical modeling of charge transport in semiconductors. We focus our attention on the models for Si and GaAs based on the maximum entropy principle which, in the framework of extended thermodynamics, leads to the definition of closed systems of moment equations starting from the Boltzmann transport equation for semiconductors.

Both the theoretical and application issues are examined.

1 Introduction

Enhanced functional integration in modern electron devices requires an increasingly accurate modeling of energy transport in semiconductors in order to describe high-field phenomena such as hot electron propagation, impact ionization and heat generation. In fact the standard drift-diffusion models cannot cope with high-field phenomena since they do not comprise energy as a dynamical variable.

Furthermore, for many applications in optoelectronics it is necessary to describe the transient interaction of electromagnetic radiation with carriers in complex semiconductor materials. Since the characteristic times are of order of the electron momentum or energy flux relaxation times, some higher moments of the carrier distribution function must be necessarily involved. These are the main reasons why more general models have been sought which incorporate energy as a dynamical variable and whose validity, at variance with the drift-diffusion model, is not restricted to quasi-stationary situations.

These models are, loosely speaking, called hydrodynamical models and they are usually derived by suitable truncation procedures, from the infinite hierarchy of the moment equations of the Boltzmann transport equation. However, most of these suffer from serious theoretical drawbacks due to the

ad hoc treatment of the closure problem [1]. Recently, in the case of silicon semiconductors, a moment approach has been introduced [2, 3] (see also [4] for a complete review) in which the closure procedure is based on the maximum entropy principle, while the conduction bands in the proximity of the local minima are described by the Kane dispersion relation. Later on, [5, 6], the same approach has been employed for GaAs. In this case both the Γ-valley and the four equivalent L-valleys have been considered. Therefore electrons in the conduction band have been treated as a mixture of two fluids, one representing electrons in the Γ-valley and the other electrons in the four equivalent L-valleys.

Both in the Si and in the GaAs case, the models comprise the balance equations of electron density, energy density, velocity and energy flux. The only difference is that for GaAs both electron populations are taken into account. These equations are coupled to the Poisson equation for the electric potential. Apart from the Poisson equation, the system is hyperbolic in the physically relevant region of the field variables.

In this paper we present a general overview of the theory underlying hydrodynamical models. In particular we investigate in depth the closure problem and present various applications both to bulk materials and to electron devices.

The considerations and the results reported in the paper are exclusively concerned with silicon and gallium arsenide.

2 General transport properties in semiconductors

Semiconductors are characterised by a sizable energy gap between the valence and the conduction bands. Upon thermal excitation, electrons from the valence band can jump to the conduction band leaving behind holes (in the language of quasi-particles). Therefore the transport of charge is achieved both through negatively charged (electrons) and positively charged (holes) carriers. The conductivity is enhanced by doping the semiconductor with donor or acceptor materials, which respectively increase the number of electrons in the conduction band or that of holes in the valence band. Therefore it is clear why the energy band structure plays a very important role in the determination of the electrical properties of the material. The energy band structure of crystals can be obtained at the cost of intensive numerical calculations (and also semiphenomenologically) by the quantum theory of solids [7]. However, for most applications, a simplified description, based on simple analytical models, is adopted to describe charge transport. In this paper we will be essentially concerned with unipolar devices in which the current is due to electrons (semiconductors doped with donor materials). Electrons which mainly contribute to the charge transport are those with energy in the neighborhoods of the lowest conduction band minima, each neighborhood being called a valley. In

silicon, there are six equivalent ellipsoidal valleys along the main crystallographic directions Δ at about 85 % from the center of the first Brilloiun zone, near the X points, which, for this reason, are termed the X-valleys. In GaAs there is an absolute minimum at the center of the Brillouin zone, the Γ-point, and local minima at the L-points along the Λ cristallographic orientations.

As mentioned above, in the simplified description employed, the energy in each valley is represented by analytical approximations. Among these, the most common are the parabolic and the Kane dispersion relation.

In the isotropic parabolic band approximation, the energy $\mathcal{E}_A$ of the A-valley, measured from the bottom of the valley $\overline{\mathcal{E}_A}$, has an expression similar to that of a classical free particle

$$\mathcal{E}_A(k_A) = \frac{\hbar^2 |\mathbf{k}_A|^2}{2m_A^*}. \tag{1}$$

In this approximation $\mathbf{k}_A$, the electron wave vector, is assumed to vary in all $\mathbb{R}^3$, m_A^* is the effective electron mass in the A-valley and $\hbar$ the reduced Planck constant.

A more appropriate analytical approximation, which takes into account the non-parabolicity at high energy, is given by the Kane dispersion relation

$$\mathcal{E}_A(k_A)\left[1 + \alpha_A \mathcal{E}_A(k_A)\right] = \frac{\hbar^2 k^2}{2m_A^*}, \quad \mathbf{k} \in \mathbb{R}, \tag{2}$$

where α_A is the non parabolicity parameter.

The electron velocity $v(\mathbf{k})$ [1] in a generic band or valley depends on the energy $\mathcal{E}$ by the relation

$$v(\mathbf{k}) = \frac{1}{\hbar} \nabla_{\mathbf{k}} \mathcal{E}.$$

Explicitly we get for parabolic band

$$v^i = \frac{\hbar k^i}{m^*}, \tag{3}$$

while in the approximation of the Kane dispersion relation

$$v^i = \frac{\hbar k^i}{m^* \left[1 + 2\alpha \mathcal{E}(k)\right]}. \tag{4}$$

In the semiclassical kinetic approach the charge transport in semiconductors is described by the *Boltzmann equation*. For electrons in the conduction band it reads

$$\frac{\partial f}{\partial t} + v^i(\mathbf{k}) \frac{\partial f}{\partial x^i} - \frac{eE^i}{\hbar} \frac{\partial f}{\partial k^i} = \mathcal{C}[f], \tag{5}$$

[1] the valley index has been omitted for simplicity

where $f(\mathbf{x}, \mathbf{k}, t)$ is the electron distribution function and $\mathcal{C}[f]$ represents the effects due to scattering with phonons, impurities and with other electrons. In a multivalley description one has to consider a transport equation for each valley.

The electric field, $\mathbf{E}$, is calculated by solving the Poisson equation for the electric potential ϕ

$$E_i = -\frac{\partial \phi}{\partial x_i}, \tag{6}$$

$$\nabla(\epsilon \nabla \phi) = -e(N_+ - N_- - n), \tag{7}$$

N_+ and N_- denote the donor and acceptor density respectively (which depend only on the position), ϵ the dielectric constant and n the electron number density

$$n = \int f d\mathbf{k}.$$

The equations (5)-(7) constitute the Boltzmann-Poisson system that is the basic semiclassical model of electron transport in semiconductors.

The main scattering mechanisms in a semiconductor are the electron-phonon interaction, the interaction with impurities, the electron-electron scatterings and the interaction with stationary imperfections of the crystal as vacancies, external and internal crystal boundaries. In many situations the electron-electron collision term can be neglected since the electron density is not too high. However in the case of high doping, electron-electron collisions must be taken into account because they might produce sizable effects. Retaining the electron-electron collision term greatly increases the complexity of the collision operator on the RHS of the semiclassical Boltzmann equation. In fact the collision operator for the electron-electron scattering is a highly nonlinear one, being quartic in the distribution function.

After a collision the electron can remain in the same valley (intravalley scattering) or be drawn in another valley (intervalley scattering).

The general form of the collision operator $\mathcal{C}[f]$ for each type of scattering mechanism is

$$\mathcal{C}[f] = \int \left[P(\mathbf{k}', \mathbf{k}) f(\mathbf{k}') \left(1 - 4\pi^3 f(\mathbf{k})\right) - P(\mathbf{k}, \mathbf{k}') f(\mathbf{k}) \left(1 - 4\pi^3 f(\mathbf{k}')\right) \right] d\mathbf{k}' \tag{8}$$

The first term in (8) represents the gain and the second one the loss. The terms $1 - 4\pi^3 f(\mathbf{k})$ account for the Pauli exclusion principle. $P(\mathbf{k}, \mathbf{k}')$ is the transition probability from the state $\mathbf{k}$ to the state $\mathbf{k}'$.

Under the assumption that the electron gas is dilute, the collision operator can be linearized with respect to f and becomes

$$\mathcal{C}[f] = \int \left[P(\mathbf{k}', \mathbf{k}) f(\mathbf{k}') - P(\mathbf{k}, \mathbf{k}') f(\mathbf{k}) \right] d\mathbf{k}'. \tag{9}$$

As we shall see at equilibrium the electron distribution must obey the Fermi-Dirac statistics

$$f_{eq} = \left[\exp\left(-\frac{\mathcal{E}-\mu}{k_B T_L}\right) + 1\right]^{-1},$$

k_B being the Boltzmannn constant, μ the chemical potential and T_L the lattice temperature which will be taken as constant.

In the dilute case, one can consider the maxwellian limit of the Fermi-Dirac distribution

$$f_{eq} \approx \exp\left(-\frac{\mathcal{E}-\mu}{k_B T_L}\right).$$

In both cases from the principle of detailed balance [8], it follows that

$$P(\mathbf{k}', \mathbf{k}) = P(\mathbf{k}, \mathbf{k}') \exp\left(-\frac{\mathcal{E}-\mathcal{E}'}{k_B T_L}\right), \tag{10}$$

where $\mathcal{E} = \mathcal{E}(\mathbf{k})$ and $\mathcal{E}' = \mathcal{E}(\mathbf{k}')$.

3 H-theorem and the null space of the collision operator

In [9, 10, 11] an H-theorem has been derived for the physical electron-phonon operator in the homogeneous case without electric field. The same problem has also been discussed in [12] in the parabolic case.

Here we review the question in the case of an arbitrary form of the energy band and in the presence of an electric field, neglecting the electron-electron interaction and assuming the electron gas sufficiently dilute to neglect the degeneracy effects. By following [13] a physical interpretation of the results is suggested.

The transition probability from the state $\mathbf{k}$ to the state $\mathbf{k}'$ has the general form [14]

$$P(\mathbf{k}, \mathbf{k}') = \mathcal{G}(\mathbf{k}, \mathbf{k}') \left[(N_B + 1)\delta(\mathcal{E}' - \mathcal{E} + \hbar\omega_q) + N_B \delta(\mathcal{E}' - \mathcal{E} - \hbar\omega_q)\right] \tag{11}$$

where $\delta(x)$ is the Dirac distribution and $\mathcal{G}(\mathbf{k}, \mathbf{k}')$ is the so-called overlap factor which depends on the band structure and the particular type of interaction [14] and enjoys the properties

$$\mathcal{G}(\mathbf{k}, \mathbf{k}') = \mathcal{G}(\mathbf{k}', \mathbf{k}) \quad \text{and} \quad \mathcal{G}(\mathbf{k}, \mathbf{k}') \geq 0.$$

N_B is the phonon distribution which obeys the Bose-Einstein statistics

$$N_B = \frac{1}{\exp(\hbar\omega_q / k_B T_L) - 1}, \tag{12}$$

where $\hbar\omega_q$ is the phonon energy.

Given an arbitary function $\psi(\mathbf{k})$ for which the following integrals exist, the chain of identities [9, 10, 11]

$$\int \mathcal{C}[f]\psi(\mathbf{k})d\mathbf{k} = \int [P(\mathbf{k}',\mathbf{k})f(\mathbf{k}') - P(\mathbf{k},\mathbf{k}')f(\mathbf{k})]\,\psi(\mathbf{k})d\mathbf{k}\,d\mathbf{k}' =$$

$$\int_{\mathcal{B}^2} P(\mathbf{k},\mathbf{k}')f(\mathbf{k})\,(\psi(\mathbf{k}') - \psi(\mathbf{k}))\,d\mathbf{k}d\,\mathbf{k}' =$$

$$\int_{\mathcal{B}^2} \mathcal{G}(\mathbf{k},\mathbf{k}')\,[(N_B+1)\delta(\mathcal{E}' - \mathcal{E} + \hbar\omega_q) + N_B\delta(\mathcal{E}' - \mathcal{E} - \hbar\omega_q)] \times$$

$$f(\mathbf{k})\,(\psi(\mathbf{k}') - \psi(\mathbf{k}))\,d\mathbf{k}d\,\mathbf{k}' =$$

$$\int_{\mathcal{B}^2} \mathcal{G}(\mathbf{k},\mathbf{k}')\delta(\mathcal{E}'-\mathcal{E}-\hbar\omega_q)\,[(N_B+1)f(\mathbf{k}')-N_Bf(\mathbf{k})]\,(\psi(\mathbf{k})-\psi(\mathbf{k}'))\,d\mathbf{k}d\,\mathbf{k}'$$

holds. By following [11] if we set without loss of generality

$$f(\mathbf{k}) = h(\mathbf{k})\exp\left(-\frac{\mathcal{E}}{k_BT_L}\right),$$

and in analogy with the case of a simple gas we take

$$\psi(\mathbf{k}) = k_B \log h(\mathbf{k}),$$

by using the definition of $\delta(x)$, one has

$$k_B\int \mathcal{C}[f]\log h(\mathbf{k})d\mathbf{k} = k_B\int \mathcal{G}(\mathbf{k},\mathbf{k}')\delta(\mathcal{E}' - \mathcal{E} - \hbar\omega_q)N_B\exp\left(-\frac{\mathcal{E}}{k_BT_L}\right)$$

$$(h(\mathbf{k}') - h(\mathbf{k}))\,(\log h(\mathbf{k}) - \log h(\mathbf{k}'))\,d\mathbf{k}d\,\mathbf{k}' \le 0. \tag{13}$$

Therefore along the characteristics of eq. (5)

$$-\int \log h(\mathbf{k})\frac{df}{dt}d\mathbf{k} = -\int \mathcal{C}[f]\log h(\mathbf{k})d\mathbf{k} \ge 0.$$

This implies that

$$\Psi = k_B\int\left(\int \log h(\mathbf{k})\,df\right)d\mathbf{k} = k_B\int\left(f\log f - f + \frac{\mathcal{E}}{k_BT_L}f\right)d\mathbf{k}. \tag{14}$$

can be considered as a Liapunov function for the Boltzmann-Poisson system (5)-(7). The first two terms are equal to the opposite of the entropy arising in the classical limit of a Fermi gas, while the last term is due to the presence of the phonons. Ψ represents the nonequilibrium counterpart of the equilibrium Helmholtz free energy, divided by the lattice temperature. It is well known in thermostatics that for a body kept at constant temperature and mechanically insulated, the equilibrium states are minima for Ψ.

A strictly related problem is the one of determining the null space of the collision operator. It consists in finding the solutions of the equation $\mathcal{C}(f) = 0$. The resulting distribution functions represent the equilibrium solutions. Physically one expects that, asymptotically in time, the solution to a given initial value problem will tend to such a solution.

The problem of determining the null space for the physical electron-phonon operator was tackled and solved in general in [11] where it was proved that the equilibrium solutions are not only the Fermi-Dirac distributions but form an infinite sequence of functions of the kind

$$f(k) = \frac{1}{1 + h(\mathbf{k}) \exp \mathcal{E}(\mathbf{k})/k_B T_L} \tag{15}$$

where $h(\mathcal{E}) = h(\mathcal{E} + \hbar\omega_q)$ is a periodic function of period $\hbar\omega_q/n$, $n \in \mathbb{N}$. This property implies a numerable set of collisional invariants and hence of conservation laws. The physical meaning is that the density of electrons whose energy $\mathcal{E}$ differs from a given value u by a multiple of $\hbar\omega_q$ is constant. However if there are several types of phonons, as in the real physical cases, and their frequencies are not commensurable, the kernel of the collision operator reduces to the Fermi-Dirac distribution.

4 Macroscopic models

4.1 Moment equations

Macroscopic models are obtained by taking the moments of the Boltzmann transport equation. In principle, all the hierarchy of the moment equations should be retained, but for practical purposes it is necessary to truncate it at a suitable order N. Such a truncation introduces two main problems due to the fact that the number of unknowns exceeds that of the equations: these are

i) the closure for higher order fluxes;

ii) the closure for the production terms.

As in gasdynamics [15], multiplying eq. (5) by a sufficiently regular function $\psi(\mathbf{k})$ and integrating over $\mathcal{B}$, the first Brillouin zone, one obtains the generic *moment equation*

$$\frac{\partial M_\psi}{\partial t} + \int \psi(\mathbf{k}) v^i(\mathbf{k}) \frac{\partial f}{\partial x^i} d\mathbf{k} - \frac{e}{\hbar} E^j \int \psi(\mathbf{k}) \frac{\partial}{\partial k^j} f d\mathbf{k} = \int \psi(\mathbf{k}) \mathcal{C}[f] d\mathbf{k}, \tag{16}$$

with

$$M_\psi = \int \psi(\mathbf{k}) f d\mathbf{k},$$

the moment relative to the weight function ψ.

Since

$$\int \psi(\mathbf{k}) \frac{\partial f}{\partial k^j} d\mathbf{k} = \int_{\partial\mathcal{B}} \psi(\mathbf{k}) f \mathbf{n} d\sigma - \int f \frac{\partial \psi(\mathbf{k})}{\partial k^j} d\mathbf{k},$$

with $\mathbf{n}$ outward unit normal field on the boundary $\partial\mathcal{B}$ of the domain $\mathcal{B}$ and $d\sigma$ surface element of $\partial\mathcal{B}$, eq. (16) becomes

$$\frac{\partial M_\psi}{\partial t} + \frac{\partial}{\partial x^i}\int f\psi(\mathbf{k})v^i(\mathbf{k})d\mathbf{k} + \frac{e}{\hbar}E^j\left[\int f\frac{\partial\psi(\mathbf{k})}{\partial k^j}d\mathbf{k} - \int_{\partial\mathcal{B}}\psi(\mathbf{k})fn_j d\sigma\right] = \int\psi(\mathbf{k})\mathcal{C}(f)d\mathbf{k}. \tag{17}$$

The term

$$\int_{\partial\mathcal{B}}\psi(\mathbf{k})f\mathbf{n}d\sigma$$

vanishes both when $\mathcal{B}$ is expanded to $\mathbb{R}^3$, as in the parabolic and Kane approximations, (because in order to guarantee the integrability condition f must tend to zero sufficiently fast as $k \mapsto \infty$) and when $\mathcal{B}$ is compact and $\psi(\mathbf{k})$ is periodic and continuous on $\partial\mathcal{B}$. This latter condition is a consequence of the periodicity of f on $\mathcal{B}$ and the symmetry of $\mathcal{B}$ with respect to the origin.

Various models employ different expressions of $\psi(\mathbf{k})$ and number of moments.

4.2 The maximum entropy principle

The maximum entropy principle (hereafter MEP) leads to a systematic way of obtaining constitutive relations on the basis of information theory (see [16, 17, 18, 19] for a review).

According to MEP if a given number of moments M_A, $A = 1, \ldots, N$, are known, the distribution function which can be used to evaluate the unknown moments of f, corresponds to the extremal, f_{ME}, of the entropy functional under the constraints that it yields exactly the known moments M_A

$$\int\psi_A f_{ME}d\mathbf{k} = M_A. \tag{18}$$

Since the electrons interact with the phonons describing the thermal vibrations of the ions placed at the points of the crystal lattice, in principle we should deal with a two component system (electrons and phonons). However, if one considers the phonon gas as a thermal bath at constant temperature T_L, only the electron component of the entropy must be maximized. Moreover, by considering the electron gas as sufficiently dilute, one can take the expression of the entropy obtained as limiting case of that arising in the Fermi statistics

$$s = -k_B\int(f\log f - f)\,d\mathbf{k}. \tag{19}$$

If we introduce the lagrangian multipliers Λ_A, the problem of maximizing s under the constraints (18) is equivalent to maximizing

$$\tilde{s} = \Lambda_A\left(M_A - \int\psi_A f d\mathbf{k}\right) - s,$$

the Legendre transform of s, without constraints,

$$\delta\tilde{s} = 0.$$

This gives

$$\left[\log f + \frac{\Lambda_A \psi^A}{k_B}\right] \delta f = 0.$$

Since the latter relation must hold for arbitrary δf, it follows

$$f_{ME} = \exp\left[-\frac{1}{k_B}\Lambda_A \psi^A\right]. \tag{20}$$

We stress that at variance with the monatomic gas, the integrability problem due to the fact that the sign of the argument in the exponential is not defined, does not arise here because the moments are obtained by integrating over the first Brillouin zone, which is a compact set of $\mathbb{R}^3$.

In order to get the dependence of the Λ_A's on the M_A's, one has to invert the constraints (18). Then by taking the moments of f_{ME} and $\mathcal{C}[f_{ME}]$, one finds the closure relations for the fluxes and the production terms appearing in the balance equations. On account of the analytical difficulties this, in general, can be achieved only with a numerical procedure. However, apart from the computational problems, the balance equations are now a closed set of partial differential equations and with standard considerations in extended thermodynamics [16], it is easy to show that they form a quasilinear hyperbolic system.

Let us set

$$\eta(f) = -k_B\left(f \log f - f\right).$$

The entropy balance equation is obtained multiplying the equation (5) by $\eta'(f) = \partial_f \eta(f)$ and afterwards integrating with respect to $\mathbf{k}$, one has

$$\frac{\partial}{\partial t}\int \eta(f) d\mathbf{k} + \frac{\partial}{\partial x^i}\int \eta(f) v^i d\mathbf{k} - \frac{e}{\hbar}E^i \int \eta'(f)\frac{\partial}{\partial k^i} f d\mathbf{k} = \int \eta'(f)\mathcal{C}[f] d\mathbf{k}.$$

By taking into account the periodicity condition of f on the first Brillouin zone, the integral

$$\int \eta'(f)\frac{\partial}{\partial k^i} f d\mathbf{k} = \int \frac{\partial \eta(f)}{\partial k^i} d\mathbf{k} = \int_{\partial B} \eta(f) n^i d\mathbf{k}$$

vanishes and the entropy balance equations assumes the usual form

$$\frac{\partial s}{\partial t} + \frac{\partial \varphi^i}{\partial x^i} = g,$$

with

$$\varphi^i = \int \eta(f) v^i d\mathbf{k} \quad \text{entropy flux}$$