Hydrodynamic modeling of electron transport in graphene

Semi-classical and Quantum corrected Hydrodynamic models

by

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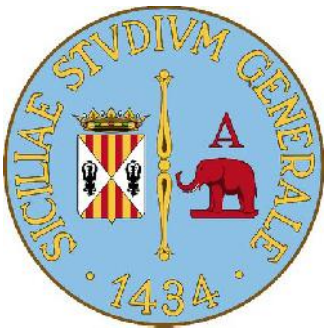

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Liliana Luca

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Introduction

Graphene, a monolayer of sp^2-bonded carbon atoms, is not only the basis for graphite but also a new material with immense potential in microelectronics for its exceptional electrical transport properties, like high conductivity and high charge mobility. Although graphene or single layers of graphite have been subject of research since the 1960s, the special and unique properties of this material have become more popular after 2004. This was mainly pushed forward by the pioneering work of Andre Geim and Konstantin Novoselov who received the Nobel Prize in Physics in 2010. Within the last years the excellent and unique electronic, optical and mechanical characteristics of graphene were systematically analyzed and explored, making this material ideally suiting for various applications. As a result of the promising properties of graphene, it seems to be an ideal candidate to take over from silicon for the next generation of faster and smaller electronic devices [21]. Yet, graphene is semi-metallic with no band gap, which severely limits its applications in electronics because - as is widely known- the electronic band gap plays a central role in modern device physics and technology and controls the performance of semiconductor devices. Moreover, it is a property inherent to semiconductors and insulators which considerably govern their transport and optical properties [69]. It has been possible to open and tune the band gap of graphene bilayers through selective control of carrier concentration in the single layers by applying an electric field [69] or by doping [53]. These results have profound implications for potential applications of graphene in electronics and for graphene-based devices modeling.

To deal with the basic kinetic transport equations remains too expensive for real life applications. Nevertheless from transport equations it is possible to derive simpler fluid dynamic equations for macroscopic quantities like particle, velocity, or energy densities. They represent a good compromise between physical accuracy and computational cost.

Recently, the Hilbert or Chapman-Enskog techniques have been applied to different situations arising in a hierarchy of macroscopic models [24]. They amounts to asymptotic expansions of the distribution function in terms of Knudsen number, i.e. the ratio of the particle mean free path to a characteristic (physical) length scale.

Close to equilibrium, simple models based on drift-diffusion equations are able to capture and

reproduce quantitatively the main particle transport characteristics. Nevertheless the description of high-field phenomena such as hot electron propagation, impact ionization and heat generation in modern electron devices requires an accurate modeling of energy transport in semiconductors which the standard drift-diffusion models cannot describe properly because they don't include - among dynamic variables - the energy. In the presence of high electric fields, in the stationary equations involved, the convective and the drift terms are dominant. This can be handled by the Scharfetter-Gummel discretization technique [62]. The key idea is to approximate the current density along each edge in a mesh by a constant, yielding an exponential approximation of the electric potential. This technique is related to mixed finite-element and finite-volume methods.

Furthermore, for many applications in optoelectronics one needs to describe the transient interaction of electromagnetic radiation with carriers in complex semiconductor materials and since the characteristic times are of order of the electron momentum or energy flux relaxation times, some higher moments of the distribution function must be necessarily involved [32]. Therefore these phenomena cannot be described within the framework of the drift-diffusion equations (which are valid only in the quasi-stationary limit) and generalizations of the drift-diffusion equations have been developed which would incorporate energy as a dynamic variable and also would not be restricted to quasi-stationary situations. These models are generally speaking called hydrodynamic models and the present work aims at formulating models of this type for a properly description of charge transport in graphene, which is extremely important for growing technological development in Computer-Aided Design (CAD) tools.

A standard approach to derive macroscopic models, like drift-diffusion, energy transport or hydrodynamic ones, is the moments method. Intrinsic to this procedure is closure condition that completes the evolution equation for the moments. To close the system, approximations for the Boltzmann equation were originally employed by Grad [22]. Grad's closure relies on an expansion of the one-particle distribution in Hermite polynomials (for more details see also [24]).

An alternative method is to choose the moments of interest and assume that the corresponding approximate distribution function be that the one with highest entropy among all those that satisfy the constraints of our prior knowledge. Moment closures obtained in this manner appear to have many desirable mathematical properties including hyperbolicity. In fact, in contrast to Grad's classical closure [22, 23], the hyperbolicity of the equations is not lost for states far from equilibrium, so that entropy-based closures can be used for the simulation of strongly non-equilibrium processes.

This approach, generally known as Maximum Entropy Principle, will be exploited to close the hierarchy of moment equations obtained in the models presented below.

The plan of the Thesis is as follows.

Chapter 1 provides an overview of the electronic band structure of graphene, while in Chapter 2 the semiclassical kinetic model is briefly recalled.

Basic elements of the Maximum Entropy Principle (hereafter MEP) are recalled in Chapter 3,

starting from the definition of "entropy". Furthermore we show as it is possible to employ it as an inference method to obtain the results achieved in the context of the statistical mechanics (see [26, 48]).
The original results of this Thesis are presented in Chapter 4 and 5.

Chapter 4 focuses on the formulation of semi-classical hydrodynamic models based on the MEP without taking into account quantum effects and it is mainly concerned with describing models formulated in [34, 35] by L. Luca, V. Romano. The models presented in this Chapter differ in the choice of moments to assume as basic field variables. Firstly main features of the semiclassical transport equation in graphene are recalled and general considerations regarding semi-classical hydrodynamic models are presented.

Then the first model analyzed is the linear hydrodynamic model formulated in [12] and a new model with the same moments has been developed in [35] but taking into account fully non linear closure relations. The comparison indicates that non-linear closure relations do not lead to a better result than the linearized ones. Secondly we try to get better results by adding further field variables. We analyze the case in which the moments added are expectation values of powers of energy [34] and it has been found that these further moments do not improve the accuracy of the model. In this last case we have considered only the linear closure relations since fully non linear closure relations lead to problems of integrability of the functions involved.

Then another model based on MEP is proposed but including - among the field variables - the deviatoric part of the stress tensor [35]. For this choice of moments both linear and non linear closure relations have been considered and it has been found that for low and moderate electric fields both models are reasonably acceptable but it is crucial to include - among the variables - the deviatoric part of the stress tensor to maintain good accuracy in a wider range of applied electric fields. Therefore apparently the results confirm that the nonlinearity is not critical for accuracy and this agrees with the literature in other fields like phonon transport [18] and radiative transport [39]. The validity of all the models presented in this Chapter is assessed by comparing the mean values of energy and velocity with those obtained from the direct solutions of the Boltzmann equation proposed in [15, 61] in the simple case of suspended monolayer graphene for several values of the Fermi energy and electric field.

To take into account quantum phenomena, in the last Chapter a quantum hydrodynamic model for charge transport in graphene is derived from a moment expansion of the Wigner-Boltzmann equation and a preliminary analysis of the mathematical structure of the model is performed [36]. The analogous formulation of MEP for the Wigner function w is not straightforward mainly because w is not a probability density function. Therefore this hydrodynamic model has been obtained under the following assumptions (see also [58]):

1. a regime in which quantum effects can be considered only a perturbation of the semiclassical model;

2. the collision term has the same form as the semiclassical case, an approximation widely

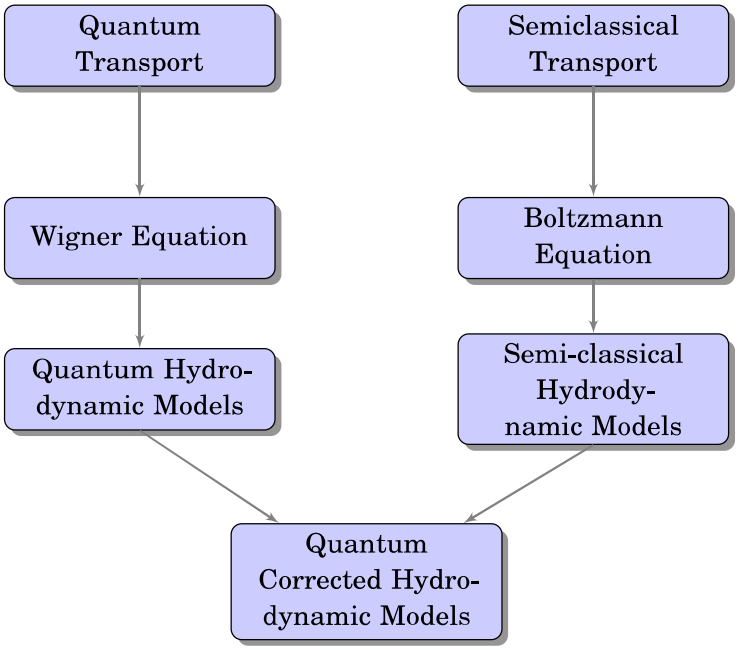

Figure 0.1: Schematic rappresentation of the strategy adopted for development of Quantum Corrected Hydrodynamic models

discussed in [56].

The needed closure relations are obtained by adding quantum corrections based on the equilibrium Wigner function to the semiclassical model formulated in [12, 34, 35] by exploiting the Maximum Entropy Principle. In other terms, the strategy adopted for formulating these models combined quantum and semi-classical approaches as shown in Fig. 0.1.

The expression of the equilibrium Wigner function which takes into account the energy band of graphene has been obtained by solving the corresponding Bloch equation. To assess the validity of the proposed model numerical simulations are under current investigation.
Lastly, starting from this hydrodynamic model a quantum energy-transport and a quantum drift-diffusion models are deduced in the long time asymptotic limit.

Some details of models are postponed in Appendices.

CHAPTER 1

THE ELECTRONIC BAND STRUCTURE OF GRAPHENE

Graphene has a honeycomb crystal lattice as shown in Fig. 1.1 (a). The four valence electrons of carbon atoms in the lattice occupies three in-plane sp^2 hybrid orbitals that are responsible for the covalent bonding, and the p_z orbital extending out of the basal plane.

The atoms in graphene form two interpenetrating triangular Bravais sub-lattices and each unit cell of graphene is defined by the 2D lattice vectors $\mathbf{a_1}$ and $\mathbf{a_2}$ [13]. There are two carbon atoms in the sublattices A and B, respectively. The vectors $\mathbf{a_1}$ and $\mathbf{a_2}$ can be espressed as

$$\mathbf{a_1} = a\left(\frac{3}{2}, \frac{\sqrt{3}}{2}\right), \qquad \mathbf{a_2} = a\left(\frac{3}{2}, -\frac{\sqrt{3}}{2}\right)$$

where $a \approx 1.42\,\text{Å}$ is the nearest-neighbour distance which is the length of covalent bonds between carbon atoms in the A and B sites. This value is close to that in the benzene molecule, and intermediate between the single (C-C) and double (C=C) bonds with lengths of $1.54\,\text{Å}$ and $1.31\,\text{Å}$.

The reciprocal lattice vectors $\mathbf{b_1}$ and $\mathbf{b_2}$ defined by the condition $\mathbf{a_i} \cdot \mathbf{b_j} = 2\pi\delta_{ij}$ are

$$\mathbf{b_1} = \frac{2\pi}{3a}\left(1, \sqrt{3}\right), \qquad \mathbf{b_2} = \frac{2\pi}{3a}\left(1, -\sqrt{3}\right).$$

From these definitions, one could notice that the first Brillouin zone of the reciprocal lattice is bounded by the planes bisecting the vectors to the nearest reciprocal lattice points. This gives a first Brillouin zone of the same form as the original hexagons of the honeycomb lattice, but rotated with respect to them by $\frac{\pi}{2}$.

The valence (π) and conduction bands (π^*) of graphene touch at high symmetric six points which include, in the first Brillouin zone, two type of the corners, generally labeled with K and K' as shown in the Fig. 1.1 (b). Explicitly, their positions in momentum space are given by

$$K = \frac{2\pi}{3a}\left(1, \frac{\sqrt{3}}{3}\right), \qquad K' = \frac{2\pi}{3a}\left(1, -\frac{\sqrt{3}}{3}\right).$$

Three nearest-neighbor vectors in real space are given by

$$\boldsymbol{\delta_1} = \frac{a}{2}(1,\sqrt{3}) \qquad \boldsymbol{\delta_2} = \frac{a}{2}(1,-\sqrt{3}) \qquad \boldsymbol{\delta_3} = -a(1,0)$$

while the six second-nearest neighbors are located at

$$\boldsymbol{\delta_1}' = \pm\mathbf{a_1} \qquad \boldsymbol{\delta_2}' = \pm\mathbf{a_2} \qquad \boldsymbol{\delta_3}' = \pm(\mathbf{a_2}-\mathbf{a_1}).$$

The valence electrons of carbon are strongly bound to the ions in graphene, and the crystalline

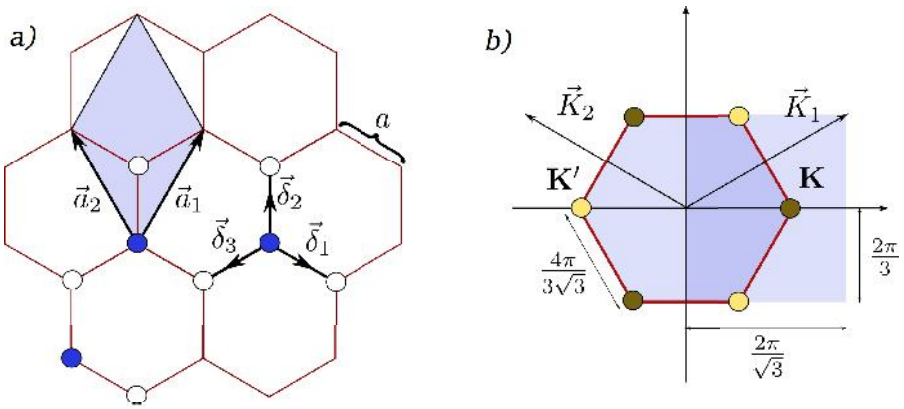

Figure 1.1: **a)** The hexagonal lattice of graphene, with the nearest neighbor $\boldsymbol{\delta_i}$ and the primitive vectors $\mathbf{a_i}$. **b)** The Brillouin zone of graphene, with the Dirac points $\mathbf{K}$ and $\mathbf{K}'$ indicated. Close to these points, the dispersion of graphene is conical and the density of states is proportional to the absolute value of the energy.

orbitals are not significantly distorted from the atomic orbitals for electrons. Consequently, the electron structures of graphene could be described through the tight-binding model, where the lattice symmetry is included as a periodic perturbation of electrons occupying the atomic orbitals.

The sp^2 hybridized states form fully occupied (empty) σ (σ^*) bands with a huge gap of ~ 12 eV, whereas the π^* (π) states form a single band with conical self-crossing points at K and K' at the corners of the Brillouin zone of graphene. The conical feature of graphene band structure with a linear dispersion at the Fermi level is the origin of its unique electronic properties.

Due to the presence of a wide gap between the bonding σ and anti-bonding σ^* bands, they are frequently neglected as they are too far away from the Fermi level to play a role and a simplified tight-binding model can be constructed by considering only the hopping of electrons between the nearest-neighbour and second-nearest-neighbour p_z orbitals in the electronic Hamiltonian, that is

$$H = -t\sum_{\langle i,j\rangle,\sigma}(a^+_{\sigma,i}b_{\sigma,j}+H.c.) - t'\sum_{\langle i,j\rangle,\sigma}(a^+_{\sigma,i}a_{\sigma,j}+b^+_{\sigma,i}b_{\sigma,j}+H.c.)$$

where $H.c.$ denotes the hermitian conjugate terms, a^+ (a) are the creation (annihilation) operators for electrons with spin σ in the sublattice A. Similarly, b^+ (b) creates (annihilates) an electron on sublattice B. $t = 2.7$ eV is the hopping parameter between nearest-neighbour orbitals in the A

and B sublattices, while t' is the hopping parameter for nearest hopping within the same A or B sublattices. This model was firstly used by Wallace in 1947 [67] to study the band structure of graphene and graphite. Solving the one-electron Schröndinger equation yields the relation between energy $\mathscr{E}$ and wave vector $\mathbf{k} = (k_x, k_y)$ is

$$\mathscr{E}_{\pm}(\mathbf{k}) = \pm t\sqrt{3 + f(\mathbf{k})} - t' f(\mathbf{k}),$$

where the function f is

$$f(\mathbf{k}) = 4\cos\left(\frac{3a}{2}k_x\right)\cos\left(\frac{a\sqrt{3}}{2}k_y\right) + 2\cos\left(a\sqrt{3}k_y\right).$$

The sign + refers to conduction band, while the sign − refers to the valence band.

A nonzero value of t' breaks the electron-hole symmetry between π and π^* bands with respect

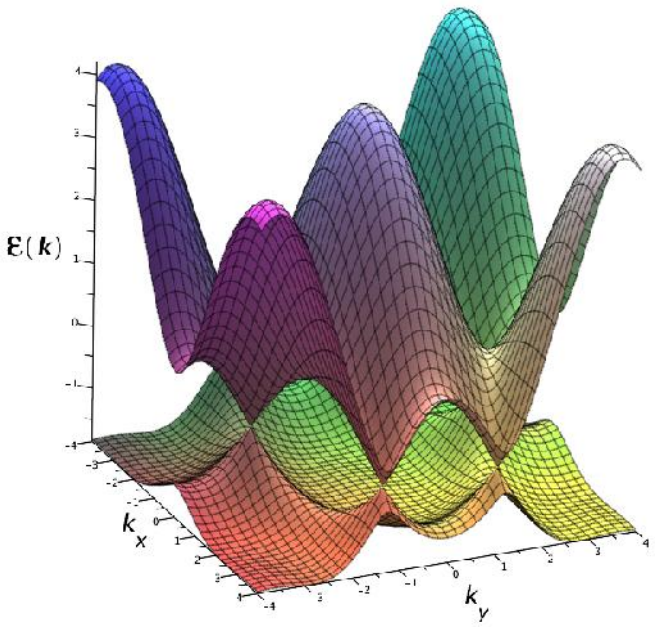

Figure 1.2: The electronic band structure calculated from the tight-binding model, with hopping parameters $t = 2.7$ eV and $t' = -0.2t$

to $\mathscr{E} = 0$, and shift the conical point from $\mathscr{E} = 0$ to $\mathscr{E} = 3t'$. In Fig. 1.2 the π (π^*) bands of electrons in graphene are plotted with t' set to be $-0.2t$, from which one could conclude that the Fermi surface is located at the K and K' points in the Brillouin zone.

For a typical semiconductor, the energy dispersion at band edge can usually be expandend as

$$\mathscr{E}_{\pm}(\mathbf{p}) = \pm\frac{p^2}{2m^*}$$

where m^* is the effective mass of an electron (hole), p is the modulus of the crystal momentum $\mathbf{p} = \hbar\mathbf{k}$ and $\hbar$ the reduced Planck's constant. The electronic velocity is

$$v = \frac{p}{m^*} = \sqrt{\frac{2\mathscr{E}}{m^*}}$$

that is a function of energy $\mathscr{E}$ and effective mass m^*, which is finite.

In contrast to the parabolic energy-momentum dispersion relation for electrons in a typical semiconductor, the linear dispersion near the Fermi level (at K and K') in graphene indicates that the electrons behave as massless Dirac fermions. This relation between $\mathscr{E}$ and $\mathbf{k}$ is known as Dirac cone, and the K (K') points in the Brillouin zone are called the Dirac points.

At these points $\mathscr{E}_{\pm}(\mathbf{k}) = 0$ and by assuming that $t' = 0$, the Hamiltonian describing the low energy excitations near the Dirac points (for $|\mathbf{k}|a << 1$) [1] can be written in the form

$$H = v_F \begin{pmatrix} 0 & p_x + ip_y \\ p_x - ip_y & 0 \end{pmatrix} \equiv v_F \hat{\boldsymbol{\sigma}} \cdot \mathbf{p}$$

where the components of the operator $\hat{\boldsymbol{\sigma}}$ are the usual Pauli matrices and $v_F = \frac{3a|t|}{2\hbar} \sim 1.1 \times 10^6 \frac{m}{s}$ is the Fermi velocity of electronic states at the Fermi surface. Hence near the Dirac points, the eigenvalues of H give the following linear dispersion relation

$$\mathscr{E}(p) = \pm v_F p \tag{1.1}$$

Electrons, which mostly contribute to the charge transport in pristine graphene, are indeed those being in the two valleys around the Dirac points. Therefore, four populations of electrons will be taken into account, which will be labeled by $\ell = K, K'$ for the valley and $A = \pi, \pi^*$ for the bands, respectively. On account of (1.1), their energy is given by

$$\mathscr{E}_{\ell,A}(\mathbf{k}) = s_A \hbar v_F |\mathbf{k} - \mathbf{k}_\ell|, \tag{1.2}$$

with $\mathbf{k}_\ell$ the position of the Dirac point ℓ and

$$s_A = \begin{cases} -1 & \text{if} \quad A = \pi \\ 1 & \text{if} \quad A = \pi^* \end{cases} .$$

If we assume $t' \neq 0$ in the tight-binding approximation, the Hamiltonian describing the energy in the proximity of Dirac points can then be written in the form

$$H = v_F \begin{pmatrix} \alpha & p_x + ip_y \\ p_x - ip_y & -\alpha \end{pmatrix}$$

with eigenvalues

$$\mathscr{E}(p) = \pm v_F \sqrt{p^2 + \alpha^2} \tag{1.3}$$

[1] For simplicity, here and in the following expressions wave vectors are measured with respect to the K (K') point

introducing an energy gap α at the Dirac points.

For the formulation of semi-classical hydrodynamic models we adopt the linear dispersion relation (1.1), while, to develop quantum corrected hydrodynamic model in the last Chapter, t' is not neglected and the regularization (1.3) is used.

CHAPTER 2

SEMI-CLASSICAL KINETIC MODEL

In a semi-classical kinetic setting, the charge transport in graphene is described by two Boltzmann equations, one for electrons in the valence (π) band and one for electrons in the conduction (π^*) band in each set of equivalent Dirac points (K or K′)

$$\frac{\partial f^A(\mathbf{r},\mathbf{k},t)}{\partial t} + \mathbf{v}^A(\mathbf{k})\cdot\nabla_{\mathbf{r}} f^A(\mathbf{r},\mathbf{k},t) - \frac{q}{\hbar}\mathbf{E}\cdot\nabla_{\mathbf{k}} f^A(\mathbf{r},\mathbf{k},t) = \mathscr{C}^A(\mathbf{r},\mathbf{k},t),\ A=\pi,\pi^*,$$

where $f^A(\mathbf{r},\mathbf{k},t)$ represents the distribution function of charge carriers in the A-band at position $\mathbf{r}$, time t and wave vector $\mathbf{k}$. To simplify explicit references to the valleys around K or K′ have been omitted.

$\nabla_{\mathbf{r}}$ and $\nabla_{\mathbf{k}}$ are the gradients with respect to the position and wave vector respectively, q is the elementary (positive) charge, while the microscopic velocity $\mathbf{v}^A$ is related to the energy band by $\mathbf{v}^A(\mathbf{k}) = \frac{1}{\hbar}\nabla_{\mathbf{k}}\mathscr{E}_{\alpha_A}(\mathbf{k}) = \alpha_A v_F \frac{\mathbf{k}}{k}$. In the models presented below the electric field $\mathbf{E}$ is assumed external and constant.

$\mathscr{C}^A$ is the collision term representing the interactions of electrons with acoustic phonons (ac), longitudinal (LO) and transversal (TO) optical phonons, and K–phonons.

The LO and TO phonons are in-plane (with respect to the plane of the lattice) modes, which give rise to electron intravalley transitions, which mostly involve phonons with wave vectors near to the center Γ of the Brillouin zone (for this reason they are also called Γ phonons). The wave vectors $\mathbf{q}$ of these phonons are near to zero and for their dispersion relations the Einstein approximation can be used, according to which $\hbar\omega \approx \texttt{const}$, with ω the phonon frequency. Such transitions can be both intraband and interband.

The K–phonons are not a real phonon branch. Their name derives from their wave vectors being close to the K or K′ point [33]. They belong to an optical branch and induce intervalley scatterings. An Einstein approximation with a mean phonon energy is used for them. Interaction

of electrons with out-of-plane phonon modes, the so-called Z phonons, or with in-plane phonons having wave vectors far from the Γ or K point is negligible [5], even though these phonons can play some role in thermal effects. For an accurate description of phonon dispersion relations and thermal conductivity in graphene, we refer to [17, 52, 55] while, for a general review about mesoscopic theories of heat transport in nanosystems, the interested reader is referred to [63].

As above, the collision term is given by summing the contributions from the several types of scatterings. The generic term due to a single scattering from a state $\mathbf{k}$ in the A-band to a state $\mathbf{k}'$ in the B-band reads (omitting the dependence on space and time for simplifying the notation)

$$\mathscr{C}_{AB}^{(s)}(\mathbf{k}) = \frac{1}{(2\pi)^2}\int_{\mathbb{R}^2}\left[w_{BA}^{(s)}(\mathbf{k}',\mathbf{k})f^B(\mathbf{k}')\left(1-f^A(\mathbf{k})\right) - w_{AB}^{(s)}(\mathbf{k},\mathbf{k}')f^A(\mathbf{k})\left(1-f^B(\mathbf{k}')\right)\right]d\mathbf{k}', \qquad s = ac, LO, TO, K, \tag{2.1}$$

where $w_{AB}^{(s)}(\mathbf{k},\mathbf{k}')$ is the transition rate. If $A = B$, there is an intra-band scattering, otherwise it is an inter-band scattering. The first Brillouin zone has been extended to all $\mathbb{R}^2$. It is important to remark that, due to the peculiar band structure, in particular the zero energy gap, the Pauli exclusion principle plays a significant role and the use of a linearized collision operator is not physically accurate.

In the case of acoustic phonons, the elastic approximation is usually considered. Therefore, the collision is intraband and can be written as

$$\mathscr{C}^A(\mathbf{k}) = \frac{1}{(2\pi)^2}\int_{\mathbb{R}^2} w^{(ac)}(\mathbf{k}',\mathbf{k})\left(f^A(\mathbf{k}') - f^A(\mathbf{k})\right)d\mathbf{k}', \tag{2.2}$$

where $w^{(ac)}(\mathbf{k}',\mathbf{k}) = A^{(ac)}(1+\cos\theta'')\delta(\mathscr{E}_{\alpha_A}(\mathbf{k}') - \mathscr{E}_{\alpha_A}(\mathbf{k}))$ with $A^{(ac)} = \dfrac{\pi D_{ac}^2 k_B T_L}{2\sigma\hbar v_{ac}^2}$. Here θ'' is the convex angle between $\mathbf{k}$ and $\mathbf{k}'$, D_{ac}^2 is the acoustic phonon coupling constant, v_{ac} is the sound speed in graphene, σ is the graphene areal density, k_B the Boltzmann constant and T_L the graphene lattice temperature, which will be kept constant.

For a generic optical phonon interaction and a K-phonon interaction from a state in band A to a state in band B the transition rate splits as

$$w_{AB}^{(s)}(\mathbf{k},\mathbf{k}') = w_{AB}^{(s,+)}(\mathbf{k},\mathbf{k}') + w_{AB}^{(s,-)}(\mathbf{k},\mathbf{k}'), \quad s = LO, TO, K,$$

where $w_{AB}^{(s,+)}(\mathbf{k},\mathbf{k}')$ and $w_{AB}^{(s,-)}(\mathbf{k},\mathbf{k}')$ represent emission and absorption processes respectively.

In the case $s = LO, TO$ we get

$$w_{AB}^{(s,\pm)}(\mathbf{k},\mathbf{k}') = A^{(s)}D_\Gamma^2\left[1-\eta_s\alpha_A\alpha_B\cos(\theta+\theta')\right]\left(N_B^s + \frac{1}{2} \pm \frac{1}{2}\right)\delta(\mathscr{E}_B(\mathbf{k}') - \mathscr{E}_A(\mathbf{k}) \pm \hbar\omega)$$

where $A^{(s)} = \pi/\sigma\omega_s$, D_Γ^2 is the optical phonon coupling constant and N_B^s is the Bose-Einstein distribution

$$N_B^s = \frac{1}{e^{\hbar\omega_s/k_B T_L} - 1}$$

with $\hbar\omega_s$ phonon energy. θ and θ' are the convex angles between $\mathbf{k}$ and $\mathbf{k}'-\mathbf{k}$ and between $\mathbf{k}'$ and $\mathbf{k}'-\mathbf{k}$. η_s is a parameter which assumes the following values

$$\eta_s = \begin{cases} 1 & \text{if} \quad s = \text{LO} \\ -1 & \text{if} \quad s = \text{TO} \end{cases}.$$

Hereafter $\hbar\omega_{LO}$ and $\hbar\omega_{TO}$, according to literature data, are considered equal with a common value denoted by $\hbar\omega_{OP}$. Therefore, the distributions of LO and TO phonons will be the same and will be denoted by N_B^{OP}.

If $s = K$ the transition rate is given by

$$w_{AB}^{(K,\pm)}(\mathbf{k},\mathbf{k}') = A^{(K)} D_K^2 \left(1 - \alpha_A \alpha_B \cos\theta''\right) \left(N_B^K + \frac{1}{2} \pm \frac{1}{2}\right) \delta(\mathscr{E}_B(\mathbf{k}') - \mathscr{E}_A(\mathbf{k}) \pm \hbar\omega_K),$$

where $A^{(K)} = \pi/\sigma\omega_K$ and D_K^2 is the K-phonon coupling constant.

At equilibrium the distribution of electrons, both in the conduction and valence band, are given by the Fermi-Dirac distribution

$$f_{FD}(\mathbf{r},\mathbf{k},t) = \frac{1}{1 + \exp\left(\dfrac{\mathscr{E}(\mathbf{k}) - \varepsilon_F}{k_B T_L}\right)}, \quad -\infty < \mathscr{E}(\mathbf{k}) < +\infty, \tag{2.3}$$

where ε_F is the Fermi energy. The lattice temperature T_L will be considered constant and equal to 300 K. In pristine graphene $\varepsilon_F = 0$ but applying a gate voltage it is possible to modify the value of ε_F creating a kind of doping like in conventional semiconductors. If ε_F is positive and high enough, there is a sort of n-doping and the only significant contribution to the current is from electrons in the conduction band. Analogously, if $\varepsilon_F < 0$ there is a sort of p-doping.

From now on, to simplify, we will only consider the conduction band but the results can be easily extended to include the valence band. Therefore we will consider a unique Boltzmann equation

$$\begin{aligned} &\frac{\partial f(\mathbf{r},\mathbf{k},t)}{\partial t} + \mathbf{v}(\mathbf{k}) \cdot \nabla_{\mathbf{r}} f(\mathbf{r},\mathbf{k},t) - \frac{q}{\hbar}\mathbf{E} \cdot \nabla_{\mathbf{k}} f(\mathbf{r},\mathbf{k},t) = \\ &= \frac{1}{(2\pi)^2} \sum_{s=ac,LO,TO,K} \int_{\mathbb{R}^2} \left[w^{(s)}(\mathbf{k}',\mathbf{k}) f(\mathbf{k}')(1 - f(\mathbf{k})) - w^{(s)}(\mathbf{k},\mathbf{k}') f(\mathbf{k}) \left(1 - f(\mathbf{k}')\right) \right] d\mathbf{k}' \end{aligned} \tag{2.4}$$

for the distribution $f(\mathbf{r},\mathbf{k},t)$ of electrons in the conduction band. Of course in the collision term only intraband scatterings are now present. In the $\mathbf{k}$-space, a reference frame centered at the Dirac point will be assumed.

CHAPTER 3

INFORMATION THEORY APPROACH TO STATISTICAL MECHANICS

In the context of the Bayesian interpretation of probability, **Maximum Entropy Principle** (MEP) is being increasingly applied to construct descriptive and predictive models of complex physical systems, from large experimental data sets. Both its wide applicability and the success it obtained in different contexts are given by its conceptual simplicity and mathematical soundness. MEP is based on the information theory of Shannon and was devised for applications in statistical physics by Jaynes [26] (for a general review of the application of MEP to semiconductors the interested reader is referred to [11, 44]). The central idea of this principle is to estimate the distribution of the particles of the system among the microstates, on the basis of the partial knowledge of some macroscopic data. The latter informations are specified in the form of some simple moment constraints. Here we concisely review the basic elements of MEP, starting from the notion of "entropy", and we show that it is possible to obtain all the expressions of statistical mechanics by maximizing it.

3.1 Definition of Entropy

Entropy is defined as the quantitative measure of disorder or randomness in a system. The notion of Entropy was first introduced by Clausius in the setting of Physics, and it deals with the transfer of heat and energy within a system. Later Boltzmann provided the statistical analogue of thermodynamic entropy linking the concept of entropy with molecular disorder or chaos with the well-known relation: Entropy S is proportional to the natural logarithm of a quantity W representing the maximum number of microscopic ways in which the macroscopic state (such as temperature, pressure, volume, etc.) can be realized, that is

$$S = k_B \ln W,$$

in which k_B is the Boltzmann constant.

In information theory in 1948, Shannon borrowed the concept of entropy from thermodynamics introducing a unique quantity H that measures the amount of uncertainty of an unknown or random quantity. Because of the similarity of the mathematical structure and physical meaning, the quantity H is also named entropy, as is the quantity S introduced in thermodynamics and statistical mechanics.
Unlike Clausius-Boltzmann entropy, since Shannon's entropy can be interpreted as a measure of our ignorance about a system, it is not a property of the system, but of our knowledge about it. Then it is dependent on the observer/experimenter interacting with the system.

First of all, let us consider the discrete case. Let X be a descrete random variable taking the values $x_1, x_2, ..., x_N$ such that

$$\sum_{k=1}^{N} p_k = 1$$

where p_k is the prior probability that X assumes the value x_k. Let us suppose that we don't know the prior probability but we have only a partial knowledge about it. Therefore we require that the measure of the uncertainty H satisfy the following three conditions

1) $H(p_1, p_2, ..., p_N)$ is a continuous function of p_i, for $i = 1, ..., N$;

2) If all p_i are equal, the quantity $H(\frac{1}{N}, ..., \frac{1}{N})$ is a monotonically increasing function of N;

3) *The composition law.* If the values are arbitrarily divided into m groups $(x_{11}, ..., x_{1k_1})$,$(x_{21}, ..., x_{2k_2})$, ..., $(x_{m1}, ..., x_{mk_m})$, and the corresponding probabilities are $w_1 = p_{11} + p_{12} + ... + p_{1k_1}$, ..., $w_m = p_{m1} + p_{m2} + ... + p_{mk_m}$, then we must have

$$H(p_1, p_2, ..., p_N) = H(w_1, w_2, ..., w_N) + w_1 H(p_{11}|w_1, ..., p_{1k_1}|w_1) + ... + w_m H(p_{m_1}|w_m, ..., p_{mk_m}|w_m) \tag{3.1}$$

where the vertical bar denotes conditional probability. The composition law is also called consistency or additivity, which means that the uncertainty measure H must be independent of the type of probabilistic test, or of the grouping of the values.

The first axiom represent just a technical assumption and the second one is a formalization of the intuitive idea that more choice means greater uncertainty. The third axiom is the least obvious. We justify it when the values of X are collected into two disjoint sets $A = \{x_1, x_2, ..., x_r\}$ and $B = \{x_{r+1}, ..., x_n\}$ by constructing a compound experiment: one of the two sets, A or B, is selected with probability w_1 and w_2 respectively. If the set A is chosen then we select x_i with the conditional probability

$$P(X = x_i|A) = \begin{cases} \frac{p_i}{w_1} & \text{if } x_i \in A \\ 0 & \text{otherwise} \end{cases}$$

Similarly if the group B is chosen.

Let Y be the result of the compound experiment. If $x_i \in A$,

$$P(Y = x_i) = P(A)P(Y = x_i|A) = w_1 \frac{p_i}{w_1} = p_i = P(X = x_i).$$

We get the same result if $x_i \in B$. Therefore X and Y have the same distribution. The uncertainty before the experiment $H(p_1, p_2, ..., p_n)$ is the sum of the amount of uncertainty $H(w_1, w_2)$ and a weighted sum of the entropies conditioned on each group. In fact when the group A or B is chosen, the remaining uncertainty is $H(\frac{p_1}{w_1}, \frac{p_2}{w_1}, ..., \frac{p_r}{w_1})$ or $H(\frac{p_{r+1}}{w_2}, \frac{p_{r+2}}{w_2}, ..., \frac{p_{r+n}}{w_2})$. Thus, after the group has been specified, the average uncertainty is

$$w_1 H\left(\frac{p_1}{w_1}, \frac{p_2}{w_1}, ..., \frac{p_r}{w_1}\right) + w_2 H\left(\frac{p_{r+1}}{w_2}, \frac{p_{r+2}}{w_2}, ..., \frac{p_{r+n}}{w_2}\right).$$

We expect that the uncertainty about the compound experiment minus that removed by selecting the group must equal the average uncertainty after the group is specified, that is

$$H(p_1, p_2, ..., p_n) - H(w_1, w_2) = w_1 H\left(\frac{p_1}{w_1}, \frac{p_2}{w_1}, ..., \frac{p_r}{w_1}\right) + w_2 H\left(\frac{p_{r+1}}{w_2}, \frac{p_{r+2}}{w_2}, ..., \frac{p_{r+n}}{w_2}\right),$$

which is the third axiom in the particular case of two subsets.

Proposition 3.1. *Let $k \in \mathbb{R}^+$ a constant depending on the unit to be used, the measure H have the unique form:*

$$H(p_1, p_2, ..., p_N) = -k \sum_{i=1}^{N} p_i \log p_i \tag{3.2}$$

where we adopt the convention that $0 \log 0 := 0$.

Different logarithmic bases result in different entropy units and the constant k is usually set to unity. The unit has no relevance in maximizing entropy. For convenience, the logarithmic base is always assumed to be e (the Nepero number) in Maximum Entropy Method. Therefore, unless otherwise specified, we assume $\log \equiv \log_e \equiv \ln$.

To prove that (3.2) is the only function satisfying the axioms 1)-3) we need the following lemma.

Lemma 3.1. *Let X be a discrete random variable uniformly distributed on the finite set $\{x_1, ..., x_N\}$. Then $H(\frac{1}{N}, ..., \frac{1}{N}) := k \ln N$ with $k \in \mathbb{R}^+$.*

Proof. Let divide the N values $\{x_1, ..., x_N\}$ into k groups. Each group contains r_i values, such that $\sum_{i=1}^{k} r_i = N$. Applying (3.1) we have

$$H\left(\frac{1}{N}, ..., \frac{1}{N}\right) = H\left(\frac{r_1}{N}, ..., \frac{r_k}{N}\right) + \sum_{i=1}^{k} \frac{r_i}{N} H\left(\frac{1}{r_i}, ..., \frac{1}{r_i}\right).$$

Now consider the special case of $r_1 = r_2 = ... = r_k = m$. Every group has m values, $mk = N$. Then

$$H\left(\frac{1}{N}, ..., \frac{1}{N}\right) = H\left(\frac{1}{k}, ..., \frac{1}{k}\right) + \sum_{i=1}^{k} \frac{m}{N} H\left(\frac{1}{m}, ..., \frac{1}{m}\right) = H\left(\frac{1}{k}, ..., \frac{1}{k}\right) + H\left(\frac{1}{m}, ..., \frac{1}{m}\right)$$

Let denote with f

$$f(k) := H\left(\frac{1}{k},...,\frac{1}{k}\right)$$

we have

$$f(N) = f(mk) = f(m) + f(k) \quad \text{with } m,k \text{ positive integers}$$

The special case in which $m = 1$ and $N = 1$ implies $f(1) = H(1) = 0$ confirming that Entropy is zero when one outcome is certain to occur. By induction it is straightforward to prove that

$$f(N^k) = kf(N). \tag{3.3}$$

Thus we observe that $f(N) = k \ln N$ where k is an arbitrary integer satisfies the previous functional equation. Let's show that it is the sole family of solutions.
Let s and t be two positive integers with $t > s > 2$. It is possible to find two integers m,n defined up to a common factor, such that

$$\frac{m}{n} \leq \frac{\ln t}{\ln s} \leq \frac{m+1}{n} \tag{3.4}$$

which implies

$$m \ln s \leq n \ln t \leq (m+1) \ln s \longrightarrow s^m \leq t^n \leq s^{m+1}.$$

From the monotonicity of the function f we have $f(s^m) \leq f(t^n) \leq f(s^{m+1})$ and applying (3.3) we obtain

$$mf(s) \leq nf(t) \leq (m+1)f(s). \tag{3.5}$$

From (3.4) and (3.5) we get

$$\left|\frac{f(t)}{f(s)} - \frac{\ln t}{\ln s}\right| \leq \frac{1}{n}, \tag{3.6}$$

Since n can be chosen arbitrarily large

$$\frac{f(t)}{f(s)} = \frac{\ln t}{\ln s} = \text{constant}. \tag{3.7}$$

■

We now prove that the only expression that satisfies the axioms 1)-3) is Shannon's entropy (3.2). Hereafter we use simplified notation $S(A)$ to indicate the entropy associated to generic random variable A. Therefore $S(AB)$ denotes the joint entropy of random variables A and B, while $S(A|B)$ denotes the conditional entropy which represents a misure of our ignorance of state internal to the system A, given the states of one or more specified other system B with which it has correlation.

Proof. Next, let us consider any rational numbers

$$p_i = \frac{g_i}{g} \qquad i = 1,...,N$$

where g_i are any positive integers and $g = \sum_{i=1}^{N} g_i$. .The system $\Omega = \{x_1, ..., x_N\}$ is assumed to be described by the probability distribution $\{p_i = \frac{g_i}{g}\}_{i=1,...,N}$.
Consider N statistically independent systems, $\mathscr{B}_1, \mathscr{B}_2, ..., \mathscr{B}_N$, each of which contains g_i equally likely states $\{b_{i1}, ..., b_{ig_i}\}$. We construct the system $\mathscr{B}$ dependent on Ω as follows. $\mathscr{B}$ contains g events which are partitioned into N groups: $\mathscr{B}_1, \mathscr{B}_2, ..., \mathscr{B}_N$ and if Ω is in the state x_i then the system $\mathscr{B}_i$ is chosen. Since $\mathscr{B}_i (1 \leq i \leq N)$ has g_i events, from Lemma A.1 $f(g_i) = H\left(\frac{1}{g_i}, ..., \frac{1}{g_i}\right) = C \ln g_i$. Let $S(B|\Omega)$ be the mean conditional entropy of the system $\mathscr{B}$ conditioned on Ω

$$S(B|\Omega) = C \sum_{i=1}^{N} p_i \ln g_i,$$

where $C > 0$ is a constant depending on the unit to be used. If we now consider the compound system $\Omega\mathscr{B}$, the joint probability to have Ω in the state x_i and $\mathscr{B}$ in a specific state of $\mathscr{B}_i$ is given by $p_i \times \frac{1}{g_i} = \frac{1}{g}$, then the system $\Omega\mathscr{B}$ has a uniform distribution with g states. This implies that $S(\Omega\mathscr{B}) = H(\frac{1}{g}, ..., \frac{1}{g}) = C \ln g$. Applying the composition law we get

$$S(\Omega\mathscr{B}) = S(\Omega) + S(\mathscr{B}|\Omega),$$

which implies

$$H(p_1, p_2, ..., p_N) = S(\Omega) = S(\Omega\mathscr{B}) - S(\mathscr{B}|\Omega) = C \ln g - C \sum_i p_i \ln g_i = -C \sum_i p_i \ln p_i.$$

By employing continuity axiom, the proof extends to the case of *real* values. ■

Proposition 3.2. *The uniform distribution on the finite set $\{x_1, ..., x_N\}$ is the maximum entropy distribution among all discrete distributions supported on this set, that is*

$$H\left(\frac{1}{N}, ..., \frac{1}{N}\right) \geq H(p_1, p_2, ..., p_n). \tag{3.8}$$

Equality holds if and only if $p_i = \frac{1}{N}$ for all $i = 1, ..., N$.

Proof. The maximum value of the entropy can be obtained calculating the maximum value of the function $H(p_1, p_2, ..., p_N)$ subject to the constraint:

$$\sum_{i=1}^{N} p_i = 1.$$

The above problem is a constrained optimization problem, which is usually addressed by the method of Lagrange. Consider the Lagrangian functional $\mathscr{L}$

$$\mathscr{L}(p_1, p_2, ..., p_n, \lambda) = H(p_1, p_2, ..., p_N) - \lambda \left(1 - \sum_{i=1}^{N} p_i\right) = -k \sum_{i=1}^{N} p_i \ln p_i - \lambda \left(1 - \sum_{i=1}^{N} p_i\right)$$

where λ is the Lagrange multiplier associated with the constraint. Maximizing the unconstraint Lagrangian $\mathscr{L}$ we obtain a solution to the constrained maximum entropy problem. This can be achieved by setting:

$$\begin{cases} \frac{\partial \mathscr{L}}{\partial p_i} = 0 & i = 1,...,N, \\ \frac{\partial \mathscr{L}}{\partial \lambda} = 0. \end{cases} \Rightarrow \begin{cases} p_i = \exp\left(\frac{\lambda}{k} - 1\right) & i = 1,...,N, \\ 1 - \sum_{i=1}^{N} p_i = 0. \end{cases}$$

Note that the probabilities p_i do not depend on index i. Therefore

$$\sum_{i=1}^{N} p_i = 1 \Rightarrow \sum_{i=1}^{N} \exp\left(\frac{\lambda}{k} - 1\right) = 1 \Rightarrow \exp\left(\frac{\lambda}{k} - 1\right) = \frac{1}{N}$$

from which it can be deduced that

$$p_i = \frac{1}{N} \qquad i = 1,....,N.$$

It follows that the uniform distribution $p_i = \frac{1}{N}$ is the only stationary distribution for $\mathscr{L}$. To see that, now we prove that the entropy is maximized by the uniform distribution, namely that

$$-\sum_{i=1}^{N} p_i \ln p_i \geq -\frac{1}{N} \sum_{i=1}^{N} \ln \frac{1}{N} = \ln N.$$

Indeed

$$\ln N + \sum_{i=1}^{N} p_i \ln p_i = \sum_{i=1}^{N} p_i \ln N + \sum_{i=1}^{N} p_i \ln p_i = \sum_{i=1}^{N} p_i (\ln N + \ln p_i) = \sum_{i=1}^{N} p_i \ln(N p_i) = \frac{1}{N} \sum_{i=1}^{N} N p_i \ln(N p_i) \geq 0.$$

The last inequality[1] follows because $x \ln x \geq x - 1$, $x \in \mathbb{R}_+$. It is obvious that the equality occurs if and only if $p_i = \frac{1}{N}$, $i = 1,...,N$. ■

Hence, given no information about a discrete distribution, the maximum entropy distribution is the uniform distribution. This result suggests a theoretical justification of the Laplace's principle of indifference (sometimes called the principle of insufficient reason) which states that given mutually exclusive and exhaustive indistinguishable possibilities, each possibility should be assigned equal probability of $\frac{1}{N}$.

Proposition 3.3. *Consider a system of two components X, Y taking on values in $\Omega = \{x_1,...,x_n\}_{n\in\mathbb{N}}$ and $\Gamma = \{y_1, y_2, ..., y_m\}_{m\in\mathbb{N}}$ respectively. Assume that X and Y have the joint probability r_{kl} that X and Y occupy the states x_k and y_l respectively. The classical (Shannon) entropy $S(XY)$ of the composite system is*

$$S(XY) = \sum_{l} S(X|Y = y_l) + S(X).$$

[1] Here we used again the convention that $0 \ln 0 := 0$

Proof. Let $\{p_1,...,p_n\}$ and $\{q_1,...,q_m\}$ be the probability distributions of X and Y respectively, such that:

$$p_k = P(X = x_k)$$
$$q_l = P(Y = y_l).$$

Let c_{kl} the conditional probability of X, given Y

$$c_{kl} = P(X = x_k|Y = y_l) = \frac{P(X = x_k, Y = y_l)}{P(Y = y_l)} = \frac{r_{kl}}{q_l}.$$

The entropy of the composite system is

$$\begin{aligned} S(XY) := H(r_{11}, r_{12}, ..., r_{nm}) = & H(c_{11}q_1, c_{12}q_2, ..., c_{nm}q_m) = -\tilde{k}\sum_{k,l} q_l c_{kl} \ln(q_l c_{kl}) = \\ & = \sum_l q_l \left(-\tilde{k}\sum_k c_{kl} \ln c_{kl}\right) - \tilde{k}\sum_l q_l \ln q_l \left(\sum_k c_{kl}\right). \end{aligned} \tag{3.9}$$

Since c_{kl} is a probability density, it satisfy $\sum_{k=1}^{n} c_{kl} = 1$, with $l = 1,...,m$.Then

$$S(XY) := \sum_l q_l \left(-\tilde{k}\sum_k c_{kl} \ln c_{kl}\right) - \tilde{k}\sum_l q_l \ln q_l. \tag{3.10}$$

Recall that the conditional entropy of X given Y is defined as the weighted sum of $S(X|Y = y_l)$ over all possible values y_l that Y may take.

$$S(X|Y) := \sum_l q_l S(X|Y = y_l) = \sum_l q_l H(c_{1l}, c_{2l}, ..., c_{nl}) = \sum_l q_l \left(-\tilde{k}\sum_k c_{kl} \ln c_{kl}\right), \tag{3.11}$$

From (3.1), (3.10) and (3.11) we get

$$S(XY) = \sum_l S(X|Y = y_l) + S(Y).$$

■

As an immediate consequence of this proposition, we have the following result.

Corollary 3.1. *If X and Y are independent random variables, then*

$$S(XY) = S(X) + S(Y).$$

Shannon's entropy is an extensive quantity for statistically independent subsystems, a well known property of the Clausius-Boltzmann entropy in classical thermodynamics.

Another property of the entropy is that it is unaffected by inclusion of the outcomes with zero probability

$$H(p_1, p_2, ..., p_{N-1}) = H(p_1, p_2, ..., p_{N-1}, 0) \qquad \text{for all } N \in \mathbb{N}.$$

We have discussed the case of discrete variables. Shannon's entropy defined for a discrete random variable can be extended to situations when the random variable X is continuous. The concept of entropy for continuous distribution was also presented in Shannon's original paper [64] and is referred to as the *differential entropy*. In this case, the distribution of X is expressed in terms of probability density function (p.d.f.) $p(x)$, which is assumed to be a continuous one for simplicity and the differential entropy is defined as

$$S(p(x)) := -C\int_{-\infty}^{+\infty} p(x)\ln p(x)dx. \tag{3.12}$$

Differential entropy retains many of the properties of its descrete counterpart, but with some important differences. For example, the entropy of a discrete random variable remains invariant under a change of variable, however with a continuous random variable the entropy does not necessarily remain invariant. Indeed if $f \in C^1(\mathbb{R})$ is an arbitrary invertible transformation of a random variable X such that $x = f(t)$ and $\frac{\partial f}{\partial t} \neq 0$ for all $t \in \mathbb{R}$ then:

$$S(p(f(t))) := -C\int_{-\infty}^{+\infty} p(f(t))\ln p(f(t))\left|\frac{\partial f}{\partial t}\right| dt$$

where $\left|\frac{\partial f}{\partial t}\right|$ is the Jacobian of the transformation. Setting $\tilde{p}(t) = p(f(t))\left|\frac{\partial f}{\partial t}\right|$, it is evident that when the Jacobian $\left|\frac{\partial f}{\partial t}\right| \neq 1$ the entropy

$$S(p(x)) = S(p(f(t))) := -C\int_{-\infty}^{+\infty} \tilde{p}(f(t))\ln p(f(t))dt$$

does not preserve the previous structure. In order to overcome this difficulty, we introduce a measure $m(x)$ in the entropy expression which may or may not be normalized and we define the so-called *relative entropy* as follow:

$$S(p(x)||m(x)) := -C\int_{-\infty}^{+\infty} p(x)\ln\left(\frac{p(x)}{m(x)}\right)dx. \tag{3.13}$$

If $p(x)$ changes, $m(x)$ also changes in the same manner so that the value of S remains unchanged. In fact setting $\tilde{m}(x) = m(f(t))\left|\frac{\partial f}{\partial t}\right|$ it is clear that

$$S(p(x)||m(x)) = -C\int_{-\infty}^{+\infty} \tilde{p}(t)\ln\left(\frac{\tilde{p}(t)}{\tilde{m}(t)}\right)dt$$

remains invariant under the generic change of variable $x = f(t)$ previously considered. In Maximum Entropy Method $m(x)$ is the so-called prior (estimate) of the solution of model.
By analogy with continuous case, the discrete version of the relative entropy is defined as follows

$$S(p||m) := -C\sum_{i=1}^{n} p_i \ln\left(\frac{p_i}{m_i}\right).$$

Remark. If $m(x)$ is assumed to be a probability distribution and consequently properly normalized and $p(x)$ is absolutely continuous with respect to m, the expression [2]

$$\overline{S}(p||m) := \int_{-\infty}^{+\infty} p(x)\ln\left(\frac{p(x)}{m(x)}\right)dx, \tag{3.14}$$

[2]Motivated by continuity, we set $0\ln\frac{0}{0} := 0$.

is known as the Kullback-Leibler divergence and represents a measure of the distance between the two probability distributions $p(x)$ and $m(x)$ over a continuous random variable X. Clearly, the discrete version is defined as follows

$$\overline{S}(p||m) := \sum_{i=1}^{n} p_i \ln\left(\frac{p_i}{m_i}\right).$$

Unlike discrete entropy, differential entropy (3.12) can takes negative values. In contrast with (3.12) the espression (3.14) remains *non-negative*. To prove this important property we have to use the well know Jensen's inequality

Proposition 3.4. *Jensen's inequality states that for any convex function $f(x)$, we have*

$$\mathbb{E}[f(x)] \geq f[\mathbb{E}(x)] \tag{3.15}$$

where $\mathbb{E}[f(x)]$ is the expected value of a random variable x after applying a convex function f to it.

Note that an analogue of Jensen's inequality exists for concave functions where the inequality simply changes sign. This inequality allows us to establish that Kullback-Leibler divergence is non-negative which is a fundamental result in information theory.

Theorem 3.1. *Given p and m probability functions for which Kullback-Leibler divergence is defined. Then*

$$\overline{S}(p(x)||m(x)) \geq 0,$$

and equality holds if and only if $p = m$ almost everywhere.

Proof. Let $\mathscr{S} = \{x : p(x) > 0\}$ be the support set of p. After observing that (3.14) is the expectated value $\mathbb{E}_m\left[-\ln\left(\frac{m(x)}{p(x)}\right)\right]$ with respect to a reference measure m, we have

$$\begin{aligned}\overline{S}(p(x)||m(x)) &= -\int_{\mathscr{S}} p(x)\ln\left(\frac{m(x)}{p(x)}\right)dx \geq -\ln\left(\int_{\mathscr{S}} p(x)\left(\frac{m(x)}{p(x)}\right)dx\right) \qquad \text{(by Jensen's inequality)} \\ &= -\ln\left(\int_{\mathscr{S}} m(x)dx\right) = 0.\end{aligned} \tag{3.16}$$

Since $\ln x$ is a strictly concave function of x, we have equality if and only if $\frac{m(x)}{p(x)} = 1$ everywhere, i.e., $p(x) = m(x)$.

■

3.2 Maximum entropy inference of a distribution: the discrete case

Let consider a discrete random variable X with n possible outcomes $x_1, x_2, ..., x_n$. Let us suppose that some averages $< f_r(x) >= \sum_{i=1}^{n} p_i f_r(x_i)$, $r = 1, 2, ..., m$ are known where $f_r : \{x_1, x_2, ..., x_n\} \longrightarrow \mathbb{R}$

are assigned functions. We want to estimate the unknown probabilities $p(x_1), p(x_2), ..., p(x_n)$ when only the knowledge of the previous mean values is available.
The maximum entropy method consists of seeking the probability distribution which maximizes the entropy of the system, subject to the previous constraints:

$$\begin{aligned} &\max_p S[p] \qquad \text{subject to} \\ &\sum_{i=1}^{n} p_i = 1, \\ &< f_r(x) >= \sum_{i=1}^{n} p_i f_r(x_i), \qquad r = 1, ..., m. \end{aligned}$$

where $p = (p_1, p_2, ..., p_n)$ ranges over the set of n-dimensional probability vectors.

This constrained optimization problem is typically solved by using the method of Lagrange multipliers. Therefore let λ_r, $r = 1, ..., m$ the Lagrange multipliers associated to the constraints, we have to solve the following unconstrained optimization problem

$$\mathscr{S}' = -C \sum_{i=1}^{n} p_i \ln \frac{p_i}{m_i} - \lambda_0 \left(\sum_{i=1}^{n} p_i - 1 \right) - \sum_{r=1}^{m} \lambda_r \left[< f_r(x) > - \sum_{i=1}^{n} p_i f_r(x_i) \right].$$

Applying the optimality condition

$$\frac{\partial \mathscr{S}'}{\partial p_i} = 0,$$

one gets

$$p_i = m_i e^{-\lambda_0 - \sum_{r=1}^{m} \lambda_r f_r(x_i)}, \tag{3.17}$$

where the constant C has been included into the multipliers by means of the trasformation $1 + \frac{\lambda_0}{C} \mapsto \lambda_0$, $\frac{\lambda_r}{C} \mapsto \lambda_r$. Using the normalizing condition and the other constraints we get

$$p_i = \frac{m_i}{Z} e^{-\sum_{r=1}^{m} \lambda_r f_r(x_i)}, \qquad \lambda_0 = \ln Z$$

where

$$Z = \sum_{i=1}^{m} m_i e^{-\sum_{r=1}^{m} \lambda_r f_r(x_i)}$$

is the partition function.
The following lemma allow us to prove that (3.17) is a maximum for S.

Lemma 3.2. *If $(p_1, p_2, ..., , p_n)$ and $(q_1, q_2, ..., q_n)$ are two probability vectors then the inequality*

$$-\sum_{i=1}^{n} q_i \ln \frac{q_i}{m_i} \leq -\sum_{i=1}^{n} q_i \ln \frac{p_i}{m_i} \tag{3.18}$$

holds.

Proof. Relation (3.18) is equivalent to

$$\sum_{i=1}^{n} q_i \ln \frac{q_i}{p_i} \geq 0.$$

From the elementary inequality $x \ln x \geq x - 1$ valid for $x \geq 0$ (the case $x = 0$ of course must be intended as limit), one has

$$\sum_{i=1}^{n} q_i \ln \frac{q_i}{p_i} = \sum_{i=1}^{n} p_i \frac{q_i}{p_i} \ln \frac{q_i}{p_i} \geq \sum_{i=1}^{n} p_i \left(\frac{q_i}{p_i} - 1 \right) = 0.$$

■

Now we can prove the following property

Theorem 3.2. *The distribution*

$$p_i = m_i e^{-\lambda_0 - \sum_{r=1}^{m} \lambda_r f_r(x_i)}$$

is a maximum for S.

Proof. for $p_i = m_i e^{-\lambda_0 - \sum_{r=1}^{m} \lambda_r f_r(x_i)}$ we obtain that the value of entropy is

$$\overline{S} = -C \sum_{i=1}^{n} p_i \ln \frac{p_i}{m_i} = -C \left(-\lambda_0 - \sum_{r=1}^{m} \lambda_r f_r(x_i) \right).$$

Let $(q_1, q_2, ..., q_n)$ an arbitrary probability vector satisfying the constraints. By the previous lemma we get

$$-C \sum_{i=1}^{n} q_i \ln \frac{q_i}{m_i} \leq -C \sum_{i=1}^{n} q_i \ln \frac{p_i}{m_i} = -C \left(-\lambda_0 - \sum_{r=1}^{m} \lambda_r f_r(x_i) \right) = \overline{S}.$$

■

Remark. *If the random variable X taking values in a countable set, often additional technical hypotheses must be necessarily introduced to ensure convergence of the series present in the maximum entropy estimator. This usually gives restriction on the choice of the functions f_r.*

3.2.1 Maximum entropy distributions in Statistical Mechanics

Now, assuming X to be some microscopic quantity of a physical system, we show, with some basic examples, how MEP has been used to derive all distributions of statistical mechanics by maximizing the entropy of the system subject to some given constraints.

3.2.1.1 Maxwell-Boltzmann distribution

In statistical mechanics, Maxwell-Boltzmann statistics describes the average distribution of identical but distinguishable non-interacting particles over various energy states in thermal equilibrium, and is applicable when the temperature is high enough or the particle density is low enough to render quantum effects negligible.

A fundamental physical assumption in statistical mechanics is that in the absence of additional information, for an isolated system of N particles at thermodynamical equilibrium, all the

accessible microstates are equally probable. Hence, a macrostate corresponding to the largest number of microstates is the most probable.

Suppose G_i distinct quantum states have the same energy ϵ_i, i.e., G_i is the degeneracy of energy level ϵ_i. It is found that the number of microstates corresponding to the distribution of particles $\{n_i\}$ is

$$W(\{n_i\}) = \frac{N!}{\prod_i n_i!} \prod_i G_i^{n_i}$$

where N is the total number of particles. Using the Stirling formula for the factorial expansion $\ln m! \approx m(\ln m - 1)\,(m >> 1)$, one gets

$$\ln W \approx N \ln N - \sum_i n_i \ln n_i + \sum_i n_i \ln G_i. \tag{3.19}$$

Maximizing $\ln W$ under the constraints

$$\sum_i n_i = N, \tag{3.20}$$

$$\sum_i \epsilon_i n_i = E, \tag{3.21}$$

yields the most probable distribution $\{n_i\}$:

$$\frac{n_i}{N} = \frac{G_i}{Z} e^{-\beta \epsilon_i} \tag{3.22}$$

where Z is the partition function,

$$Z = \sum_i G_i e^{-\beta \epsilon_i}. \tag{3.23}$$

Equation (3.22) are the Boltzmann distribution of particles among energy levels. Now we present how this distribution is predicted by applying the maximum-entropy principle. Let p_i be the probability that a particle is found to be in energy level ϵ_i (i.e., in anyone of the G_i quantum states) and let $\tilde{S}$ be the relative entropy defined as

$$\tilde{S} = -\sum_i p_i \ln \frac{p_i}{G_i} \tag{3.24}$$

with m_i as G_i (the degeneracy of ϵ_i). Defining the average energy as $\bar{\epsilon} = \frac{E}{N}$ the constraints read

$$\sum_i p_i = 1, \tag{3.25}$$

$$\sum_i p_i \epsilon_i = \bar{\epsilon}. \tag{3.26}$$

To maximize the entropy (3.24) under the constraints (3.25) and (3.26), we introduce the Lagrange multipliers, λ and β and we look for the maximum of the auxiliary function:

$$\mathscr{L}(p_1, p_2, ..., p_n) = -\sum_i p_i \ln \frac{p_i}{G_i} + \lambda \left(\sum_i p_i - 1 \right) - \beta \left(\sum_i \epsilon_i p_i - \bar{\epsilon} \right).$$

Applying the optimality condition, we get

$$\frac{\partial \mathscr{L}}{\partial p_i} = -\left(\ln \frac{p_i}{G_i} + 1\right) + \lambda - \beta\epsilon_i = 0.$$

The solution is

$$\frac{p_i}{G_i} = e^{\lambda - 1} e^{-\beta\epsilon_i}. \tag{3.27}$$

The constants λ and β are then obtained from the constraints:

$$\sum_i p_i = 1 \Longrightarrow \sum_i G_i e^{\lambda - 1} e^{-\beta\epsilon_i} = 1,$$

whence

$$e^{\lambda - 1} = \frac{1}{\sum_i G_i e^{-\beta\epsilon_i}}. \tag{3.28}$$

If we denote the partition function as

$$Z = \sum_i G_i e^{-\beta\epsilon_i}, \tag{3.29}$$

from (3.27) and (3.28) we have

$$p_i = \frac{G_i}{Z} e^{-\beta\epsilon_i}, \tag{3.30}$$

which is the same form as (3.22).

In the thermodynamic limit ($N \longrightarrow \infty$ and the number density of particles remains constant), by the law of large numbers the proportion $\frac{n_i}{N}$ is approximately equal to the probability p_i, and (3.30) is equivalent to (3.22). The constraints (3.25),(3.26) are also equivalent to (3.20),(3.21). Equation (3.19) becomes

$$\ln W \approx -N \sum_i \frac{n_i}{N} \ln\left(\left(\frac{n_i}{N}\right)/G_i\right) \approx -N \sum_i p_i \ln(p_i/G_i) = N\tilde{S} \tag{3.31}$$

where $\tilde{S}$ is the relative entropy per particle, $N\tilde{S}$ is the relative entropy of the system. For a system in equilibrium, both $\ln W$ and $N\tilde{S}$ attain the maximum values. On the other hand, according to the Boltzmann relation, for the thermodynamic entropy S, it holds that

$$S = k_B \ln W$$

where k_B is the Boltzmann constant. Combining the last two expressions yields the relation

$$S = k_B N \tilde{S}. \tag{3.32}$$

From previous considerations we see that maximizing $\ln W$ and maximizing $N\tilde{S}$ are equivalent. Therefore the two methods give the same results but the second approach is based on fewer assumptions and is more systematic.

3.2.1.2 Fermi-Dirac and Bose-Einstein distributions

Consider a system consisting of particles identical and indistinguishable (nonlocalized), and hence Fermi-Dirac or Bose-Einstein statistics applies. The method used here also relies on the assumption of equiprobabilities. Under the constraints of the total number of particles and the total energy, (3.20) and (3.21), the most probable distribution $\{n_i\}$ is determined by maximizing the corresponding number of quantum states. Being different from the situation in deriving the Boltzmann distribution, particles here are not only identical but also indistinguishable. In addition, for a system consisting of Fermions Pauli's exclusion principle takes effect: a single quantum state can contain at most one particle. The number of quantum states corresponding to the distribution $\{n_i\}$ of particles is given by the following expressions

$$W_{FD}(\{n_i\}) = \prod_i \frac{G_i!}{n_i!(G_i - n_i)!} \qquad \text{(Fermion system)},$$

$$W_{BE}(\{n_i\}) = \prod_i \frac{(n_i + G_i - 1)!}{n_i!(G_i - 1)!} \qquad \text{(Boson system)}.$$

Using the Stirling formula, one gets

$$\ln W_{FD} \approx \sum_i -n_i \ln n_i + G_i \ln G_i - (G_i - n_i)\ln(G_i - n_i) \qquad \text{(Fermion system)}, \tag{3.33}$$

$$\ln W_{BE} \approx \sum_i -n_i \ln n_i - G_i \ln G_i + (G_i - n_i)\ln(G_i - n_i) \qquad \text{(Boson system)}. \tag{3.34}$$

Then, after some algebra similar to that in deriving the Boltzmann distribution, we obtain that the most probable distributions $\{n_i\}$ are

$$n_i = \frac{G_i}{e^{\lambda + \beta\epsilon_i} + 1} \qquad \text{(Fermion system)} \tag{3.35}$$

$$n_i = \frac{G_i}{e^{\lambda + \beta\epsilon_i} - 1} \qquad \text{(Boson system)} \tag{3.36}$$

where λ and β are the Lagrange multipliers introduced to take into account the constraints (3.20)-(3.21).

Now we show how to obtain these distributions by applying the maximum-entropy principle. Let p_{ijn} be the probability that the j-th quantum state of the energy level ϵ_i contains n particles. The average number of particles in the energy level ϵ_i is

$$< n_i >= \sum_{j=1}^{G_i} \sum_n p_{ijn} n. \tag{3.37}$$

Maximizing the following expression of entropy of the system

$$\tilde{S} = -\sum_i \sum_{j=1}^{G_i} \sum_n p_{ijn} \ln p_{ijn} \tag{3.38}$$

subject to the constraints

$$\sum_i \sum_{j=1}^{G_i} \sum_n p_{ijn} n = N, \tag{3.39}$$

$$\sum_i \sum_{j=1}^{G_i} \sum_n p_{ijn} n\epsilon_i = E, \tag{3.40}$$

we obtain that the probability that the j-th quantum state of the energy level ϵ_i contains n particles is given by

$$p_{ijn} = \frac{e^{-(\lambda_1+\lambda_2\epsilon_i)n}}{\sum_m e^{-(\lambda_1+\lambda_2\epsilon_i)m}} \tag{3.41}$$

where λ_1 and λ_2 are the Lagrange multipliers associated with the constraints (3.39)-(3.40), respectively.

In the specific case of *Fermi-Dirac Distribution*, according to Pauli's exclusion principle, $n = 0, 1$. Therefore (3.41) becomes

$$p_{ijn} = \frac{e^{-(\lambda_1+\lambda_2\epsilon_i)n}}{1 + e^{-(\lambda_1+\lambda_2\epsilon_i)}} \tag{3.42}$$

The Maximum Entropy solution $\{< n_i >\}$ is obtained by substituting (3.42) in (3.37):

$$< n_i >= \sum_{j=1}^{G_i} \frac{e^{-(\lambda_1+\lambda_2\epsilon_i)}}{1 + e^{-(\lambda_1+\lambda_2\epsilon_i)}} = \frac{G_i e^{-(\lambda_1+\lambda_2\epsilon_i)}}{1 + e^{-(\lambda_1+\lambda_2\epsilon_i)}} = \frac{G_i}{e^{\lambda_1+\lambda_2\epsilon_i} + 1}, \tag{3.43}$$

where the spin is included in the degeneracy factor G_i. We observe that in this case it must be $n_i \leq G_i$.

Furthermore, substituting (3.42) in (3.38) (with $n = 0, 1$) and utilizing Stirling's formula yields the entropy of the system,

$$\tilde{S} = -\sum_i < n_i > \ln < n_i > -G_i \ln G_i + (G_i - < n_i >) \ln(G_i - < n_i >). \tag{3.44}$$

Comparing (3.43) with (3.35), we see that in the thermodynamic limit ($n_i \approx < n_i >$) the Maximum Entropy solution is the same as those in statistical mechanics. Furthermore, comparing (3.44) with (3.33), we see that the entropy $\tilde{S}$ and $\ln W_{FD}$ are equal. From the Boltzmann relation $S = k_B \ln W$, it follows that $S = k_B \tilde{S}$.

Similarly, we derive the *Bose-Einstein distribution* for a system of indistinguishable bosons which are particles that do not obey the Pauli Exclusion Principle. Thus an unlimited number of bosons can co-exist simultaneously in the same quantum state. Since in this case $n = 0, 1, 2, ...$ (3.41) becomes

$$p_{ijn} = \frac{e^{-(\lambda_1+\lambda_2\epsilon_i)n}}{\sum_{m=0}^{+\infty} e^{-(\lambda_1+\lambda_2\epsilon_i)m}}. \tag{3.45}$$

The Maximum Entropy solution $\{< n_i >\}$ is obtained by substituting (3.45) in (3.37):

$$< n_i >= \sum_{j=1}^{G_i} \frac{\sum_{n=0}^{+\infty} e^{-(\lambda_1+\lambda_2\epsilon_i)n} n}{\sum_{n=0}^{+\infty} e^{-(\lambda_1+\lambda_2\epsilon_i)n}}. \tag{3.46}$$

By applying the following formulae

$$\sum_{n=0}^{+\infty} e^{-an} = \frac{1}{1-e^{-a}}, \qquad \sum_{n=0}^{+\infty} n e^{-an} = \frac{e^{-a}}{(1-e^{-a})^2}, \qquad a > 0,$$

the solution (3.46) reads

$$< n_i >= \frac{G_i}{e^{\lambda_1+\lambda_2\epsilon_i} - 1}. \tag{3.47}$$

provided that $\lambda_1 + \lambda_2\epsilon_i > 0$.

Furthermore, substituting (3.45) in (3.38) (with $n = 0, 1, ...$) and using Stirling's formula yields the entropy of the system,

$$\tilde{S} = -\sum_i < n_i > \ln < n_i > + G_i \ln G_i - (G_i - < n_i >)\ln(G_i - < n_i >). \tag{3.48}$$

Comparing (3.47) with (3.36), we see that in the thermodynamic limit the Maximum Entropy solution is the same as those in statistical mechanics. Furthermore, comparing (3.48) with (3.34), we see that the entropy $\tilde{S}$ and $\ln W_{FD}$ are equal. From the Boltzmann relation $S = k_B \ln W$, it follows that $S = k_B \tilde{S}$.

The Lagrange multipliers λ_1 and λ_2 introduced in the above distributions are determined from the constraints (3.39) and (3.40) and they can be related to the thermodynamic temperature T, so that if we set

$$\lambda_1 = -\frac{\mu}{k_B T},$$
$$\lambda_2 = \frac{1}{k_B T},$$

where μ is the chemical potential, we get the classical Fermi-Dirac or Bose-Einstein distribution in the discrete form

$$f(\epsilon_i) = \frac{n_i}{G_i} = \frac{1}{e^{\lambda_1+\lambda_2\epsilon_i} \pm 1} = \frac{1}{e^{\frac{\epsilon_i-\mu}{k_B T}} \pm 1}, \tag{3.49}$$

where the sign "+" refers to fermions and the sign "-" to bosons. The expression $\frac{n_i}{G_i}$ represents the i-th occupation number. It is clear that for fermions this number is always less or equal to one.

These examples show that the Maximum Entropy Principle and the conventional statistical mechanics method give exactly the same results. In addition we observe that, applying the Maximum Entropy Principle, the well known results of statistical mechanics are obtained with a fewer number of physical assumptions.

3.3 Maximum entropy inference of a distribution: the continuous case

The above results can be extended in the case of continuous random variables. Here the probability distribution is expressed in terms of probability density function (p.d.f.) $f : \mathbb{R}^n \longrightarrow R_0^+$, which is assumed to be a continuous one for simplicity. Let consider the following weight functions

$$\psi_A : \mathbb{R}^n \longrightarrow \mathbb{R}^{d_A}, \qquad A = 1,...,N$$

with d_A and N integers, such that the mean values defined as

$$< \psi_A >= \int_{\mathbb{R}^n} \psi_A(x) f(x) dx \qquad A = 1,...,N$$

there exist and are finite.

We want to estimate the unknown probability density f based on the knowledge of some of averages $< \psi_A >$, $A = 1,...,N$. Let introduce the following functional space

$$\mathscr{F}_\psi = \left\{ g : \mathbb{R}^n \longrightarrow R_0^+ \quad \text{such that} \int_{\mathbb{R}^n} \psi_A(x) g(x) dx, \quad A = 1,...,N, \text{ there exist and are finite} \right\}.$$

On the analogy of the discrete case, we estimate f by maximizing the (relative) entropy

$$S[g] = -\int_{\mathbb{R}^n} g(x) \ln \frac{g(x)}{m(x)} dx \qquad \text{with } g \in \mathscr{F}_\psi$$

subject to constraints

$$< \psi_A >= \int_{\mathbb{R}^n} \psi_A(x) g(x) dx \qquad A = 1,...,N.$$

As usual, this constrained maximization problem is solved by the Lagrange multiplier method. Specifically, let introduce the objective functional $\mathscr{L}$

$$\mathscr{L}[g] = S[g] - \sum_{A=1}^{N} \lambda_A \left(< \psi_A > - \int_{\mathbb{R}^n} \psi_A(x) g(x) dx \right)$$

where λ_A, $A = 1,...,\mathscr{I}_n$ are the Lagrange multipliers associated with the constraint. Let the variation of $\mathscr{L}$ with respect to $g(x)$ be zero, i. e.,

$$0 = \delta \mathscr{L} = -\int_{\mathbb{R}^n} \left[1 + \ln \frac{g(x)}{m(x)} + \sum_{A=1}^{\mathscr{I}_n} \lambda_A \psi_A(x) \right] \delta g \, dx.$$

Since δg is arbitrary, the quantity in the square brackets must be zero. Therefore we get the Maximum Entropy Estimator

$$f_{MEP}(x) = m(x) \exp \left(-1 - \sum_{A=1}^{\mathscr{I}_n} \lambda_A \psi_A(x) \right).$$

where the Lagrange multipliers $\lambda_A, A = 1,...,N$ are determined by the constraints

$$< \psi_A >= \int_{\mathbb{R}^n} \psi_A(x) f_{MEP}(x) dx \qquad A = 1,...,N.$$

Clearly, to obtain an integrable solution, the weight functions ψ_A have to be chosen appropriately.

CHAPTER 4

SEMI-CLASSICAL HYDRODYNAMIC MODELS BASED ON THE MAXIMUM ENTROPY PRINCIPLE

This Chapter is based on [34, 35].

4.1 Semi-classical Hydrodynamic models: general considerations

The starting point for the derivation of semi-classical hydrodynamic models is the semi-classical Boltzmann equation (2.4).
Numerical solutions of eq.(2.4) can be obtained, for example, via Direct Monte Carlo Simulation (DSMC)[15, 61] or by finite difference schemes [33] or by discontinuous Galerkin (DG) methods [15]. However, these simulations have been obtained for simple cases like pristine graphene under the effect of a constant external electric field. With a view to more complex situations, like those represented by a metal-oxide-semiconductor field-effect transistor (MOSFET) with a graphene channel, it is better to benefit from simpler models like drift-diffusion, energy transport or hydrodynamic ones. These directly provide balance equations for macroscopic quantities like electron density, average velocity or current, average energy, etc., and, therefore, are more suited as models for CAD tools.

The macroscopic quantities are related to the distribution function because they represent average values of some functions of the wave vector $\mathbf{k}$. For example, the density $n(\mathbf{r},t)$ is given by

$$n(\mathbf{r},t) = \frac{2}{(2\pi)^2}\int_{\mathbb{R}^2} f(\mathbf{r},\mathbf{k},t)d\mathbf{k}.$$

Similarly the average energy $W(\mathbf{r},t)$ is given by the relation

$$n(\mathbf{r},t)W(\mathbf{r},t) = \frac{2}{(2\pi)^2}\int_{\mathbb{R}^2} f(\mathbf{r},\mathbf{k},t)\mathscr{E}(\mathbf{k})d\mathbf{k}.$$

Generally speaking, given a weight function $\psi(\mathbf{k})$, the corresponding macroscopic quantity is the expectation value

$$M(\mathbf{r},t) = \frac{2}{(2\pi)^2}\int_{\mathbb{R}^2} \psi(\mathbf{k}) f(\mathbf{r},\mathbf{k},t) d\mathbf{k},$$

where the factor 2 is included to take into account the two states of spin, whereas the valley degeneracy is disregarded.
The evolution equation for $M(\mathbf{r},t)$ is deduced by multiplying eq.(2.4) for $\psi(\mathbf{k})$ and by integrating with respect to $\mathbf{k}$

$$\frac{\partial M}{\partial t} \quad + \quad \nabla_{\mathbf{r}} \cdot \int_{\mathbb{R}^2} f \frac{2\psi(\mathbf{k})}{(2\pi)^2} \mathbf{v}(\mathbf{k}) d\mathbf{k} - \frac{q}{\hbar}\mathbf{E} \cdot \int_{\mathbb{R}^2} f \nabla_{\mathbf{k}} \frac{2\psi(\mathbf{k})}{(2\pi)^2} d\mathbf{k} = \int_{\mathbb{R}^2} \frac{2\psi(\mathbf{k})}{(2\pi)^2} C[f] d\mathbf{k}. \tag{4.1}$$

Note that the moment equations depend only on the independent variables $\mathbf{r}, t$. This considerably reduces numerical complexity.

The macroscopic models differ in the different expressions of $\psi(\mathbf{k})$ employed in the moment equations, e.g. the drift-diffusion models only use the balance equation for density while the energy-transport models use, in addition, the balance equation for energy. Analogous to fluid-dynamics, we talk about hydrodynamic models if, at least, the balance equations for density, velocity and energy are included.

The main issue related to any model based on balance equations deduced as moment equations of type (4.1) is that there are more unknowns than introduced moments in the evolution equations, and the so-called *closure problem* arises. This arises from expressing the additional unknowns, that is the extra fluxes and production terms

$$\int_{\mathbb{R}^2} f \frac{2\psi(\mathbf{k})}{(2\pi)^2} \mathbf{v}(\mathbf{k}) d\mathbf{k}, \quad \int_{\mathbb{R}^2} f \nabla_{\mathbf{k}} \frac{2\psi(\mathbf{k})}{(2\pi)^2} d\mathbf{k}, \quad \int_{\mathbb{R}^2} \frac{2\psi(\mathbf{k})}{(2\pi)^2} C[f] d\mathbf{k},$$

as functions of the basic moments.

A systematic way to get the needed closure relations is employing the Maximum Entropy Principle (MEP). Firstly, we have to determine the expression of entropy in the continuum approximation. To achieve this, recalling that $f_i = \frac{n_i}{G_i}$ we observe that the entropy for fermions in the discrete case is given by

$$\begin{aligned} S[f] =& k_B \left[\sum_i G_i \ln G_i - \sum_i n_i \ln n_i - \sum_i (G_i - n_i) \ln(G_i - n_i) \right] = \\ =& k_B \left[\sum_i G_i \ln G_i - \sum_i (f_i G_i) \ln(f_i G_i) - \sum_i (G_i - f_i G_i) \ln(G_i - f_i G_i) \right] = \\ =& -k_B \sum_i G_i [f_i \ln f_i + (1-f_i) \ln(1-f_i)]. \end{aligned}$$

In the continuum limit, we resort the following standard formula valid for any regular enough function $h(k)$ [25]

$$\sum_i h(k_i) G_i \longrightarrow \frac{2V}{(2\pi)^2} \int_{\mathscr{B}_r} h(\mathbf{k}) d\mathbf{k}$$

where V is the spatial volume (that of the crystal in the case of semiconductors). The sum must be intended over all the discrete wave vectors k_i inside the first Brillouin zone. Therefore the entropy of the system in the semi-classical approximation reads

$$S[f] = -\frac{2k_B}{(2\pi)^2}\int_{\mathbb{R}^2}[f\ln f + (1-f)\ln(1-f)]\,d\mathbf{k}. \tag{4.2}$$

Let us suppose that a certain number of moments $M_A(\mathbf{r},t)$, $A = 1,2,\cdots,N$, relative to the weight functions $\psi_A(\mathbf{k})$, are known. According to MEP, the electron distribution function is estimated with the distribution f_{MEP} obtained by solving the following constrained optimization problem: for fixed $\mathbf{r}$ and t,

$$\max_{f\in\mathscr{F}} S[f] \quad \text{subject to the constraints:}$$

$$0 < f < 1, \tag{4.3}$$

$$M_A = \frac{2}{(2\pi)^2}\int_{\mathbb{R}^2}\psi_A(\mathbf{k})f(\mathbf{r},\mathbf{k},t)d\mathbf{k}, \quad A = 1,2,\cdots,N, \tag{4.4}$$

where $S[f]$ is the entropy of the system (4.2). Recall that $\mathscr{F}$ is the space of the function $g(\mathbf{k})$ such that $\psi_A(\mathbf{k})g(\mathbf{k}) \in L^1(\mathbb{R}^2)$ for $A = 1,2,\cdots,N$.

Here with $L^1(\mathbb{R}^2)$ we have denoted the usual Banach space of the summable functions defined over $\mathbb{R}^2$.

To take into account bilateral constraints let us introduce the Lagrange multipliers λ_A, $A = 1,2,\cdots,N$, and the Legendre transform of S

$$S' = S + \sum_A \lambda_A\left(M_A - \frac{2}{(2\pi)^2}\int_{\mathbb{R}^2} f\psi_A(\mathbf{k})d\mathbf{k}\right).$$

Let the variation of S' with respect to f be zero, i.e.,

$$0 = \delta S' = -\frac{2k_B}{(2\pi)^2}\int_{\mathbb{R}^2}\left[\ln f - \ln(1-f) + \frac{1}{k_B}\sum_A \psi_A(\mathbf{k})\lambda_A\right]\delta f\,d\mathbf{k}.$$

Since δf is arbitrary, the quantity in the square brackets must be zero; we get

$$f_{MEP}(\mathbf{r},\mathbf{k},t) = \frac{1}{1+\exp\left[\sum_A \psi_A(\mathbf{k})\lambda_A(\mathbf{r},t)\right]},$$

which also fulfills the unilateral constraints (4.3).

The multiplicative constant $\frac{1}{k_B}$ has been included into the multipliers for simplicity.

To complete the optimization procedure, it is necessary to invert the relations (4.4) and express the Lagrangian multipliers as functions of the basic variables. This can generally be achieved only numerically or by some approximation, e.g. expanding around the equilibrium state.

Apart from the above problem of inversion, once one gets f_{MEP}, the needed closure relations are obtained by evaluating the extra fluxes and production terms with f_{MEP} instead of f.

It should be mentioned that full non-linear closure, when it is inserted in the moment equations, leads to a hyperbolic system in the time direction [27, 48]. If f_{MEP} is obtained in an approximate form, the hyperbolicity of the moment equations has to be checked case by case.

The goodness of the models obtained with different choices of basic moments can be assessed by comparing the results obtained by directly integrating the transport equation.

In the Appendix A we recall a known uniforme convergence result by Borwein and Huang [8] for truncated moment problems defined on a compact set as the Brillouin zone, when the Fermi-Dirac type entropy is used as objective function. Nevertheless, while the case of moment problems defined on a compact support was known long before [6, 8], similar problems, as those considered in this Thesis, with unbounded support (or unbounded moments a_i) are usually difficult and still studied. Specifically, in the models formulated below, the weight functions chosen are not necessarily on $L^\infty(\mathscr{B}_r)$ and the Brillouin zone is extended to all space $\mathbb{R}^2$. Consequently the integrals involved are defined on the unbounded domain $\mathbb{R}^2$. We will see that numerical computations seem to suggest heuristically that for similar problems with unbounded support (or unbounded moments ψ_A) the Maximum Entropy estimator converges to the unknown density function f, although theoretical convergence is still an open problem, see [2].

In the next sections several models will be analyzed for homogeneous graphene in a constant electric field, by considering both linear and non-linear closure relations.

4.2 Comparing linear and non-linear 6-moment models

A hydrodynamic model based on the maximum entropy principle (MEP) has been formulated in [12] using a set of field variables which has been proved to be successful for traditional semiconductors like silicon [30, 31, 40, 43, 49, 57, 58], gallium arsernide [39, 40], silicon carbide [1]. Here we compare the solutions obtained with such a model with the direct simulation of the Boltzmann equation provided by the DG method proposed in [15, 61]. The results are quite acceptable for low and moderate electric fields but not completely satisfactory for higher fields.

The model is based on the following moments

$$n = \frac{2}{(2\pi)^2}\int_{\mathbb{R}^2} f(\mathbf{r},\mathbf{k},t)d\mathbf{k} \quad \text{density,} \tag{4.5}$$

$$nW = \frac{2}{(2\pi)^2}\int_{\mathbb{R}^2} f(\mathbf{r},\mathbf{k},t)\mathscr{E}(\mathbf{k})d\mathbf{k} \quad \text{energy density,} \tag{4.6}$$

$$n\mathbf{V} = \frac{2}{(2\pi)^2}\int_{\mathbb{R}^2} f(\mathbf{r},\mathbf{k},t)\mathbf{v}(\mathbf{k})d\mathbf{k} \quad \text{linear momentum density,} \tag{4.7}$$

$$n\mathbf{S} = \frac{2}{(2\pi)^2}\int_{\mathbb{R}^2} f(\mathbf{r},\mathbf{k},t)\mathscr{E}(\mathbf{k})\mathbf{v}(\mathbf{k})d\mathbf{k} \quad \text{energy-flux density.} \tag{4.8}$$

The corresponding evolution equations are given by

$$\begin{aligned}
&\frac{\partial}{\partial t} n + \nabla_{\mathbf{r}} (n\,\mathbf{V}) = 0,\\
&\frac{\partial}{\partial t} (n\,W) + \nabla_{\mathbf{r}} (n\,\mathbf{S}) + q\,n\,\mathbf{E}\cdot\mathbf{V} = n\,C_W,\\
&\frac{\partial}{\partial t} (n\,\mathbf{V}) + \nabla_{\mathbf{r}} \left(n\,\mathbf{F}^{(0)}\right) + q\,n\,\mathbf{G}^{(0)} : \mathbf{E} = n\,C_{\mathbf{v}},\\
&\frac{\partial}{\partial t} (n\,\mathbf{S}) + \nabla_{\mathbf{r}} \left(n\,\mathbf{F}^{(1)}\right) + q\,n\,\mathbf{G}^{(1)} : \mathbf{E} = n\,C_{\mathbf{S}}.
\end{aligned}$$

Besides the average densities, velocities, energies and energy fluxes, additional quantities appear[1]

$$\begin{aligned}
&n\,C_n = \frac{2}{(2\pi)^2} \int_{\mathbb{R}^2} \mathscr{C}(\mathbf{k})\,d\,\mathbf{k}, \quad n\,C_{\mathbf{v}} = \frac{2}{(2\pi)^2} \int_{\mathbb{R}^2} \mathbf{v}(\mathbf{k})\mathscr{C}(\mathbf{k})\,d\,\mathbf{k},\\
&n\,C_W = \frac{2}{(2\pi)^2} \int_{\mathbb{R}^2} \mathscr{E}(\mathbf{k})\mathscr{C}(\mathbf{k})\,d\,\mathbf{k}, \quad n\,C_{\mathbf{S}} = \frac{2}{(2\pi)^2} \int_{\mathbb{R}^2} \mathscr{E}(\mathbf{k})\mathbf{v}(\mathbf{k})\mathscr{C}(\mathbf{k})\,d\,\mathbf{k}\\
&n \begin{pmatrix} \mathbf{F}^{(0)} \\ \mathbf{F}^{(1)} \end{pmatrix} = \frac{2}{(2\pi)^2} \int_{\mathbb{R}^2} \begin{pmatrix} 1 \\ \mathscr{E}(\mathbf{k}) \end{pmatrix} \mathbf{v}(\mathbf{k}) \otimes \mathbf{v}(\mathbf{k}) f(\mathbf{r},\mathbf{k},t)\,d\mathbf{k},\\
&n \begin{pmatrix} \mathbf{G}^{(0)} \\ \mathbf{G}^{(1)} \end{pmatrix} = \frac{2}{\hbar(2\pi)^2} \int_{\mathbb{R}^2} f(\mathbf{r},\mathbf{k},t) \nabla_{\mathbf{k}} \begin{pmatrix} \mathbf{v}(\mathbf{k}) \\ \mathscr{E}(\mathbf{k})\mathbf{v}(\mathbf{k}) \end{pmatrix} d\mathbf{k},
\end{aligned}$$

which must be expressed as a function of the basic variables n, $\mathbf{V}$, W, $\mathbf{S}$.

Regarding the production terms, they are given by summing the contributions from the different types of phonon scattering

$$C_M = C_M^{(ac)} + \sum_{s=LO,TO,K} C_M^{(s)},$$

with $M = n, W, \mathbf{V}, \mathbf{S}$.
In [12] the following expression of the distribution function deduced by MEP

$$f_{MEP}(\mathbf{r},\mathbf{k},t) = \frac{1}{1+\exp(\lambda(\mathbf{r},t) + \lambda_w(\mathbf{r},t)\mathscr{E}(\mathbf{k}) + (\lambda_{\mathbf{V}}(\mathbf{r},t) + \mathscr{E}(\mathbf{k})\lambda_{\mathbf{S}}(\mathbf{r},t))\cdot\mathbf{v}(\mathbf{k}))} \tag{4.9}$$

has been used in the linearized form [2]

$$f_{MEP}(\mathbf{r},\mathbf{k},t) \approx \frac{1}{1+e^{\lambda+\lambda_w\mathscr{E}}} - \frac{e^{\lambda+\lambda_w\mathscr{E}}}{(1+e^{\lambda+\lambda_w\mathscr{E}})^2}(\lambda_{\mathbf{V}} + \mathscr{E}\lambda_{\mathbf{S}})\cdot\mathbf{v}. \tag{4.10}$$

Explicit closure relations have been obtained in [12] in the case of f_{MEP} linearized with respect to the vectorial Lagrange multipliers.
For better readability, the non-linear closure relations obtained in the case of non-linear f_{MEP}, are summarized in the Appendix B.

The linear model has been proved [14] to be hyperbolic in the physical relevant region $W > 0$.

[1] the symbol $\otimes$ denotes the tensor product of vectors

[2] In the following the explicit dependence on $\mathbf{r},\mathbf{k},t$ is omitted for the sake of simplifying the notation.

To evaluate the soundness of the model we consider the simple case of pristine graphene in a constant electric field $\mathbf{E}$. The physical situation we simulate is that of a strip of graphene which is infinitely long in the transversal direction with respect to that of the electric field (see Fig. 4.1). This allows to look for solutions which are not depending on space and to avoid any effect related to the boundary conditions.

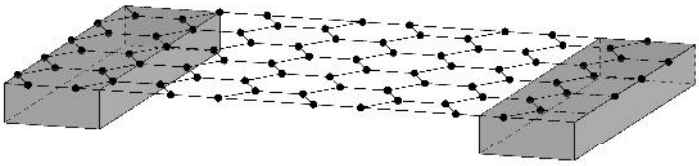

Figure 4.1: Schematic representation of a suspended monolayer graphene. In the direction orthogonal to the contacts the material is infinitely long. In each contact there is a constant electrostatic potential.

The evolution equations are reduced to a system of ordinary differential equations (ODE's). The only significant component of each equation is along direction of $\mathbf{E}$. If we choose a reference frame such that $\mathbf{E}$ is parallel to the x-axis, the evolution equations read

$$\frac{d}{dt}n = 0, \tag{4.11}$$

$$\frac{d}{dt}(nW) = -q\,n\,\mathbf{E}\cdot\mathbf{V} + nC_W, \tag{4.12}$$

$$\frac{d}{dt}(n\mathbf{V}) = -q\,n\,\mathbf{G}^{(0)} : \mathbf{E} + nC_{\mathbf{v}}, \tag{4.13}$$

$$\frac{d}{dt}(n\mathbf{S}) = -q\,n\,\mathbf{G}^{(1)} : \mathbf{E} + nC_{\mathbf{S}}. \tag{4.14}$$

As initial conditions we assume thermodynamic equilibrium. As a consequence, the initial conditions for the macroscopic variables are

$$n(0) = \frac{2}{(2\pi)^2}\int_{\mathbb{R}^2} f_{FD}(\mathbf{k})d\mathbf{k}, \tag{4.15}$$

$$n(0)W(0) = \frac{2}{(2\pi)^2}\int_{\mathbb{R}^2} f_{FD}(\mathbf{k})\mathscr{E}d\mathbf{k}, \tag{4.16}$$

$$n(0)\mathbf{V}(0) = \mathbf{0}, \tag{4.17}$$

$$n(0)\mathbf{S}(0) = \mathbf{0}, \tag{4.18}$$

where $f_{FD}(\mathbf{k})$ is the Fermi-Dirac distribution (2.3).

In Fig. 4.2, for several values of the Fermi energy and electric field, we compare the results obtained with the linearized 6-moment model (L6MM) and those obtained by a direct simulation of the Boltzmann equation with the approach based on the Discontinuous Galerkin (DG) method proposed in [15, 61]. First the case $\varepsilon_F = 0.4$ eV has been analyzed. Regarding average energy, the results of the MEP model are quite satisfactory. In the steady regime the maximum relative error

is about 2.8 % and is reached when $E = 6$ kV/cm. In the other cases we have a relative error of 1.6 % for $E = 4$ kV/cm, 0.04 % for $E = 2$ kV/cm.

The relative error for the velocity is greater. The discrepancy has a maximum for $E = 6$ kV/cm of about 19.5 %. For $E = 4$ kV/cm the relative error is 15.2 %, for $E = 2$ kV/cm 8 %. It is evident that the model is quite acceptable for low and moderate fields but less adequate at high fields.

To understand if the Fermi energy influences the accuracy of the MEP model, we performed similar simulations with $\varepsilon_F = 0.6$ eV (Fig. 4.3). The qualitative behaviour is similar to the case $\varepsilon_F = 0.4$ eV but with a better agreement between the DG and hydrodynamic results. One finds a relative error for the energy not greater than 1 % while the error in the velocity is 9 % if $E = 6$ kV/cm, 7 % if $E = 4$ kV/cm, 0.8 % if $E = 2$ kV/cm. Apparently, increasing the Fermi energy, or equivalently the electron density, improves the performance of the hydrodynamic model. This seems to agree with classical gasdynamics where the higher density, the more accurate are fluid-dynamic equations.

Although the overall discrepancy is reasonable for the applications, it is likely that some non-linear terms need to be included in the velocity and energy-flux or additional moments.

As a first attempt, the full non-linear 6-moment model (6MM), obtained with the full non-linear distribution function (4.9), is numerically solved to assess the influence of the linear approximation. Inverting the basic moments-Lagrange multipliers can be performed numerically but such a cumbersome numerical procedure was avoided by assuming the Lagrange multipliers as field variables, therefore

$$\frac{d}{dt}\begin{pmatrix} n \\ W \\ \mathbf{V} \\ \mathbf{S} \end{pmatrix} = \begin{pmatrix} \frac{\partial n}{\partial \lambda} & \frac{\partial n}{\partial \lambda_w} & \frac{\partial n}{\partial \lambda_V} & \frac{\partial n}{\partial \lambda_{\mathbf{S}}} \\ \frac{\partial W}{\partial \lambda} & \frac{\partial W}{\partial \lambda_w} & \frac{\partial W}{\partial \lambda_V} & \frac{\partial W}{\partial \lambda_{\mathbf{S}}} \\ \frac{\partial \mathbf{V}}{\partial \lambda} & \frac{\partial \mathbf{V}}{\partial \lambda_w} & \frac{\partial \mathbf{V}}{\partial \lambda_{\mathbf{V}}} & \frac{\partial \mathbf{V}}{\partial \lambda_{\mathbf{S}}} \\ \frac{\partial \mathbf{S}}{\partial \lambda} & \frac{\partial \mathbf{S}}{\partial \lambda_w} & \frac{\partial \mathbf{S}}{\partial \lambda_{\mathbf{V}}} & \frac{\partial \mathbf{S}}{\partial \lambda_{\mathbf{S}}} \end{pmatrix} \frac{d}{dt}\begin{pmatrix} \lambda \\ \lambda_w \\ \lambda_{\mathbf{V}} \\ \lambda_{\mathbf{S}} \end{pmatrix}. \tag{4.19}$$

The components of the Jacobian matrix were obtained by differentiating under the integral sign thanks to the integrability conditions of f_{MEP}. The numerical evaluation of the integrals was performed with Gaussian quadrature formulas.

The results are reported in Figs. 4.2, 4.3 where the same cases for the linear model were considered. It is evident that the non-linear terms do not help in improving the model.

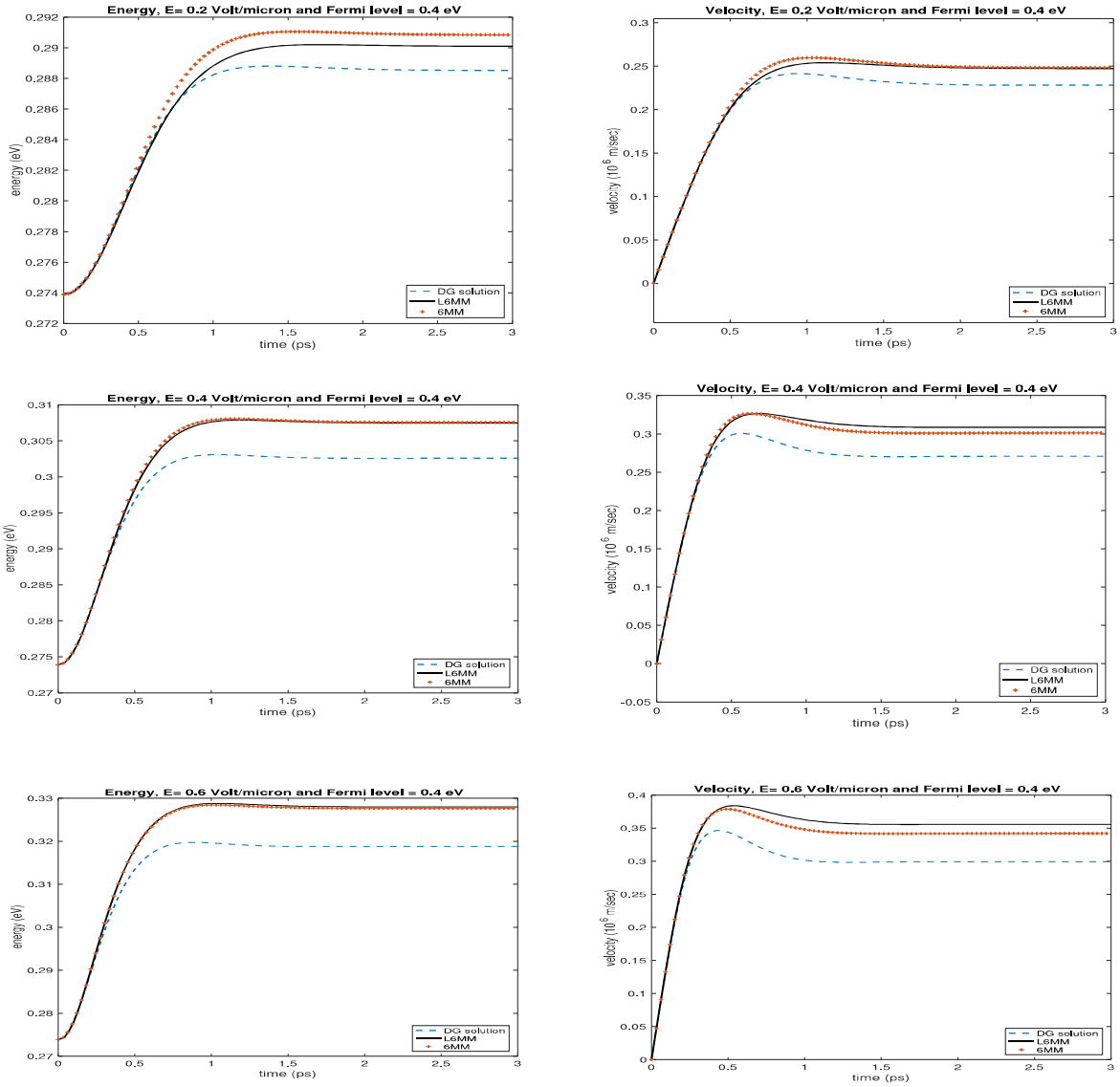

Figure 4.2: Comparing the energy and velocity obtained with a direct solution of the Boltzmann equation (DG method) (dashed lines), the 6MM (crossed lines) and its linearized version (L6MM) (continuous line) for the electric fields $E = 2$ kV/cm, $E = 4$ kV/cm, $E = 6$ kV/cm by considering a constant lattice temperature of 300 K and a Fermi energy equal to 0.4 eV.

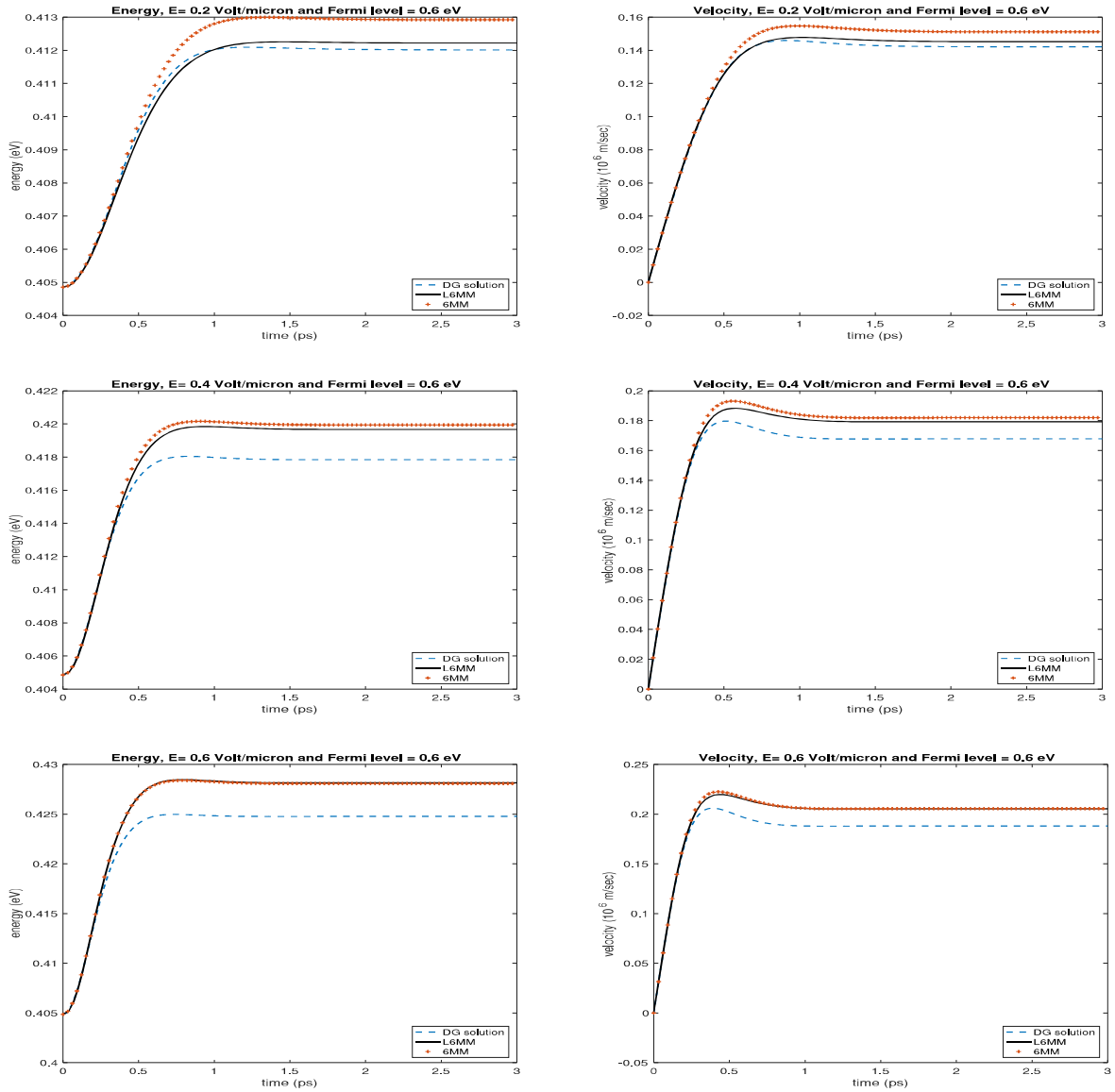

Figure 4.3: Comparing the energy and velocity obtained with a direct solution of the Boltzmann equation (DG method) (dashed lines), the 6MM (crossed lines) and its linearized version (L6MM) (continuous line) for the electric fields $E = 2$ kV/cm, $E = 4$ kV/cm, $E = 6$ kV/cm by considering a constant lattice temperature of 300 K and a Fermi energy equal to 0.6 eV.

4.3 The case of moments based on energy powers.

In the previous section a 6-moment model has been formulated by taking as fundamental variables the electron density, linear momentum, energy and energy flux. Numerical results show, however, that this choise of moments is, in case of high electric fields, not sufficient for accurate modeling. Here we try to get better results by including additional moments which are

averages involving higher powers of energy. Explicitly, we consider the following weight functions $\{1, \mathscr{E}(\mathbf{k}), v, \mathscr{E}(\mathbf{k})v(\mathbf{k}), \mathscr{E}^2(\mathbf{k})v(\mathbf{k}), ..., \mathscr{E}^N(\mathbf{k})v(\mathbf{k})\}$ to which the following moments

$$
\begin{aligned}
n &= \frac{2}{(2\pi)^2}\int_{\mathbb{R}^2} f(\mathbf{r},\mathbf{k},t)d\mathbf{k}, && (4.20)\\
nW &= \frac{2}{(2\pi)^2}\int_{\mathbb{R}^2} f(\mathbf{r},\mathbf{k},t)\mathscr{E}(\mathbf{k})d\mathbf{k}, && (4.21)\\
n\mathbf{V} &= \frac{2}{(2\pi)^2}\int_{\mathbb{R}^2} f(\mathbf{r},\mathbf{k},t)\mathbf{v}(\mathbf{k})d\mathbf{k}, && (4.22)\\
n\mathbf{S} &= \frac{2}{(2\pi)^2}\int_{\mathbb{R}^2} f(\mathbf{r},\mathbf{k},t)\mathscr{E}(\mathbf{k})\mathbf{v}(\mathbf{k})d\mathbf{k}, && (4.23)\\
n\mathbf{S}^{(2)} &= \frac{2}{(2\pi)^2}\int_{\mathbb{R}^2} f(\mathbf{r},\mathbf{k},t)\mathscr{E}^2(\mathbf{k})\mathbf{v}(\mathbf{k})d\mathbf{k} && (4.24)
\end{aligned}
$$

$$\vdots$$

$$
n\mathbf{S}^{(N)} = \frac{2}{(2\pi)^2}\int_{\mathbb{R}^2} f(\mathbf{r},\mathbf{k},t)\mathscr{E}^N(\mathbf{k})\mathbf{v}(\mathbf{k})d\mathbf{k} \qquad (4.25)
$$

correspond. Their evolution equations are obtained by taking the moments of the Boltzmann equation with respect to weight functions and they read

$$
\begin{aligned}
&\frac{\partial}{\partial t}n + \nabla_{\mathbf{r}}(n\,\mathbf{V}) = n\,C_n\,, && (4.26)\\
&\frac{\partial}{\partial t}(nW) + \nabla_{\mathbf{r}}(n\,\mathbf{S}) + qn\,\mathbf{E}\cdot\mathbf{V} = n\,C_W, && (4.27)\\
&\frac{\partial}{\partial t}(n\mathbf{V}) + \nabla_{\mathbf{r}}\left(n\,\mathbf{F}^{(0)}\right) + qn\,\mathbf{G}^{(0)}:\mathbf{E} = n\,C_{\mathbf{V}}, && (4.28)\\
&\frac{\partial}{\partial t}(n\mathbf{S}) + \nabla_{\mathbf{r}}\left(n\,\mathbf{F}^{(1)}\right) + qn\,\mathbf{G}^{(1)}:\mathbf{E} = n\,C_{\mathbf{S}}, && (4.29)\\
&\frac{\partial}{\partial t}(n\mathbf{S}^{(2)}) + \nabla_{\mathbf{r}}\left(n\,\mathbf{F}^{(2)}\right) + qn\,\mathbf{G}^{(2)}:\mathbf{E} = n\,C_{\mathbf{S}}^{(2)}, && (4.30)
\end{aligned}
$$

$$\vdots$$

$$
\frac{\partial}{\partial t}(n\mathbf{S}^{(N)}) + \nabla_{\mathbf{r}}\left(n\,\mathbf{F}^{(N)}\right) + qn\,\mathbf{G}^{(N)}:\mathbf{E} = n\,C_{\mathbf{S}}^{(N)}. \qquad (4.31)
$$

The additional quantities, appearing in the previous balance equations and must be expressed in terms of n, W,$\mathbf{V}$, $\mathbf{S}$, $\mathbf{S}^{(2)}$,...,$\mathbf{S}^{(N)}$, are the production terms

$$
\begin{aligned}
nC_n &= \frac{2}{(2\pi)^2}\int_{\mathbb{R}^2} C(\mathbf{k})d\mathbf{k}, && (4.32)\\
nC_W &= \frac{2}{(2\pi)^2}\int_{\mathbb{R}^2} \mathscr{E}(\mathbf{k})C(\mathbf{k})d\mathbf{k}, && (4.33)\\
nC_{\mathbf{V}} &= \frac{2}{(2\pi)^2}\int_{\mathbb{R}^2} \mathbf{v}(\mathbf{k})C(\mathbf{k})d\mathbf{k}, && (4.34)\\
nC_{\mathbf{S}} &= \frac{2}{(2\pi)^2}\int_{\mathbb{R}^2} \mathscr{E}(\mathbf{k})\mathbf{v}(\mathbf{k})C(\mathbf{k})d\mathbf{k}, && (4.35)\\
nC_{\mathbf{S}}^{(2)} &= \frac{2}{(2\pi)^2}\int_{\mathbb{R}^2} \mathscr{E}^2(\mathbf{k})\mathbf{v}(\mathbf{k})C(\mathbf{k})d\mathbf{k}, && (4.36)
\end{aligned}
$$

$$\vdots$$

$$n\,C_{\mathbf{S}}^{(N)} = \frac{2}{(2\pi)^2}\int_{\mathbb{R}^2} \mathscr{E}^N(\mathbf{k})\mathbf{v}(\mathbf{k})C(\mathbf{k})d\mathbf{k}, \tag{4.37}$$

and the fluxes[3]

$$n\,\mathbf{G}^{(0)} = \frac{2}{\hbar(2\pi)^2}\int_{\mathbb{R}^2} f(\mathbf{r},\mathbf{k},t)\nabla_{\mathbf{k}}\mathbf{V}(\mathbf{k})d\mathbf{k}, \tag{4.38}$$

$$n\,\mathbf{G}^{(1)} = \frac{2}{\hbar(2\pi)^2}\int_{\mathbb{R}^2} f(\mathbf{r},\mathbf{k},t)\nabla_{\mathbf{k}}(\mathscr{E}(\mathbf{k})\mathbf{v}(\mathbf{k}))d\mathbf{k}, \tag{4.39}$$

$$n\,\mathbf{G}^{(2)} = \frac{2}{\hbar(2\pi)^2}\int_{\mathbb{R}^2} f(\mathbf{r},\mathbf{k},t)\nabla_{\mathbf{k}}(\mathscr{E}^2(\mathbf{k})\mathbf{v}(\mathbf{k}))d\mathbf{k}, \tag{4.40}$$

$$\vdots$$

$$n\,\mathbf{G}^{(N)} = \frac{2}{\hbar(2\pi)^2}\int_{\mathbb{R}^2} f(\mathbf{r},\mathbf{k},t)\nabla_{\mathbf{k}}(\mathscr{E}^N(\mathbf{k})\mathbf{v}(\mathbf{k}))d\mathbf{k}, \tag{4.41}$$

$$n\,\mathbf{F}^{(0)} = \frac{2}{(2\pi)^2}\int_{\mathbb{R}^2} \mathbf{v}(\mathbf{k})\otimes\mathbf{v}(\mathbf{k})f(\mathbf{r},\mathbf{k},t)d\mathbf{k}, \tag{4.42}$$

$$n\,\mathbf{F}^{(1)} = \frac{2}{(2\pi)^2}\int_{\mathbb{R}^2} \mathscr{E}(\mathbf{k})\mathbf{v}(\mathbf{k})\otimes\mathbf{v}(\mathbf{k})f(\mathbf{r},\mathbf{k},t)d\mathbf{k}, \tag{4.43}$$

$$n\,\mathbf{F}^{(2)} = \frac{2}{(2\pi)^2}\int_{\mathbb{R}^2} \mathscr{E}^2(\mathbf{k})\mathbf{v}(\mathbf{k})\otimes\mathbf{v}(\mathbf{k})f(\mathbf{r},\mathbf{k},t)d\mathbf{k}, \tag{4.44}$$

$$\vdots$$

$$n\,\mathbf{F}^{(N)} = \frac{2}{(2\pi)^2}\int_{\mathbb{R}^2} \mathscr{E}^N(\mathbf{k})\mathbf{v}(\mathbf{k})\otimes\mathbf{v}(\mathbf{k})f(\mathbf{r},\mathbf{k},t)d\mathbf{k}. \tag{4.45}$$

Regarding the production terms, they are given by summing the contributions from the different types of phonon scattering

$$n\,C_M = n\,C_M^{(ac)} + \sum_{s=LO,TO,K} n\,C_M^{(s)}$$

with $M = n, W, \mathbf{V}, \mathbf{S}, \mathbf{S}^{(2)}, ..., \mathbf{S}^{(N)}$.

By exploiting MEP, the following estimator of the distribution function is obtained

$$f_{MEP}(\mathbf{r},\mathbf{k},t) = \frac{1}{1+\exp\left(\lambda(\mathbf{r},t)+\lambda_w(\mathbf{r},t)\mathscr{E}(\mathbf{k})+(\lambda_{\mathbf{V}}(\mathbf{r},t)+\mathscr{E}(\mathbf{k})\lambda_{\mathbf{S}}(\mathbf{r},t)+\mathscr{E}^2(\mathbf{k})\lambda_{\mathbf{S}^{(2)}}(\mathbf{r},t))\cdot\mathbf{v}(\mathbf{k})+...+\mathscr{E}^N(\mathbf{k})\lambda_{\mathbf{S}^{(N)}}(\mathbf{r},t))\cdot\mathbf{v}(\mathbf{k})\right)}, \tag{4.46}$$

where λ, λ_w, $\lambda_{\mathbf{S}}$, $\lambda_{\mathbf{S}}^{(2)}$, ..., $\lambda_{\mathbf{S}}^{(N)}$ are the set of Lagrange multipliers relative to the basic fields.

If one linearizes by considering the vectorial quantities as first order terms because they vanish at equilibrium, the MEP estimator can be written as [4]

$$f_{MEP}(\mathbf{r},\mathbf{k},t) \approx \frac{1}{1+e^{\lambda+\lambda_w\mathscr{E}}} - \frac{e^{\lambda+\lambda_w\mathscr{E}}}{(1+e^{\lambda+\lambda_w\mathscr{E}})^2}(\lambda_{\mathbf{V}}+\mathscr{E}\lambda_{\mathbf{S}}+\mathscr{E}^2\lambda_{\mathbf{S}}^{(2)}+...+\mathscr{E}^N\lambda_{\mathbf{S}}^{(N)})\cdot\mathbf{v}. \tag{4.47}$$

This is the expression we will use in the following and for the sake of clarity the closure relations obtained by adopting this distribution function are postponed to the Appendix C.

[3] the symbol $\otimes$ denotes the tensor product of vectors

[4] The explicit dependence on $\mathbf{r},\mathbf{k},t$ is omitted for the sake of simplifying the notation.

4.3.1 Mathematical structure of the model with 8 moments

Before investigating the accuracy of the model and presenting some numerical results, we deduce its main mathematical features taking into account the particular case of 8 moment model with the flux of the squared power of energy. A generalization of this study in the case of a model with an arbitrary number of moments is under current investigation.

Explicitly, we consider the following weight functions $\{1, \mathscr{E}(\mathbf{k}), v, \mathscr{E}(\mathbf{k})v(\mathbf{k}), \mathscr{E}^2(\mathbf{k})v(\mathbf{k})\}$ to which the following moments

$$n = \frac{2}{(2\pi)^2}\int_{\mathbb{R}^2} f(\mathbf{r},\mathbf{k},t)d\mathbf{k}, \tag{4.48}$$

$$nW = \frac{2}{(2\pi)^2}\int_{\mathbb{R}^2} f(\mathbf{r},\mathbf{k},t)\mathscr{E}(\mathbf{k})d\mathbf{k}, \tag{4.49}$$

$$n\mathbf{V} = \frac{2}{(2\pi)^2}\int_{\mathbb{R}^2} f(\mathbf{r},\mathbf{k},t)\mathbf{v}(\mathbf{k})d\mathbf{k}, \tag{4.50}$$

$$n\mathbf{S} = \frac{2}{(2\pi)^2}\int_{\mathbb{R}^2} f(\mathbf{r},\mathbf{k},t)\mathscr{E}(\mathbf{k})\mathbf{v}(\mathbf{k})d\mathbf{k}, \tag{4.51}$$

$$n\mathbf{S}^{(2)} = \frac{2}{(2\pi)^2}\int_{\mathbb{R}^2} f(\mathbf{r},\mathbf{k},t)\mathscr{E}^2(\mathbf{k})\mathbf{v}(\mathbf{k})d\mathbf{k} \tag{4.52}$$

correspond. Their evolution equations are

$$\frac{\partial}{\partial t}n + \nabla_{\mathbf{r}}(n\,\mathbf{V}) = n\,C_n\,, \tag{4.53}$$

$$\frac{\partial}{\partial t}(nW) + \nabla_{\mathbf{r}}(n\,\mathbf{S}) + qn\,\mathbf{E}\cdot\mathbf{V} = n\,C_W, \tag{4.54}$$

$$\frac{\partial}{\partial t}(n\mathbf{V}) + \nabla_{\mathbf{r}}\left(n\,\mathbf{F}^{(0)}\right) + qn\,\mathbf{G}^{(0)}:\mathbf{E} = n\,C_{\mathbf{V}}, \tag{4.55}$$

$$\frac{\partial}{\partial t}(n\mathbf{S}) + \nabla_{\mathbf{r}}\left(n\,\mathbf{F}^{(1)}\right) + qn\,\mathbf{G}^{(1)}:\mathbf{E} = n\,C_{\mathbf{S}}, \tag{4.56}$$

$$\frac{\partial}{\partial t}(n\mathbf{S}^{(2)}) + \nabla_{\mathbf{r}}\left(n\,\mathbf{F}^{(2)}\right) + qn\,\mathbf{G}^{(2)}:\mathbf{E} = n\,C_{\mathbf{S}}^{(2)}, \tag{4.57}$$

To study its main proprieties let introduce the following quantities

$$J_n(\lambda,\lambda_w) := \int_0^{+\infty} \frac{\mathscr{E}^n e^{\lambda+\lambda_w\mathscr{E}}}{\left(1+e^{\lambda+\lambda_w\mathscr{E}}\right)^2}\,d\mathscr{E}, \quad K_n(\lambda,\lambda_w) := \frac{1}{2\pi\hbar^2 v_F}J_n(\lambda,\lambda_w).$$

Theorem 4.1. *There is a local one-to-one correspondence between Lagrange multipliers and field variables.*

Proof. Let us introduce the vectors $\mathbf{U^{(1)}} = (n, W)$ and $\mathbf{U}_l^{(1)} = (\lambda, \lambda_w)$. The Jacobian matrix is given by

$$B = \frac{\partial(n,W)}{\partial(\lambda,\lambda_w)} = -\frac{1}{\pi\hbar^2 v_F^2}\begin{pmatrix} J_1 & J_2 \\ J_2 & J_3 \end{pmatrix}.$$

Let us consider the quadratic form associated to the matrix B

$$g(\xi) = (\xi_1,\xi_2)B(\xi_1,\xi_2)^T \quad \forall \xi = (\xi_1,\xi_2) \in \mathbb{R}^2.$$

One has

$$g(\xi) = -\frac{1}{\pi\hbar^2 v_F^2}\int_0^{+\infty}\frac{\mathscr{E}e^{\lambda+\lambda_w\mathscr{E}}}{(1+e^{\lambda+\lambda_w\mathscr{E}})^2}\left(\xi_1+\mathscr{E}\xi_2\right)^2 d\mathscr{E}.$$

Since $\xi_1+\mathscr{E}\xi_2$ is zero at most in a set of zero measure, g is negative definite and there is a local one-to-one correspondence between $\mathbf{U^{(1)}}$ and $\mathbf{U}_l^{(1)}$.

Regarding the vectorial fields, one finds

$$\begin{pmatrix} n\mathbf{V} \\ n\mathbf{S} \\ n\mathbf{S}^{(2)} \end{pmatrix} = -\frac{1}{2\pi\hbar^2}\begin{pmatrix} J_1(\lambda,\lambda_w) & J_2(\lambda,\lambda_w) & J_3(\lambda,\lambda_w) \\ J_2(\lambda,\lambda_w) & J_3(\lambda,\lambda_w) & J_4(\lambda,\lambda_w) \\ J_3(\lambda,\lambda_w) & J_4(\lambda,\lambda_w) & J_5(\lambda,\lambda_w) \end{pmatrix}\begin{pmatrix} \lambda_{\mathbf{V}} \\ \lambda_{\mathbf{S}} \\ \lambda_{\mathbf{S}}^{(2)} \end{pmatrix} := C\begin{pmatrix} \lambda_{\mathbf{V}} \\ \lambda_{\mathbf{S}} \\ \lambda_{\mathbf{S}}^{(2)} \end{pmatrix}.$$

Let us consider the quadratic form associated to the matrix C

$$h(\xi) = (\xi_1,\xi_2,\xi_3)C(\xi_1,\xi_2,\xi_3)^T \quad \forall \xi = (\xi_1,\xi_2,\xi_3)\in\mathbb{R}^3.$$

One has

$$h(\xi) = -\frac{1}{2\pi\hbar^2}\int_0^{+\infty}\frac{\mathscr{E}e^{\lambda+\lambda_w\mathscr{E}}}{(1+e^{\lambda+\lambda_w\mathscr{E}})^2}\left(\xi_1+\mathscr{E}\xi_2+\mathscr{E}^2\xi_3\right)^2 d\mathscr{E}.$$

Since $\xi_1+\mathscr{E}\xi_2++\mathscr{E}^2\xi_3$ is zero at most in a set of zero measure, h is negative definite and there is a local one-to-one correspondence between Lagrange multipliers and field variables. □

Theorem 4.2. *The evolution equations closed with MEP form a hyperbolic system of balance laws in the time direction.*

Proof. Thanks to the previous theorem, we can use the Lagrange multipliers as field variables. In term of the Lagrange multipliers the evolution equations become

$$\frac{d}{dt}\begin{pmatrix} \lambda \\ \lambda_w \\ \lambda_{\mathbf{V}} \\ \lambda_{\mathbf{S}} \\ \lambda_{\mathbf{S}}^{(2)} \end{pmatrix} = \begin{pmatrix} B & O_{2\times 3} \\ O_{3\times 2} & C \end{pmatrix}^{-1}\mathscr{G}, \tag{4.58}$$

where $O_{m\times n}$ denote the zero matrix of size m by n and

$$\mathscr{G} = \begin{bmatrix} -qn\begin{pmatrix} 0 \\ \mathbf{V} \\ \mathbf{G^{(0)}} \\ \mathbf{G^{(1)}} \\ \mathbf{G^{(2)}} \end{pmatrix}\cdot\mathbf{E} + n\begin{pmatrix} C_n \\ C_W \\ C_{\mathbf{V}} \\ C_{\mathbf{S}} \\ C_{\mathbf{S}}^{(2)} \end{pmatrix} \end{bmatrix}.$$

Denoting with (x_1,x_2) the spatial variables, the evolution equations can be written in the form

$$\mathscr{A}_0\frac{\partial\Lambda}{\partial t} + \mathscr{A}_1\frac{\partial\Lambda}{\partial x_1} + \mathscr{A}_2\frac{\partial\Lambda}{\partial x_2} = \mathscr{G} \tag{4.59}$$

where

$$\Lambda = (\lambda, \lambda_w, \lambda_{V_1}, \lambda_{S_1}, \lambda_{S_1^{(2)}}, \lambda_{V_2}, \lambda_{S_2}, \lambda_{S_2^{(2)}})^T,$$

$$\begin{aligned}
\mathscr{A}_0 &= \nabla_\Lambda \mathscr{F}_0 \quad \text{with} \quad \mathscr{F}_0 = (n, nW, nV_1, nS_1, nS_1^{(2)}, nV_2, nS_2, nS_2^{(2)})^T, \\
\mathscr{A}_1 &= \nabla_\Lambda \mathscr{F}_1 \quad \text{with} \quad \mathscr{F}_1 = (nV_1, nS_1, nF_{11}^{(0)}, nF_{11}^{(1)}, nF_{11}^{(2)}, nF_{21}^{(0)}, nF_{21}^{(1)}, F_{21}^{(2)})^T, \\
\mathscr{A}_2 &= \nabla_\Lambda \mathscr{F}_2 \quad \text{with} \quad \mathscr{F}_2 = (nV_2, nS_2, nF_{12}^{(0)}, nF_{12}^{(1)}, nF_{12}^{(2)}, nF_{22}^{(0)}, nF_{22}^{(1)}, nF_{22}^{(2)})^T.
\end{aligned}$$

Here V_i and S_i $i = 1,2$ are the components of $\mathbf{V}$ and $\mathbf{S}$ and $F_{ij}^{(0)}$, $F_{ij}^{(1)}$,$F_{ij}^{(2)}$ $i,j = 1,2$ are the components of the tensors $\mathbf{F}^{(0)}$, $\mathbf{F}^{(1)}$ and $\mathbf{F}^{(2)}$ respectively.

We prove that $\det(\mathscr{A}_0) \neq 0$. Omitting the dependence on Lagrangian multipliers λ and λ_w for the sake of simplicity, explicitly $\mathscr{A}_0$ reads

$$\mathscr{A}_0 = \begin{pmatrix}
-\frac{2}{v_F}K_1 & -\frac{2}{v_F}K_2 & 0 & 0 & 0 & 0 & 0 & 0 \\
-\frac{2}{v_F}K_2 & -\frac{2}{v_F}K_3 & 0 & 0 & 0 & 0 & 0 & 0 \\
\frac{\partial nV_1}{\partial \lambda} & \frac{\partial nV_1}{\partial \lambda_w} & -v_F K_1 & -v_F K_2 & -v_F K_3 & 0 & 0 & 0 \\
\frac{\partial nS_1}{\partial \lambda} & \frac{\partial nS_1}{\partial \lambda_w} & -v_F K_2 & -v_F K_3 & -v_F K_4 & 0 & 0 & 0 \\
\frac{\partial nS_1^{(2)}}{\partial \lambda} & \frac{\partial nS_1^{(2)}}{\partial \lambda_w} & -v_F K_3 & -v_F K_4 & -v_F K_5 & 0 & 0 & 0 \\
\frac{\partial nV_2}{\partial \lambda} & \frac{\partial nV_2}{\partial \lambda_w} & 0 & 0 & 0 & -v_F K_1 & -v_F K_2 & -v_F K_3 \\
\frac{\partial nS_2}{\partial \lambda} & \frac{\partial nS_2}{\partial \lambda_w} & 0 & 0 & 0 & -v_F K_2 & -v_F K_3 & -v_F K_4 \\
\frac{\partial nS_2^{(2)}}{\partial \lambda} & \frac{\partial nS_2^{(2)}}{\partial \lambda_w} & 0 & 0 & 0 & -v_F K_3 & -v_F K_4 & -v_F K_5
\end{pmatrix}.$$

We can factorize the determinant of $\mathscr{A}_0$ as

$$\frac{1}{64} \frac{\left(J_1 J_3 J_5 - J_1 {J_4}^2 + 2 J_2 J_4 J_3 - {J_2}^2 J_5 - {J_3}^3\right)^2 \left(J_1 J_3 - {J_2}^2\right)}{\pi^8 h^{16} v^4}.$$

Since the two matrices

$$\begin{pmatrix} J_1 & J_2 \\ J_2 & J_3 \end{pmatrix}, \quad \begin{pmatrix} J_1 & J_2 & J_3 \\ J_2 & J_3 & J_4 \\ J_3 & J_4 & J_5 \end{pmatrix}$$

are positive definite, in virtue of theorem 4.1, it follows that $\det(\mathscr{A}_0) > 0$ for any value of the fields. For arbitrary $\mathbf{n} = (n_1, n_2)$ belonging to the unit circle of $\mathbb{R}^2$, the eigenvalue equation is

$$\det\left(n_1 \mathscr{A}_1 + n_2 \mathscr{A}_2 - \mu \mathscr{A}_0\right) = 0$$

which has the following roots:

$$\begin{aligned}
\mu_1 &= 0 \quad \text{with multiplicity four,} \\
\mu_{2,3} &= \pm \frac{\sqrt{2}}{2} v_F \quad \text{both with multiplicity two.}
\end{aligned}$$

To complete the analysis of the hyperbolicity, we study the rank of the matrix $M(\mu) = n_1\mathscr{A}_1 + n_2\mathscr{A}_2 - \mu\mathscr{A}_0$ which explicitly is given by

$$\begin{pmatrix}
\sum_{i=1}^{2} n_i \frac{\partial}{\partial\lambda}(nV_i) + \frac{2\mu}{v_F}K_1 & \sum_{i=1}^{2} n_i \frac{\partial}{\partial\lambda_w}(nV_i) + \frac{2\mu}{v_F}K_2 & -n_1K_1 & -n_1K_2 & -n_1K_3 & -n_2K_1 & -n_2K_2 & -n_2K_3 \\
\sum_{i=1}^{2} n_i \frac{\partial}{\partial\lambda}(nS_i) + \mu\frac{1}{\pi\hbar^2 v_F^2}J_2 & \sum_{i=1}^{2} n_i \frac{\partial}{\partial\lambda_w}(nS_i) + \mu\frac{1}{\pi\hbar^2 v_F^2}J_3 & -n_1K_2 & -n_1K_3 & -n_1K_4 & -n_2K_2 & -n_2K_3 & -n_2K_4 \\
n_1\frac{\partial}{\partial\lambda}(nF_{11}^{(0)}) - \mu\frac{\partial nV_1}{\partial\lambda} & n_1\frac{\partial}{\partial\lambda_w}(nF_{11}^{(0)}) - \mu\frac{\partial nV_1}{\partial\lambda_w} & \mu K_1 & \mu K_2 & \mu K_3 & 0 & 0 & 0 \\
n_1\frac{\partial}{\partial\lambda}(nF_{11}^{(1)}) - \mu\frac{\partial nS_1}{\partial\lambda} & n_1\frac{\partial}{\partial\lambda_w}(nF_{11}^{(1)}) - \mu\frac{\partial nS_1}{\partial\lambda_w} & \mu K_2 & \mu K_3 & \mu K_4 & 0 & 0 & 0 \\
n_1\frac{\partial}{\partial\lambda}(nF_{11}^{(2)}) - \mu\frac{\partial nS_1^{(2)}}{\partial\lambda} & n_1\frac{\partial}{\partial\lambda_w}(nF_{11}^{(2)}) - \mu\frac{\partial nS_1^{(2)}}{\partial\lambda_w} & \mu K_3 & \mu K_4 & \mu K_5 & 0 & 0 & 0 \\
n_2\frac{\partial}{\partial\lambda}(nF_{22}^{(0)}) - \mu\frac{\partial nV_2}{\partial\lambda} & n_2\frac{\partial}{\partial\lambda_w}(nF_{22}^{(0)}) - \mu\frac{\partial nV_2}{\partial\lambda_w} & 0 & 0 & 0 & \mu K_1 & \mu K_2 & \mu K_3 \\
n_2\frac{\partial}{\partial\lambda}(nF_{22}^{(1)}) - \mu\frac{\partial nS_2}{\partial\lambda} & n_2\frac{\partial}{\partial\lambda_w}(nF_{22}^{(1)}) - \mu\frac{\partial nS_2}{\partial\lambda_w} & 0 & 0 & 0 & \mu K_2 & \mu K_3 & \mu K_4 \\
n_2\frac{\partial}{\partial\lambda}(nF_{22}^{(2)}) - \mu\frac{\partial nS_2^{(2)}}{\partial\lambda} & n_2\frac{\partial}{\partial\lambda_w}(nF_{22}^{(2)}) - \mu\frac{\partial nS_2^{(2)}}{\partial\lambda_w} & 0 & 0 & 0 & \mu K_3 & \mu K_4 & \mu K_5
\end{pmatrix}$$

Let us denote by m_{ij} the generic element of the matrix $M(\mu)$.

1. Case $\mu = 0$.

   By taking into account the fact that $nF_{11}^{(k)} = nF_{22}^{(k)}$, $k = 1,2$, from the definition of J_n it follows that the third, fourth and fifth rows of the matrix $M(0)$ are proportional to the sixth, seventh and eighth rows, respectively. In fact

$$\begin{aligned}
&n_2(m_{31},...,m_{3j},...,m_{38}) - n_1(m_{61},...,m_{6j},...,m_{68}) = 0,\\
&n_2(m_{41},...,m_{4j},...,m_{48}) - n_1(m_{71},...,m_{7j},...,m_{78}) = 0,\\
&n_2(m_{51},...,m_{5j},...,m_{58}) - n_1(m_{81},...,m_{8j},...,m_{88}) = 0.
\end{aligned}$$

   Therefore, the rank is not greater than six. Moreover, the determinant of the minor of order four obtained by eliminating the last four rows and the last four columns is equal to

$$\frac{1}{16}\frac{{n_1}^4\left(J_1J_3 - {J_2}^2\right)^2}{\pi^4\hbar^8}$$

   which is different from zero because we have previously proved that the quantity $J_1J_3 - {J_2}^2$ is positive. Therefore, apart from the case $\frac{\partial}{\partial\lambda}(nF_{11}^{(k)}) = \frac{\partial}{\partial\lambda}(nF_{22}^{(k)}) = 0$, $k = 1,2$, the rank of $M(0)$ is four. From a direct verification, the expressions $\frac{\partial}{\partial\lambda}(nF_{11}^{(k)})$ and $\frac{\partial}{\partial\lambda}(nF_{22}^{(k)})$, $k = 1,2$, obtained with MEP, are different from zero. Therefore the rank of $M(0)$ is always four.

2. Case $\mu = \frac{\sqrt{2}}{2}v_F$.

   By taking into account the fact that $nF_{11}^{(k)} = nF_{22}^{(k)}$, $k = 1,2$, from the definition of J_n it follows that the third row of the matrix $M(\frac{\sqrt{2}}{2}v_F)$ is a linear combination of the first and sixth rows while the fourth is a linear combination of the second and seventh ones. In fact one has

$$\begin{aligned}
&n_1(m_{31},...,m_{3j},...,m_{38}) + \mu(m_{11},...,m_{1j},...,m_{18}) + n_2(m_{61},...,m_{6j},...,m_{68}) = 0,\\
&n_1(m_{41},...,m_{4j},...,m_{48}) + \mu(m_{21},...,m_{2j},...,m_{28}) + n_2(m_{71},...,m_{7j},...,m_{78}) = 0.
\end{aligned}$$

Moreover, the determinant of the sub-matrix obtained by eliding the first two rows and the first two columns is

$$\frac{1}{512}\frac{v^6\left(J_1J_3J_5-J_1{J_4}^2+2J_2J_4J_3-{J_2}^2J_5-{J_3}^3\right)^2}{\pi^6h^{12}},$$

which is different from zero because the matrix of C of theorem 4.1 is positive definite. Therefore the rank of $M(\frac{\sqrt{2}}{2}v_F)$ is six.

3. Case $\mu=-\frac{\sqrt{2}}{2}v_F$. The same considerations of the previous case hold.

□

4.3.2 Numerical results of 8 moments model

As already done for the previous model, to assess the validity of the model, we consider the case of pristine suspended graphene under the effect of a constant electric field $\mathbf{E}$. The evolution equations are reduced to a system of Ordinary Differential Equations (ODE's). The only significant component of each equation is that along the direction of $\mathbf{E}$. Therefore, the evolution equations read

$$\frac{d}{dt}n=0, \tag{4.60}$$

$$\frac{d}{dt}(n\,W)=-q\,n\,\mathbf{E}\cdot\mathbf{V}+n\,C_W, \tag{4.61}$$

$$\frac{d}{dt}(n\,\mathbf{V})=-q\,n\,\mathbf{G}^{(0)}:\mathbf{E}+n\,C_{\mathbf{V}}, \tag{4.62}$$

$$\frac{d}{dt}(n\,\mathbf{S})=-q\,n\,\mathbf{G}^{(1)}:\mathbf{E}+n\,C_{\mathbf{S}}, \tag{4.63}$$

$$\frac{d}{dt}(n\,\mathbf{S}^{(2)})=-q\,n\,\mathbf{G}^{(2)}:\mathbf{E}+n\,C^{(2)}_{\mathbf{S}}. \tag{4.64}$$

We assume initially thermodynamic equilibrium and the results are plotted in Fig.s 4.4, 4.5 for Fermi energy 0.4 eV and in Fig.s 4.10, 4.11 for Fermi energy 0.6 eV. We have compared the results obtained with the 8-moment model (8MM) presented in this section with those obtained with the 6-moment model (6MM) in [12]. As reference solutions we have taken those given by a direct numerical integration of the Boltzmann equation with the Discontinuous Galerkin approach proposed in [15, 61].

For low electric fields the velocity predicted by 6MM is more accurate than that obtained with 8MM. In the presence of higher electric fields, the difference between 6MM and 8MM is smaller but in any case 6MM performs better or no worse than 8MM. Differences are smaller in energy but again 6MM reveals no worse than 8MM. These considerations do not depend on the Fermi energy. Moreover, the hydrodynamic results systematically overestimate those obtained by the direct solution of the Boltzmann equation. It is likely that this effect is due to an underestimation of the dissipative character of the collision terms.

It is clear that the inclusion of the variable $\mathbf{S^{(2)}}$ does not improve the model. We have tried to get better results by adding further moments like $\mathbf{S^{(3)}}$ and $\mathbf{S^{(4)}}$ but from a qualitative point of view no real improvements are obtained. There is a strong numerical evidence that increasing the hierarchy of the field variables with additional terms of the type

$$n\,\mathbf{S^{(N)}} = \frac{2}{(2\pi)^2}\int_{\mathbb{R}^2} f(\mathbf{r},\mathbf{k},t)\mathscr{E}^N\mathbf{v}d\mathbf{k},$$

with N a positive integer, is not promising.

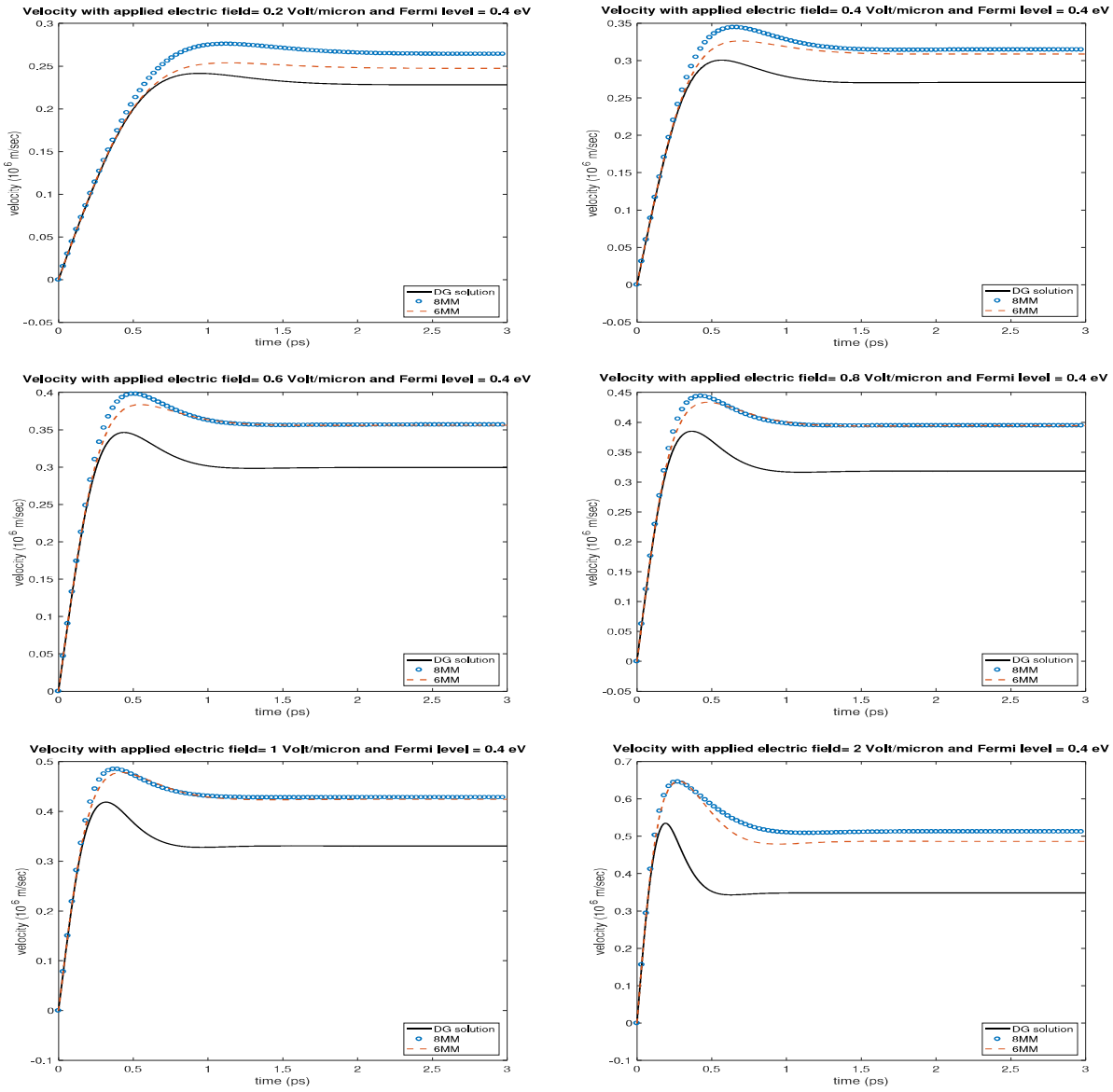

Figure 4.4: Comparison of the average velocity obtained with a direct solution of the Boltzmann equation (DG method) (continuous line), the 8MM (circled line) and the 6MM (dashed lines) for electric fields $E = 2$ kV/cm, $E = 4$ kV/cm, $E = 6$ kV/cm, $E = 8$ kV/cm, $E = 10$ kV/cm, $E = 20$ kV/cm by considering a constant lattice temperature of 300 K and a Fermi energy equal to 0.4 eV.

In summary a hydrodynamic model for charge transport in graphene has been presented trying to improve the results in [12] with the inclusion of additional moments related to quadratic power of energy. In pristine graphene, the numerical solutions given by such a model have been compared with those of the semiclassical Boltzmann equation obtained by a DG method. Apparently no real improvement is achieved with respect to the model in [12]. Therefore, the formulation of models more accurate than that in [12] has to be based on a different set of weight

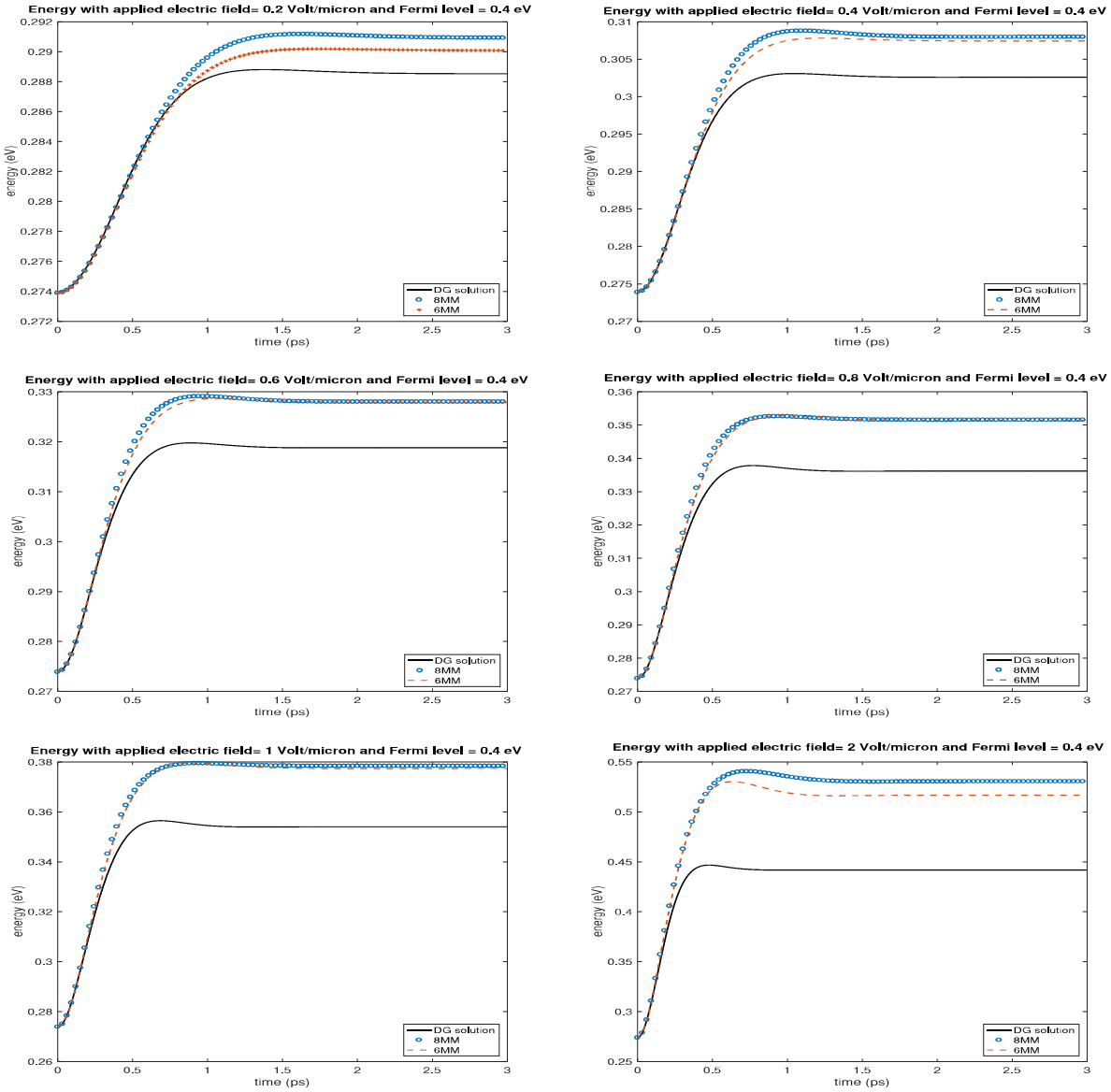

Figure 4.5: Comparison of the average energy obtained with a direct solution of the Boltzmann equation (DG method) (continuous line), the 8MM (circled line) and the 6MM (dashed lines) for electric fields $E = 2$ kV/cm, $E = 4$ kV/cm, $E = 6$ kV/cm, $E = 8$ kV/cm, $E = 10$ kV/cm, $E = 20$ kV/cm by considering a constant lattice temperature of 300 K and a Fermi energy equal to 0.4 eV.

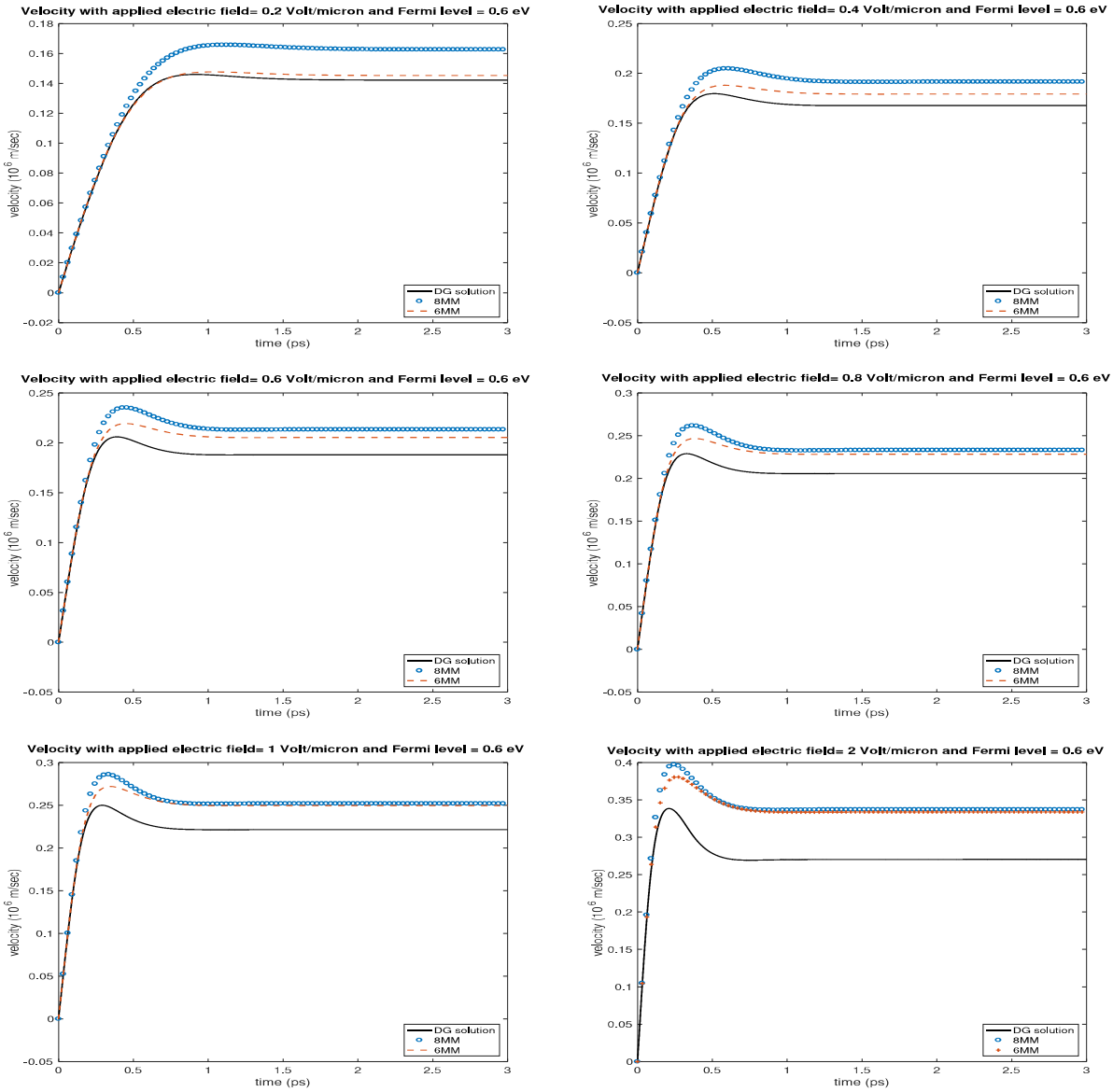

Figure 4.6: Comparison of the average velocity obtained with a direct solution of the Boltzmann equation (DG method) (continuous line), the 8MM (circled line) and the 6MM (dashed lines) for electric fields $E = 2$ kV/cm, $E = 4$ kV/cm, $E = 6$ kV/cm, $E = 8$ kV/cm, $E = 10$ kV/cm, $E = 20$ kV/cm by considering a constant lattice temperature of 300 K and a Fermi energy equal to 0.6 eV.

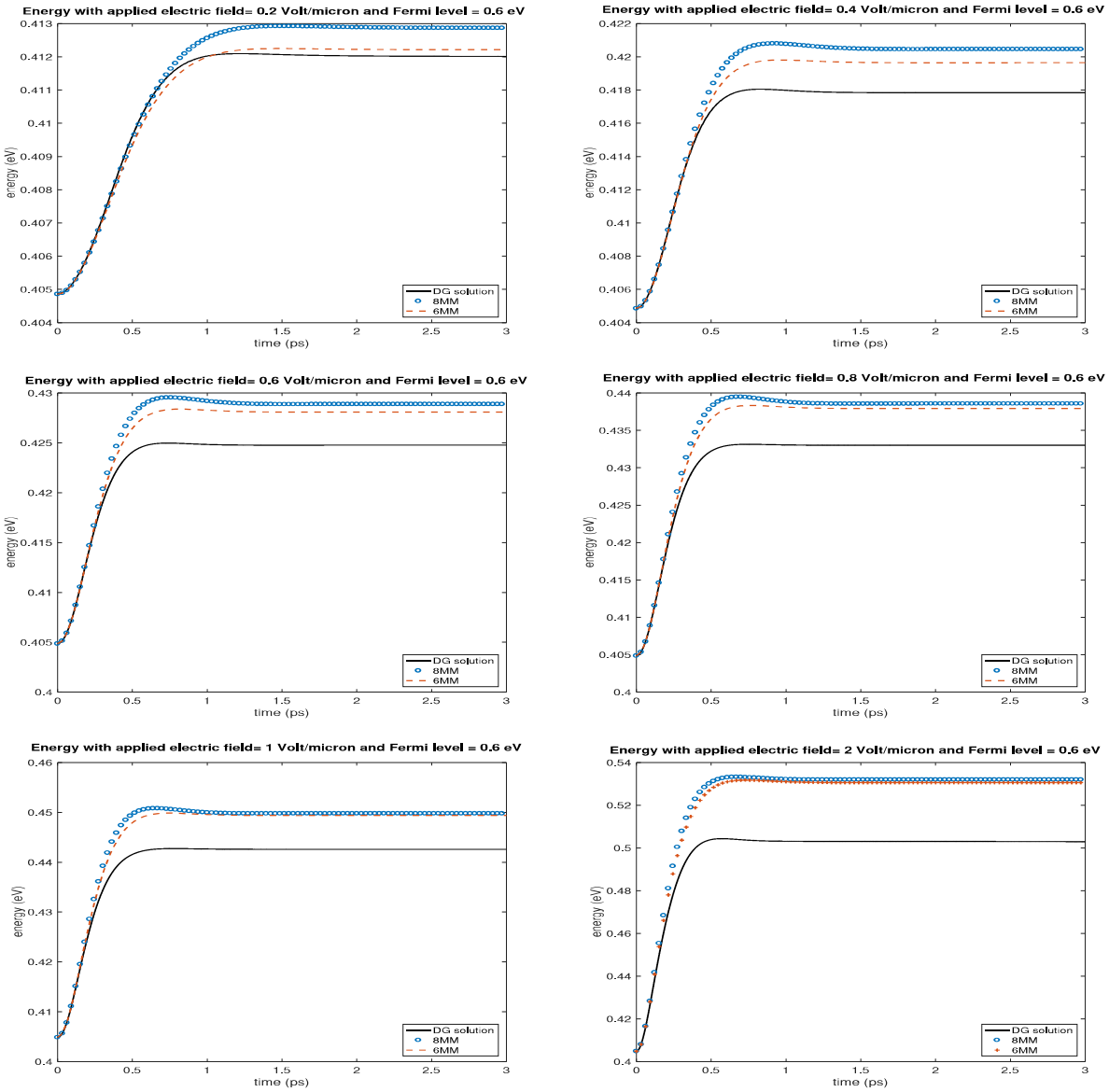

Figure 4.7: Comparison of the average energy obtained with a direct solution of the Boltzmann equation (DG method) (continuous line), the 8MM (circled line) and the 6MM (dashed lines) for electric fields $E = 2$ kV/cm, $E = 4$ kV/cm, $E = 6$ kV/cm, $E = 8$ kV/cm, $E = 10$ kV/cm, $E = 20$ kV/cm by considering a constant lattice temperature of 300 K and a Fermi energy equal to 0.6 eV.

function, for example including higher-order terms in the velocity as will be shown in the next section.

4.4 The case of moments based on velocity powers

In this section a new 8-moment model based on MEP is obtained by adding a further field variable representing the average value of the tensorial product of the microscopic velocity. Let us consider the weight functions $\{1, \mathscr{E}, \mathbf{v}, \mathscr{E}\mathbf{v}, \mathbf{v}\otimes\mathbf{v}\}$ to which the following average quantities correspond

$$n = \frac{2}{(2\pi)^2}\int_{\mathbb{R}^2} f(\mathbf{r},\mathbf{k},t)d\mathbf{k}, \tag{4.65}$$

$$nW = \frac{2}{(2\pi)^2}\int_{\mathbb{R}^2} f(\mathbf{r},\mathbf{k},t)\mathscr{E}d\mathbf{k}, \tag{4.66}$$

$$n\mathbf{V} = \frac{2}{(2\pi)^2}\int_{\mathbb{R}^2} f(\mathbf{r},\mathbf{k},t)\mathbf{v}d\mathbf{k}, \tag{4.67}$$

$$n\mathbf{S} = \frac{2}{(2\pi)^2}\int_{\mathbb{R}^2} f(\mathbf{r},\mathbf{k},t)\mathscr{E}\mathbf{v}d\mathbf{k}, \tag{4.68}$$

$$n\mathbf{T} = \frac{2}{(2\pi)^2}\int_{\mathbb{R}^2} f(\mathbf{r},\mathbf{k},t)\mathbf{v}\otimes\mathbf{v}d\mathbf{k}, \tag{4.69}$$

where the new field $\mathbf{T}$ is the stress tensor.

To have the independent field variables, since the trace of $n\mathbf{T}$ is given by nv_F^2, we consider its deviatoric part

$$n\mathbf{D} = \frac{2}{(2\pi)^2}\int_{\mathbb{R}^2} f(\mathbf{r},\mathbf{k},t)\mathbf{v}\otimes\mathbf{v}d\mathbf{k} - \frac{1}{2}nv_F^2\mathbf{I}, \tag{4.70}$$

where $\mathbf{I}$ is the identity tensor. It is enough to consider the evolution of the components nD_{11} and nD_{12} because $nD_{11} + nD_{22} = 0$.

The balance equations are now

$$\frac{\partial}{\partial t}n + \nabla_{\mathbf{r}}(n\mathbf{V}) = nC_n, \tag{4.71}$$

$$\frac{\partial}{\partial t}nW + \nabla_{\mathbf{r}}(n\mathbf{S}) + qn\mathbf{E}\cdot\mathbf{V} = nC_W, \tag{4.72}$$

$$\frac{\partial}{\partial t}n\mathbf{V} + \nabla_{\mathbf{r}}(n\mathbf{F}^{(0)}) + qn\mathbf{G}^{(0)}:\mathbf{E} = nC_{\mathbf{V}}, \tag{4.73}$$

$$\frac{\partial}{\partial t}n\mathbf{S} + \nabla_{\mathbf{r}}(n\mathbf{F}^{(1)}) + qn\mathbf{G}^{(1)}:\mathbf{E} = nC_{\mathbf{S}}, \tag{4.74}$$

$$\frac{\partial}{\partial t}n\mathbf{D} + \nabla_{\mathbf{r}}(n\mathbf{H}^{(0)}) + qn\mathbf{L}^{(0)}:\mathbf{E} = nC_{\mathbf{D}}, \tag{4.75}$$

where

$$
\begin{aligned}
n\mathbf{F}^{(0)} &= \frac{2}{(2\pi)^2}\int_{\mathbb{R}^2}\mathbf{v}\otimes\mathbf{v}f(\mathbf{r},\mathbf{k},t)d\mathbf{k},\\
n\mathbf{F}^{(1)} &= \frac{2}{(2\pi)^2}\int_{\mathbb{R}^2}\mathscr{E}\mathbf{v}\otimes\mathbf{v}f(\mathbf{r},\mathbf{k},t)d\mathbf{k},\\
n\mathbf{H}^{(0)} &= \frac{2}{(2\pi)^2}\int_{\mathbb{R}^2}\mathbf{v}\otimes\left(\mathbf{v}\otimes\mathbf{v}-\frac{1}{2}v_F^2\mathbf{I}\right)f(\mathbf{r},\mathbf{k},t)d\mathbf{k}=\frac{2}{(2\pi)^2}\int_{\mathbb{R}^2}\mathbf{v}\otimes\mathbf{v}\otimes\mathbf{v}f(\mathbf{r},\mathbf{k},t)d\mathbf{k}\\
&\quad -\frac{1}{2}v_F^2 n\mathbf{V}\otimes\mathbf{I},\\
n\mathbf{G}^{(0)} &= \frac{2}{\hbar(2\pi)^2}\int_{\mathbb{R}^2}f(\mathbf{r},\mathbf{k},t)\nabla_{\mathbf{k}}\mathbf{v}(\mathbf{k})d\mathbf{k},\\
n\mathbf{G}^{(1)} &= \frac{2}{\hbar(2\pi)^2}\int_{\mathbb{R}^2}f(\mathbf{r},\mathbf{k},t)\nabla_{\mathbf{k}}(\mathscr{E}(\mathbf{k})\mathbf{v}(\mathbf{k}))d\mathbf{k},\\
n\mathbf{L}^{(0)} &= \frac{2}{\hbar(2\pi)^2}\int_{\mathbb{R}^2}f(\mathbf{r},\mathbf{k},t)\nabla_{\mathbf{k}}(\mathbf{v}\otimes\mathbf{v})d\mathbf{k},
\end{aligned}
$$

and similar definitions for the production terms.

Also in this case, the production terms are given by summing the contributions from the different types of phonon scattering

$$C_M = C_M^{(ac)} + \sum_{s=LO,TO,K} C_M^{(s)}$$

with $M = n, W, \mathbf{V}, \mathbf{S}, \mathbf{D}$.

The MEP distribution function corresponding to the previous choice of weight functions is given by

$$f_{MEP}(\mathbf{r},\mathbf{k},t) = \frac{1}{1+\exp(\lambda+\lambda_w\mathscr{E}+(\lambda_{\mathbf{V}}+\mathscr{E}\lambda_{\mathbf{S}})\cdot\mathbf{v}+\sum_{i,j=1}^{2}\lambda_{ij}(v_iv_j-\frac{1}{2}v_F^2\delta_{ij}))}, \tag{4.76}$$

where v_i are the components of $\mathbf{v}$.

On account of the symmetry of tensor $\mathbf{D}$, $\lambda_{ij} = \lambda_{ji}$. Moreover, it is convenient to introduce $\lambda_D = \lambda_{11} - \lambda_{22}$ and consider as independent components λ_D and λ_{12} by taking into account that $\mathbf{D}$ is traceless.

In view of the numerical application, we evaluate the closure relations according to the hypothesis that $\lambda_{\mathbf{V}}$, $\lambda_{\mathbf{S}}$ are parallel. This holds true in the case of 1D problems as we will consider in the next section. For the sake of better readability, non-linear closure relations are summarized in Appendix D.1.

4.4.0.1 Numerical results

We again consider the 1D case. Let us introduce the field variables

$$\mathbf{U} = (n, nW, nD_{11}, nD_{12}, nV, nS)^T$$

and the relative Lagrange multipliers $\mathbf{\Lambda} = (\lambda, \lambda_w, \lambda_D, \lambda_{12}, \lambda_V, \lambda_S)^T$ where V and S are the significant components of $\mathbf{V}$ and $\mathbf{S}$ and D_{11} and D_{12} the significant components of the tensor $\mathbf{D}$. Moreover, let us denote by B the Jacobian matrix

$$B = \frac{\partial(n, nW, nD_{11}, nD_{12}, nV, nS)}{\partial(\lambda, \lambda_w, \lambda_D, \lambda_{12}, \lambda_V, \lambda_S)}. \tag{4.77}$$

From general theory it follows that B is invertible and the evolution equations can be written in the form

$$\frac{d}{dt}\mathbf{U} = -qn \begin{pmatrix} 0 \\ V \\ L_{11}^{(0)} \\ L_{12}^{(0)} \\ G^{(0)} \\ G^{(1)} \end{pmatrix} E + n\mathbf{C} \tag{4.78}$$

where $\mathbf{C} = (C_n, C_W, C_{D_{11}}, C_{D_{12}}, C_V, C_S)^T$.
If we introduce the quantity $\mathscr{G}$:

$$\mathscr{G} = -qn \begin{pmatrix} 0 \\ V \\ L_{11}^{(0)} \\ L_{12}^{(0)} \\ G^{(0)} \\ G^{(1)} \end{pmatrix} E + n\mathbf{C},$$

we have

$$\frac{d}{dt}\mathbf{\Lambda} = B^{-1}\mathscr{G}. \tag{4.79}$$

We compare the results obtained by the 8-moment model (8MM) with those obtained by the direct solution of the transport equation through the DG method and we also include the results obtained by the linearized version (L8MM) deduced by linearizing the MEP distribution function as follows [5]

$$f_{MEP}(\mathbf{r}, \mathbf{k}, t) \approx f^{(i)} + f^{(a)}, \tag{4.80}$$

where

$$f^{(i)} = \frac{1}{1 + e^{\lambda + \lambda_w \mathscr{E}}},\ f^{(a)} = -\frac{e^{\lambda + \lambda_w \mathscr{E}}}{(1 + e^{\lambda + \lambda_w \mathscr{E}})^2} \left[(\lambda_{\mathbf{v}} + \mathscr{E}\lambda_{\mathbf{S}}) \cdot \mathbf{v} + \sum_{i,j=1}^{2} \lambda_{ij} \left(v_i v_j - \frac{1}{2} v_F^2 \delta_{ij} \right) \right].$$

For clarity, the closure relations obtained by adopting the previous distribution function are postponed to Appendix D.2.

The results are plotted in Figs. 4.8, 4.9 for Fermi energy 0.4 eV and in Figs. 4.10, 4.11 for Fermi energy 0.6 eV. The improvement, compared to the previous models, is evident. A significant

[5] In the one dimensional case $\lambda_{12} = 0$.

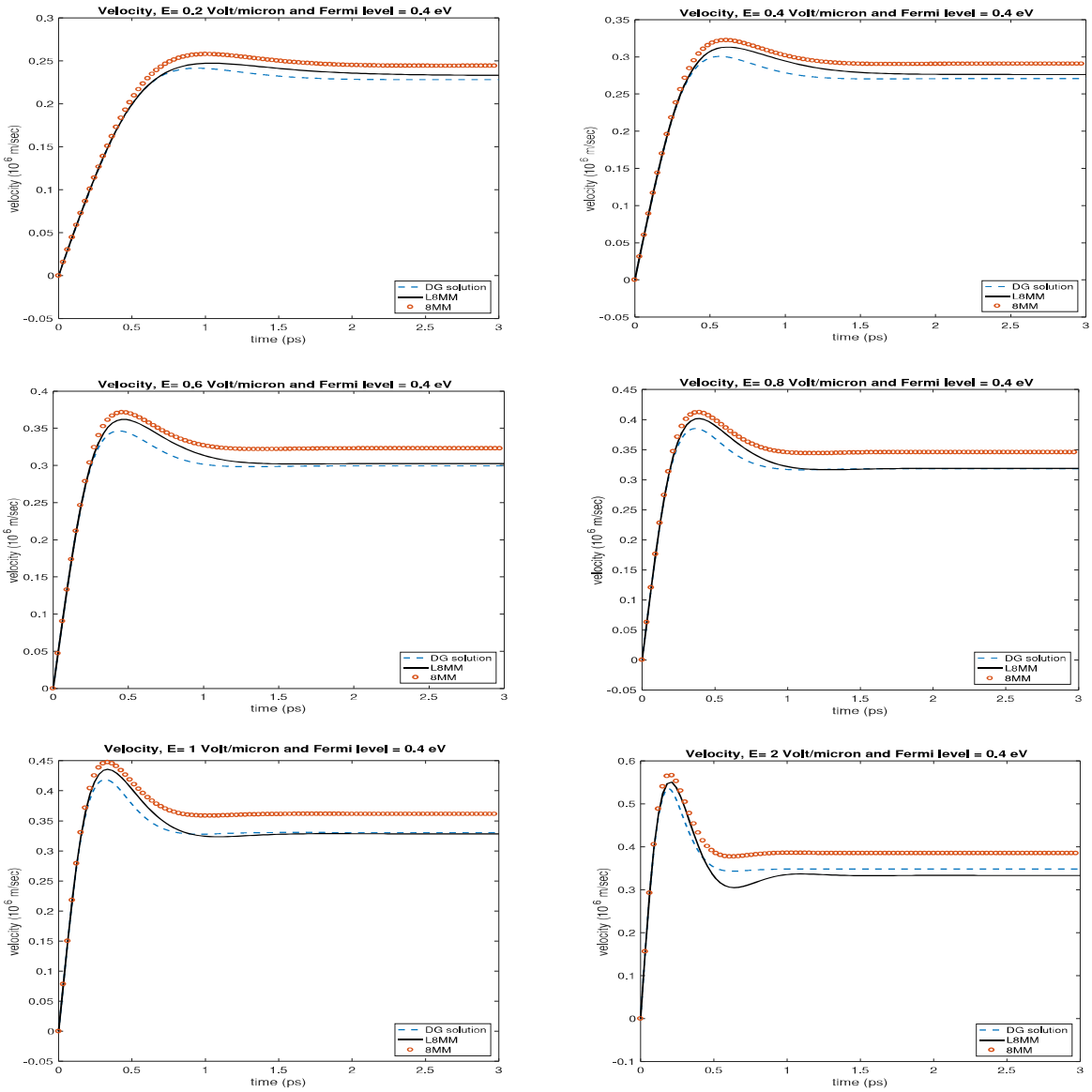

Figure 4.8: Comparing the average velocity obtained with a direct solution of the Boltzmann equation (DG method) (dashed lines), the 8MM (circles lines) and its linearized version (L8MM) (continuous line) for electric fields $E = 2$ kV/cm, $E = 4$ kV/cm, $E = 6$ kV/cm, $E = 8$ kV/cm, $E = 10$ kV/cm, $E = 20$ kV/cm by considering a constant lattice temperature of 300 K and a Fermi energy equal to 0.4 eV.

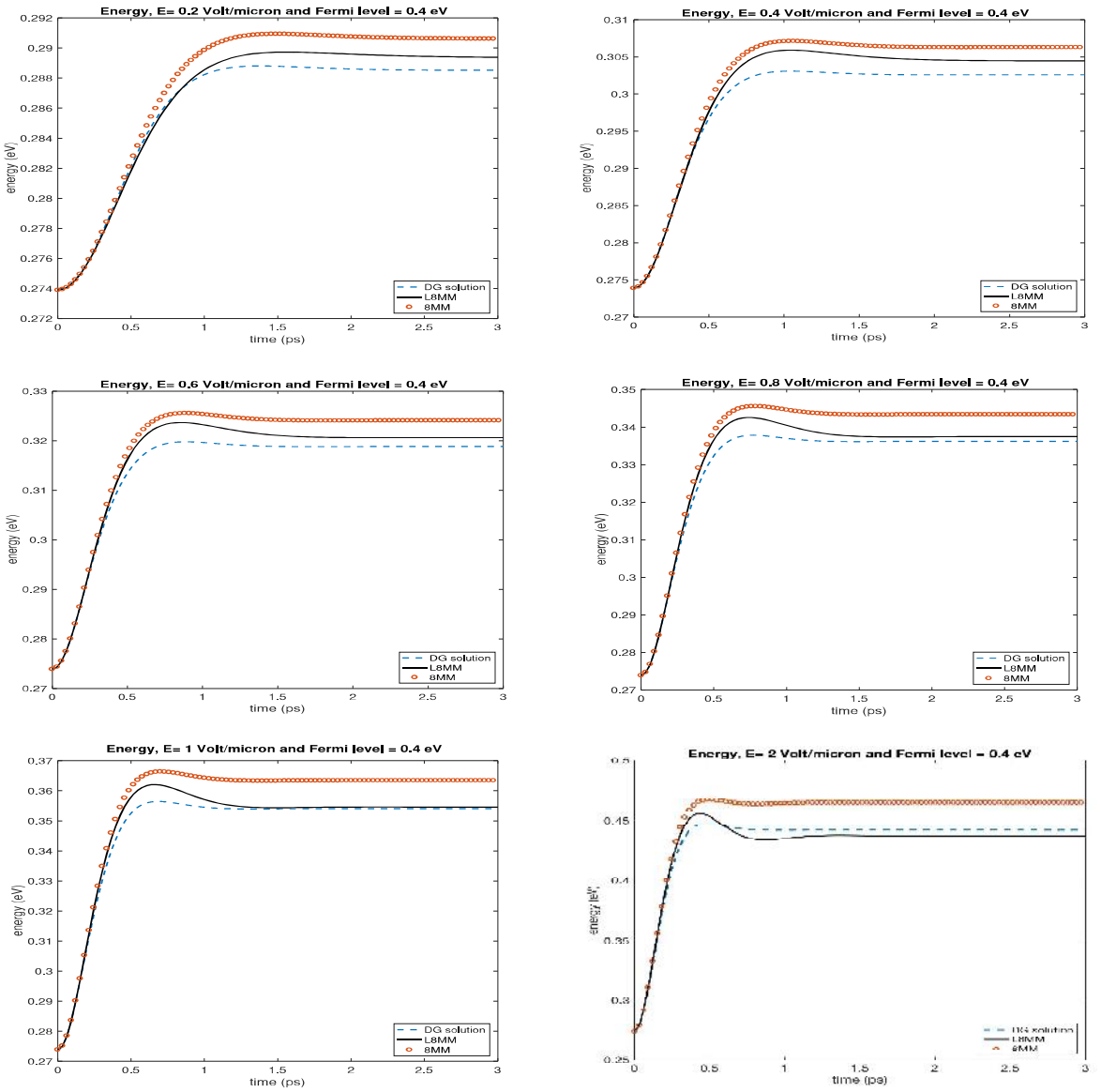

Figure 4.9: Comparing the average energy obtained with a direct solution of the Boltzmann equation (DG method) (dashed lines), the 8MM (circles lines) and its linearized version (L8MM) (continuous line) for electric fields $E = 2$ kV/cm, $E = 4$ kV/cm, $E = 6$ kV/cm, $E = 8$ kV/cm, $E = 10$ kV/cm, $E = 20$ kV/cm by considering a constant lattice temperature of 300 K and a Fermi energy equal to 0.4 eV.

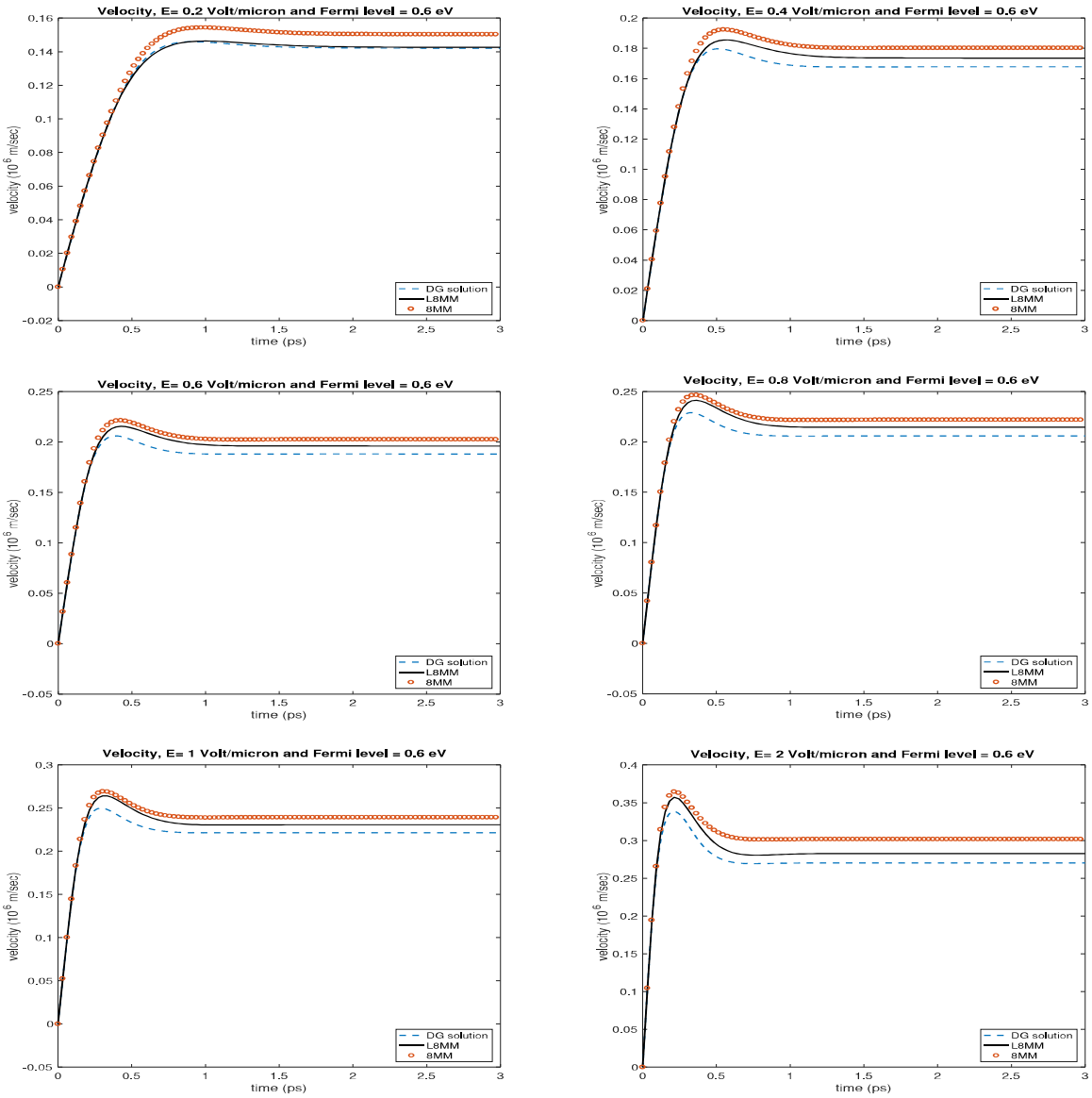

Figure 4.10: Comparing the average velocity obtained with a direct solution of the Boltzmann equation (DG method) (dashed lines), the 8MM (circles lines) and its linearized version (L8MM) (continuous line) for electric fields $E = 2$ kV/cm, $E = 4$ kV/cm, $E = 6$ kV/cm, $E = 8$ kV/cm, $E = 10$ kV/cm, $E = 20$ kV/cm by considering a constant lattice temperature of 300 K and a Fermi energy equal to 0.6 eV.

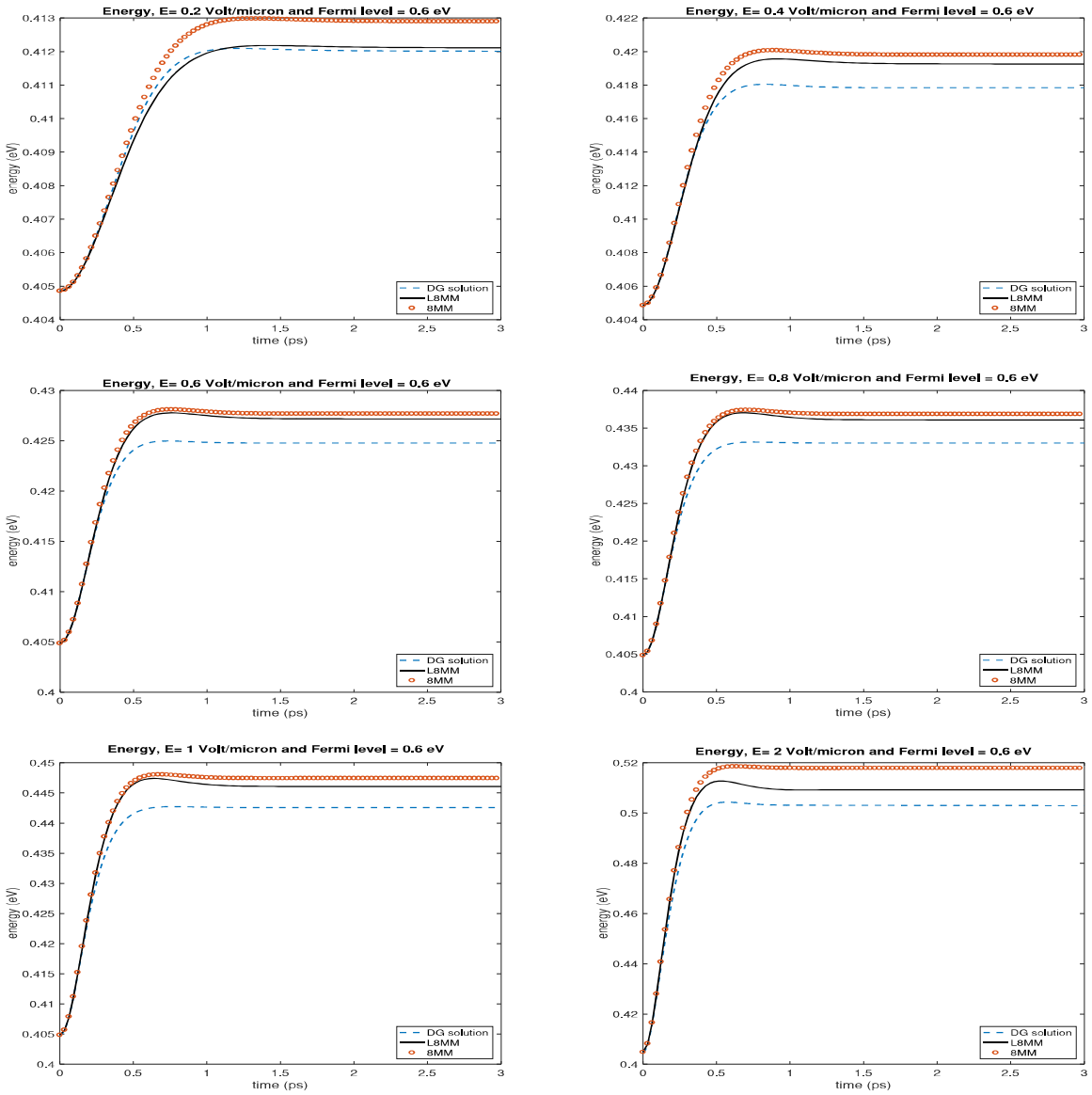

Figure 4.11: Comparing the average energy obtained with a direct solution of the Boltzmann equation (DG method) (dashed lines), the 8MM (circles lines) and its linearized version (L8MM) (continuous line) for electric fields $E = 2$ kV/cm, $E = 4$ kV/cm, $E = 6$ kV/cm, $E = 8$ kV/cm, $E = 10$ kV/cm, $E = 20$ kV/cm by considering a constant lattice temperature of 300 K and a Fermi energy equal to 0.6 eV.

point is that the non-linear model again does not present better performance compared to the linear one. At higher Fermi energy the agreement is better.

As expected, at low electric fields the difference between 8MM and L8MM is slight. At higher electric fields L8MM is more accurate. Apparently, L8MM can be considered a good compromise to reasonably simulate charge transport in graphene by a hydrodynamic model. Of course, additional tensorial quantities of higher order in the velocity could be added but we believe that L8MM presented above is already a good model from a computational point of view. A very high number of field variables increases computational complexity and a hydrodynamic model is viable only if the numerical effort for integrating it remains appreciably lower than that required for the original transport equation.

The last important issue is that in the general non-linear case the hyperbolicity of the model is assured while in the linearized version it must be checked. A good model should have a wide enough hyperbolicity region to cover the physically significant part of the field variable domain. Hence, let us analyze the hyperbolicity condition in the linear 1D case.

Denoting the spatial variable by x, the evolution equations become

$$\mathscr{A}_0 \frac{\partial \Lambda}{\partial t} + \mathscr{A} \frac{\partial \Lambda}{\partial x} = \mathscr{G} \tag{4.81}$$

where

$$\begin{aligned} \mathscr{A}_0 &= \nabla_\Lambda \mathscr{F}_0 \quad \text{with} \quad \mathscr{F}_0 = (n, nW, nD_{11}, nV, nS)^T \\ \mathscr{A} &= \nabla_\Lambda \mathscr{F}_1 \quad \text{with} \quad \mathscr{F}_1 = (nV, nS, nH_{111}, nF_{11}^{(0)}, nF_{11}^{(1)})^T. \end{aligned}$$

By setting

$$\begin{aligned} J_n(\lambda, \lambda_w) &= \int_0^{+\infty} \frac{\mathscr{E}^n e^{\lambda + \lambda_w \mathscr{E}}}{(1 + e^{\lambda + \lambda_w \mathscr{E}})^2} d\mathscr{E}, \\ K_n(\lambda, \lambda_w) &= \int_0^{+\infty} \frac{\mathscr{E}^n e^{\lambda + \lambda_w \mathscr{E}}}{(1 + e^{\lambda + \lambda_w \mathscr{E}})^2} - 2 \int_0^{+\infty} \frac{\mathscr{E}^n e^{2(\lambda + \lambda_w \mathscr{E})}}{(1 + e^{\lambda + \lambda_w \mathscr{E}})^3} d\mathscr{E}, \end{aligned}$$

explicitly $\mathscr{A}_0$ reads

$$\mathscr{A}_0 = \begin{pmatrix} -\frac{1}{\pi\hbar^2 v_F^2} J_1(\lambda, \lambda_w) & -\frac{1}{\pi\hbar^2 v_F^2} J_2(\lambda, \lambda_w) & 0 & 0 & 0 \\ -\frac{1}{\pi\hbar^2 v_F^2} J_2(\lambda, \lambda_w) & -\frac{1}{\pi\hbar^2 v_F^2} J_3(\lambda, \lambda_w) & 0 & 0 & 0 \\ -\frac{v_F^2}{8\pi\hbar^2} \lambda_D K_1(\lambda, \lambda_w) & -\frac{v_F^2}{8\pi\hbar^2} \lambda_D K_2(\lambda, \lambda_w) & -\frac{v_F^2}{8\pi\hbar^2} J_1(\lambda, \lambda_w) & 0 & 0 \\ \frac{\partial nV_1}{\partial \lambda} & \frac{\partial nV_1}{\partial \lambda_w} & 0 & -\frac{1}{2\pi\hbar^2} J_1(\lambda, \lambda_w) & -\frac{1}{2\pi\hbar^2} J_2(\lambda, \lambda_w) \\ \frac{\partial nS_1}{\partial \lambda} & \frac{\partial nS_1}{\partial \lambda_w} & 0 & -\frac{1}{2\pi\hbar^2} J_2(\lambda, \lambda_w) & -\frac{1}{2\pi\hbar^2} J_3(\lambda, \lambda_w) \end{pmatrix}. \tag{4.82}$$

Omitting the dependence on Lagrangian multipliers λ and λ_w for simplicity, we can factorize the determinant of $\mathscr{A}_0$ as

$$\det(\mathscr{A}_0) = -\frac{1}{v_F^2} \left(\frac{1}{2\pi\hbar^2} \right)^5 J_1 \left(J_1 J_3 - J_2^2 \right)^2.$$

Since $J_1 > 0$ and

$$\begin{pmatrix} J_1 & J_2 \\ J_2 & J_3 \end{pmatrix}$$

is positive definite, it follows that $\det(\mathscr{A}_0) < 0$ for any value of the fields. The eigenvalue equation

$$\det\left(\mu\mathscr{A}_0 - \mathscr{A}\right) = 0$$

has the following roots:

$$\mu_1 = 0, \mu_{2,3} = \pm\frac{\sqrt{3}}{2}v_F,$$
$$\mu_{4,5} = \pm\frac{1}{4}\frac{\sqrt{2}\,v_F}{\sqrt{J_1\left(J_1J_3 - {J_2}^2\right)}}\sqrt{{v_F}^2\lambda_D\left(K_3J_1^2 + K_1J_2^2 - 2J_1J_2K_2\right) + 4J_1\left(J_1J_3 - {J_2}^2\right)}.$$

The eigenvalues are all real if and only if the quantity

$$g = {v_F}^2\lambda_D\left(K_3J_1^2 + K_1J_2^2 - 2J_1J_2K_2\right) + 4J_1\left(J_1J_3 - {J_2}^2\right)$$

is non negative.

The high non-linearity of such an expression makes it very difficult to prove analytically that these eigenvalues are real for all significant values of the field variables. To estimate this, we evaluated the function g and found that it is always positive along the solutions of Figs. 4.8-4.11. Moreover the eigenvalues are distinct; in fact with a very good approximation $\mu_{4,5} \approx \pm\frac{\sqrt{2}}{2}v_F$. This is a strong index of the hyperbolicity of the L8MM at least in the simulated cases.

CHAPTER 5

QUANTUM CORRECTED HYDRODYNAMIC MODELS

Introduction

Nanoscale semiconductor devices are playing an increasingly important role in advanced microelectronic applications, including multiple-state logic and memory devices. Therefore, in modeling and simulations of semiconductor devices of ultra-small size (say nano-size) in a strong electric field, quantum mechanical effects have to be taken into account. Graphene, consisting of an isolated single atomic layer of graphite, is an ideal candidate for the channel of ultimate scaled electron devices.

In this Chapter, based on [36] by L.Luca and V.Romano, the typical physical situation we want to describe is the case when the main contribution to the charge transport can be considered semiclassical while the quantum effects can be assumed to enter as small perturbations. For example, this is reasonable for devices like MOSFETs of characteristic length of about ten nanometers under the effect of strong electric fields.

To take into account quantum phenomena, the semiclassical Boltzmann equation is not enough to describe charge transport. As a starting point for deriving of the quantum corrections to the semiclassical model, we consider the Wigner equation. At zero order we recover the semiclassical models developed in [12, 34, 35, 45] by exploiting the Maximum Entropy Principle (MEP). By following the idea developed in [58] for silicon, $\hbar^2$ order corrections are obtained from the scaling of high field and collision dominated regime. In the limit of high collisional frequency of the quantum correction to the collision operator, this is equivalent to determine the $\hbar^2$ order corrections with the equilibrium Wigner function, similarly to what done in [19]. The problem to find out the equilibrium Wigner function in the case of an arbitrary energy band has been discussed in [60] where the corresponding Bloch equation is written and solved for sil-

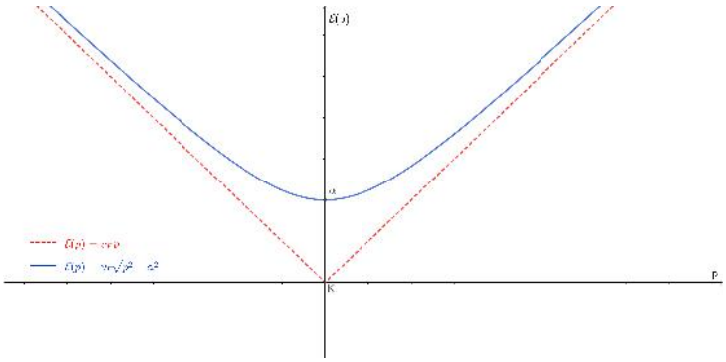

Figure 5.1: Qualitative behaviour of the energy dispersion relation.

icon in the Kane dispersion relation approximation. Here the same approach is used for graphene.

One important issue is related to the conical shape of the energy band around the Dirac points of the first Brillouin zone. This fact makes singular some term of the expansion if a sharp zero gap between the conduction and the valence band is assumed. However, see for example [13], from a theoretical point of view it is possible the presence, although very small, of a gap which is related to the first and second neighbourd hopping energy. Therefore, around the Dirac points we employ a regularized energy band. Explicit formulas are obtained and the resulting model is given by a set of dispersive PDEs.

Other approaches for formulating quantum hydrodynamic models can be found for example in [3, 4, 46, 47] where asymptotic expansions, like the Chapman-Enskog one, are employed along with a quantum version of MEP. Of course it is also possile to try to numerically solve directly the Wigner equation but major computational difficulties arise and at the present time it seems far from being a standard feasible tool for the design of electron devices. The interested reader can see the monograph [56] and the paper [15, 50, 61] for recent advances of the algoritms in stochastic approaches.

In this Chapter explicit result for a quantum corrected six moment model are obtained and a preliminary analysis of the mathematical structure of the model is performed. Some details are postponed in the Appendix E. To develop this model t' must not be neglected, hence the symmetry between the valence and the conduction bands is broken and a gap appears. To take into account such an effects but still retaining an analytical expression useful for the purposes of devising hydrodynamic models, we modify the gapless expression of the dispersion relation and adopt the following regularization (see Fig. 5.1)

$$\mathscr{E}(p) \approx v_F \sqrt{p^2 + \alpha^2},$$

where α is a small parameter related to the nearest-neighbour and next nearest-neighbour hopping energies and p is the modulus of the crystal momentum $\mathbf{p} = \hbar\mathbf{k}$. Hence, the components

of the electron velocity $\mathbf{v}$ are given by

$$v_i = \frac{\partial \mathscr{E}}{\partial p_i} \approx v_F \frac{p_i}{\sqrt{p^2+\alpha^2}}$$

and the higher-order derivatives are approximated in the following way

$$\frac{\partial^2 \mathscr{E}(p)}{\partial p_i \partial p_j} \approx v_F \left(-\frac{p_i p_j}{(p^2+\alpha^2)^{3/2}} + \frac{\delta_{ij}}{\sqrt{p^2+\alpha^2}} \right),$$

$$\frac{\partial^3 \mathscr{E}(p)}{\partial p_i \partial p_j \partial p_k} \approx v_F \left(-\frac{1}{(p^2+\alpha^2)^{3/2}} \left(p_i \delta_{jk} + p_j \delta_{ik} + p_k \delta_{ij} \right) + 3 \frac{p_i p_j p_k}{(p^2+\alpha^2)^{5/2}} \right),$$

$$\frac{\partial^4 \mathscr{E}(p)}{\partial p_i \partial p_j \partial p_k \partial p_l} \approx v_F \left(\frac{3}{(\alpha^2+p^2)^{5/2}} (p_i p_l \delta_{jk} + p_j p_l \delta_{ik} + p_k p_l \delta_{ij} + \delta_{il} p_j p_k + \delta_{jl} p_i p_k + \delta_{kl} p_i p_j) - \right.$$

$$\left. - \frac{1}{(\alpha^2+p^2)^{3/2}} (\delta_{il}\delta_{jk} + \delta_{jl}\delta_{ik} + \delta_{lk}\delta_{ij}) - 15 \frac{p_i p_j p_k p_l}{(\alpha^2+p^2)^{7/2}} \right),$$

where δ_{ij} is the Kronecker delta.
Note that if $\alpha \neq 0$ the modulus v of the velocity is no longer constant and electrons don't behave as massless Dirac fermions.

5.1 Derivation of Quantum corrected hydrodynamic model

Let us introduce the single-particle density matrix, $\rho(\mathbf{r},\mathbf{s},t)$ which is related to the wave function ψ by

$$\rho(\mathbf{r},\mathbf{s},t) = \psi(\mathbf{r},t)\overline{\psi}(\mathbf{s},t) \quad \text{for any} \quad \mathbf{r},\mathbf{s} \in \mathbb{R}^2. \tag{5.1}$$

It satisfies the relation

$$\rho(\mathbf{r},\mathbf{r},t) = n(\mathbf{r},t), \tag{5.2}$$

with $n(\mathbf{r},t)$ the (average) electron density.

The time evolution of the density matrix is described by the von Neumann equation

$$i\hbar \frac{\partial}{\partial t} \rho(\mathbf{r},\mathbf{s},t) = (H_{\mathbf{r}} - H_{\mathbf{s}}) \rho(\mathbf{r},\mathbf{s},t) \tag{5.3}$$

where $H_{\mathbf{r}}$ and $H_{\mathbf{s}}$ represent the Hamiltonians acting with respect to the $\mathbf{r}$ and $\mathbf{s}$ variables respectively.

If $\mathscr{E}(\mathbf{p})$ is the energy band in terms of the crystal momentum $\mathbf{p} = \hbar\mathbf{k}$, the symbol of the Hamiltonian reads

$$H(\mathbf{r},\mathbf{p}) = \mathscr{E}(\mathbf{p}) - q\,\Phi(\mathbf{r},t) \tag{5.4}$$

where the external potential $\Phi(\mathbf{r},t)$ here is assumed to be real. Moreover, we assume that $\mathscr{E}(\mathbf{p})$ is a even function of the modulus of $\mathbf{p}$.

On account of the quantum mechanics correspondence principle $\mathbf{p} \longrightarrow -i\hbar\nabla_{\mathbf{r}}$, the von Neumann equation reads

$$i\hbar \frac{\partial}{\partial t} \rho(\mathbf{r},\mathbf{s},t) = (\mathscr{E}(-i\hbar\nabla_{\mathbf{r}}) - \mathscr{E}(-i\hbar\nabla_{\mathbf{s}})) \rho(\mathbf{r},\mathbf{s},t) - q(\Phi(\mathbf{r},t) - \Phi(\mathbf{s},t)) \rho(\mathbf{r},\mathbf{s},t). \tag{5.5}$$

We have to specify the meaning of the operator $\mathscr{E}(-i\hbar\nabla_{\mathbf{r}})$.

Given a function $g \in L^1(\mathbb{R}^2)$ let us denote by $\mathscr{F}[g](\boldsymbol{\eta})$ its Fourier transform

$$\mathscr{F}[g](\boldsymbol{\eta}) = \int_{\mathbb{R}^2_{\mathbf{v}}} g(\mathbf{v}) e^{-i\mathbf{v}\cdot\boldsymbol{\eta}} d\mathbf{v}, \tag{5.6}$$

and let us denote by $\mathscr{F}^{-1}$ the inverse Fourier transform

$$\mathscr{F}^{-1}[h(\boldsymbol{\eta})] = \frac{1}{(2\pi)^2} \int_{\mathbb{R}^2_{\boldsymbol{\eta}}} h(\boldsymbol{\eta}) e^{i\mathbf{v}\cdot\boldsymbol{\eta}} d\boldsymbol{\eta}. \tag{5.7}$$

The operator $\mathscr{E}(-i\hbar\nabla_{\mathbf{r}})\rho(\mathbf{r},\mathbf{s},t)$ is defined as a multiplication operator in the Fourier transform space and then mapped back in the $\mathbf{r}$-space

$$\mathscr{E}(-i\hbar\nabla_{\mathbf{r}})\rho(\mathbf{r},\mathbf{s},t) = \frac{1}{(2\pi\hbar)^2} \int_{\mathbb{R}^2\times\mathbb{R}^2} \mathscr{E}(\boldsymbol{\eta})\rho(\mathbf{r}',\mathbf{s},t) e^{-i\boldsymbol{\eta}\cdot\frac{(\mathbf{r}'-\mathbf{r})}{\hbar}} d\boldsymbol{\eta} d\mathbf{r}'. \tag{5.8}$$

where $\boldsymbol{\eta}$ is the momentum conjugate to $\mathbf{r}'$.

In order to derive a transport equation, let us introduce the single electron Wigner quasi-distribution $w(\mathbf{x},\mathbf{p},t)$, depending on the position $\mathbf{x}$, momentum $\mathbf{p}$ and time t, defined as

$$w(\mathbf{x},\mathbf{p},t) = \mathscr{F}\left[\rho\left(\mathbf{x}+\frac{\mathbf{y}}{2},\mathbf{x}-\frac{\mathbf{y}}{2},t\right)\right](\mathbf{x},\mathbf{p},t) = \int_{\mathbb{R}^2} \rho\left(\mathbf{x}+\frac{\mathbf{y}}{2},\mathbf{x}-\frac{\mathbf{y}}{2},t\right) e^{-i\mathbf{p}\cdot\mathbf{y}/\hbar} d\mathbf{y} \tag{5.9}$$

If we set $u(\mathbf{x},\mathbf{y},t) := \rho\left(\mathbf{x}+\frac{\mathbf{y}}{2},\mathbf{x}-\frac{\mathbf{y}}{2},t\right)$ then $w = \mathscr{F}[u]$ and of course

$$u(\mathbf{x},\mathbf{y},t) = \mathscr{F}^{-1}[w] = \frac{1}{(2\pi\hbar)^2} \int_{\mathbb{R}^2} w(\mathbf{x},\mathbf{p},t) e^{i\mathbf{p}\cdot\mathbf{y}/\hbar} d\mathbf{p}. \tag{5.10}$$

Now we are denoting with $\mathbf{p}$ the momentum conjugate with $\mathbf{y}$. Using the change of coordinates

$$\mathbf{r} = \mathbf{x} + \frac{\mathbf{y}}{2}, \qquad \mathbf{s} = \mathbf{x} - \frac{\mathbf{y}}{2},$$

and after observing that

$$\mathbf{x} = \frac{\mathbf{r}+\mathbf{s}}{2}, \qquad \mathbf{y} = \mathbf{r}-\mathbf{s},$$

the expressions of $\nabla_{\mathbf{r}}$ and $\nabla_{\mathbf{s}}$ are

$$\nabla_{\mathbf{r}} = \frac{1}{2}\nabla_{\mathbf{x}} + \nabla_{\mathbf{y}}, \quad \nabla_{\mathbf{s}} = \frac{1}{2}\nabla_{\mathbf{x}} - \nabla_{\mathbf{y}},$$

and the symbols associated to $\mathscr{E}(-i\hbar\nabla_{\mathbf{r}})$ and $\mathscr{E}(-i\hbar\nabla_{\mathbf{s}})$ become

$$\mathscr{E}(-i\hbar\nabla_{\mathbf{r}}) = \mathscr{E}\left(\mathbf{p}+\frac{1}{2}\boldsymbol{\eta}\right), \quad \mathscr{E}(-i\hbar\nabla_{\mathbf{s}}) = \mathscr{E}\left(\mathbf{p}-\frac{1}{2}\boldsymbol{\eta}\right),$$

where the fact that $\mathscr{E}$ is an even function has been used.

Fourier transforming eq. (5.5) gives

$$i\hbar\frac{\partial}{\partial t}\mathscr{F}[u](\mathbf{x},\mathbf{p},t) = \mathscr{F}\left[\left(\mathscr{E}\left(\mathbf{p}+\frac{1}{2}\boldsymbol{\eta}\right) - \mathscr{E}\left(\mathbf{p}-\frac{1}{2}\boldsymbol{\eta}\right)\right)u(\mathbf{x},\mathbf{y},t) - q(\Phi(\mathbf{r},t)-\Phi(\mathbf{s},t))u(\mathbf{x},\mathbf{y},t)\right](\mathbf{x},\mathbf{p},t).$$

From (5.8) and (5.9), one has

$$\begin{aligned}
&\mathscr{F}\left[\left(\mathscr{E}\left(\mathbf{p}+\frac{1}{2}\boldsymbol{\eta}\right)-\mathscr{E}\left(\mathbf{p}-\frac{1}{2}\boldsymbol{\eta}\right)\right)u(\mathbf{x},\mathbf{y},t)\right](\mathbf{x},\mathbf{p},t)=\\
&=\frac{1}{(2\pi\hbar)^2}\mathscr{F}\left[\int_{\mathbb{R}^2_{\mathbf{x}'}\times\mathbb{R}^2_{\boldsymbol{\eta}}}\left(\mathscr{E}\left(\mathbf{p}+\frac{1}{2}\boldsymbol{\eta}\right)-\mathscr{E}\left(\mathbf{p}-\frac{1}{2}\boldsymbol{\eta}\right)\right)u(\mathbf{x}',\mathbf{y},t)e^{i\boldsymbol{\eta}\cdot\frac{(\mathbf{x}-\mathbf{x}')}{\hbar}}d\boldsymbol{\eta}d\mathbf{x}'\right]=\\
&=\frac{1}{(2\pi\hbar)^2}\int_{\mathbb{R}^2_{\mathbf{x}'}\times\mathbb{R}^2_{\boldsymbol{\eta}}\times\mathbb{R}^2_{\mathbf{y}}}\left(\mathscr{E}\left(\mathbf{p}+\frac{1}{2}\boldsymbol{\eta}\right)-\mathscr{E}\left(\mathbf{p}-\frac{1}{2}\boldsymbol{\eta}\right)\right)u(\mathbf{x}',\mathbf{y},t)e^{i\boldsymbol{\eta}\cdot\frac{(\mathbf{x}-\mathbf{x}')}{\hbar}}e^{-i\mathbf{p}\cdot\mathbf{y}/\hbar}d\boldsymbol{\eta}d\mathbf{x}'d\mathbf{y}=\\
&=\frac{1}{(2\pi\hbar)^2}\int_{\mathbb{R}^2_{\mathbf{x}'}\times\mathbb{R}^2_{\boldsymbol{\eta}}}\left(\mathscr{E}\left(\mathbf{p}+\frac{1}{2}\boldsymbol{\eta}\right)-\mathscr{E}\left(\mathbf{p}-\frac{1}{2}\boldsymbol{\eta}\right)\right)w(\mathbf{x}',\mathbf{p},t)e^{i\boldsymbol{\eta}\cdot\frac{(\mathbf{x}-\mathbf{x}')}{\hbar}}d\boldsymbol{\eta}d\mathbf{x}',
\end{aligned}\tag{5.11}$$

and

$$\begin{aligned}
&\mathscr{F}\left[\left(\Phi\left(\mathbf{x}+\frac{\mathbf{y}}{2}\right)-\Phi\left(\mathbf{x}-\frac{\mathbf{y}}{2}\right)\right)u(\mathbf{x},\mathbf{y},t)\right](\mathbf{x},\mathbf{p},t)=\\
&=\frac{1}{(2\pi\hbar)^2}\mathscr{F}\left[\int_{\mathbb{R}^2_{\mathbf{p}'}}\left(\Phi\left(\mathbf{x}+\frac{\mathbf{y}}{2}\right)-\Phi\left(\mathbf{x}-\frac{\mathbf{y}}{2}\right)\right)w(\mathbf{x},\mathbf{p}',t)e^{i\mathbf{p}'\cdot\mathbf{y}/\hbar}d\mathbf{p}'\right]=\\
&=\frac{1}{(2\pi\hbar)^2}\int_{\mathbb{R}^2_{\mathbf{y}}\times\mathbb{R}^2_{\mathbf{p}'}}\left(\Phi\left(\mathbf{x}+\frac{\mathbf{y}}{2}\right)-\Phi\left(\mathbf{x}-\frac{\mathbf{y}}{2}\right)\right)u(\mathbf{x},\mathbf{y},t)e^{i(\mathbf{p}'-\mathbf{p})\cdot\mathbf{y}/\hbar}d\mathbf{p}'d\mathbf{y}.
\end{aligned}\tag{5.12}$$

Altogether, the Wigner function satisfies the equation

$$\frac{\partial w(\mathbf{x},\mathbf{p},t)}{\partial t}+S[\mathscr{E}]w(\mathbf{x},\mathbf{p},t)-q\theta[\mathscr{E}]w(\mathbf{x},\mathbf{p},t)=C[w]\tag{5.13}$$

which is the quantum counterpart of the semiclassical Boltzmann transport equation. $S[\mathscr{E}]$ and $\theta[\mathscr{E}]$ represent the pseudo-differential operators

$$S[\mathscr{E}]w(\mathbf{x},\mathbf{p},t)=\frac{i}{\hbar(2\pi)^2}\int_{\mathbb{R}^2_{\mathbf{x}'}\times\mathbb{R}^2_{\boldsymbol{\nu}}}\left[\mathscr{E}\left(\mathbf{p}+\frac{\hbar}{2}\boldsymbol{\nu},t\right)-\mathscr{E}\left(\mathbf{p}-\frac{\hbar}{2}\boldsymbol{\nu},t\right)\right]w(\mathbf{x}',\mathbf{p},t)e^{-i(\mathbf{x}'-\mathbf{x})\cdot\boldsymbol{\nu}}d\mathbf{x}'d\boldsymbol{\nu},\tag{5.14}$$

$$\theta[\mathscr{E}]w(\mathbf{x},\mathbf{p},t)=\frac{i}{\hbar(2\pi)^2}\int_{\mathbb{R}^2_{\mathbf{p}'}\times\mathbb{R}^2_{\boldsymbol{\eta}}}\left[\Phi\left(\mathbf{x}+\frac{\hbar}{2}\boldsymbol{\eta},t\right)-\Phi\left(\mathbf{x}-\frac{\hbar}{2}\boldsymbol{\eta},t\right)\right]w(\mathbf{x},\mathbf{p}',t)e^{i(\mathbf{p}'-\mathbf{p})\cdot\boldsymbol{\eta}}d\mathbf{p}'d\boldsymbol{\eta}.\tag{5.15}$$

The Wigner equation must be augmented with the Poisson one for the electrostatic potential[1]

$$\nabla\cdot(\varepsilon\nabla\Phi)=-q(N_D-n).\tag{5.16}$$

Approximating with the Taylor expansion centered at $\hbar=0$ we get

$$\mathscr{E}\left(\mathbf{p}+\frac{\hbar}{2}\boldsymbol{\nu},t\right)-\mathscr{E}\left(\mathbf{p}-\frac{\hbar}{2}\boldsymbol{\nu},t\right)=\nabla_{\mathbf{p}}\mathscr{E}(p)\cdot\hbar\boldsymbol{\nu}+\frac{1}{24}\frac{\partial^3\mathscr{E}(p)}{\partial p_ip_jp_k}\hbar^3\nu_i\nu_j\nu_k+O(\hbar^5),\tag{5.17}$$

$$\Phi\left(\mathbf{x}+\frac{\hbar}{2}\boldsymbol{\eta},t\right)-\Phi\left(\mathbf{x}-\frac{\hbar}{2}\boldsymbol{\eta},t\right)=\nabla_{\mathbf{x}}\Phi(\mathbf{x})\cdot\hbar\boldsymbol{\eta}+\frac{1}{24}\frac{\partial^3\Phi(\mathbf{x})}{\partial x_i\partial x_j\partial x_k}\hbar^3\eta_i\eta_j\eta_k+O(\hbar^5).\tag{5.18}$$

[1]The unipolar case with a positive Fermi energy is considered. Obvious changes must be introduced in the bipolar case.

Substituting the previous relations into (5.14) and (5.15) we obtain

$$\begin{aligned} S[\mathscr{E}]w(\mathbf{x},\mathbf{p},t) &\approx \frac{i}{\hbar(2\pi)^2}\int_{\mathbb{R}^2_{\mathbf{x}'}\times\mathbb{R}^2_{\nu}}\left[\nabla_{\mathbf{p}}\mathscr{E}(p)\cdot\hbar\boldsymbol{\nu}+\frac{1}{24}\frac{\partial^3\mathscr{E}(p)}{\partial p_i\partial p_j\partial p_k}\hbar^3\nu_i\nu_j\nu_k\right]w(\mathbf{x}',\mathbf{p},t)e^{-i(\mathbf{x}'-\mathbf{x})\cdot\boldsymbol{\nu}}d\mathbf{x}'d\boldsymbol{\nu} \\ &= \frac{i}{(2\pi)^2}\nabla_{\mathbf{p}}\mathscr{E}(p)\cdot\int_{\mathbb{R}^2_{\mathbf{x}'}\times\mathbb{R}^2_{\nu}}\boldsymbol{\nu}w(\mathbf{x}',\mathbf{p},t)e^{-i(\mathbf{x}'-\mathbf{x})\cdot\boldsymbol{\nu}}d\mathbf{x}'d\boldsymbol{\nu} \\ &+ \frac{i}{(2\pi)^2}\frac{1}{24}\frac{\partial^3\mathscr{E}(p)}{\partial p_i\partial p_j\partial p_k}\hbar^2\int_{\mathbb{R}^2_{\mathbf{x}'}\times\mathbb{R}^2_{\nu}}\nu_i\nu_j\nu_k w(\mathbf{x}',\mathbf{p},t)e^{-i(\mathbf{x}'-\mathbf{x})\cdot\nu}d\mathbf{x}'d\boldsymbol{\nu} \\ &= \nabla_{\mathbf{p}}\mathscr{E}(p)\cdot\nabla_{\mathbf{x}}w(\mathbf{x},\mathbf{p},t)-\frac{\hbar^2}{24}\frac{\partial^3\mathscr{E}(p)}{\partial p_i\partial p_j\partial p_k}\frac{\partial^3 w(\mathbf{x},p,t)}{\partial x_i\partial x_j\partial x_k} \end{aligned} \tag{5.19}$$

and

$$\begin{aligned} \theta[\mathscr{E}]w(\mathbf{x},\mathbf{p},t) &\approx \frac{i}{\hbar(2\pi)^2}\int_{\mathbb{R}^2_{\mathbf{p}'}\times\mathbb{R}^2_{\boldsymbol{\eta}}}\left[\nabla_{\mathbf{x}}\Phi(\mathbf{x})\cdot\hbar\boldsymbol{\eta}+\frac{1}{24}\frac{\partial^3\Phi(\mathbf{x})}{\partial x_i\partial x_j\partial x_k}\hbar^3\eta_i\eta_j\eta_k\right]w(\mathbf{x},\mathbf{p}',t)e^{i(\mathbf{p}'-\mathbf{p})\cdot\boldsymbol{\eta}}d\mathbf{p}'d\boldsymbol{\eta} \\ &= -\nabla_{\mathbf{x}}\Phi(\mathbf{x})\cdot\nabla_p w(\mathbf{x},\mathbf{p},t)+\frac{\hbar^2}{24}\frac{\partial^3\Phi(\mathbf{x})}{\partial x_i\partial x_j\partial x_k}\frac{\partial^3 w(\mathbf{x},p,t)}{\partial p_i\partial p_j\partial p_k}. \end{aligned} \tag{5.20}$$

We suppose that the expansion

$$w = w^{(0)}+\hbar^2 w^{(1)}+O(\hbar^4)$$

holds. By proceeding in a formal way, as $\hbar\longrightarrow 0$ the Wigner equation gives the semiclassical Boltzmann equation, therefore we identify $w^{(0)}(\mathbf{x},\mathbf{p},t)$ with the semiclassical distribution (4.10)

$$w^{(0)}(\mathbf{x},\mathbf{p},t)\approx f_{MEP}(\mathbf{x},\mathbf{p},t).$$

At first order in $\hbar^2$ one finds

$$\begin{aligned} &\frac{\partial w^{(1)}(\mathbf{x},\mathbf{p},t)}{\partial t}+\mathbf{v}\cdot\nabla_{\mathbf{x}}w^{(1)}(\mathbf{x},\mathbf{p},t)-\frac{1}{24}\frac{\partial^3\mathscr{E}(p)}{\partial p_i\partial p_j\partial p_k}\frac{\partial^3 w^{(0)}(\mathbf{x},\mathbf{p},t)}{\partial x_i\partial x_j\partial x_k}+q\nabla_{\mathbf{x}}\Phi(\mathbf{x})\cdot\nabla_{\mathbf{p}}w^{(1)}(\mathbf{x},\mathbf{p},t)- \\ &-\frac{q}{24}\frac{\partial^3\Phi(\mathbf{x})}{\partial x_i\partial x_j\partial x_k}\frac{\partial^3 w^{(0)}(\mathbf{x},\mathbf{p},t)}{\partial p_i\partial p_j\partial p_k}=\mathscr{C}[w^{(1)}](\mathbf{x},\mathbf{p},t). \end{aligned} \tag{5.21}$$

To go on we need an approximation for $w^{(1)}$ and for $\mathscr{C}[w^{(1)}]$. We expand the collision term up to second order in $\hbar$

$$\mathscr{C}[w]\approx\mathscr{C}[w^{(0)}]+\hbar^2\mathscr{C}[w^{(1)}],$$

where $\mathscr{C}[w^{(0)}]$ is the semiclassical collision operator. Following [58] we model the second term as follows

$$\mathscr{C}[w^{(1)}]=-\nu\left(w^{(1)}-w^{(1)}_{eq}\right).$$

where $w^{(1)}_{eq}$ is the second order term in $\hbar$ of the equilibrium Wigner function and ν plays the role of a collision frequency which in general can depend on $\mathbf{p}$.

In the limit $\nu \mapsto +\infty$ one formally gets $w^{(1)} = w^{(1)}_{eq}$. Hereafter, we will suppose that $w^{(1)} = w^{(1)}_{eq}$ with a good approximation (a similar assumption was made also in [19]). Therefore, it is necessary to find out the expression of $w^{(1)}_{eq}$.

5.2 Equilibrium Wigner function

Let us denote with $\hat{\rho}$ the density matrix operator. It is related to ρ by the relation

$$(\hat{\rho}\,\phi)(\mathbf{x},t) = \int_{\mathbb{R}^2} \rho(\mathbf{x},\mathbf{y},t)\phi(\mathbf{y})d\mathbf{y},$$

for any suitable test function ϕ. In other words, $\rho(\mathbf{x},\mathbf{y},t)$ is the kernel of $\hat{\rho}$. This solves the operatorial Liouville von-Neumann equation

$$i\hbar\frac{\partial}{\partial t}\hat{\rho} = [H,\hat{\rho}],$$

where $[H,\hat{\rho}] = H\hat{\rho} - \hat{\rho}H$ is the commutator. In a steady state, and in particular at equilibrium, $\frac{\partial}{\partial t}\hat{\rho} = 0$ and therefore $[H,\hat{\rho}] = 0$, that is H commutes with $\hat{\rho}$. As well-known, if one assumes for simplicity a Boltzmann statistics, the equilibrium density matrix operator is given by [20]

$$\hat{\rho}_{eq} = \exp(-\beta(H-\varphi_F)), \tag{5.22}$$

where φ_F is the quasi-Fermi potential and $\beta = \frac{1}{k_B T_L}$, T_L being the lattice temperature (here assumed constant). We will denote by $\rho_{eq}(\mathbf{r},\mathbf{s},\beta)$ the density matrix at equilibrium. The dependence on β has been explicitly included.

Observe that the factor $\exp(\varphi_F)$ plays only the role of a normalization factor. Therefore, one first can consider the case $\varphi_F = 0$ and then rescales by multiplying by $\exp(\varphi_F)$. Let φ_F be zero.

Expanding $\exp(-\beta H)$ it is possible to get an approximation of $\rho_{eq}(\mathbf{r},\mathbf{s},\beta)$ at different orders in $\hbar$. An alternative approach is based on the Bloch equation as follows. By deriving with respect to β, one has

$$\frac{\partial\hat{\rho}_{eq}}{\partial\beta} = -H\hat{\rho}_{eq} = -\frac{1}{2}(H\hat{\rho}_{eq} + \hat{\rho}_{eq}H),$$

where the commutation relation between H and $\hat{\rho}_{eq}$ has been used. For any suitable test function ϕ, we have

$$\int_{\mathbb{R}^2}\frac{\partial\rho_{eq}(\mathbf{r},\mathbf{s},\beta)}{\partial\beta}\phi(\mathbf{s})d\mathbf{s} = -\frac{1}{2}\int_{\mathbb{R}^2}[H_{\mathbf{r}}\rho_{eq}(\mathbf{r},\mathbf{s},\beta)\phi(\mathbf{s}) + \rho_{eq}(\mathbf{r},\mathbf{s},\beta)H_{\mathbf{s}}\phi(\mathbf{s})]d\mathbf{s}.$$

From general considerations in quantum mechanics, we require that H must be self-adjoint

$$\int_{\mathbb{R}^2}\rho_{eq}(\mathbf{r},\mathbf{s},\beta)H_{\mathbf{s}}\phi(\mathbf{s})\,d\mathbf{s} = \int_{\mathbb{R}^2}H_{\mathbf{s}}\rho_{eq}(\mathbf{r},\mathbf{s},\beta)\phi(\mathbf{s})\,d\mathbf{s}$$

and therefore from the previous relations we get the Bloch equation

$$\frac{\partial\rho_{eq}(\mathbf{r},\mathbf{s},\beta)}{\partial\beta} = -\frac{1}{2}[H_{\mathbf{r}}\rho_{eq}(\mathbf{r},\mathbf{s},\beta) + H_{\mathbf{s}}\rho_{eq}(\mathbf{r},\mathbf{s},\beta)].$$

Let consider a Hamiltonian of the general form (5.4). After the change of variable

$$\mathbf{r} = \mathbf{x} + \frac{\hbar}{2}\boldsymbol{\eta} \qquad \mathbf{s} = \mathbf{x} - \frac{\hbar}{2}\boldsymbol{\eta},$$

and by Fourier transforming, the Bloch equation reads

$$\begin{aligned}\frac{\partial w_{eq}(\mathbf{x},\mathbf{p},\beta)}{\partial\beta} = -\frac{1}{2}\Bigg\{\frac{1}{(2\pi)^2}\int_{\mathbb{R}^2_{\mathbf{x}'}\times\mathbb{R}^2_{\boldsymbol{\nu}}} \mathscr{E}\left(\mathbf{p}+\frac{\hbar}{2}\boldsymbol{\nu}\right)+\mathscr{E}\left(\mathbf{p}-\frac{\hbar}{2}\boldsymbol{\nu}\right) w_{eq}(\mathbf{x}',\mathbf{p},\beta)e^{-i(\mathbf{x}'-\mathbf{x})\cdot\boldsymbol{\nu}}d\mathbf{x}'\,d\boldsymbol{\nu}- \\ -\frac{q}{(2\pi)^2}\int_{\mathbb{R}^2_{\mathbf{p}'}\times\mathbb{R}^2_{\boldsymbol{\eta}}} \Phi\left(\mathbf{x}+\frac{\hbar}{2}\eta\right)+\Phi\left(\mathbf{x}-\frac{\hbar}{2}\boldsymbol{\eta}\right) w_{eq}(\mathbf{x},\mathbf{p}',\beta)e^{i(\mathbf{p}'-\mathbf{p})\cdot\boldsymbol{\eta}}d\mathbf{p}'\,d\boldsymbol{\eta}\Bigg\},\end{aligned} \tag{5.23}$$

where $w_{eq}(\mathbf{x},\mathbf{p},\beta)$ is the equilibrium Wigner function.

Since for $\beta = 0$ we must have $\hat{\rho}_{eq} = 1$, it follows

$$\int_{\mathbb{R}^2} \rho(\mathbf{r},\mathbf{s},0)\phi(\mathbf{s})d\mathbf{s} = \phi(\mathbf{r}),$$

which implies [2]

$$\rho(\mathbf{r},\mathbf{s},0) = \delta(\mathbf{s}-\mathbf{r}),$$

wherefrom

$$w_{eq}(\mathbf{x},\mathbf{p},0) = 1. \tag{5.24}$$

Eq. (5.23) augmented with (5.24) allows us to determine w_{eq}. In view of the application in the next sections, we look for solution of the form

$$w_{eq}(\mathbf{x},\mathbf{p},\beta) = w^{(0)}_{eq}(\mathbf{x},\mathbf{p},\beta) + \hbar^2 w^{(1)}_{eq}(\mathbf{x},\mathbf{p},\beta).$$

By taking into account that

$$\mathscr{E}\left(\mathbf{p}+\frac{\hbar}{2}\nu\right)+\mathscr{E}\left(\mathbf{p}-\frac{\hbar}{2}\nu\right) = 2\mathscr{E}(\mathbf{p}) + \frac{1}{4}\frac{\partial^2\mathscr{E}(\mathbf{p})}{\partial p_i\partial p_j}\nu_i\nu_j\hbar^2 + o(\hbar^2), \tag{5.25}$$

$$\Phi\left(\mathbf{x}+\frac{\hbar}{2}\eta\right)+\Phi\left(\mathbf{x}-\frac{\hbar}{2}\eta\right) = 2\Phi(\mathbf{x}) + \frac{1}{4}\frac{\partial^2\Phi(\mathbf{x})}{\partial x_i\partial x_j}\eta_i\eta_j\hbar^2 + o(\hbar^2), \tag{5.26}$$

at first-order approximation in $\hbar^2$ the Bloch equation reads

$$\begin{aligned}\frac{\partial w_{eq}(\mathbf{x},\mathbf{p},\beta)}{\partial\beta} = -\mathscr{E}(\mathbf{p})w_{eq}(\mathbf{x},\mathbf{p},\beta) + \frac{\hbar^2}{8}\frac{\partial^2\mathscr{E}(\mathbf{p})}{\partial p_i\partial p_j}\frac{\partial^2 w_{eq}(\mathbf{x},\mathbf{p},\beta)}{\partial x_i\partial x_j} + q\Phi(\mathbf{x})w_{eq}(\mathbf{x},\mathbf{p},\beta)+ \\ -\frac{q\hbar^2}{8}\frac{\partial^2\Phi(\mathbf{x})}{\partial x_i\partial x_j}\frac{\partial^2 w_{eq}(\mathbf{x},\mathbf{p},\beta)}{\partial p_i\partial p_j}.\end{aligned} \tag{5.27}$$

At zero order one has

$$\frac{\partial w^{(0)}_{eq}(\mathbf{x},\mathbf{p},\beta)}{\partial\beta} = -\mathscr{E}(\mathbf{p})w^{(0)}_{eq}(\mathbf{x},\mathbf{p},\beta) + q\Phi(\mathbf{x})w^{(0)}_{eq}(\mathbf{x},\mathbf{p},\beta) \tag{5.28}$$

[2] we let δ denote the Dirac distribution.

whose solution with $w^{(0)}_{eq}(\mathbf{x},\mathbf{p},0)=1$ is

$$w^{(0)}_{eq}(\mathbf{x},\mathbf{p},\beta)=\exp\left[-\beta E(\mathbf{p})+q\beta\Phi(\mathbf{x})\right].$$

At first order in $\hbar^2$ one has

$$\begin{aligned}\frac{\partial w^{(1)}_{eq}(\mathbf{x},\mathbf{p},\beta)}{\partial\beta}&=-\mathscr{E}(\mathbf{p})w^{(1)}_{eq}(\mathbf{x},\mathbf{p},\beta)+\frac{1}{8}\frac{\partial^2\mathscr{E}(\mathbf{p})}{\partial p_i\partial p_j}\frac{\partial^2 w^{(0)}_{eq}(\mathbf{x},\mathbf{p},\beta)}{\partial x_i\partial x_j}+q\Phi(\mathbf{x})w^{(1)}_{eq}(\mathbf{x},\mathbf{p},\beta)+\\&-\frac{q}{8}\frac{\partial^2\Phi(\mathbf{x})}{\partial x_i\partial x_j}\frac{\partial^2 w^{(0)}_{eq}(\mathbf{x},\mathbf{p},\beta)}{\partial p_i\partial p_j}.\end{aligned}\tag{5.29}$$

We solve the last equation via separation of variables by looking for solution of the form

$$w^{(1)}_{eq}(\mathbf{x},\mathbf{p},\beta)=w^{(0)}_{eq}(\mathbf{x},\mathbf{p},\beta)g(\mathbf{x},\mathbf{p},\beta)\tag{5.30}$$

with the function g satisfying the equation

$$\frac{\partial g(\mathbf{x},\mathbf{p},\beta)}{\partial\beta}=\frac{1}{8w^{(0)}_{eq}(\mathbf{x},\mathbf{p},\beta)}\left[\frac{\partial^2\mathscr{E}(\mathbf{p})}{\partial p_i\partial p_j}\frac{\partial^2 w^{(0)}_{eq}(\mathbf{x},\mathbf{p},\beta)}{\partial x_i\partial x_j}-q\frac{\partial^2\Phi(\mathbf{x})}{\partial x_i\partial x_j}\frac{\partial^2 w^{(0)}_{eq}(\mathbf{x},\mathbf{p},\beta)}{\partial p_i\partial p_j}\right],\tag{5.31}$$

and the initial condition $g(\mathbf{x},\mathbf{p},0)=0$.

One finds

$$g(\mathbf{x},\mathbf{p},\beta)=\frac{q\beta^2}{8}\frac{\partial^2\mathscr{E}(\mathbf{p})}{\partial p_i\partial p_j}\frac{\partial^2\Phi(\mathbf{x})}{\partial x_i\partial x_j}+\frac{\beta^3 q}{24}\left[q\frac{\partial^2\mathscr{E}(\mathbf{p})}{\partial p_i\partial p_j}\frac{\partial\Phi(\mathbf{x})}{\partial x_i}\frac{\partial\Phi(\mathbf{x})}{\partial x_j}-\frac{\partial^2\Phi(\mathbf{x})}{\partial x_i\partial x_j}v_iv_j\right]\tag{5.32}$$

where v_i are the components of $\mathbf{v}$ (we recall that $\mathbf{v}=\nabla_{\mathbf{p}}E(\mathbf{p})$ is the electron velocity).
Altogether, including now also the presence of a nonzero quasi-Fermi potential, we get the equilibrium Wigner function in the case of a general energy band

$$w_{eq}(\mathbf{x},\mathbf{p},\beta)=w^{(0)}_{eq}(\mathbf{x},\mathbf{p},\beta)+\hbar^2 w^{(1)}_{eq}(\mathbf{x},\mathbf{p},\beta)+o(\hbar^2)\tag{5.33}$$

where

$$w^{(0)}_{eq}(\mathbf{x},\mathbf{p},\beta)=\exp(q\Phi(\mathbf{x})\beta)\exp(-\beta(\mathscr{E}(p)-\varphi_F))\tag{5.34}$$

$$\begin{aligned}w^{(1)}_{eq}(\mathbf{x},\mathbf{p},\beta)&=\exp(q\Phi(\mathbf{x})\beta)\exp(-\beta(\mathscr{E}(p)-\varphi_F))\left\{\frac{q\beta^2}{8}\frac{\partial^2\mathscr{E}(p)}{\partial p_i\partial p_j}\frac{\partial^2\Phi(\mathbf{x})}{\partial x_i\partial x_j}+\right.\\&\left.+\frac{\beta^3\hbar^2}{24}\left[q^2\frac{\partial^2\mathscr{E}(p)}{\partial p_i\partial p_j}\frac{\partial\Phi(\mathbf{x})}{\partial x_i}\frac{\partial\Phi(\mathbf{x})}{\partial x_j}-q\frac{\partial^2\Phi(\mathbf{x})}{\partial x_i\partial x_j}v_iv_j\right]\right\}.\end{aligned}\tag{5.35}$$

Note that for a quadratic energy band the expression already found by Wigner [68] is recovered.

Remark. The zero order term of the equilibrium Wigner function does not coincide with the Fermi Dirac distribution but gives the Boltzmann-Maxwell low density limit. In the following we will make use only of the $\hbar^2$ term and the previous concern will not really matter. However, from a theoretical point of view we would address a bit better the issue.

The expression (5.22) of the equilibrium density matrix operator stems from the expression of the quantum entropy according to von Neumann [51] $S_q=-k_B\mathrm{Tr}(\hat{\rho}\log\hat{\rho})$, where Tr is the

trace operator. Indeed, (5.22) maximizes such a quantum entropy. One of the main matter of debate is the fact that the von Neumann entropy does not include the Fermi or the Bose statistics. Moreover, as pointed out in recent papers [54, 65], in a closed system S_q must be conserved because the evolution of the system is described by unitary operators. Instead, in a open system, like a semiconductor electron device, there is a fast decay of the off-diagonal terms and practically only the diagonal contribution to S_q survives. Arguing on such a remark, Polkovnikov [54] has suggested to use as entropy only the diagonal contribution S_d and has proved that it increase in time according to the second law of thermodynamics. A further modification, pointed out in [65], could be used to introduce a new definition of entropy

$$-k_B \sum_k \left[< \hat{\rho}_{kk} \log < \hat{\rho}_{kk} > \mp (1 \pm < \hat{\rho}_{kk} >) \log(1 \pm < \hat{\rho}_{kk} >) \right], \tag{5.36}$$

where the $< \hat{\rho}_{kk} >$'s are the expectation values of the diagonal elements of $\hat{\rho}_{kk}$ which can be interpreted as occupation numbers, the upper sign being valid for Bosons and the lower one for Fermions .

This could solve the problem of the limit of the equilibrium Wigner function but the needed calculations become much more involved to carry out analytically. We are confident that the quantum correction given by (5.35) is good enough for determining the quantum extension of the semiclassical hydrodynamic model. These issues are under current investigation and will be the subject of a forthcoming article.

5.3 A 6-moment model with quantum corrections

In this section we consider a 6-moment model obtained by choosing as weight functions $\{1, \mathscr{E}, \mathbf{v}, \mathscr{E}\mathbf{v}\}$. Explicit closure relation has been obtained in [12] and [45] the crystal heating effects have been also included. Comparisons with Direct Simulation Monte Carlo [15, 16, 37, 38, 61] have shown a good accuracy of the model. In this Section the general guideline for getting quantum corrections to the semiclassical hydryodynamic models will be delineated. The model is based on the same moments (4.5)-(4.8) as in the semiclassical case but defined now as

$$n(\mathbf{x},t) = \frac{2}{(2\pi\hbar)^2} \int_{\mathbb{R}^2} w(\mathbf{x},\mathbf{p},t)\, d\mathbf{p}, \tag{5.37}$$

$$n(\mathbf{x},t) W(\mathbf{x},t) = \frac{2}{(2\pi\hbar)^2} \int_{\mathbb{R}^2} w(\mathbf{x},\mathbf{p},t) \mathscr{E}(\mathbf{p})\, d\mathbf{p}, \tag{5.38}$$

$$n(\mathbf{x},t) \mathbf{V}(\mathbf{x},t) = \frac{2}{(2\pi\hbar)^2} \int_{\mathbb{R}^2} w(\mathbf{x},\mathbf{p},t) \mathbf{v}(\mathbf{p})\, d\mathbf{p}, \tag{5.39}$$

$$n(\mathbf{x},t) \mathbf{S}(\mathbf{x},t) = \frac{2}{(2\pi\hbar)^2} \int_{\mathbb{R}^2} w(\mathbf{x},\mathbf{p},t) \mathscr{E}(\mathbf{p}) \mathbf{v}(\mathbf{p})\, d\mathbf{p}, \tag{5.40}$$

where $w(\mathbf{x},\mathbf{p},t) \approx f_{MEP}(\mathbf{x},\mathbf{p},t) + \hbar^2 w_{eq}^{(1)}(\mathbf{x},\mathbf{p},t)$ is the Wigner function instead of the distribution function[3].

[3]From now on, f_{MEP} is expressed in terms of the crystal momentum $\mathbf{p}$ instead of the wave-vector $\mathbf{k}$.

The corresponding evolution equations, obtained by taking the moments of the Wigner equation, up to $\hbar^2$ terms, are given by

$$\frac{\partial}{\partial t}n(\mathbf{x},t)+\frac{\partial}{\partial x_i}\left(n(\mathbf{x},t)V_i(\mathbf{x},t)-\frac{\hbar^2}{24}\frac{\partial^2\left(n(\mathbf{x},t)T^{(0)}_{ijk}(\mathbf{x},t)\right)}{\partial x_j\partial x_k}\right)=0, \tag{5.41}$$

$$\begin{aligned}&\frac{\partial}{\partial t}(n(\mathbf{x},t)W(\mathbf{x},t))+\frac{\partial}{\partial x_i}\left(n(\mathbf{x},t)S_i(\mathbf{x},t)-\frac{\hbar^2}{24}\frac{\partial^2\left(n(\mathbf{x},t)T^{(1)}_{ijk}(\mathbf{x},t)\right)}{\partial x_j\partial x_k}\right)+\\&-q\frac{\partial\Phi(\mathbf{x})}{\partial x_i}\cdot n(\mathbf{x},t)V_i(\mathbf{x},t)+\frac{q\hbar^2}{24}\frac{\partial^3\Phi(\mathbf{x})}{\partial x_i\partial x_j\partial x_k}n(\mathbf{x},t)T^{(0)}_{ijk}(\mathbf{x},t)=nC_W[w^{(0)}](\mathbf{x},t),\end{aligned} \tag{5.42}$$

$$\begin{aligned}&\frac{\partial}{\partial t}(n(\mathbf{x},t)V_i(\mathbf{x},t))+\frac{\partial}{\partial x_j}\left(n(\mathbf{x},t)F^{(0)}_{ij}(\mathbf{x},t)-\frac{\hbar^2}{24}\frac{\partial^2\left(n(\mathbf{x},t)H^{(0)}_{ijkl}(\mathbf{x},t)\right)}{\partial x_k\partial x_l}\right)+\\&-q\frac{\partial\Phi(\mathbf{x})}{\partial x_j}\cdot n(\mathbf{x},t)G^{(0)}_{ij}(\mathbf{x},t)+\frac{q\hbar^2}{24}\frac{\partial^3\Phi(\mathbf{x})}{\partial x_j\partial x_k\partial x_l}n(\mathbf{x},t)L^{(0)}_{ijkl}=nC_{V_i}[w^{(0)}](\mathbf{x},t),\end{aligned} \tag{5.43}$$

$$\begin{aligned}&\frac{\partial}{\partial t}(n(\mathbf{x},t)S_i(\mathbf{x},t))+\frac{\partial}{\partial x_j}\left(n(\mathbf{x},t)F^{(1)}_{ij}(\mathbf{x},t)-\frac{\hbar^2}{24}\frac{\partial^2\left(n(\mathbf{x},t)H^{(1)}_{ijkl}(\mathbf{x},t)\right)}{\partial x_k\partial x_l}\right)+\\&-q\frac{\partial\Phi(\mathbf{x})}{\partial x_j}\cdot n(\mathbf{x},t)G^{(1)}_{ij}(\mathbf{x},t)+\frac{q\hbar^2}{24}\frac{\partial^3\Phi(\mathbf{x})}{\partial x_j\partial x_k\partial x_l}n(\mathbf{x},t)L^{(1)}_{ijkl}(\mathbf{x},t)=nC_{S_i}[w^{(0)}](\mathbf{x},t),\end{aligned} \tag{5.44}$$

supplemented by the Poisson equation for the electric potential

$$\nabla\cdot(\varepsilon\nabla\Phi)=-q(N_D-n). \tag{5.45}$$

Note that the production terms are identical to the semiclassical case. A discussion about the regime of validity of such approximation can be found, for example, in [56].

Besides the average densities, velocities, energies and energy fluxes, the additional quantities appear

$$\begin{aligned}n(\mathbf{x},t)\begin{pmatrix}T^{(0)}_{ijk}(\mathbf{x},t)\\T^{(1)}_{ijk}(\mathbf{x},t)\end{pmatrix}&=\frac{2}{(2\pi\hbar)^2}\int_{\mathbb{R}^2}\begin{pmatrix}1\\\mathscr{E}(p)\end{pmatrix}w^{(0)}(\mathbf{x},\mathbf{p},t)\frac{\partial^3\mathscr{E}(p)}{\partial p_i\partial p_j\partial p_k}\,d\mathbf{p},\\n(\mathbf{x},t)\begin{pmatrix}H^{(0)}_{ijkl}(\mathbf{x},t)\\H^{(1)}_{ijkl}(\mathbf{x},t)\end{pmatrix}&=\frac{2}{(2\pi\hbar)^2}\int_{\mathbb{R}^2}\begin{pmatrix}1\\\mathscr{E}(p)\end{pmatrix}w^{(0)}(\mathbf{x},\mathbf{p},t)\frac{\partial^3\mathscr{E}(p)}{\partial p_i\partial p_j\partial p_k}v_l\,d\mathbf{p},\\n(\mathbf{x},t)\begin{pmatrix}G^{(0)}_{ij}(\mathbf{x},t)\\G^{(1)}_{ij}(\mathbf{x},t)\end{pmatrix}&=\frac{2}{(2\pi\hbar)^2}\int_{\mathbb{R}^2}\begin{pmatrix}1\\\mathscr{E}(p)\end{pmatrix}w(\mathbf{x},\mathbf{p},t)\frac{\partial^2\mathscr{E}(p)}{\partial p_i\partial p_j}\,d\mathbf{p},\\n(\mathbf{x},t)\begin{pmatrix}L^{(0)}_{ijkl}(\mathbf{x},t)\\L^{(1)}_{ijkl}(\mathbf{x},t)\end{pmatrix}&=\frac{2}{(2\pi\hbar)^2}\int_{\mathbb{R}^2}\begin{pmatrix}1\\\mathscr{E}(p)\end{pmatrix}w^{(0)}(\mathbf{x},\mathbf{p},t)\frac{\partial^4\mathscr{E}(p)}{\partial p_i\partial p_j\partial p_k\partial p_l}\,d\mathbf{p},\\n(\mathbf{x},t)\begin{pmatrix}F^{(0)}_{ij}(\mathbf{x},t)\\F^{(1)}_{ij}(\mathbf{x},t)\end{pmatrix}&=\frac{2}{(2\pi\hbar)^2}\int_{\mathbb{R}^2}\begin{pmatrix}1\\\mathscr{E}(p)\end{pmatrix}w(\mathbf{x},\mathbf{p},t)v_i\,v_j\,d\mathbf{p}.\end{aligned}$$

that must be expressed as function of the basic variables n, W, $\mathbf{V}$, $\mathbf{S}$. The closure relations are obtained by inserting $w(\mathbf{x},\mathbf{p},t)\approx f_{MEP}(\mathbf{x},\mathbf{p},t)+\hbar^2 w^{(1)}_{eq}(\mathbf{x},\mathbf{p},t)$ into the previous relations. For the

sake of better readability, the closure relations are summarized in the Appendix E. The results can be extended to the bipolar case in a straightforward way with similar considerations.

We observe that regarding the production terms, they are given by summing the contributions from different types of phonon scattering.

Further moments can be added, e.g. the deviatoric part of the stress tensor as in [35], and corresponding closure relations can be obatined with the same procedure.

5.4 Preliminary classification of the 1D quantum hydrodynamic equations in the six moment case

Here, a prelimary analysis of the mathematical properties of the six moment quantum hydrodynamic model is performed in the 1D case. If we denote by x_1 the only relevant space variable, the $\hbar^2$ term of the equilibrium Wigner function becomes

$$w_{eq}^{(1)}(\mathbf{x},\mathbf{p},\beta) = \exp(q\Phi(\mathbf{x})\beta)\exp(-\beta(\mathscr{E}(p)-\varphi_F)) \left\{\left(\frac{q\beta^2}{8}\frac{\partial^2\mathscr{E}(p)}{\partial p_1^2}\frac{\partial^2\Phi(\mathbf{x})}{\partial x_1^2}+\frac{\beta^3}{24}\left[q^2\frac{\partial^2\mathscr{E}(p)}{\partial p_1^2}\left(\frac{\partial\Phi(\mathbf{x})}{\partial x_1}\right)^2-q\frac{\partial^2\Phi(\mathbf{x})}{\partial x_1^2}v_1^2\right]\right)\right\} \tag{5.46}$$

and the 1D evolution equations reads

$$\frac{\partial}{\partial t}n(\mathbf{x},t)+\frac{\partial}{\partial x_1}n(\mathbf{x},t)V_1(\mathbf{x},t)-\frac{h^2}{24}\frac{\partial^3(n(\mathbf{x},t)T_{111}^{(0)}(\mathbf{x},t))}{\partial x_1^3}=0, \tag{5.47}$$

$$\frac{\partial}{\partial t}n(\mathbf{x},t)W(\mathbf{x},t)+\frac{\partial}{\partial x_1}n(\mathbf{x},t)S_1(\mathbf{x},t)-\frac{h^2}{24}\frac{\partial^3(n(\mathbf{x},t)T_{111}^{(1)}(\mathbf{x},t))}{\partial x_1^3}+ -q\frac{\partial\Phi(\mathbf{x})}{\partial x_1}\cdot n(\mathbf{x},t)V_1(\mathbf{x},t)+\frac{q\hbar^2}{24}\frac{\partial^3\Phi(\mathbf{x})}{\partial x_1^3}n(\mathbf{x},t)T_{111}^{(0)}(\mathbf{x},t)=nC_W[w^{(0)}](\mathbf{x},t), \tag{5.48}$$

$$\frac{\partial}{\partial t}n(\mathbf{x},t)V_1(\mathbf{x},t)+\frac{\partial}{\partial x_1}n(\mathbf{x},t)F_{11}^{(0)}(\mathbf{x},t)-\frac{\hbar^2}{24}\frac{\partial^3(n(\mathbf{x},t)H_{1111}^{(0)}(\mathbf{x},t))}{\partial x_1^3}+ -q\frac{\partial\Phi(\mathbf{x})}{\partial x_1}\cdot n(\mathbf{x},t)G_{11}^{(0)}(\mathbf{x},t)+\frac{q\hbar^2}{24}\frac{\partial^3\Phi(\mathbf{x})}{\partial x_1^3}n(\mathbf{x},t)L_{1111}^{(0)}(\mathbf{x},t)=nC_{V_i}[w^{(0)}](\mathbf{x},t), \tag{5.49}$$

$$\frac{\partial}{\partial t}n(\mathbf{x},t)S_1(\mathbf{x},t)+\frac{\partial}{\partial x_1}n(\mathbf{x},t)F_{11}^{(1)}(\mathbf{x},t)-\frac{\hbar^2}{24}\frac{\partial^3(n(\mathbf{x},t)H_{1111}^{(1)}(\mathbf{x},t))}{\partial x_1^3}+ -q\frac{\partial\Phi(\mathbf{x})}{\partial x_1}\cdot n(\mathbf{x},t)G_{11}^{(1)}(\mathbf{x},t)+\frac{q\hbar^2}{24}\frac{\partial^3\Phi(\mathbf{x})}{\partial x_1^3}n(\mathbf{x},t)L_{1111}^{(1)}(\mathbf{x},t)=nC_{S_i}[w^{(0)}](\mathbf{x},t). \tag{5.50}$$

Let us introduce the vector of the field variables

$$\mathbf{U}=(n,nW,nV_1,nS_1)^T$$

and the relative Lagrange multipliers $\mathbf{\Lambda}=\left(\lambda,\lambda_w,\lambda_{V_1},\lambda_{S_1}\right)^T$. Moreover, let us denote by A_0 the Jacobian matrix

$$A_0=\frac{\partial(n,nW,nV_1,nS_1)}{\partial\left(\lambda,\lambda_w,\lambda_{V_1},\lambda_{S_1}\right)}. \tag{5.51}$$

From the general theory it follows that A_0 is invertible (for more details see [12, 34, 35]) and the evolution equations can be written in the form

$$\frac{\partial}{\partial t}\mathbf{U}+\frac{\partial}{\partial x_1}\begin{pmatrix} nV_1 \\ nS_1 \\ nF^{(0)}_{11} \\ nF^{(1)}_{11}\end{pmatrix}=\mathscr{G}+\begin{pmatrix} 0 \\ nC_W \\ nC_{V_i} \\ nC_{S_i}\end{pmatrix}, \tag{5.52}$$

where

$$\mathscr{G}=\frac{\hbar^2}{24}\frac{\partial^3}{\partial x_1^3}\begin{pmatrix} nT^{(0)}_{111} \\ nT^{(1)}_{111} \\ nH^{(0)}_{1111} \\ nH^{(1)}_{1111}\end{pmatrix}+q\frac{\partial\Phi(x)}{\partial x_1}\begin{pmatrix} 0 \\ nV_1 \\ nG^{(0)}_{11} \\ nG^{(1)}_{11}\end{pmatrix}-\frac{q\hbar^2}{24}\frac{\partial^3\Phi(x)}{\partial x_1^3}\begin{pmatrix} 0 \\ nT^{(0)}_{111} \\ nL^{(0)}_{1111} \\ nL^{(1)}_{1111}\end{pmatrix}.$$

Let us consider the case of zero electric field. Hence

$$\mathscr{G}=\frac{\hbar^2}{24}\frac{\partial^3}{\partial x_1^3}\begin{pmatrix} nT^{(0)}_{111} \\ nT^{(1)}_{111} \\ nH^{(0)}_{1111} \\ nH^{(1)}_{1111}\end{pmatrix}.$$

Moreover we assume that the relaxation times of energy, velocity and energy flux are much longer than the characteristic time of the evolution of the system and, in consequence, we neglect the production terms $C_W[w^{(0)}](\mathbf{x},t)$, $C_{V_i}[w^{(0)}](\mathbf{x},t)$, $C_{S_i}[w^{(0)}](\mathbf{x},t)$. Indeed, the production terms are not relevant to the aim of classifying the nature of the PDEs.

The resulting evolution equations can be written in the form

$$A_0\frac{\partial\mathbf{\Lambda}}{\partial t}+A_1\frac{\partial\mathbf{\Lambda}}{\partial x}=\mathscr{G}$$

where $A_1=\nabla_\Lambda\mathscr{F}_1$, with $\mathscr{F}_1=(nV_1,nS_1,nF^{(0)}_{11},nF^{(1)}_{11})$.

Let $(\overline{\lambda},\overline{\lambda}_w,\overline{\lambda}_{V_1},\overline{\lambda}_{S_1})=(-\frac{\varepsilon_F}{k_BT_L},\frac{1}{k_BT_L},0,0)$ be the equilibrium solution at assigned Fermi level ε_F.

Now, we perturb the equilibrium solution with a Fourier mode and linearize the partial differential equations (PDEs) with respect to the perturbation. Set

$$\begin{pmatrix}\lambda \\ \lambda_w \\ \lambda_{V_1} \\ \lambda_{S_1}\end{pmatrix}=\begin{pmatrix}\overline{\lambda} \\ \overline{\lambda}_w \\ \overline{\lambda}_{V_1} \\ \overline{\lambda}_{S_1}\end{pmatrix}+e^{-\sigma t+i\mathbf{k}\cdot\mathbf{x}}\begin{pmatrix}\delta\lambda \\ \delta\lambda_w \\ \delta\lambda_{V_1} \\ \delta\lambda_{S_1}\end{pmatrix}.$$

To go on it is necessary to linearize the macroscopic variable n,nW,nV_1,nS_1. For example, the density is approximated in this way

$$n=N_D+e^{-\sigma t+i\mathbf{k}\cdot\mathbf{x}}\left(\frac{\partial n(\bar{\Lambda})}{\partial\lambda}\delta\lambda+\frac{\partial n(\bar{\Lambda})}{\partial\lambda_w}\delta\lambda_w\right) \tag{5.53}$$

and similarly

$$nW = nW(\bar{\Lambda}) + e^{-\sigma t + i\mathbf{k}\cdot\mathbf{x}}\left(\frac{\partial(nW(\bar{\Lambda}))}{\partial\lambda}\delta\lambda + \frac{\partial(nW(\bar{\Lambda}))}{\partial\lambda_w}\delta\lambda_w\right), \tag{5.54}$$

$$nV_1 = nV_1(\bar{\Lambda}) + e^{-\sigma t + i\mathbf{k}\cdot\mathbf{x}}\left(\frac{\partial(nV_1(\bar{\Lambda}))}{\partial\lambda_{V_1}}\delta\lambda_{V_1} + \frac{\partial(nV_1(\bar{\Lambda}))}{\partial\lambda_{S_1}}\delta\lambda_{S_1}\right), \tag{5.55}$$

$$nS_1 = nS_1(\bar{\Lambda}) + e^{-\sigma t + i\mathbf{k}\cdot\mathbf{x}}\left(\frac{\partial(nS_1(\bar{\Lambda}))}{\partial\lambda_{V_1}}\delta\lambda_{V_1} + \frac{\partial(nS_1(\bar{\Lambda}))}{\partial\lambda_{S_1}}\delta\lambda_{S_1}\right). \tag{5.56}$$

Denoting by λ_A the generic component of Λ, we write the linearized model as follows:

$$-\sigma\left(\frac{\partial n(\bar{\Lambda})}{\partial\lambda}\delta\lambda + \frac{\partial n(\bar{\Lambda})}{\partial\lambda_w}\delta\lambda_w\right) + i\mathbf{k}\sum_A \frac{\partial(nV_1(\bar{\Lambda}))}{\partial\lambda_A}\delta\lambda_A + i\mathbf{k}^3\frac{h^2}{24}\sum_A \frac{\partial(nT^{(0)}_{111}(\bar{\Lambda}))}{\partial\lambda_A}\delta\lambda_A = 0, \tag{5.57}$$

$$-\sigma\left(\frac{\partial nW(\bar{\Lambda})}{\partial\lambda}\delta\lambda + \frac{\partial nW(\bar{\Lambda})}{\partial\lambda_w}\delta\lambda_w\right) + i\mathbf{k}\sum_A \frac{\partial(nS_1(\bar{\Lambda}))}{\partial\lambda_A}\delta\lambda_A + i\mathbf{k}^3\frac{h^2}{24}\sum_A \frac{\partial(nT^{(1)}_{111}(\bar{\Lambda}))}{\partial\lambda_A}\delta\lambda_A = 0, \tag{5.58}$$

$$-\sigma\sum_A \frac{\partial(nV_1(\bar{\Lambda}))}{\partial\lambda_A}\delta\lambda_A + i\mathbf{k}\sum_A \frac{\partial(nF^{(0)}_{11}(\bar{\Lambda}))}{\partial\lambda_A}\delta\lambda_A + i\mathbf{k}^3\frac{h^2}{24}\sum_A \frac{\partial(nH^{(0)}_{1111}(\bar{\Lambda}))}{\partial\lambda_A}\delta\lambda_A = 0 \tag{5.59}$$

$$-\sigma\sum_A \frac{\partial(nS_1(\bar{\Lambda}))}{\partial\lambda_A}\delta\lambda_A + i\mathbf{k}\sum_A \frac{\partial(nF^{(1)}_{11}(\bar{\Lambda}))}{\partial\lambda_A}\delta\lambda_A + i\mathbf{k}^3\frac{h^2}{24}\sum_A \frac{\partial(nH^{(1)}_{1111}(\bar{\Lambda}))}{\partial\lambda_A}\delta\lambda_A = 0, \tag{5.60}$$

which in compact form reads

$$\mathscr{L}[\delta\lambda, \delta\lambda_w, \delta\lambda_{V_1}, \delta\lambda_{S_1}]^T = 0, \tag{5.61}$$

where $\mathscr{L}$ is the matrix representing the symbol of the linearized system (5.57)-(5.60).

The roots of the determinant $P(\sigma)$ of the matrix $\mathscr{L}$ determine the mathematical type of the PDE system. There are two physically interesting cases to consider:

1) $\hbar = 0$ (semi-classical model). The roots of $P(\sigma)$ and corresponding modes are

$$+ik\frac{\sqrt{2}}{2} \qquad \text{hyperbolic, multiplicity 2}$$

$$-ik\frac{\sqrt{2}}{2} \qquad \text{hyperbolic, multiplicity 2}$$

for all ε_F and $\alpha < 1$.

2) $\hbar \neq 0$ (quantum corrected model).

a) If $|\mathbf{k}| \longrightarrow \infty$ the dispersive modes are dominant

$$+iC(\alpha, \varepsilon_F)\hbar^2 k^3 \qquad \text{hyperbolic dispersion, multiplicity 2}$$

$$-iC(\alpha, \varepsilon_F)\hbar^2 k^3 \qquad \text{hyperbolic dispersion, multiplicity 2}$$

where $C(\alpha, \varepsilon_F)$ is a constant depending on the numerical value of parameters α and ε_F.

b) If $|\mathbf{k}| \longrightarrow 0$ the hyperbolic modes are dominant

$$+iD(\alpha,\varepsilon_F)\hbar k^2 \qquad \text{hyperbolic, multiplicity 2}$$

$$-iD(\alpha,\varepsilon_F)\hbar k^2 \qquad \text{hyperbolic, multiplicity 2}$$

where $D(\alpha,\varepsilon_F)$ is a constant depending on the numerical value of parameters α and ε_F.

c) If $0 < |\mathbf{k}| < +\infty$ the corresponding modes are

$$\pm k\, c_1(\alpha,\varepsilon_F)\Big[c_2(\alpha,\varepsilon_F)\hbar^4k^4 + c_3(\alpha\varepsilon_F)\hbar^2k^2 + c_4(\alpha,\varepsilon_F) + \hbar^2k^2\sqrt{\hbar^4k^4c_5(\alpha,\varepsilon_F) + \hbar^2k^2c_6(\alpha,\varepsilon_F) + c_7(\alpha,\varepsilon_F)}\Big]^{1/2},$$

with multiplicity 2.

$c_1(\alpha,\varepsilon_F)$, $c_2(\alpha,\varepsilon_F)$, $c_3(\alpha,\varepsilon_F)$, $c_4(\alpha,\varepsilon_F)$, $c_5(\alpha,\varepsilon_F)$, $c_6(\alpha,\varepsilon_F)$, $c_7(\alpha,\varepsilon_F)$ are constants depending on the numerical value of parameters α and ε_F.The high nonlinearity of such expression makes very difficult to assess analytically the sign of the argument of the roots for all positive α. To have a guess about that, we have numerically evaluated, the functions

$$f(\alpha,\hbar,k) = c_2(\alpha)\hbar^4k^4 + c_3(\alpha)\hbar^2k^2 + c_4(\alpha) + \hbar^2k^2\sqrt{\hbar^4k^4c_5(\alpha) + \hbar^2k^2c_6(\alpha) + c_7(\alpha)}$$

and

$$g(\alpha,\hbar,k) = \hbar^4k^4c_5(\alpha) + \hbar^2k^2c_6(\alpha) + c_7(\alpha)$$

for meaningfull values of ε_F, α and $\hbar k$. It has been found that f is always negative, while g is always positive. For example in Fig.5.2 the case of Fermi level $\varepsilon_F = 0.4$ eV is shown. Similar results have been obtained for other values of ε_F.

This leads to be confident that also in this last case the modes are pure immaginary.

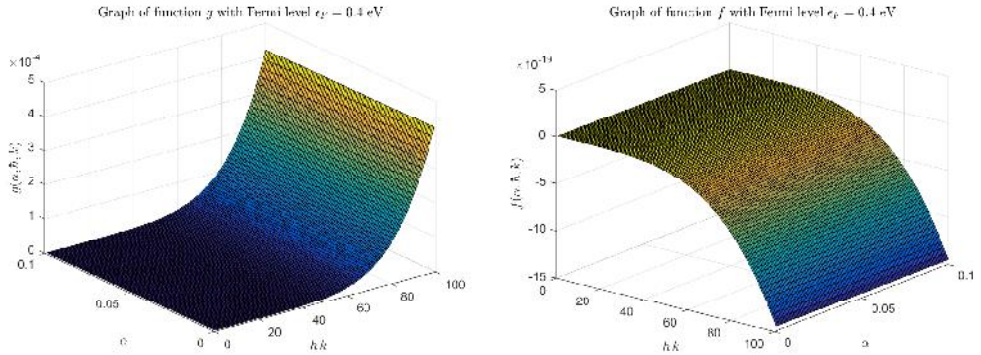

Figure 5.2: Graphics of g (on the left) and f (on the right) with Fermi level $\varepsilon_F = 0.4$ eV, for $\alpha \in [10^{-3}, 10^{-1}]$ and $\hbar k \in [0, 100]$.

5.5 Energy-transport and drift-diffusion limit models

From the hydrodynamic model it is possible to deduce an energy-transport one under a suitable scaling. In the semiclassical case the advantages of the energy-transport formulation are a better regularity of the solutions and the possibility of applying efficient numerical schemes like the Scharfetter-Gummel one [57]. In the presence of quantum corrections we expect also better features of solutions and a better performance of the numerical scheme. If we consider a long time scaling, the evolution equations (5.63)-(5.64) tend to the stationary case. In particular, the equations for $n\mathbf{V}$ and $n\mathbf{S}$ become a linear system for these variables

$$n\begin{pmatrix} c_{11} & c_{12} \\ c_{21} & c_{22} \end{pmatrix}\begin{pmatrix} nV_i \\ nS_i \end{pmatrix} = \begin{pmatrix} b_i^{(0)} \\ b_i^{(1)} \end{pmatrix},$$

where the coefficients c_{ij} depends on the energy W (for explicit expressions see [35]) while

$$\begin{aligned} b_i^{(0)} &= \frac{\partial}{\partial x_j}\left(n(\mathbf{x},t)F_{ij}^{(0)} - \frac{\hbar^2}{24}\frac{\partial^2\left(n(\mathbf{x},t)H_{ijkl}^{(0)}\right)}{\partial x_k \partial x_l}\right) - q\frac{\partial}{\partial x_j}\Phi(\mathbf{x})\cdot n(\mathbf{x},t)G_{ij}^{(0)} \\ &\quad + \frac{q\hbar^2}{24}\frac{\partial^3\Phi(\mathbf{x})}{\partial x_j \partial x_k \partial x_l}n(\mathbf{x},t)L_{ijkl}^{(0)}, \\ b_i^{(1)} &= \frac{\partial}{\partial x_j}\left(n(\mathbf{x},t)F_{ij}^{(1)} - \frac{\hbar^2}{24}\frac{\partial^2\left(n(\mathbf{x},t)H_{ijkl}^{(1)}\right)}{\partial x_k \partial x_l}\right) - q\frac{\partial}{\partial x_j}\Phi(\mathbf{x})\cdot n(\mathbf{x},t)V_j\cdot n(\mathbf{x},t)G_{ij}^{(1)} \\ &\quad + \frac{q\hbar^2}{24}\frac{\partial^3\Phi(\mathbf{x})}{\partial x_j \partial x_k \partial x_l}n(\mathbf{x},t)L_{ijkl}^{(1)}. \end{aligned}$$

One gets

$$\begin{pmatrix} nV_i \\ nS_i \end{pmatrix} = \frac{1}{c_{11}c_{22}-c_{12}c_{21}}\begin{pmatrix} c_{22} & -c_{12} \\ -c_{21} & c_{11} \end{pmatrix}\begin{pmatrix} b_i^{(0)} \\ b_i^{(1)} \end{pmatrix} \tag{5.62}$$

and by inserting these relations into the equations for n and nW, one obtains the following *stationary quantum energy-transport model*

$$\frac{\partial}{\partial x_i}\left[\frac{1}{c_{11}c_{22}-c_{12}c_{21}}\left(c_{22}b_i^{(0)} - c_{21}b_i^{(1)}\right) - \frac{\hbar^2}{24}\frac{\partial^2\left(n(\mathbf{x},t)T_{ijk}^{(0)}\right)}{\partial x_j \partial x_k}\right] = 0, \tag{5.63}$$

$$\begin{aligned} &\frac{\partial}{\partial x_i}\left(\frac{1}{c_{11}c_{22}-c_{12}c_{21}}\left(-c_{12}b_i^{(0)} + c_{11}b_i^{(1)}\right) - \frac{\hbar^2}{24}\frac{\partial^2\left(n(\mathbf{x},t)T_{ijk}^{(1)}\right)}{\partial x_j \partial x_k}\right) \\ &-q\frac{\partial}{\partial x_i}\Phi(\mathbf{x})\cdot n(\mathbf{x},t)V_i + \frac{q\hbar^2}{24}\frac{\partial^3\Phi(\mathbf{x})}{\partial x_i \partial x_j \partial x_k}n(\mathbf{x},t)T_{ijk}^{(0)} = C_W[w]. \end{aligned} \tag{5.64}$$

Moreover, let us model the energy collision term in the relaxation approximation

$$C_W[w] = -\frac{W - W_0}{\tau_W},$$

with τ_W the energy relaxation time and W_0 the equilibrium energy.

In the limit the scaled τ_W tend to zero, from the equation (5.64) one has formally $W = W_0$ and remain only the equation (5.63) which is equivalent to the conservation of the total current $\mathbf{J}$, i. e.

$$J_i = \frac{1}{c_{11}c_{22} - c_{12}c_{21}} \left(c_{22} b_i^{(0)} - c_{21} b_i^{(1)} \right) - \frac{\hbar^2}{24} \frac{\partial^2 \left(n(\mathbf{x}, t) T_{ijk}^{(0)} \right)}{\partial x_j \partial x_k} = \bar{J}_i, \; i = 1, 2, \tag{5.65}$$

$\bar{J}_i$ being constant values. Equation (5.65) coupled with the Poisson equation for the electrostatic potential constitutes the limiting *stationary drift-diffusion model* deduced from the energy-transport one. It is a generalization of the standard quantum model based on the Bohm potential (see [28] for a review of the current models known in the literature).

The quantities involving (5.65) can be explicitly evaluated in terms of the Fermi energy ϵ_F and the electrostatic potential Φ (we omit the details of the derivation. The interested reader can get it starting from the results in [36]).

Conclusions and Future Work

Semi-classical hydrodynamic models for charge transport in graphene have been presented. In pristine graphene, the numerical solutions given by those models have been compared with those of the semiclassical Boltzmann equation obtained by a DG method. Apparently the nonlinearity does not improve the results. This agrees with literature in other fields like phonon transport [18] and radiative transport [39]. Moreover it has been found that it is crucial to include - among the variables - the deviatoric part of the stress tensor in order to maintain a good accuracy in a wider range of applied electric fields.

Then to include quantum effects, the proposed models can be extended by incorporating the first quantum corrections. Therefore in the last chapter an example of quantum hydrodynamic model for charge transport in graphene has been formulated. It is composed of the semicassical model presented in [12, 34, 35] augmented with quantum corrections at $\hbar^2$ order deduced by exploiting the equilibrium Wigner function obtained by solving the Bloch equation in the case of graphene. As $\hbar \rightarrowtail 0$, the proposed model of course reduces to the semiclassical one which turned out to be accurate enough by comparison with DSMC results [34, 35]. Several strategies can be found in the literature for devising quantum hydrodynamic models (the interested reader is referred to [28] for a comprehensive review) but usually strong approximations on the collision terms or on the energy bands are introduced and the semiclassical limit leads to semiclassical models whose soundness is questionable. To asses the validity of the proposed model numerical simulations are under current investigation and they will be presented in a forthcoming article. Furthermore, quantum energy-transport and drift-diffusion models have been formally derived from the quantum hydrodynamic equations in the long time asymptotic limit. In analogy with the semiclassical case we are confident that the energy-transport and drift-diffusion models have mathematical properties which allow an easier numerical treatment.

APPENDIX A

UNIFORM CONVERGENCE FOR MOMENT PROBLEMS WITH FERMI-DIRAC TYPE ENTROPIES

Using the maximum entropy method to solve a moment problem requires maximizing a measure of entropy/information, a convex integral functional of probability density function f subject to given moment constraints. We show that under certain assumptions on the objective functional, as the number n of moments increases to infinity, the estimates f_n converges in L^∞ norm to the unknown density function f.

By introducing a convex integrand as the entropic objective for a truncated moment problem, we have to solve the following optimization problem:

$$(\mathscr{P}_n)\begin{cases}\max\limits_{f\in\mathscr{F}} S[f] \\ s.t. \quad M_A - \frac{2}{(2\pi)^2}\int_{\mathscr{B}r}\psi_A(\mathbf{k})f(\mathbf{r},\mathbf{k},t)\,d\mathbf{k}=0 \qquad A=1,2,...,\mathscr{I}_n \\ f\in L^1(\mathscr{B}r)\end{cases} \tag{A.1}$$

where $\mathscr{B}r$ is the Brillouin zone, which is a complete finite misure space, $\psi_A \in L^\infty(\mathscr{B}r)$ for $A=1,2,...,\mathscr{I}_n$ (an increasing sequence of finite index sets). The entropy $S[f]$ can be written as

$$S[f]=\int_{\mathscr{B}r}\phi(f(\mathbf{r},\mathbf{k},t))d\mathbf{k},$$

where

$$\phi(f)=-\frac{2k_B}{(2\pi)^2}[f\ln f+(1-f)\ln(1-f)]. \tag{A.2}$$

Note that ϕ is a Fermi-Dirac type entropy which satisfies:

1) $dom(\phi)=(0,1)$;

2) The function ϕ is strictly convex and differentiable on $dom(\phi)$, with the derivative satisfying

$$\lim_{f\longrightarrow 0^+}\phi'(f)=-\infty \qquad \lim_{f\longrightarrow 1^-}\phi'(f)=+\infty.$$

The conjugate function of ϕ is defined as

$$\phi^*(g) := \max_{g \in dom(\phi)} \{fg - \phi(f)\}.$$

When the function ϕ satisfies the above assumptions, the conjugate function is everywhere finite, strictly convex and differentiable on $dom(\phi)$, with a very useful property $\phi^{*'} \equiv (\phi')^{-1}$. The dual problem for $(\mathscr{P}_n)$ is then an unconstrained minimization problem:

$$(\mathscr{D}_n) \begin{cases} \min \int_{\mathscr{B}r} \left[\sum_{A=1}^{\mathscr{I}_n} \lambda_A(\mathbf{r},t)\psi_A(\mathbf{k}) f(\mathbf{r},\mathbf{k},t)) - \phi^*(\sum_{A=1}^{\mathscr{I}_n} \lambda_A(\mathbf{r},t)\psi_A(\mathbf{k})) \right] d\mathbf{k} \\ \lambda_A(\mathbf{r},t) \in \mathbb{R}^{\kappa(A)}. \end{cases} \tag{A.3}$$

where $\kappa(A)$ is the order of corresponding tensor M_A. Of course $\kappa(A)$ may not be exactly n.

Hereafter we assume $\mathbf{r}$ and t fixed. By well-known duality results (see [7]) the optima of both $(\mathscr{P}_n)$ and $(\mathscr{D}_n)$ are attained and equal, provided that the following form of a constraint qualification holds:

$$(CQ) \begin{cases} \text{there exists } \tilde{f} \in L^1(\mathscr{B}r) \text{ such that} \\ M_A = \int_{\mathscr{B}r} \psi_A(\mathbf{k}) \tilde{f}(\mathbf{k}) d\mathbf{k}, \quad A = 1, ..., \mathscr{I}_n \\ 0 < \tilde{f} < 1, \qquad \text{a.e. on } \mathscr{B}r \\ \int_{\mathscr{B}_r} \phi(\tilde{f}) d\mathbf{k} < +\infty. \end{cases} \tag{A.4}$$

Moreover, if $\overline{\Lambda} = (\overline{\lambda}_1, \overline{\lambda}_2, ..., \overline{\lambda}_{\mathscr{I}_n})$ is an optimal solution to $(\mathscr{D}_n)$, then the unique solution to $(\mathscr{P}_n)$ can be reconstructed by

$$f_n = \phi^{*'} \left(\sum_{A=1}^{\mathscr{I}_n} \overline{\lambda}_A \psi_A \right).$$

The uniqueness of the solution follows from the strict convexity of ϕ.

Note that we have $\phi'(f_n) \in \text{span}\{\psi_A, A = 1, ..., \mathscr{I}_n\}$, which implies

$$0 < f_n(\mathbf{k}) < 1, \quad \text{a.e. on } \mathscr{B}r$$

We will discuss the uniform norm of $f_n - f$, which is defined as

$$\| f_n - f \|_\infty = \text{ess sup}\{|f_n(\mathbf{k}) - f(\mathbf{k})| : \mathbf{k} \in \mathscr{B}r\}.$$

A.0.1 Some Inequalities

First of all some preliminary definitions and known results in convex analysis are recalled. Let X be a real Banach space and X^* be the topological dual space of X. The set of subgradients of f at $x_0 \in dom(f)$ is defined to be

$$\partial f(x_0) := \{x^* \in X^* | < x^*, x - x_0 > \leq f(x) - f(x_0), \text{for all } x \in X\}.$$

It has the following properties.

Proposition A.1. *If a convex function f is continuous at $x_0 \in dom(f)$, then $\partial f(x_0)$ is a nonempty, convex, and weak*-compact subset in X^*.*

For any functional $f : X \longrightarrow]-\infty, +\infty[$ and its convex conjugate $f^* : X^* \longrightarrow]-\infty, +\infty[$, Fenchel's inequality (also known as the Fenchel-Young inequality) holds for any $x \in X$ and $x \in X^*$:

$$f^*(x^*) + f(x) \geq < x, x^* > \tag{A.5}$$

The proof of (A.5) follows immediately from the definition of convex conjugate and the equality holds exactly for $x^* \in \partial f(x)$.

Definition A.1. For $x \in dom(f)$, $h \in X$, if the limit

$$\delta F(x;h) = \lim_{\alpha \longrightarrow 0} \frac{1}{\alpha}[F(x+\alpha h) - F(x)]$$

exists, it is called the Gateaux differential of F at x with increment h. If the above limit exists for each $h \in X$, then F is said to be Gateaux differentiable at x and the Gateaux differential will be denoted by $F'(x)$.

Definition A.2. If $\delta F(x;\cdot) \longrightarrow \mathbb{R}$ is linear and continuous such that

$$\lim_{\|h\| \longrightarrow 0} \frac{\|F(x+h) - F(x) - \delta F(x;h)\|}{\|h\|} = 0,$$

then F is said to be Frechet differentiable at x.

It is obvious that the Frechet differentiability implies the Gateaux differentiability but not usually vice versa. For a lower semicontinuous convex function on a Banach space, the Gateaux differential is always linear and continuous and we have

$$\partial F(x) = \{F'(x)\}.$$

In this case, the Fenchel-Young inequality becomes

$$< F'(x), x > = F(x) + F^*(F'(x)). \tag{A.6}$$

We will use this property frequently in proving theorems we will present below.

Given an integer n and $g \in L^\infty(\mathscr{B}r)$, for our convenience, the best approximation of g by $\{\psi_A, A = 1, ..., \mathscr{I}_n\}$ is the number defined as

$$E_n(g) := \inf\left\{ \left\| \sum_{A=1}^{\mathscr{I}_n} \psi_A \lambda_A - g \right\|_\infty, \lambda_A \in \mathbb{R}^{\kappa(A)} \right\}$$

For a given choice of ϕ and a density function f, we write:

$$E_n := \begin{cases} E_n(\phi'(f)) & \text{If } \phi'(f) \in L^\infty(\mathscr{B}r) \\ +\infty & \text{otherwise.} \end{cases} \tag{A.7}$$

Let denote by $V(\mathscr{P}_n)$ and $V(\mathscr{D}_n)$ the optimal values of problems $(\mathscr{P}_n)$ and $(\mathscr{D}_n)$ respectively. Then we can prove the following inequalities.

Theorem A.1. *(weak duality)*

$$V(\mathscr{P}_n) \geq V(\mathscr{D}_n). \tag{A.8}$$

Proof. This follows directly from the convexity of ϕ and the Fenchel-Young inequality (A.5)

$$V(\mathscr{P}_n) = \int_{\mathscr{B}r} \phi(f) d\mathbf{k} \geq \int_{\mathscr{B}r} \sum_{A=1}^{\mathscr{I}_n} \lambda_A(\mathbf{r},t)\psi_A f(\mathbf{r},\mathbf{k},t) - \phi^*\left(\sum_{A=1}^{\mathscr{I}_n} \lambda_A(\mathbf{r},t)\psi_A(\mathbf{k})\right) d\mathbf{k} = V(\mathscr{D}_n).$$

■

Theorem A.2. *Let $E_n < +\infty$ then*

$$V(\mathscr{D}_n) \geq \int_{\mathscr{B}r} \phi(f) d\mathbf{k} - mis(\mathscr{B}r) E_n \tag{A.9}$$

Proof. Since $E_n < +\infty$, the function $\phi(f)$ is almost everywhere finite.
From Fenchel-Young equality (A.6), for almost $\mathbf{k} \in \mathscr{B}r$, we have that $\phi'(f(\mathbf{k}))$ is finite, and so

$$\phi(f) + \phi^*(\phi'(f)) = f\phi'(f)$$

For each n, we can find $\lambda_A^n \in \mathbb{R}^{\kappa(A)}, A = 1,2,...,\mathscr{I}_n$ such that

$$\begin{aligned}
\int_{\mathscr{B}r} \phi(f) d\mathbf{k} - V(\mathscr{D}_n) &= \int_{\mathscr{B}r} \left[\phi(f) + \phi^*\left(\sum_{A=1}^{\mathscr{I}_n} \lambda_A^n \psi_A\right) - f \sum_{A=1}^{\mathscr{I}_n} \lambda_A^n \psi_A\right] d\mathbf{k} = \\
&= \int_{\mathscr{B}r} \left[f\phi'(f) - \phi^*(\phi'(f)) + \phi^*\left(\sum_{A=1}^{\mathscr{I}_n} \lambda_A^n \psi_A\right) - f \sum_{A=1}^{\mathscr{I}_n} \lambda_A^n \psi_A\right] d\mathbf{k} = \\
&= \int_{\mathscr{B}r} \left[f\left(\phi'(f) - \sum_{A=1}^{\mathscr{I}_n} \lambda_A^n \psi_A\right) - \left(\phi^*(\phi'(f)) - \phi^*\left(\sum_{A=1}^{\mathscr{I}_n} \lambda_A^n \psi_A\right)\right)\right] d\mathbf{k}.
\end{aligned}$$

Since ϕ^* is strictly convex, it follows

$$\begin{aligned}
&\int_{\mathscr{B}r} \left[f\left(\phi'(f) - \sum_{A=1}^{\mathscr{I}_n} \lambda_A^n \psi_A\right) - \left(\phi^*(\phi'(f)) - \phi^*\left(\sum_{A=1}^{\mathscr{I}_n} \lambda_A^n \psi_A\right)\right)\right] d\mathbf{k} \leq \\
&\leq \int_{\mathscr{B}r} \left[f\left(\phi'(f) - \sum_{A=1}^{\mathscr{I}_n} \lambda_A^n \psi_A\right) - \phi^{*'}\left(\sum_{A=1}^{\mathscr{I}_n} \lambda_A^n \psi_A\right)\left(\phi'(f) - \sum_{A=1}^{\mathscr{I}_n} \lambda_A^n \psi_A\right)\right] d\mathbf{k} = \\
&= \int_{\mathscr{B}r} \left[\left(\phi'(f) - \sum_{A=1}^{\mathscr{I}_n} \lambda_A^n \psi_A\right)\left(f - \phi^{*'}\left(\sum_{A=1}^{\mathscr{I}_n} \lambda_A^n \psi_A\right)\right)\right] d\mathbf{k} \leq E_n mis(\mathscr{B}r).
\end{aligned}$$

The last inequality comes from the definition of E_n and the property that $\phi^{*'} = (\phi')^{-1} \in [0,1]$. Therefore,

$$\int_{\mathscr{B}r} \phi(f) d\mathbf{k} - V(\mathscr{D}_n) \leq E_n mis(\mathscr{B}r).$$

■

Corollary A.1. *Suppose that ϕ^* is twice differentiable and its second derivative is bounded above by some constant $J > 0$ on $\mathbb{R}$,Then*

$$V(\mathscr{D}_n) \geq \int_{\mathscr{B}r} \phi(f) d\mathbf{k} - J mis(\mathscr{B}r) E_n^2 \tag{A.10}$$

Proof. As in the proof of Theorem A.2, for $\lambda_A^n \in \mathbb{R}^{\kappa(A)}$, $A = 1, ..., \mathscr{I}_n$, we have

$$\int_{\mathscr{B}r} \phi(f) d\mathbf{k} - V(\mathscr{D}_n) \le \int_{\mathscr{B}r} \left[\left(\phi'(f) - \sum_{A=1}^{\mathscr{I}_n} \lambda_A^n \psi_A \right) \left(f - \phi^{*'} \left(\sum_{A=1}^{\mathscr{I}_n} \lambda_A^n \psi_A \right) \right) \right] d\mathbf{k} \le$$

$$\le E_n \int_{\mathscr{B}r} \left| f - \phi^{*'} \left(\sum_{A=1}^{\mathscr{I}_n} \lambda_A^n \psi_A \right) \right| d\mathbf{k} = E_n \int_{\mathscr{B}r} \left| \phi^{*'}(\phi'(f)) - \phi^{*'} \left(\sum_{A=1}^{\mathscr{I}_n} \lambda_A^n \psi_A \right) \right| d\mathbf{k} =$$

for some $v(\mathbf{k}) \in \left\{ \phi'(f), \sum_{A=1}^{\mathscr{I}_n} \lambda_A^n \psi_A \right\}$ using the Mean Value Theorem

$$= E_n \int_{\mathscr{B}r} \left| \phi^{*''}(v(\mathbf{k})) \left(\phi'(f) - \sum_{A=1}^{\mathscr{I}_n} \lambda_A^n \psi_A \right) \right| d\mathbf{k} \le J E_n \int_{\mathscr{B}r} \left| \phi'(f) - \sum_{A=1}^{\mathscr{I}_n} \lambda_A^n \psi_A \right| d\mathbf{k} \le J E_n^2 \, mis(\mathscr{B}r).$$

■

The proof of the next Theorem can be found in [6]. It supplies a necessary condition for f_n to be an optimum of $(\mathscr{P}_n)$.

Theorem A.3. *Suppose f_n is the optimal solution to $(\mathscr{P}_n)$. Let $\tilde{f}$ be any feasible solution for $(\mathscr{P}_n)$, then*

$$\int_{\mathscr{B}r} \phi'(f_n(\mathbf{k}))(\tilde{f}(\mathbf{k}) - f_n(\mathbf{k})) d\mathbf{k} \ge 0. \tag{A.11}$$

In particular, we have

$$\int_{\mathscr{B}r} \phi'(f_n(\mathbf{k}))(f(\mathbf{k}) - f_n(\mathbf{k})) d\mathbf{k} \ge 0. \tag{A.12}$$

If we further assume that (CQ) holds (stated in (A.4)), then equality holds in the above inequalities.

Theorems on norm convergence, in the sense of

$$\| f_n - f \|_p := \left(\int_{\mathscr{B}r} |f_n(\mathbf{k}) - f|^p d\mathbf{k} \right)^{\frac{1}{p}} \longrightarrow 0, \qquad 1 < p < +\infty \tag{A.13}$$

has been proved in [6, 66] assuming the strict convexity of the integral functional $I_\phi := \int_{\mathscr{B}_r} \phi(\mathbf{k}) d\mathbf{k}$. Here we want to prove a uniform convergence theorem for moment problems considered in this work. In the next result, we require the function ϕ to be in $C^2([0,1])$

Theorem A.4. *Let ϕ be twice continuously differentiable on $[0,1]$. Assume that for some constant $\eta > 0$, we have*

$$\phi''(g) \ge 2\eta, \quad \forall g \in [0,1].$$

Let f_n be the optimal solution to $(\mathscr{P}_n)$. Then

$$\int_{\mathscr{B}r} [\phi(f) - \phi(f_n)] d\mathbf{k} \ge \eta \| f - f_n \|_2^2 \tag{A.14}$$

Proof. By Theorem A.3 and the Mean Value Theorem,

$$\int_{\mathscr{B}r}[\phi(f)-\phi(f_n)]d\mathbf{k} \geq \int_{\mathscr{B}r}[\phi(f)-\phi(f_n)-\phi'(f_n(\mathbf{k}))(f(\mathbf{k})-f_n(\mathbf{k}))]d\mathbf{k} =$$
$$= \frac{1}{2}\int_{\mathscr{B}r}\phi''(\xi(\mathbf{k}))(f_n(\mathbf{k})-f(\mathbf{k}))^2 d\mathbf{k} \geq \eta\int_{\mathscr{B}r}(f_n(\mathbf{k})-f(\mathbf{k}))^2 d\mathbf{k} = \eta\|f_n-f\|_2^2,$$

for some $\xi \in \{f_n(\mathbf{k}), f(\mathbf{k})\} \subset (0,1)$.

■

A.0.2 Main Theorem

To relate norm convergence to uniform convergence, for given $\{\psi_A, A=1,...,\mathscr{I}_n\}$ and each $n \in \mathbb{N}$, we define some *renorming constants*

$$\Delta_{n,p} := \sup\left\{\frac{\|g\|_\infty}{\|g\|_p}, g \in span\{\psi_A, A=1,...,\mathscr{I}_n\}, g \neq 0\right\}. \tag{A.15}$$

Noting that

$$\|g\|_p \leq \|g\|_\infty (mis(\mathscr{B}r))^{\frac{1}{p}}$$

it is always true that

$$\Delta_{n,p} \geq (mis(\mathscr{B}r))^{-\frac{1}{p}} > 0 \tag{A.16}$$

Here, we will use only $\Delta_{n,2}$.

To obtain uniform bounds for $\{f_n - f\}$, we not only require (in Theorem A.4) ϕ to have the second derivative bounded below by $2\eta > 0$, but also must require ϕ^* to satisfy the following assumptions: for each fixed number $M > 0$, there exists a strictly positive and non increasing function $\Gamma_M : \mathbb{R}^+ \longrightarrow \mathbb{R}^+$, with

$$\liminf_{\xi \longrightarrow \infty} \Gamma_M(\xi)\xi > 0 \tag{A.17}$$

such that

$$|\phi^{*'}(u) - \phi^{*'}(v)| \geq \Gamma_M(|v|)|u-v|, \tag{A.18}$$

for any $u, v \in \mathbb{R}$, $|u| \leq M$.

Before establishing the main Theorem, we prove a Lemma.

Lemma A.1. *Let ϕ^* satisfy (A.17) and (A.18), let $u_n, v_n \in span\{\psi_A, A=1,...,\mathscr{I}_n\}$, and $\|u_n\|_\infty \leq M$, for some $M > 0$ and large enough n. Further suppose*

$$\Delta_{n,2}\|\phi^{*'}(u_n) - \phi^{*'}(v_n)\|_2 \longrightarrow 0 \qquad as\ n \longrightarrow \infty. \tag{A.19}$$

Then

$$\Delta_{n,2}\|u_n - v_n\|_2 \longrightarrow 0 \qquad as\ n \longrightarrow \infty. \tag{A.20}$$

Proof. By (A.18), for each $\mathbf{k} \in \mathscr{B}r$, we have

$$\begin{aligned} |\phi^{*'}(u_n(\mathbf{k})) - \phi^{*'}(v_n(\mathbf{k}))| &\geq \Gamma_M(|v_n(\mathbf{k})|)|u_n(\mathbf{k}) - v_n(\mathbf{k})| \geq \\ &\geq \Gamma_M(|v_n(\mathbf{k})| + \|u_n - v_n\|_\infty)|u_n(\mathbf{k}) - v_n(\mathbf{k})| \\ &\text{since } \Gamma_M \text{is nonincreasing} \\ &\geq \Gamma_M(|v_n(\mathbf{k})| + \Delta_{n,2}\|u_n - v_n\|_p)|u_n(\mathbf{k}) - v_n(\mathbf{k})| \\ &\text{by the definition of } \Delta_{n,2}. \end{aligned} \tag{A.21}$$

Then

$$\Delta_{n,2}\|\phi^{*'}(u_n) - \phi^{*'}(v_n)\|_2 \geq \Gamma_M(|v_n(\mathbf{k})| + \Delta_{n,2}\|u_n - v_n\|_p)\Delta_{n,2}\|u_n(\mathbf{k}) - v_n(\mathbf{k})\|_2. \tag{A.22}$$

Now we claim that $\{\Delta_{n,2}\|u_n(\mathbf{k}) - v_n(\mathbf{k})\|_2\}$ is boundend. If not, for some subsequence $\{n_i\}$ we have

$$\Delta_{n,2}\|u_{n_i}(\mathbf{k}) - v_{n_i}(\mathbf{k})\|_2 \longrightarrow \infty, \qquad \text{as } n_i \longrightarrow \infty \tag{A.23}$$

and hence

$$M + \Delta_{n,2}\|u_{n_i}(\mathbf{k}) - v_{n_i}(\mathbf{k})\|_2 \longrightarrow \infty. \qquad \text{as } n_i \longrightarrow \infty \tag{A.24}$$

By (A.17)

$$\liminf_{i \longrightarrow \infty} \Gamma_M(M + \Delta_{n,2}\|u_{n_i}(\mathbf{k}) - v_{n_i}(\mathbf{k})\|_2)(M + \Delta_{n,2}\|u_{n_i}(\mathbf{k}) - v_{n_i}(\mathbf{k})\|_2) > \liminf_{\xi \longrightarrow \infty} \Gamma(\xi)\xi > 0. \tag{A.25}$$

By (A.23) and since Γ_M is a nonincreasing function we obtain

$$\liminf_{i \longrightarrow \infty} \Gamma_M(M + \Delta_{n,2}\|u_{n_i}(\mathbf{k}) - v_{n_i}(\mathbf{k})\|_2)(\Delta_{n,2}\|u_{n_i}(\mathbf{k}) - v_{n_i}(\mathbf{k})\|_2) > 0$$

which is in contradiction with (A.19) and (A.22). Therefore $\{\Delta_{n,2}\|u_n - v_n\|_2\}$ is bounded, that is to say there exists $\overline{M}$ such that

$$\Delta_{n,2}\|u_n - v_n\|_2 \leq \overline{M}.$$

Therefore

$$\Gamma_M(\Delta_{n,2}\|u_{n_i}(\mathbf{k}) - v_{n_i}(\mathbf{k})\|_2) > \Gamma_M(\overline{M}) > 0$$

and consequently

$$\Gamma_M(M + \Delta_{n,2}\|u_{n_i}(\mathbf{k}) - v_{n_i}(\mathbf{k})\|_2) > \Gamma_M(M + \overline{M}) > 0.$$

Finally, from (A.19) and (A.22) we deduce

$$\Delta_{n,2}\|u_n - v_n\|_2 \longrightarrow 0 \qquad \text{as } n \longrightarrow \infty.$$

■

We are now able to prove the main Theorem.

Theorem A.5. *In problem (A.1) suppose that is the Fermi-Dirac type entropic function with its second derivative bounded below by $2\eta > 0$. Suppose that for each $M > 0$ there is a function $\Gamma_M : \mathbb{R}^+ \longrightarrow \mathbb{R}^+$ satisfying (A.17) and (A.18). Assume $f \in L^1(\mathscr{B}r)$, $\phi'(f) \in L^\infty(\mathscr{B}r)$, and*

$$\Delta_{n,2} E_n \longrightarrow 0, \qquad as\ n \longrightarrow \infty. \tag{A.26}$$

Let f_n be the optimal solution to $(\mathscr{P}_n)$. Then

$$\|\phi'(f) - \phi'(f_n)\|_\infty \longrightarrow 0, \qquad as\ n \longrightarrow \infty, \tag{A.27}$$

and also

$$\|f - f_n\|_\infty \longrightarrow 0, \qquad as\ n \longrightarrow \infty. \tag{A.28}$$

Proof. We choose $\lambda_A^n \in \mathbb{R}^{\kappa(A)}, A = 1, 2, ..., n$ so that

$$\left\| \phi'(f) - \sum_A \lambda_A^n \psi_A \right\|_\infty = E_n \tag{A.29}$$

then

$$\left\| \sum_A \lambda_A^n \psi_A \right\|_\infty \leq E_n + \|\phi'(f)\|_\infty. \tag{A.30}$$

By Theorem A.4

$$\int_{\mathscr{B}r} [\phi(f) - \phi(f_n)] d\mathbf{k} \geq \eta \|f - f_n\|_2^2. \tag{A.31}$$

Note that $\phi'' \geq \eta > 0$ implies $\phi^{*''} \leq \frac{1}{\eta} < \infty$ from the property $\phi^{*'} \equiv (\phi')^{-1}$. As in the proof of corollary A.1, we have

$$\int_{\mathscr{B}r} \phi(f) d\mathbf{k} - V(\mathscr{D}_n) \leq \int_{\mathscr{B}r} \left[\left(\phi'(f) - \sum_{A=1}^{\mathscr{I}_n} \lambda_A^n \psi_A \right) \left(f - \phi^{*'} \left(\sum_{A=1}^{\mathscr{I}_n} \lambda_A^n \psi_A \right) \right) \right] d\mathbf{k} \leq$$

$$\leq E_n \int_{\mathscr{B}r} \left| f - \phi^{*'} \left(\sum_{A=1}^{\mathscr{I}_n} \lambda_A^n \psi_A \right) \right| d\mathbf{k} = E_n \int_{\mathscr{B}r} \left| \phi^{*'}(\phi'(f)) - \phi^{*'} \left(\sum_{A=1}^{\mathscr{I}_n} \lambda_A^n \psi_A \right) \right| d\mathbf{k} =$$

for some $v(\mathbf{k}) \in \left\{ \phi'(f), \sum_{A=1}^{\mathscr{I}_n} \lambda_A^n \psi_A \right\}$ using the Mean Value Theorem

$$= E_n \int_{\mathscr{B}r} \left| \phi^{*''}(v(\mathbf{k})) \left(\phi'(f) - \sum_{A=1}^{\mathscr{I}_n} \lambda_A^n \psi_A \right) \right| d\mathbf{k} \leq \frac{1}{\eta} E_n \int_{\mathscr{B}r} \left| \phi'(f) - \sum_{A=1}^{\mathscr{I}_n} \lambda_A^n \psi_A \right| d\mathbf{k} \leq \frac{1}{\eta} E_n^2\, mis(\mathscr{B}r).$$

Since $V(\mathscr{P}_n) \geq V(\mathscr{D}_n)$ and f_n is the optimal solution to $(\mathscr{P}_n)$ then

$$\int_{\mathscr{B}r} \phi(f) d\mathbf{k} - V(\mathscr{P}_n) = \int_{\mathscr{B}r} (\phi(f) - \phi(f_n)) d\mathbf{k} \leq \frac{1}{\eta} E_n^2\, mis(\mathscr{B}r). \tag{A.32}$$

Then (A.31), (A.32) lead to

$$\eta^2 \|f - f_n\|_2^2 \leq E_n^2\, mis(\mathscr{B}r),$$

consequently

$$\Delta_{n,2} \eta \|f - f_n\|_2 \leq \Delta_{n,2} E_n \sqrt{mis(\mathscr{B}r)}. \tag{A.33}$$

From (A.26) we get

$$\Delta_{n,2}\|f-f_n\|_2 \longrightarrow 0 \qquad \text{as } n \longrightarrow \infty. \tag{A.34}$$

Let consider the following quantity

$$\Delta_{n,2}\left\|\phi^{*'}(\phi'(f_n))-\phi^{*'}\left(\sum_{A=1}^{\mathscr{I}_n}\lambda_A^n\psi_A\right)\right\|_2.$$

Since $\phi^{*'}=(\phi')^{-1}$ we have

$$\Delta_{n,2}\left\|\phi^{*'}(\phi'(f_n))-\phi^{*'}\left(\sum_{A=1}^{\mathscr{I}_n}\lambda_A^n\psi_A\right)\right\|_2=\Delta_{n,2}\left\|f_n-\phi^{*'}\left(\sum_{A=1}^{\mathscr{I}_n}\lambda_A^n\psi_A\right)\right\|_2\leq$$

$$\leq\Delta_{n,2}\left(\|f_n-f\|_2+\left\|f-\phi^{*'}\left(\sum_{A=1}^{\mathscr{I}_n}\lambda_A^n\psi_A\right)\right\|_2\right)=\Delta_{n,2}\left(\|f_n-f\|_2+\left\|\phi^{*'}(\phi'(f))-\phi^{*'}\left(\sum_{A=1}^{\mathscr{I}_n}\lambda_A^n\psi_A\right)\right\|_2\right)\leq$$

by the Mean Value Theorem there exists $\xi(\mathbf{k})\in\{\phi'(f),\sum_{A=1}^{\mathscr{I}_n}\lambda_A^n\psi_A\}$ such that

$$\leq\Delta_{n,2}\left(\|f_n-f\|_2+\left\|\phi^{*''}(\xi(\mathbf{k}))\left(\phi'(f)-\left(\sum_{A=1}^{\mathscr{I}_n}\lambda_A^n\psi_A\right)\right)\right\|_2\right)\leq\Delta_{n,2}\left(\|f_n-f\|_2+\frac{1}{\eta}E_n^2\,mis(\mathscr{B}r)\right).$$

Using (A.26) and (A.34) we get

$$\Delta_{n,2}\left\|\phi^{*'}(\phi'(f_n))-\phi^{*'}\left(\sum_{A=1}^{\mathscr{I}_n}\lambda_A^n\psi_A\right)\right\|_2\longrightarrow 0 \qquad \text{as } n\longrightarrow\infty. \tag{A.35}$$

Since $\phi'(f_n),\sum_A\lambda_A^n\psi_A\in span(\psi_A,A=1,...,\mathscr{I}_n)$ and

$$\left\|\sum_{A=1}^{\mathscr{I}_n}\lambda_A\psi_A\right\|_\infty\leq\|\phi'(f)\|_\infty+E_n<+\infty, \tag{A.36}$$

using Lemma (A.1) we have

$$\Delta_{n,2}\left\|\phi'(f_n)-\sum_A\lambda_A^n\psi_A\right\|_2\longrightarrow 0,\text{as } n\longrightarrow\infty. \tag{A.37}$$

By definition of $\Delta_{n,2}$

$$\left\|\phi'(f_n)-\sum_A\lambda_A^n\psi_A\right\|_\infty\leq\Delta_{n,2}\left\|\phi'(f_n)-\sum_A\lambda_A^n\psi_A\right\|_2. \tag{A.38}$$

Hence

$$\left\|\phi'(f_n)-\sum_A\lambda_A^n\psi_A\right\|_\infty\longrightarrow 0,\text{as } n\longrightarrow\infty. \tag{A.39}$$

Therefore, since

$$\|\phi'(f_n)-\phi'(f)\|_\infty\leq\left\|\phi'(f_n)-\sum_A\lambda_A^n\psi_A\right\|_\infty+\left\|\sum_A\lambda_A^n\psi_A-\phi'(f)\right\|_\infty=\left\|\phi'(f_n)-\sum_A\lambda_A^n\psi_A\right\|_\infty+E_n$$

by (A.39) we have

$$\left\|\phi'(f_n)-\phi'(f)\right\|_\infty \longrightarrow 0 \qquad \text{as } n \longrightarrow \infty. \tag{A.40}$$

In order to prove (A.40) we had to require $E_n \longrightarrow 0$ which is true if $\phi'(f) \in \overline{span}\{\psi_A, A \in \cup_{n=0}^{\infty}\mathscr{I}_n\} \supset L^1(\mathscr{B}_r)$.

In conclusion, applying the Mean Value Theorem and $\phi^{*''} \leq \frac{1}{\eta} < \infty$ we obtain

$$\|f_n - f\|_\infty = \left\|\phi^{*'}(\phi'(f_n)) - \phi^{*'}(\phi'(f))\right\|_\infty \leq \frac{1}{\eta}\left\|\phi'(f_n)-\phi'(f)\right\|_\infty. \tag{A.41}$$

Using (A.40) we have

$$\|f_n - f\|_\infty \longrightarrow 0 \qquad \text{as } n \longrightarrow \infty.$$

■

In our case, it easy to check that

$$\phi''(f) = \frac{1}{f} + \frac{1}{1-f} \geq 4.$$

To make Theorem A.5 applicable, we only need to check the existence of Γ_M which satisfies (A.17) and (A.18). We can derive following inequality using elementary calculations.

Lemma A.2. *For any $C > 0$, $T_0 > 0$, the following inequality is true for $|t| \leq T_0$:*

$$\frac{|1-e^t|}{C+e^t} \geq \frac{|t|}{(C+1)(T_0+1)}. \tag{A.42}$$

Proof. Recall that

$$e^t \geq t-1 \qquad \text{for all} t \in \mathbb{R} \tag{A.43}$$

For fixed values of $C > 0$ and $T_0 > 0$ such that $|t| \leq T_0$:

- If $t \geq 0$, using the relation (A.43) we get

$$\frac{|1-e^t|}{C+e^t} = \frac{e^t-1}{C+e^t} = 1 - \frac{C+1}{C+e^t} \geq 1 - \frac{C+1}{C+t+1} = \frac{t}{C+t+1} \geq \frac{t}{(C+T_0)(T_0+1)}.$$

  The last inequality follows because $C+t+1 \leq C+T_0+1 \leq C+CT_0+T_0+1$.

- If $t < 0$ the same considerations of the previous case hold.

■

Proposition A.2. *For ϕ defined in (A.2) there exists a function Γ_M satisfying (A.17) and (A.18).*

Proof. We computed that

$$\phi^*(g) = \ln(1+e^g)$$

and

$$\phi^{*'}(g) = \frac{e^g}{1+e^g}$$

for any $h, g \in \mathbb{R}$ and $|h| \le M$, we have

$$|\phi^{*'}(h) - \phi^{*'}(g)| = \left|\frac{e^h}{1+e^h} - \frac{e^g}{1+e^g}\right| = \frac{1}{1+e^h}\left|\frac{e^h - e^g}{1+e^g}\right| = \frac{1}{1+e^h}\left|\frac{1-e^{g-h}}{e^{-h}+e^{g-h}}\right| \ge$$
$$\frac{1}{1+e^M}\left|\frac{1-e^{g-h}}{e^M+e^{g-h}}\right| \ge \frac{1}{(1+e^M)^2}\frac{|g-h|}{M+|h|+1} := \Gamma_M(|h|)\,|g-h|$$

The last inequalities is given by applying the previous Lemma with $t = g-h$, $T_0 = M+|h|$ and $C = e^M$.

It easy to see that Γ_M is a nonnegative and decreasing function and

$$\lim_{\xi \to \infty} \Gamma_M(\xi)\xi = \frac{1}{(1+e^M)^2} > 0,$$

and (A.17) follows.

■

APPENDIX B

NON-LINEAR CLOSURE RELATIONS FOR THE 6 MOMENT MODEL

Assuming that the Lagrangian multipliers $\lambda_{\mathbf{V}}$ and $\lambda_{\mathbf{S}}$ are collinear, we choose a reference frame $(\mathbf{e_1}, \mathbf{e_2})$ in a way that $\lambda_{\mathbf{V}} = \lambda_V \, \mathbf{e_1}$, $\lambda_{\mathbf{S}} = \lambda_S \, \mathbf{e_1}$, $\mathbf{E} = E \, \mathbf{e_1}$ and introduce polar coordinates $(\mathscr{E}, \phi)$; taking into account the dispersion relation (1.2), the wave vector $\mathbf{k}$ can be written in terms of the energy $\mathscr{E}$ and the angle ϕ

$$\mathbf{k} = \frac{\mathscr{E}}{\hbar v_F} \left(\cos\phi \, \mathbf{e_1} + \sin\phi \, \mathbf{e_2} \right).$$

Therefore

$$d\mathbf{k} = k \, dk \, d\phi = \frac{\mathscr{E}}{(\hbar v_F)^2} d\mathscr{E} \, d\phi$$

with $\mathscr{E} \in [0, +\infty[$ and $\phi \in [0, 2\pi]$.

Explicitly we have

$$f_{MEP}(\mathbf{r}, \mathbf{k}, t) = \frac{1}{1 + \exp(\lambda + \lambda_w \mathscr{E} + v_F \cos\phi (\lambda_{\mathbf{V}} + \mathscr{E} \lambda_{\mathbf{S}}))} \tag{B.1}$$

where $\mathbf{v} = v_F \cos\phi \, \mathbf{e_1} + v_F \sin\phi \, \mathbf{e_2}$.

The constraints read

$$n = \frac{2}{(2\pi\hbar v_F)^2} \int_0^{2\pi} d\phi \int_0^{+\infty} \frac{\mathscr{E} d\mathscr{E}}{1 + exp(\lambda + \lambda_w \mathscr{E} + v_F \cos\phi (\lambda_{\mathbf{V}} + \mathscr{E} \lambda_{\mathbf{S}})}, \tag{B.2}$$

$$nW = \frac{2}{(2\pi\hbar v_F)^2} \int_0^{2\pi} d\phi \int_0^{+\infty} \frac{\mathscr{E}^2 d\mathscr{E}}{1 + exp(\lambda + \lambda_w \mathscr{E} + v_F \cos\phi (\lambda_{\mathbf{V}} + \mathscr{E} \lambda_{\mathbf{S}})}, \tag{B.3}$$

$$n\mathbf{V} = \frac{2}{(2\pi\hbar)^2 v_F} \int_0^{2\pi} d\phi \int_0^{+\infty} \frac{\mathscr{E} \cos\phi d\mathscr{E}}{1 + exp(\lambda + \lambda_w \mathscr{E} + v_F \cos\phi (\lambda_{\mathbf{V}} + \mathscr{E} \lambda_{\mathbf{S}})} \mathbf{e_1}, \tag{B.4}$$

$$n\mathbf{S} = \frac{2}{(2\pi\hbar)^2 v_F} \int_0^{2\pi} d\phi \int_0^{+\infty} \frac{\mathscr{E}^2 \cos\phi d\mathscr{E}}{1 + exp(\lambda + \lambda_w \mathscr{E} + v_F \cos\phi (\lambda_{\mathbf{V}} + \mathscr{E} \lambda_{\mathbf{S}})} \mathbf{e_1}, \tag{B.5}$$

The other terms of the evolution equations can be estimated by f_{MEP} as

$$n\mathbf{G}^{(0)} : E\mathbf{e_1} = \frac{E}{2\hbar^2\pi^2}\int_0^{2\pi} d\phi \int_0^{+\infty} \frac{d\mathscr{E}\sin^2\phi}{1+\exp(\lambda+\lambda_w\mathscr{E}+v_F\cos\phi(\lambda_{\mathbf{V}}+\mathscr{E}\lambda_{\mathbf{S}})}\mathbf{e_1}, \tag{B.6}$$

$$n\mathbf{G}^{(1)} : E\mathbf{e_1} = \frac{E}{2\hbar^2\pi^2}\int_0^{2\pi} d\phi \int_0^{+\infty} \frac{\mathscr{E}d\mathscr{E}}{1+\exp(\lambda+\lambda_w\mathscr{E}+v_F\cos\phi(\lambda_{\mathbf{V}}+\mathscr{E}\lambda_{\mathbf{S}})}\mathbf{e_1}. \tag{B.7}$$

B.0.0.1 Production terms

Regarding the production terms, the estimators listed below are obtained.

The productions arising from the scattering with acoustic phonons are

$$nC_n^{(ac)} = 0, \tag{B.8}$$

$$nC_W^{(ac)} = 0, \tag{B.9}$$

$$nC_{\mathbf{V}}^{(ac)} = -\frac{A^{(ac)}}{8\pi^3\hbar^4 v_F^3}\left\{\int_0^{+\infty} d\mathscr{E}\int_0^{2\pi}\cos\psi\mathscr{E}^2 f(\mathscr{E},\psi,t)d\psi\right\}\mathbf{e_1}, \tag{B.10}$$

$$nC_{\mathbf{S}}^{(ac)} = -\frac{A^{(ac)}}{8\pi^3\hbar^4 v_F^3}\left\{\int_0^{+\infty} d\mathscr{E}\int_0^{2\pi}\cos\psi\mathscr{E}^3 f(\mathscr{E},\psi,t)d\psi\right\}\mathbf{e_1}, \tag{B.11}$$

where $\psi = \phi + \theta''$ and, recalling that θ'' is the angle between $\mathbf{k}$ and $\mathbf{k}'$,

$$\mathbf{k}' = \frac{\mathscr{E}'}{\hbar v_F}\left[\cos(\phi+\theta'')\mathbf{e_1} + \sin(\phi+\theta'')\mathbf{e_2}\right].$$

We set $\beta = \dfrac{1}{k_B T_L}$ and denote by H the Heaviside function. The productions arising from the scattering with optical phonons are

$$nC_n^{(OP)} = 0, \tag{B.12}$$

$$\begin{aligned} nC_W^{(OP)} = &\frac{A^{OP}D_\Gamma^2 N_B^{OP}}{4\hbar^4 v_F^4\pi^4}\int_0^{2\pi} d\phi\int_0^{+\infty}\mathscr{E}^2 d\mathscr{E}\int_0^{2\pi} d\theta''\{[f(\mathscr{E}-\hbar\omega,\mathbf{e}')(1-f(\mathscr{E},\mathbf{e}))(\mathscr{E}-\hbar\omega)H(\mathscr{E}-\hbar\omega)\\ &+ e^{\beta\hbar\omega}f(\mathscr{E}+\hbar\omega,\mathbf{e}')(1-f(\mathscr{E},\mathbf{e}))(\mathscr{E}+\hbar\omega)\Big]\\ &-\Big[e^{\beta\hbar\omega}f(\mathscr{E},\mathbf{e})(1-f(\mathscr{E}-\hbar\omega,\mathbf{e}'))(\mathscr{E}-\hbar\omega)H(\mathscr{E}-\hbar\omega)\\ &+ f(\mathscr{E},\mathbf{e})(1-f(\mathscr{E}+\hbar\omega,\mathbf{e}'))(\mathscr{E}+\hbar\omega)]\}, \end{aligned} \tag{B.13}$$

$$\begin{aligned} nC_{\mathbf{V}}^{(OP)} = &\frac{A^{OP}D_\Gamma^2 N_B^{OP}}{4\hbar^4 v_F^3\pi^4}\int_0^{2\pi} d\phi\int_0^{+\infty}\mathscr{E}d\mathscr{E}\int_0^{2\pi}\cos\phi\, d\theta''\{[f(\mathscr{E}-\hbar\omega,\mathbf{e}')(1-f(\mathscr{E},\mathbf{e}))(\mathscr{E}-\hbar\omega)H(\mathscr{E}-\hbar\omega)\\ &+ e^{\beta\hbar\omega}f(\mathscr{E}+\hbar\omega,\mathbf{e}')(1-f(\mathscr{E},\mathbf{e}))(\mathscr{E}+\hbar\omega)\Big]\\ &-\Big[e^{\beta\hbar\omega}f(\mathscr{E},\mathbf{e})(1-f(\mathscr{E}-\hbar\omega,\mathbf{e}'))(\mathscr{E}-\hbar\omega)H(\mathscr{E}-\hbar\omega)\\ &+ f(\mathscr{E},\mathbf{e})(1-f(\mathscr{E}+\hbar\omega,\mathbf{e}'))(\mathscr{E}+\hbar\omega)]\}\mathbf{e_1}, \end{aligned} \tag{B.14}$$

$$\begin{aligned} nC_{\mathbf{S}}^{(OP)} = &\frac{A^{OP}D_\Gamma^2 N_B^{OP}}{4\hbar^4 v_F^3\pi^4}\int_0^{2\pi} d\phi\int_0^{+\infty}\mathscr{E}^2 d\mathscr{E}\int_0^{2\pi}\cos\phi\, d\theta''\{[f(\mathscr{E}-\hbar\omega,\mathbf{e}')(1-f(\mathscr{E},\mathbf{e}))(\mathscr{E}-\hbar\omega)H(\mathscr{E}-\hbar\omega)\\ &+ e^{\beta\hbar\omega}f(\mathscr{E}+\hbar\omega,\mathbf{e}')(1-f(\mathscr{E},\mathbf{e}))(\mathscr{E}+\hbar\omega)\Big]\\ &-\Big[e^{\beta\hbar\omega}f(\mathscr{E},\mathbf{e})(1-f(\mathscr{E}-\hbar\omega,\mathbf{e}'))(\mathscr{E}-\hbar\omega)H(\mathscr{E}-\hbar\omega)\\ &+ f(\mathscr{E},\mathbf{e})(1-f(\mathscr{E}+\hbar\omega,\mathbf{e}'))(\mathscr{E}+\hbar\omega)]\}\mathbf{e_1}, \end{aligned} \tag{B.15}$$

In the previous relations $\mathbf{e} = \cos\phi\,\mathbf{e_1} + \sin\phi\,\mathbf{e_2}$ while $\mathbf{e}' = \cos\psi\,\mathbf{e_1} + \sin\psi\,\mathbf{e_2}$.

The productions arising from the scattering with K-phonons are

$$nC_n^{(K)} = 0, \tag{B.16}$$

$$\begin{aligned} nC_W^{(K)} = {} & \frac{A^K D_K^2 N_B^K}{8\pi^4\hbar^4 v_F^4}\int_0^{2\pi} d\phi \int_0^{+\infty} d\mathscr{E}\,\left\{\int_0^{2\pi} d\theta''(1-\cos\theta'')\left[\mathscr{E}^2(\mathscr{E}-\hbar\omega)f(\mathscr{E}-\hbar\omega,\mathbf{e}')(1-f(\mathscr{E},\mathbf{e}))H(\mathscr{E}-\hbar\omega)\right.\right. \\ & \left. +\mathscr{E}^2 e^{\beta\hbar\omega}(\mathscr{E}+\hbar\omega)f(\mathscr{E}+\hbar\omega,\mathbf{e}')(1-f(\mathscr{E},\mathbf{e}))\right] \\ & \left. -\int_0^{2\pi} d\theta''(1-\cos\theta'')\left[\mathscr{E}^2 e^{\beta\hbar\omega} f(\mathscr{E},\mathbf{e})(1-f(\mathscr{E}-\hbar\omega),\mathbf{e}')(\mathscr{E}-\hbar\omega)H(\mathscr{E}-\hbar\omega)+\mathscr{E}^2 f(\mathscr{E},\mathbf{e})(1-f(\mathscr{E}+\hbar\omega,\mathbf{e}'))(\mathscr{E}+\hbar\omega)\right]\right\}, \end{aligned} \tag{B.17}$$

$$\begin{aligned} nC_{\mathbf{V}}^{(K)} = {} & \frac{A^K D_K^2 N_B^K}{8\pi^4\hbar^4 v_F^2}\int_0^{2\pi} d\phi \int_0^{+\infty} \left\{\int_0^{2\pi} d\theta''(1-\cos\theta'')\left[(\mathscr{E}-\hbar\omega)f(\mathscr{E}-\hbar\omega,\mathbf{e}')(1-f(\mathscr{E},\mathbf{e}))H(\mathscr{E}-\hbar\omega)\right.\right. \\ & \left. + e^{\beta\hbar\omega}(\mathscr{E}+\hbar\omega)f(\mathscr{E}+\hbar\omega,\mathbf{e}')(1-f(\mathscr{E},\mathbf{e}))\right] \\ & \left. -\int_0^{2\pi} d\theta''(1-\cos\theta'')\left[e^{\beta\hbar\omega} f(\mathscr{E},\mathbf{e})(1-f(\mathscr{E}-\hbar\omega),\mathbf{e}')(\mathscr{E}-\hbar\omega)H(\mathscr{E}-\hbar\omega)+f(\mathscr{E},\mathbf{e})(1-f(\mathscr{E}+\hbar\omega,\mathbf{e}'))(\mathscr{E}+\hbar\omega)\right]\right\}\mathscr{E}\cos\phi\,d\mathscr{E}\mathbf{e_1}, \end{aligned} \tag{B.18}$$

$$\begin{aligned} nC_{\mathbf{S}}^{(K)} = {} & \frac{A^K D_K^2 N_B^K}{8\pi^4\hbar^4 v_F^2}\int_0^{2\pi} d\phi \int_0^{+\infty} \left\{\int_0^{2\pi} d\theta''(1-\cos\theta'')\left[(\mathscr{E}-\hbar\omega)f(\mathscr{E}-\hbar\omega,\mathbf{e}')(1-f(\mathscr{E},\mathbf{e}))H(\mathscr{E}-\hbar\omega)\right.\right. \\ & \left. +e^{\beta\hbar\omega}(\mathscr{E}+\hbar\omega)f(\mathscr{E}+\hbar\omega,\mathbf{e}')(1-f(\mathscr{E},\mathbf{e}))\right] \\ & \left. -\int_0^{2\pi} d\theta''(1-\cos\theta'')\left[e^{\beta\hbar\omega} f(\mathscr{E},\mathbf{e})(1-f(\mathscr{E}-\hbar\omega),\mathbf{e}')(\mathscr{E}-\hbar\omega)H(\mathscr{E}-\hbar\omega)+f(\mathscr{E},\mathbf{e})(1-f(\mathscr{E}+\hbar\omega,\mathbf{e}'))(\mathscr{E}+\hbar\omega)\right]\right\}\mathscr{E}^2\cos\phi\,d\mathscr{E}\mathbf{e_1}, \end{aligned} \tag{B.19}$$

APPENDIX C

CLOSURE RELATIONS FOR MODEL WITH AN ARBITRARY NUMBER OF MOMENTS: THE CASE OF MOMENTS BASED ON ENERGY POWERS

One of the advantages of linearization lies in the fact that the field variables can be expressed as the sum of integrals. Therefore it is possible to calculate each addend with respect to a suitable base, greatly simplifying the calculations. For example, the average velocity

$$n\mathbf{V} = \frac{2}{(2\pi)^2}\int_{\mathbb{R}^2}\left(\frac{1}{1+e^{\lambda+\lambda_w\mathscr{E}}} - \frac{e^{\lambda+\lambda_w\mathscr{E}}}{(1+e^{\lambda+\lambda_w\mathscr{E}})^2}(\lambda_{\mathbf{V}} + \mathscr{E}\lambda_{\mathbf{S}} + \mathscr{E}^2\lambda_{\mathbf{S}}^{(2)} + \ldots + \mathscr{E}^N\lambda_{\mathbf{S}}^{(N)})\right)\mathbf{v}(\mathbf{k})d\mathbf{k},$$

can be written in this way

$$\begin{aligned} n\mathbf{V} = \frac{2}{(2\pi)^2}\Bigg(&\int_{\mathbb{R}^2}\frac{1}{1+e^{\lambda+\lambda_w\mathscr{E}}}\mathbf{v}(\mathbf{k})d\mathbf{k} - \int_{\mathbb{R}^2}\frac{e^{\lambda+\lambda_w\mathscr{E}}}{(1+e^{\lambda+\lambda_w\mathscr{E}})^2}\lambda_{\mathbf{V}}\cdot\mathbf{v}(\mathbf{k})d\mathbf{k} - \int_{\mathbb{R}^2}\frac{e^{\lambda+\lambda_w\mathscr{E}}}{(1+e^{\lambda+\lambda_w\mathscr{E}})^2}\lambda_{\mathbf{S}}\cdot\mathscr{E}\mathbf{v}(\mathbf{k})d\mathbf{k} + \ldots \\ &+ \int_{\mathbb{R}^2}\frac{e^{\lambda+\lambda_w\mathscr{E}}}{(1+e^{\lambda+\lambda_w\mathscr{E}})^2}\lambda_{\mathbf{S}^{(N)}}\cdot\mathscr{E}^N\mathbf{v}(\mathbf{k})d\mathbf{k}\Bigg). \end{aligned} \tag{C.1}$$

The integral

$$\int_{\mathbb{R}^2}\frac{e^{\lambda+\lambda_w\mathscr{E}}}{(1+e^{\lambda+\lambda_w\mathscr{E}})^2}\lambda_{\mathbf{V}}\cdot\mathbf{v}(\mathbf{k})d\mathbf{k},$$

can be evaluated by using a base adapted to $\lambda_{\mathbf{V}}$, i.e. we introduce a reference frame $(\mathbf{e_1},\mathbf{e_2})$ such that $\lambda_{\mathbf{V}} = \lambda_V\mathbf{e_1}$ and we use adapted polar coordinates for $\mathbf{v}$:

$$\mathbf{v} = v_F cos\phi\mathbf{e_1} + v_F\sin\phi\mathbf{e_2}.$$

Analogously the addend

$$\int_{\mathbb{R}^2}\frac{e^{\lambda+\lambda_w\mathscr{E}}}{(1+e^{\lambda+\lambda_w\mathscr{E}})^2}\lambda_{\mathbf{S}}\cdot\mathscr{E}\mathbf{v}(\mathbf{k})d\mathbf{k},$$

can be evaluated by using a base adapted to $\lambda_{\mathbf{S}}$. The same considerations holds to the remaining addends.

Thus, the relations between fields and Lagrange multipliers are given by

$$n = \frac{1}{\pi\hbar^2 v_F^2}\int_0^{+\infty}\frac{\mathscr{E}}{1+e^{\lambda+\lambda_w\mathscr{E}}}\,d\mathscr{E}, \tag{C.2}$$

$$nW = \frac{1}{\pi\hbar^2 v_F^2}\int_0^{+\infty}\frac{\mathscr{E}^2}{1+e^{\lambda+\lambda_w\mathscr{E}}}\,d\mathscr{E}, \tag{C.3}$$

$$\begin{aligned} n\mathbf{V} &= -\frac{1}{2\pi\hbar^2 v_F}\int_0^{+\infty}\frac{\mathscr{E}e^{\lambda+\lambda_w\mathscr{E}}}{(1+e^{\lambda+\lambda_w\mathscr{E}})^2}(\lambda_{\mathbf{V}}+\mathscr{E}\lambda_{\mathbf{S}}+\mathscr{E}^2\lambda_{\mathbf{S^{(2)}}}+\cdots+\mathscr{E}^N\lambda_{\mathbf{S^{(N)}}})d\mathscr{E} = \\ &= -\frac{1}{2\pi\hbar^2 v_F}\left\{\int_0^{+\infty}\frac{\mathscr{E}e^{\lambda+\lambda_w\mathscr{E}}}{(1+e^{\lambda+\lambda_w\mathscr{E}})^2}d\mathscr{E}\lambda_{\mathbf{V}}+\int_0^{+\infty}\frac{\mathscr{E}^2e^{\lambda+\lambda_w\mathscr{E}}}{(1+e^{\lambda+\lambda_w\mathscr{E}})^2}d\mathscr{E}\lambda_{\mathbf{S}}+\right. \\ &\left.+\int_0^{+\infty}\frac{\mathscr{E}^3e^{\lambda+\lambda_w\mathbb{E}}}{(1+e^{\lambda+\lambda_w\mathscr{E}})^2}d\mathscr{E}\lambda_{\mathbf{S^{(2)}}}+\cdots+\int_0^{+\infty}\frac{\mathscr{E}^{N+1}e^{\lambda+\lambda_w\mathscr{E}}}{(1+e^{\lambda+\lambda_w\mathscr{E}})^2}d\mathscr{E}\lambda_{\mathbf{S^{(N)}}}\right\} \end{aligned} \tag{C.4}$$

$$\begin{aligned} n\mathbf{S} &= -\frac{1}{2\pi\hbar^2}\int_0^{+\infty}\frac{\mathscr{E}^2e^{\lambda+\lambda_w\mathscr{E}}}{(1+e^{\lambda+\lambda_w\mathscr{E}})^2}(\lambda_{\mathbf{V}}+\mathscr{E}\lambda_{\mathbf{S}}+\mathscr{E}^2\lambda_{\mathbf{S^{(2)}}}+\cdots+\mathscr{E}^N\lambda_{\mathbf{S^{(N)}}})d\mathscr{E} = \\ &= -\frac{1}{2\pi\hbar^2 v_F}\left\{\int_0^{+\infty}\frac{\mathscr{E}^2e^{\lambda+\lambda_w\mathscr{E}}}{(1+e^{\lambda+\lambda_w\mathscr{E}})^2}d\mathscr{E}\lambda_{\mathbf{V}}+\int_0^{+\infty}\frac{\mathscr{E}^3e^{\lambda+\lambda_w\mathscr{E}}}{(1+e^{\lambda+\lambda_w\mathscr{E}})^2}d\mathscr{E}\lambda_{\mathbf{S}}+\right. \\ &\left.+\int_0^{+\infty}\frac{\mathscr{E}^4e^{\lambda+\lambda_w\mathscr{E}}}{(1+e^{\lambda+\lambda_w\mathscr{E}})^2}d\mathscr{E}\lambda_{\mathbf{S^{(2)}}}+\cdots+\int_0^{+\infty}\frac{\mathscr{E}^{N+2}e^{\lambda+\lambda_w\mathscr{E}}}{(1+e^{\lambda+\lambda_w\mathscr{E}})^2}d\mathscr{E}\lambda_{\mathbf{S^{(N)}}}\right\} \end{aligned} \tag{C.5}$$

$$\begin{aligned} n\mathbf{S^{(2)}} &= -\frac{1}{2\pi\hbar^2}\int_0^{+\infty}\frac{\mathscr{E}^3e^{\lambda+\lambda_w\mathscr{E}}}{(1+e^{\lambda+\lambda_w\mathscr{E}})^2}(\lambda_{\mathbf{V}}+\mathscr{E}\lambda_{\mathbf{S}}+\mathscr{E}^2\lambda_{\mathbf{S^{(2)}}}+\cdots+\mathscr{E}^N\lambda_{\mathbf{S^{(N)}}})d\mathscr{E} = \\ &= -\frac{1}{2\pi\hbar^2 v_F}\left\{\int_0^{+\infty}\frac{\mathscr{E}^3e^{\lambda+\lambda_w\mathscr{E}}}{(1+e^{\lambda+\lambda_w\mathscr{E}})^2}d\mathscr{E}\lambda_{\mathbf{V}}+\int_0^{+\infty}\frac{\mathscr{E}^4e^{\lambda+\lambda_w\mathscr{E}}}{(1+e^{\lambda+\lambda_w\mathscr{E}})^2}d\mathscr{E}\lambda_{\mathbf{S}}+\right. \\ &\left.+\int_0^{+\infty}\frac{\mathscr{E}^5e^{\lambda+\lambda_w\mathscr{E}}}{(1+e^{\lambda+\lambda_w\mathscr{E}})^2}d\mathscr{E}\lambda_{\mathbf{S^{(2)}}}+\cdots+\int_0^{+\infty}\frac{\mathscr{E}^{N+3}e^{\lambda+\lambda_w\mathscr{E}}}{(1+e^{\lambda+\lambda_w\mathscr{E}})^2}d\mathscr{E}\lambda_{\mathbf{S^{(N)}}}\right\} \end{aligned} \tag{C.6}$$

$$\vdots$$

$$\begin{aligned} n\mathbf{S^{(m)}} &= -\frac{1}{2\pi\hbar^2}\int_0^{+\infty}\frac{\mathscr{E}^{m+1}e^{\lambda+\lambda_w\mathscr{E}}}{(1+e^{\lambda+\lambda_w\mathscr{E}})^2}(\lambda_{\mathbf{V}}+\mathscr{E}\lambda_{\mathbf{S}}+\mathscr{E}^2\lambda_{\mathbf{S^{(2)}}}+\cdots+\mathscr{E}^N\lambda_{\mathbf{S^{(N)}}})d\mathscr{E} = \\ &= -\frac{1}{2\pi\hbar^2 v_F}\left\{\int_0^{+\infty}\frac{\mathscr{E}^{m+1}e^{\lambda+\lambda_w\mathscr{E}}}{(1+e^{\lambda+\lambda_w\mathscr{E}})^2}d\mathscr{E}\lambda_{\mathbf{V}}+\int_0^{+\infty}\frac{\mathscr{E}^{m+2}e^{\lambda+\lambda_w\mathscr{E}}}{(1+e^{\lambda+\lambda_w\mathscr{E}})^2}d\mathscr{E}\lambda_{\mathbf{S}}+\right. \\ &\left.+\int_0^{+\infty}\frac{\mathscr{E}^{m+3}e^{\lambda+\lambda_w\mathscr{E}}}{(1+e^{\lambda+\lambda_w\mathscr{E}})^2}d\mathscr{E}\lambda_{\mathbf{S^{(2)}}}+\cdots+\int_0^{+\infty}\frac{\mathscr{E}^{N+m+1}e^{\lambda+\lambda_w\mathscr{E}}}{(1+e^{\lambda+\lambda_w\mathscr{E}})^2}d\mathscr{E}\lambda_{\mathbf{S^{(N)}}}\right\} \end{aligned} \tag{C.7}$$

$$\vdots$$

$$\begin{aligned} n\mathbf{S^{(N)}} &= -\frac{1}{2\pi\hbar^2}\int_0^{+\infty}\frac{\mathscr{E}^{N+1}e^{\lambda+\lambda_w\mathscr{E}}}{(1+e^{\lambda+\lambda_w\mathscr{E}})^2}(\lambda_{\mathbf{V}}+\mathscr{E}\lambda_{\mathbf{S}}+\mathscr{E}^2\lambda_{\mathbf{S^{(2)}}}+\cdots+\mathscr{E}^N\lambda_{\mathbf{S^{(N)}}})d\mathscr{E} = \\ &= -\frac{1}{2\pi\hbar^2 v_F}\left\{\int_0^{+\infty}\frac{\mathscr{E}^{N+1}e^{\lambda+\lambda_w\mathscr{E}}}{(1+e^{\lambda+\lambda_w\mathscr{E}})^2}d\mathscr{E}\lambda_{\mathbf{V}}+\int_0^{+\infty}\frac{\mathscr{E}^{N+2}e^{\lambda+\lambda_w\mathscr{E}}}{(1+e^{\lambda+\lambda_w\mathscr{E}})^2}d\mathscr{E}\lambda_{\mathbf{S}}+\right. \\ &\left.+\int_0^{+\infty}\frac{\mathscr{E}^{N+3}e^{\lambda+\lambda_w\mathscr{E}}}{(1+e^{\lambda+\lambda_w\mathscr{E}})^2}d\mathscr{E}\lambda_{\mathbf{S^{(2)}}}+\cdots+\int_0^{+\infty}\frac{\mathscr{E}^{2n+1}e^{\lambda+\lambda_w\mathscr{E}}}{(1+e^{\lambda+\lambda_w\mathscr{E}})^2}d\mathscr{E}\lambda_{\mathbf{S^{(N)}}}\right\}. \end{aligned} \tag{C.8}$$

These relations have been obtained by writing the wave vector $\mathbf{k}$ in terms of energy $\mathscr{E}$ and the angle ϕ.

Regarding the relevant components of fluxes we have

$$\begin{aligned} nF_{11}^{(0)} &= \frac{2}{(2\pi)^2}\int_{\mathbb{R}^2} v_1 v_1 f_{MEP}(\mathbf{r},\mathbf{k},t)d^2\mathbf{k} = \frac{2v_F^2}{(2\pi\hbar v_F)^2}\int_0^{2\pi} d\phi \int_0^{+\infty} \mathscr{E}\, d\mathscr{E}\cos^2\phi f_{MEP}(\mathbf{r},\mathbf{k},t) \\ &\approx \frac{2\pi v_F^2}{(2\pi\hbar v_F)^2}\left\{\int_0^{+\infty}\frac{\mathscr{E}}{1+e^{\lambda+\lambda_w\mathscr{E}}}d\mathscr{E}\right\}, \end{aligned} \tag{C.9}$$

$$\begin{aligned} nF_{11}^{(1)} &= \frac{2}{(2\pi)^2}\int_{\mathbb{R}^2} \mathscr{E} v_1 v_1 f_{MEP}(\mathbf{r},\mathbf{k},t)d^2\mathbf{k} = \frac{2v_F^2}{(2\pi\hbar v_F)^2}\int_0^{2\pi} d\phi \int_0^{+\infty} \mathscr{E}^2\, d\mathscr{E}\cos^2\phi f_{MEP}(\mathbf{r},\mathbf{k},t) \\ &\approx \frac{2\pi v_F^2}{(2\pi\hbar v_F)^2}\left\{\int_0^{+\infty}\frac{\mathscr{E}^2}{1+e^{\lambda+\lambda_w\mathscr{E}}}d\mathscr{E}\right\}, \end{aligned} \tag{C.10}$$

$$\begin{aligned} nF_{11}^{(2)} &= \frac{2}{(2\pi)^2}\int_{\mathbb{R}^2} \mathscr{E}^2 v_1 v_1 f_{MEP}(\mathbf{r},\mathbf{k},t)d^2\mathbf{k} = \frac{2v_F^2}{(2\pi\hbar v_F)^2}\int_0^{2\pi} d\phi \int_0^{+\infty} \mathscr{E}^3\, d\mathscr{E}\cos^2\phi f_{MEP}(\mathbf{r},\mathbf{k},t) \\ &\approx \frac{2\pi v_F^2}{(2\pi\hbar v_F)^2}\left\{\int_0^{+\infty}\frac{\mathscr{E}^3}{1+e^{\lambda+\lambda_w\mathscr{E}}}d\mathscr{E}\right\}, \end{aligned} \tag{C.11}$$

$$\vdots$$

$$\begin{aligned} nF_{11}^{(N)} &= \frac{2}{(2\pi)^2}\int_{\mathbb{R}^2} \mathscr{E}^N v_1 v_1 f_{MEP}(\mathbf{r},\mathbf{k},t)d^2\mathbf{k} = \frac{2v_F^2}{(2\pi\hbar v_F)^2}\int_0^{2\pi} d\phi \int_0^{+\infty} \mathscr{E}^{N+1}\, d\mathscr{E}\cos^2\phi f_{MEP}(\mathbf{r},\mathbf{k},t) \\ &\approx \frac{2\pi v_F^2}{(2\pi\hbar v_F)^2}\left\{\int_0^{+\infty}\frac{\mathscr{E}^{N+1}}{1+e^{\lambda+\lambda_w\mathscr{E}}}d\mathscr{E}\right\}, \end{aligned} \tag{C.12}$$

$$nF_{12}^{(0)} = \frac{2}{(2\pi)^2}\int_{\mathbb{R}^2} v_1 v_2 f_{MEP}(\mathbf{r},\mathbf{k},t)d^2\mathbf{k} \approx 0, \tag{C.13}$$

$$nF_{12}^{(1)} = \frac{2}{(2\pi)^2}\int_{\mathbb{R}^2} \mathscr{E} v_1 v_2 f_{MEP}(\mathbf{r},\mathbf{k},t)d^2\mathbf{k} \approx 0, \tag{C.14}$$

$$nF_{12}^{(2)} = \frac{2}{(2\pi)^2}\int_{\mathbb{R}^2} \mathscr{E}^2 v_1 v_2 f_{MEP}(\mathbf{r},\mathbf{k},t)d^2\mathbf{k} \approx 0, \tag{C.15}$$

$$\vdots$$

$$nF_{12}^{(N)} = \frac{2}{(2\pi)^2}\int_{\mathbb{R}^2} \mathscr{E}^N v_1 v_2 f_{MEP}(\mathbf{r},\mathbf{k},t)d^2\mathbf{k} \approx 0, \tag{C.16}$$

$$\begin{aligned} nF_{22}^{(0)} &= \frac{2}{(2\pi)^2}\int_{\mathbb{R}^2} v_2 v_2 f_{MEP}(\mathbf{r},\mathbf{k},t)d^2\mathbf{k} = \frac{2v_F^2}{(2\pi\hbar v_F)^2}\int_0^{2\pi} d\phi \int_0^{+\infty} \mathscr{E}\, d\mathscr{E}\sin^2\phi f_{MEP}(\mathbf{r},\mathbf{k},t) \\ &\approx \frac{2\pi v_F^2}{(2\pi\hbar v_F)^2}\left\{\int_0^{+\infty}\frac{\mathscr{E}}{1+e^{\lambda+\lambda_w\mathscr{E}}}d\mathscr{E}\right\}, \end{aligned} \tag{C.17}$$

$$nF_{22}^{(1)} = \frac{2}{(2\pi)^2}\int_{\mathbb{R}^2} \mathscr{E} v_2 v_2 f_{MEP}(\mathbf{r},\mathbf{k},t) d^2\mathbf{k} = \frac{2v_F^2}{(2\pi\hbar v_F)^2}\int_0^{2\pi} d\phi \int_0^{+\infty} \mathscr{E}^2 d\mathscr{E} \sin^2\phi f_{MEP}(\mathbf{r},\mathbf{k},t)$$
$$\approx \frac{2\pi v_F^2}{(2\pi\hbar v_F)^2}\left\{\int_0^{+\infty} \frac{\mathscr{E}^2}{1+e^{\lambda+\lambda_w\mathscr{E}}} d\mathscr{E}\right\}, \tag{C.18}$$

$$nF_{22}^{(2)} = \frac{2}{(2\pi)^2}\int_{\mathbb{R}^2} \mathscr{E}^2 v_2 v_2 f_{MEP}(\mathbf{r},\mathbf{k},t) d^2\mathbf{k} = \frac{2v_F^2}{(2\pi\hbar v_F)^2}\int_0^{2\pi} d\phi \int_0^{+\infty} \mathscr{E}^3 d\mathscr{E} \sin^2\phi f_{MEP}(\mathbf{r},\mathbf{k},t)$$
$$\approx \frac{2\pi v_F^2}{(2\pi\hbar v_F)^2}\left\{\int_0^{+\infty} \frac{\mathscr{E}^3}{1+e^{\lambda+\lambda_w\mathscr{E}}} d\mathscr{E}\right\} \tag{C.19}$$

$$\vdots$$

$$nF_{22}^{(N)} = \frac{2}{(2\pi)^2}\int_{\mathbb{R}^2} \mathscr{E}^N v_2 v_2 f_{MEP}(\mathbf{r},\mathbf{k},t) d^2\mathbf{k} = \frac{2v_F^2}{(2\pi\hbar v_F)^2}\int_0^{2\pi} d\phi \int_0^{+\infty} \mathscr{E}^{N+1} d\mathscr{E} \sin^2\phi f_{MEP}(\mathbf{r},\mathbf{k},t)$$
$$\approx \frac{2\pi v_F^2}{(2\pi\hbar v_F)^2}\left\{\int_0^{+\infty} \frac{\mathscr{E}^{N+1}}{1+e^{\lambda+\lambda_w\mathscr{E}}} d\mathscr{E}\right\}, \tag{C.20}$$

where v_i are the components of $\mathbf{v}$.

The drift terms are estimated as follows

$$n\mathbf{G}^{(0)} : E\mathbf{e_1} = nG_{11}^{(0)}E = \frac{E}{2\hbar^2\pi}\int_0^{+\infty} \frac{1}{1+e^{\lambda+\lambda_w\mathscr{E}}} d\mathscr{E}, \tag{C.21}$$

$$n\mathbf{G}^{(1)} : E\mathbf{e_1} = nG_{11}^{(1)}E = \frac{E}{\hbar^2\pi}\int_0^{+\infty} \frac{\mathscr{E}}{1+e^{\lambda+\lambda_w\mathscr{E}}} d\mathscr{E}, \tag{C.22}$$

$$n\mathbf{G}^{(2)} : E\mathbf{e_1} = nG_{11}^{(2)}E = \frac{3E}{2\hbar^2\pi}\int_0^{+\infty} \frac{\mathscr{E}^2}{1+e^{\lambda+\lambda_w\mathscr{E}}} d\mathscr{E}, \tag{C.23}$$

$$\vdots$$

$$n\mathbf{G}^{(N)} : E\mathbf{e_1} = nG_{11}^{(N)}E = \frac{E(n+1)}{2\hbar^2\pi}\int_0^{+\infty} \frac{\mathscr{E}^N}{1+e^{\lambda+\lambda_w\mathscr{E}}} d\mathscr{E}. \tag{C.24}$$

C.0.0.1 Production terms

Regarding the production terms, the estimators listed below are obtained.

The productions arising from the scattering with acoustic phonons are given by

$$nC_n^{(ac)} = 0, \tag{C.25}$$

$$nC_W^{(ac)} = 0, \tag{C.26}$$

$$nC_{\mathbf{V}}^{(ac)} = \frac{1}{8\pi^2\hbar^4 v_F^2} A^{(ac)} \int_0^{+\infty} \frac{\mathscr{E}^2 e^{\lambda+\lambda_w\mathscr{E}}}{(1+e^{\lambda+\lambda_w\mathscr{E}})^2} (\lambda_{\mathbf{V}} + \mathscr{E}\lambda_{\mathbf{S}} + \mathscr{E}^2\lambda_{\mathbf{S^{(2)}}} + \cdots + \mathscr{E}^N\lambda_{\mathbf{S^N}}) d\mathscr{E} \tag{C.27}$$

$$nC_{\mathbf{S}}^{(ac)} = \frac{1}{8\pi^2\hbar^4 v_F^2} A^{(ac)} \int_0^{+\infty} \frac{\mathscr{E}^3 e^{\lambda+\lambda_w\mathscr{E}}}{(1+e^{\lambda+\lambda_w\mathscr{E}})^2} (\lambda_{\mathbf{V}} + \mathscr{E}\lambda_{\mathbf{S}} + \mathscr{E}^2\lambda_{\mathbf{S^{(2)}}} + \cdots + \mathscr{E}^N\lambda_{\mathbf{S^N}}) d\mathscr{E} \tag{C.28}$$

$$nC_{\mathbf{S^{(2)}}}^{(ac)} = \frac{1}{8\pi^2\hbar^4 v_F^2} A^{(ac)} \int_0^{+\infty} \frac{\mathscr{E}^4 e^{\lambda+\lambda_w\mathscr{E}}}{(1+e^{\lambda+\lambda_w\mathscr{E}})^2} (\lambda_{\mathbf{V}} + \mathscr{E}\lambda_{\mathbf{S}} + \mathscr{E}^2\lambda_{\mathbf{S^{(2)}}} + \cdots + \mathscr{E}^N\lambda_{\mathbf{S^N}}) d\mathscr{E} \tag{C.29}$$

$$\vdots$$

$$nC_{\mathbf{S^{(m)}}}^{(ac)} = \frac{1}{8\pi^2\hbar^4 v_F^2} A^{(ac)} \int_0^{+\infty} \frac{\mathscr{E}^{m+2} e^{\lambda+\lambda_w\mathscr{E}}}{(1+e^{\lambda+\lambda_w\mathscr{E}})^2} (\lambda_{\mathbf{V}} + \mathscr{E}\lambda_{\mathbf{S}} + \mathscr{E}^2\lambda_{\mathbf{S^{(2)}}} + \cdots + \mathscr{E}^N\lambda_{\mathbf{S^N}}) d\mathscr{E} \tag{C.30}$$

$$\vdots$$

$$nC_{\mathbf{S^{(N)}}}^{(ac)} = \frac{1}{8\pi^2\hbar^4 v_F^2} A^{(ac)} \int_0^{+\infty} \frac{\mathscr{E}^{N+2} e^{\lambda+\lambda_w\mathscr{E}}}{(1+e^{\lambda+\lambda_w\mathscr{E}})^2} (\lambda_{\mathbf{V}} + \mathscr{E}\lambda_{\mathbf{S}} + \mathscr{E}^2\lambda_{\mathbf{S^{(2)}}} + \cdots + \mathscr{E}^N\lambda_{\mathbf{S^N}}) d\mathscr{E} \tag{C.31}$$

If we set $\beta = \dfrac{1}{k_B T_L}$, the productions arising from the scattering with optical phonons read

$$nC_n^{(OP)} = 0, \tag{C.32}$$

$$nC_W^{(OP)} = \frac{A^{OP} D_\Gamma^2 N_B^{OP}}{\hbar^4 v_F^4 \pi^2} \hbar\omega (e^{\lambda_w \hbar\omega} - e^{\beta\hbar\omega}) \int_0^{+\infty} f^{(i)}(\mathscr{E}+\hbar\omega) \left(\frac{e^{\lambda+\lambda_w\mathscr{E}}}{1+e^{\lambda+\lambda_w\mathscr{E}}} \right) \mathscr{E}(\mathscr{E}+\hbar\omega) d\mathscr{E}, \tag{C.33}$$

$$\begin{aligned} nC_{\mathbf{V}}^{(OP)} = {} & \frac{A^{OP} D_\Gamma^2 N_B}{2\hbar^4 v_F^2 \pi^2} \left\{ \int_0^{+\infty} \left[f^{(i)}(\mathscr{E}) + \left(1 - f^{(i)}(\mathscr{E})\right) e^{\beta\hbar\omega} \right] \left(\frac{e^{\lambda+\lambda_w(\mathscr{E}+\hbar\omega)}}{(1+e^{\lambda+\lambda_w(\mathscr{E}+\hbar\omega)})^2} (\lambda_{\mathbf{V}} + (\mathscr{E}+\hbar\omega)\lambda_{\mathbf{S}} + \cdots + (\mathscr{E}+\hbar\omega)^N \lambda_{\mathbf{S(N)}}) \right) \mathscr{E}(\mathscr{E}+\hbar\omega) d\mathscr{E} + \right. \\ & + \left. \int_0^{+\infty} \left[e^{\beta\hbar\omega} f^{(i)}(\mathscr{E}+\hbar\omega) + \left(1 - f^{(i)}(\mathscr{E}+\hbar\omega)\right) \right] \left(\frac{e^{\lambda+\lambda_w\mathscr{E}}}{(1+e^{\lambda+\lambda_w\mathscr{E}})^2} (\lambda_{\mathbf{V}} + \mathscr{E}\lambda_{\mathbf{S}} + \cdots + \mathscr{E}^N \lambda_{\mathbf{S(N)}}) \right) (\mathscr{E}+\hbar\omega) \mathscr{E} d\mathscr{E} \right\} \end{aligned} \tag{C.34}$$

$$\begin{aligned} nC_{\mathbf{S}}^{(OP)} = {} & \frac{A^{OP} D_\Gamma^2 N_B}{2\hbar^4 v_F^2 \pi^2} \left\{ \int_0^{+\infty} \left[f^{(i)}(\mathscr{E}) + \left(1 - f^{(i)}(\mathscr{E})\right) e^{\beta\hbar\omega} \right] \left(\frac{e^{\lambda+\lambda_w(\mathscr{E}+\hbar\omega)}}{(1+e^{\lambda+\lambda_w(\mathscr{E}+\hbar\omega)})^2} (\lambda_{\mathbf{V}} + (\mathscr{E}+\hbar\omega)\lambda_{\mathbf{S}} + \cdots + (\mathscr{E}+\hbar\omega)^N \lambda_{\mathbf{S(N)}}) \right) \mathscr{E}(\mathscr{E}+\hbar\omega)^2 d\mathscr{E} + \right. \\ & + \left. \int_0^{+\infty} \left[e^{\beta\hbar\omega} f^{(i)}(\mathscr{E}+\hbar\omega) + \left(1 - f^{(i)}(\mathscr{E}+\hbar\omega)\right) \right] \left(\frac{e^{\lambda+\lambda_w\mathscr{E}}}{(1+e^{\lambda+\lambda_w\mathscr{E}})^2} (\lambda_{\mathbf{V}} + \mathscr{E}\lambda_{\mathbf{S}} + \cdots + \mathscr{E}^N \lambda_{\mathbf{S(N)}}) \right) (\mathscr{E}+\hbar\omega) \mathscr{E}^2 d\mathscr{E} \right\} \end{aligned} \tag{C.35}$$

$$\begin{aligned} nC_{\mathbf{S^{(2)}}}^{(OP)} = {} & \frac{A^{OP} D_\Gamma^2 N_B}{2\hbar^4 v_F^2 \pi^2} \left\{ \int_0^{+\infty} \left[f^{(i)}(\mathscr{E}) + \left(1 - f^{(i)}(\mathscr{E})\right) e^{\beta\hbar\omega} \right] \left(\frac{e^{\lambda+\lambda_w(\mathscr{E}+\hbar\omega)}}{(1+e^{\lambda+\lambda_w(\mathscr{E}+\hbar\omega)})^2} (\lambda_{\mathbf{V}} + (\mathscr{E}+\hbar\omega)\lambda_{\mathbf{S}} + \cdots + (\mathscr{E}+\hbar\omega)^N \lambda_{\mathbf{S(N)}}) \right) \mathscr{E}(\mathscr{E}+\hbar\omega)^3 d\mathscr{E} + \right. \\ & + \left. \int_0^{+\infty} \left[e^{\beta\hbar\omega} f^{(i)}(\mathscr{E}+\hbar\omega) + \left(1 - f^{(i)}(\mathscr{E}+\hbar\omega)\right) \right] \left(\frac{e^{\lambda+\lambda_w\mathscr{E}}}{(1+e^{\lambda+\lambda_w\mathscr{E}})^2} (\lambda_{\mathbf{V}} + \mathscr{E}\lambda_{\mathbf{S}} + \cdots + \mathscr{E}^N \lambda_{\mathbf{S(N)}}) \right) (\mathscr{E}+\hbar\omega) \mathscr{E}^3 d\mathscr{E} \right\}, \end{aligned} \tag{C.36}$$

$$\vdots$$

$$\begin{aligned} nC_{\mathbf{S^{(m)}}}^{(OP)} = {} & \frac{A^{OP} D_\Gamma^2 N_B}{2\hbar^4 v_F^2 \pi^2} \left\{ \int_0^{+\infty} \left[f^{(i)}(\mathscr{E}) + \left(1 - f^{(i)}(\mathscr{E})\right) e^{\beta\hbar\omega} \right] \left(\frac{e^{\lambda+\lambda_w(\mathscr{E}+\hbar\omega)}}{(1+e^{\lambda+\lambda_w(\mathscr{E}+\hbar\omega)})^2} (\lambda_{\mathbf{V}} + (\mathscr{E}+\hbar\omega)\lambda_{\mathbf{S}} + \cdots + (\mathscr{E}+\hbar\omega)^N \lambda_{\mathbf{S(N)}}) \right) \mathscr{E}(\mathscr{E}+\hbar\omega)^{m+1} d\mathscr{E} + \right. \\ & + \left. \int_0^{+\infty} \left[e^{\beta\hbar\omega} f^{(i)}(\mathscr{E}+\hbar\omega) + \left(1 - f^{(i)}(\mathscr{E}+\hbar\omega)\right) \right] \left(\frac{e^{\lambda+\lambda_w\mathscr{E}}}{(1+e^{\lambda+\lambda_w\mathscr{E}})^2} (\lambda_{\mathbf{V}} + \mathscr{E}\lambda_{\mathbf{S}} + \cdots + \mathscr{E}^N \lambda_{\mathbf{S(N)}}) \right) (\mathscr{E}+\hbar\omega) \mathscr{E}^{m+1} d\mathscr{E} \right\}, \end{aligned} \tag{C.37}$$

$$\vdots$$

$$\begin{aligned} nC^{(OP)}_{\mathbf{S(N)}} = \; & \frac{A^{OP}D_{\Gamma}^2 N_B}{2\hbar^4 v_F^2 \pi^2}\left\{\int_0^{+\infty}\left[f^{(i)}(\mathscr{E})+\left(1-f^{(i)}(\mathscr{E})\right)e^{\beta\hbar\omega}\right]\left(\frac{e^{\lambda+\lambda_W(\mathscr{E}+\hbar\omega)}}{(1+e^{\lambda+\lambda_W(\mathscr{E}+\hbar\omega)})^2}(\lambda_{\mathbf{V}}+(\mathscr{E}+\hbar\omega)\lambda_{\mathbf{S}}+\cdots+(\mathscr{E}+\hbar\omega)^N\lambda_{\mathbf{S(N)}})\right)\mathscr{E}(\mathscr{E}+\hbar\omega)^{N+1}d\mathscr{E}+\right. \\ + \; & \left.\int_0^{+\infty}\left[e^{\beta\hbar\omega}f^{(i)}(\mathscr{E}+\hbar\omega)+\left(1-f^{(i)}(\mathscr{E}+\hbar\omega)\right)\right]\left(\frac{e^{\lambda+\lambda_W\mathscr{E}}}{(1+e^{\lambda+\lambda_W\mathscr{E}})^2}(\lambda_{\mathbf{V}}+\mathscr{E}\lambda_{\mathbf{S}}+\cdots+\mathscr{E}^N\lambda_{\mathbf{S(N)}})\right)(\mathscr{E}+\hbar\omega)\mathscr{E}^{N+1}d\mathscr{E}\right\}. \end{aligned} \tag{C.38}$$

The productions arising from the scattering with K-phonons can be written as

$$nC_n^{(K)} = 0, \tag{C.39}$$

$$nC^{(K)}_{W} = \frac{A^K D_K^2 N_B^K}{2\hbar^4 v_F^4 \pi^2}(e^{\lambda_W\hbar\omega}-e^{\beta\hbar\omega})\hbar\omega\int_0^{+\infty}f^{(i)}(\mathscr{E})\left(\frac{e^{\lambda+\lambda_W\mathscr{E}}}{1+e^{\lambda+\lambda_W(\mathscr{E}+\hbar\omega)}}\right)\mathscr{E}(\mathscr{E}+\hbar\omega)d\mathscr{E}, \tag{C.40}$$

$$\begin{aligned} nC^{(K)}_{\mathbf{V}} = \; & \frac{3A^K D_K^2 N_B^K}{8\pi^2\hbar^4 v_F^2}\left\{\int_0^{+\infty}\left(\frac{e^{\lambda+\lambda_W(\mathscr{E}+\hbar\omega)}}{(1+e^{\lambda+\lambda_W(\mathscr{E}+\hbar\omega)})^2}(\lambda_{\mathbf{V}}+(\mathscr{E}+\hbar\omega)\lambda_{\mathbf{S}}+\cdots+(\mathscr{E}+\hbar\omega)^N\lambda_{\mathbf{S(N)}})\right)(\mathscr{E}+\hbar\omega)\mathscr{E}\left\{f^{(i)}(\mathscr{E})+(1-f^{(i)}(\mathscr{E}))e^{\beta\hbar\omega}\right\}d\mathscr{E}+\right. \\ + \; & \left.\int_0^{+\infty}\left(\frac{e^{\lambda+\lambda_W\mathscr{E}}}{(1+e^{\lambda+\lambda_W\mathscr{E}})^2}(\lambda_{\mathbf{V}}+\mathscr{E}\lambda_{\mathbf{S}}+\cdots+\mathscr{E}^N\lambda_{\mathbf{S(N)}})\right)(\mathscr{E}+\hbar\omega)\mathscr{E}\left\{1-f^{(i)}(\mathscr{E}+\hbar\omega)+f^{(i)}(\mathscr{E}+\hbar\omega)e^{\beta\hbar\omega}\right\}d\mathscr{E}\right\}, \end{aligned} \tag{C.41}$$

$$\begin{aligned} nC^{(K)}_{\mathbf{S}} = \; & \frac{A^K D_K^2 N_B^K}{8\pi^2\hbar^4 v_F^2}\left\{\int_0^{+\infty}(3\mathscr{E}+2\hbar\omega)\left(\frac{e^{\lambda+\lambda_W(\mathscr{E}+\hbar\omega)}}{(1+e^{\lambda+\lambda_W(\mathscr{E}+\hbar\omega)})^2}(\lambda_{\mathbf{V}}+(\mathscr{E}+\hbar\omega)\lambda_{\mathbf{S}}+\cdots+(\mathscr{E}+\hbar\omega)^N\lambda_{\mathbf{S(N)}})\right)(\mathscr{E}+\hbar\omega)\mathscr{E}\left\{f^{(i)}(\mathscr{E})+(1-f^{(i)}(\mathscr{E}))e^{\beta\hbar\omega}\right\}d\mathscr{E}+\right. \\ + \; & \left.\int_0^{+\infty}(3\mathscr{E}+\hbar\omega)\left(\frac{e^{\lambda+\lambda_W\mathscr{E}}}{(1+e^{\lambda+\lambda_W\mathscr{E}})^2}(\lambda_{\mathbf{V}}+\mathscr{E}\lambda_{\mathbf{S}}+\cdots+\mathscr{E}^N\lambda_{\mathbf{S(N)}})\right)(\mathscr{E}+\hbar\omega)\mathscr{E}\left\{1-f^{(i)}(\mathscr{E}+\hbar\omega)+f^{(i)}(\mathscr{E}+\hbar\omega)e^{\beta\hbar\omega}\right\}d\mathscr{E}\right\} \end{aligned} \tag{C.42}$$

$$\begin{aligned} nC^{(K)}_{\mathbf{S(2)}} = \; & \frac{A^K D_K^2 N_B^K}{8\pi^2\hbar^4 v_F^2}\left\{\int_0^{+\infty}(2(\mathscr{E}+\hbar\omega)^2+\mathscr{E}^2)\left(\frac{e^{\lambda+\lambda_W(\mathscr{E}+\hbar\omega)}}{(1+e^{\lambda+\lambda_W(\mathscr{E}+\hbar\omega)})^2}(\lambda_{\mathbf{V}}+(\mathscr{E}+\hbar\omega)\lambda_{\mathbf{S}}+\cdots+(\mathscr{E}+\hbar\omega)^N\lambda_{\mathbf{S(N)}})\right)(\mathscr{E}+\hbar\omega)\mathscr{E}\left\{f^{(i)}(\mathscr{E})+(1-f^{(i)}(\mathscr{E}))e^{\beta\hbar\omega}\right\}d\mathscr{E}+\right. \\ + \; & \left.\int_0^{+\infty}((\mathscr{E}+\hbar\omega)^2+2\mathscr{E}^2)\left(\frac{e^{\lambda+\lambda_W\mathscr{E}}}{(1+e^{\lambda+\lambda_W\mathscr{E}})^2}(\lambda_{\mathbf{V}}+\mathscr{E}\lambda_{\mathbf{S}}+\cdots+\mathscr{E}^N\lambda_{\mathbf{S(N)}})\right)(\mathscr{E}+\hbar\omega)\mathscr{E}\left\{1-f^{(i)}(\mathscr{E}+\hbar\omega)+f^{(i)}(\mathscr{E}+\hbar\omega)e^{\beta\hbar\omega}\right\}d\mathscr{E}\right\} \end{aligned} \tag{C.43}$$

$$\vdots$$

$$\begin{aligned} nC^{(K)}_{\mathbf{S(m)}} = \; & \frac{A^K D_K^2 N_B^K}{8\pi^2\hbar^4 v_F^2}\left\{\int_0^{+\infty}(2(\mathscr{E}+\hbar\omega)^m+\mathscr{E}^m)\left(\frac{e^{\lambda+\lambda_W(\mathscr{E}+\hbar\omega)}}{(1+e^{\lambda+\lambda_W(\mathscr{E}+\hbar\omega)})^2}(\lambda_{\mathbf{V}}+(\mathscr{E}+\hbar\omega)\lambda_{\mathbf{S}}+\cdots+(\mathscr{E}+\hbar\omega)^N\lambda_{\mathbf{S(N)}})\right)(\mathscr{E}+\hbar\omega)\mathscr{E}\left\{f^{(i)}(\mathscr{E})+(1-f^{(i)}(\mathscr{E}))e^{\beta\hbar\omega}\right\}d\mathscr{E}+\right. \\ + \; & \left.\int_0^{+\infty}((\mathscr{E}+\hbar\omega)^m+2\mathscr{E}^m)\left(\frac{e^{\lambda+\lambda_W\mathscr{E}}}{(1+e^{\lambda+\lambda_W\mathscr{E}})^2}(\lambda_{\mathbf{V}}+\mathscr{E}\lambda_{\mathbf{S}}+\cdots+\mathscr{E}^N\lambda_{\mathbf{S(N)}})\right)(\mathscr{E}+\hbar\omega)\mathscr{E}\left\{1-f^{(i)}(\mathscr{E}+\hbar\omega)+f^{(i)}(\mathscr{E}+\hbar\omega)e^{\beta\hbar\omega}\right\}d\mathscr{E}\right\} \end{aligned} \tag{C.44}$$

$$\vdots$$

$$\begin{aligned} nC^{(K)}_{\mathbf{S(N)}} = \; & \frac{A^K D_K^2 N_B^K}{8\pi^2\hbar^4 v_F^2}\left\{\int_0^{+\infty}(2(\mathscr{E}+\hbar\omega)^N+\mathscr{E}^N)\left(\frac{e^{\lambda+\lambda_W(\mathscr{E}+\hbar\omega)}}{(1+e^{\lambda+\lambda_W(\mathscr{E}+\hbar\omega)})^2}(\lambda_{\mathbf{V}}+(\mathscr{E}+\hbar\omega)\lambda_{\mathbf{S}}+\cdots+(\mathscr{E}+\hbar\omega)^N\lambda_{\mathbf{S(N)}})\right)(\mathscr{E}+\hbar\omega)\mathscr{E}\left\{f^{(i)}(\mathscr{E})+(1-f^{(i)}(\mathscr{E}))e^{\beta\hbar\omega}\right\}d\mathscr{E}+\right. \\ + \; & \left.\int_0^{+\infty}((\mathscr{E}+\hbar\omega)^N+2\mathscr{E}^N)\left(\frac{e^{\lambda+\lambda_W\mathscr{E}}}{(1+e^{\lambda+\lambda_W\mathscr{E}})^2}(\lambda_{\mathbf{V}}+\mathscr{E}\lambda_{\mathbf{S}}+\cdots+\mathscr{E}^N\lambda_{\mathbf{S(N)}})\right)(\mathscr{E}+\hbar\omega)\mathscr{E}\left\{1-f^{(i)}(\mathscr{E}+\hbar\omega)+f^{(i)}(\mathscr{E}+\hbar\omega)e^{\beta\hbar\omega}\right\}d\mathscr{E}\right\} \end{aligned} \tag{C.45}$$

APPENDIX D

CLOSURE RELATIONS FOR THE 8 MOMENT MODEL: THE CASE OF MOMENTS BASED ON VELOCITY POWERS

D.1 Non-linear closure relations

Assuming that the Lagrangian multipliers $\lambda_{\mathbf{V}}$ and $\lambda_{\mathbf{S}}$ are collinear, we choose a reference frame $(\mathbf{e_1}, \mathbf{e_2})$ in a way that $\lambda_{\mathbf{V}} = \lambda_V \, \mathbf{e_1}$, $\lambda_{\mathbf{S}} = \lambda_S \, \mathbf{e_1}$, $\mathbf{E} = E \, \mathbf{e_1}$ and introduce polar coordinates. Explicitly we have

$$f_{MEP}(\mathbf{r}, \mathbf{k}, t) = \frac{1}{1 + \exp(\lambda + \lambda_w \mathscr{E} + v_F \cos\phi(\lambda_{\mathbf{V}} + \mathscr{E}\lambda_{\mathbf{S}}) + \lambda_D(v_F^2 \cos^2\phi - \frac{1}{2}v_F^2) + 2\lambda_{12} v_F^2 \cos\phi \sin\phi)} \tag{D.1}$$

where $\mathbf{v} = v_F \cos\phi \, \mathbf{e_1} + v_F \sin\phi \, \mathbf{e_2}$.

The constraints read

$$n = \frac{2}{(2\pi\hbar v_F)^2} \int_0^{2\pi} d\phi \int_0^{+\infty} \frac{\mathscr{E} d\mathscr{E}}{1 + exp(\lambda + \lambda_w \mathscr{E} + v_F \cos\phi(\lambda_{\mathbf{V}} + \mathscr{E}\lambda_{\mathbf{S}}) + \lambda_D(v_F^2 \cos^2\phi - \frac{1}{2}v_F^2) + 2\lambda_{12} v_F^2 \cos\phi \sin\phi)}, \tag{D.2}$$

$$nW = \frac{2}{(2\pi\hbar v_F)^2} \int_0^{2\pi} d\phi \int_0^{+\infty} \frac{\mathscr{E}^2 d\mathscr{E}}{1 + exp(\lambda + \lambda_w \mathscr{E} + v_F \cos\phi(\lambda_{\mathbf{V}} + \mathscr{E}\lambda_{\mathbf{S}}) + \lambda_D(v_F^2 \cos^2\phi - \frac{1}{2}v_F^2) + 2\lambda_{12} v_F^2 \cos\phi \sin\phi)}, \tag{D.3}$$

$$n\mathbf{V} = \frac{2}{(2\pi\hbar)^2 v_F} \int_0^{2\pi} d\phi \int_0^{+\infty} \frac{\mathscr{E} \cos\phi d\mathscr{E}}{1 + exp(\lambda + \lambda_w \mathscr{E} + v_F \cos\phi(\lambda_{\mathbf{V}} + \mathscr{E}\lambda_{\mathbf{S}}) + \lambda_D(v_F^2 \cos^2\phi - \frac{1}{2}v_F^2) + 2\lambda_{12} v_F^2 \cos\phi \sin\phi)} \mathbf{e_1}, \tag{D.4}$$

$$n\mathbf{S} = \frac{2}{(2\pi\hbar)^2 v_F} \int_0^{2\pi} d\phi \int_0^{+\infty} \frac{\mathscr{E}^2 \cos\phi d\mathscr{E}}{1 + exp(\lambda + \lambda_w \mathscr{E} + v_F \cos\phi(\lambda_{\mathbf{V}} + \mathscr{E}\lambda_{\mathbf{S}}) + \lambda_D(v_F^2 \cos^2\phi - \frac{1}{2}v_F^2) + 2\lambda_{12} v_F^2 \cos\phi \sin\phi)} \mathbf{e_1}, \tag{D.5}$$

$$\begin{aligned} nD_{11} = \frac{2}{(2\pi\hbar)^2} \Bigg\{ & \int_0^{2\pi} \int_0^{+\infty} \frac{\mathscr{E} d\mathscr{E} \cos^2\phi}{1 + \exp(\lambda + \lambda_w \mathscr{E} + v_F \cos\phi(\lambda_{\mathbf{V}} + \mathscr{E}\lambda_{\mathbf{S}}) + \lambda_D(v_F^2 \cos^2\phi - \frac{1}{2}v_F^2) + 2\lambda_{12} v_F^2 \cos\phi \sin\phi)} \\ & - \frac{1}{2} v_F^2 \int_0^{2\pi} \int_0^{+\infty} \frac{\mathscr{E} d\mathscr{E}}{1 + \exp(\lambda + \lambda_w \mathscr{E} + v_F \cos\phi(\lambda_{\mathbf{V}} + \mathscr{E}\lambda_{\mathbf{S}}) + \lambda_D(v_F^2 \cos^2\phi - \frac{1}{2}v_F^2) + 2\lambda_{12} v_F^2 \cos\phi \sin\phi)} \Bigg\}, \end{aligned} \tag{D.6}$$

$$nD_{12} = \frac{2}{(2\pi\hbar)^2} \left\{ \int_0^{2\pi} \int_0^{+\infty} \frac{\mathscr{E} d\mathscr{E} \sin\phi \cos\phi}{1 + \exp(\lambda + \lambda_w \mathscr{E} + v_F \cos\phi(\lambda_{\mathbf{V}} + \mathscr{E}\lambda_{\mathbf{S}}) + \lambda_D(v_F^2 \cos^2\phi - \frac{1}{2}v_F^2) + 2\lambda_{12} v_F^2 \cos\phi \sin\phi)} \right\}. \tag{D.7}$$

The other terms of the evolution equations can be estimated by f_{MEP} as

$$n\mathbf{G}^{(0)} : E\mathbf{e_1} = \frac{E}{2h^2\pi^2} \int_0^{2\pi} d\phi \int_0^{+\infty} \frac{d\mathscr{E} \sin^2\phi}{1 + \exp(\lambda + \lambda_w \mathscr{E} + v_F \cos\phi(\lambda_{\mathbf{V}} + \mathscr{E}\lambda_{\mathbf{S}}) + \lambda_D(v_F^2 \cos^2\phi - \frac{1}{2}v_F^2) + 2\lambda_{12} v_F^2 \cos\phi \sin\phi)} \mathbf{e_1}, \tag{D.8}$$

$$n\mathbf{G}^{(1)}:E\mathbf{e_1}=\frac{E}{2\hbar^2\pi^2}\int_0^{2\pi}d\phi\int_0^{+\infty}\frac{\mathscr{E}d\mathscr{E}}{1+\exp(\lambda+\lambda_w\mathscr{E}+v_F\cos\phi(\lambda_{\mathbf{V}}+\mathscr{E}\lambda_{\mathbf{S}})+\lambda_D(v_F^2\cos^2\phi-\frac{1}{2}v_F^2)+2\lambda_{12}v_F^2\cos\phi\sin\phi)}\mathbf{e_1}. \tag{D.9}$$

$$(nL^{(0)}:\mathbf{E})_{11} = \frac{v_FE}{\hbar^2\pi^2}\int_0^{+\infty}d\mathscr{E}\int_0^{2\pi}d\phi f_{MEP}(\mathbf{r},\mathbf{k},t)\left(\cos\phi-\cos^3\phi\right), \tag{D.10}$$

$$(nL^{(0)}:\mathbf{E})_{12} = \frac{v_FE}{2\hbar^2\pi^2}\int_0^{+\infty}d\mathscr{E}\int_0^{2\pi}d\phi f_{MEP}(\mathbf{r},\mathbf{k},t)\left(-2\cos^2\phi\sin\phi+\sin\phi\right), \tag{D.11}$$

$$\begin{aligned} nH_{111} &= \frac{2}{(2\pi)^2}\int_{\mathbb{R}^2}v_1v_1v_1f_{MEP}(\mathbf{r},\mathbf{k},t)d^2\mathbf{k}-\frac{1}{2}nV_1 \\ &= \frac{2v_F^3}{(2\pi\hbar v_F)^2}\int_0^{2\pi}d\phi\int_0^{+\infty}\mathscr{E}\,d\mathscr{E}\cos^3\phi\,f_{MEP}(\mathbf{r},\mathbf{k},t)-\frac{1}{2}nV_1, \end{aligned} \tag{D.12}$$

$$nH_{112} = \frac{2}{(2\pi)^2}\int_{\mathbb{R}^2}v_1v_1v_2f_{MEP}(\mathbf{r},\mathbf{k},t)d^2\mathbf{k}=\frac{2v_F^3}{(2\pi\hbar v_F)^2}\int_0^{2\pi}d\phi\int_0^{+\infty}\mathscr{E}\,d\mathscr{E}\sin\phi\cos^2\phi f_{MEP}(\mathbf{r},\mathbf{k},t), \tag{D.13}$$

where the wave vector $\mathbf{k}$ must be written in terms of the energy $\mathscr{E}$ and the angle ϕ

$$\mathbf{k}=\frac{\mathscr{E}}{\hbar v_F}\left(\cos\phi\,\mathbf{e_1}+\sin\phi\,\mathbf{e_2}\right).$$

D.1.0.1 Production terms

Regarding the production terms, general expressions of $nC_t^{(s)}$ with $t=n,W,\mathbf{V},\mathbf{S}$ and $s=ac,OP,K$ are the same as those introduced in Appendix B for non-linear 6 moments model, now evaluated with the expression (D.1) of f_{MEP}.

The new production terms, added in this model, arising from the scattering with acoustic phonons are

$$nC_{D_{11}}^{(ac)}=\frac{A^{(ac)}}{8\pi^3\hbar^4v_F^2}\left\{\int_0^{+\infty}\int_0^{2\pi}\mathscr{E}^2f(\mathscr{E},\psi,t)(1-2\cos^2\psi)d\psi\right\}, \tag{D.14}$$

$$nC_{D_{12}}^{(ac)}=0, \tag{D.15}$$

where $\psi=\phi+\theta''$ and, recalling that θ'' is the angle between $\mathbf{k}$ and $\mathbf{k}'$,

$$\mathbf{k}'=\frac{\mathscr{E}'}{\hbar v_F}\left[\cos(\phi+\theta'')\,\mathbf{e_1}+\sin(\phi+\theta'')\,\mathbf{e_2}\right].$$

We set $\beta=\dfrac{1}{k_BT_L}$ and denote by H the Heaviside function. The new productions arising from the scattering with optical phonons are

$$\begin{aligned} nC_{D_{11}}^{(OP)} =& \frac{A^{OP}D_\Gamma^2N_B^{OP}}{4\hbar^4v_F^2\pi^4}\int_0^{2\pi}d\phi\int_0^{+\infty}\mathscr{E}d\mathscr{E}\int_0^{2\pi}\cos^2\phi d\theta''\{[f(\mathscr{E}-\hbar\omega,\mathbf{e}')(1-f(\mathscr{E},\mathbf{e}))(\mathscr{E}-\hbar\omega)H(\mathscr{E}-\hbar\omega) \\ &+e^{\beta\hbar\omega}f(\mathscr{E}+\hbar\omega,\mathbf{e}')(1-f(\mathscr{E},\mathbf{e}))(\mathscr{E}+\hbar\omega)\Big] \\ &-\Big[e^{\beta\hbar\omega}f(\mathscr{E},\mathbf{e})(1-f(\mathscr{E}-\hbar\omega,\mathbf{e}'))(\mathscr{E}-\hbar\omega)H(\mathscr{E}-\hbar\omega) \\ &+f(\mathscr{E},\mathbf{e})(1-f(\mathscr{E}+\hbar\omega,\mathbf{e}'))(\mathscr{E}+\hbar\omega)]\}, \end{aligned} \tag{D.16}$$

$$\begin{aligned} nC_{D_{12}}^{(OP)} =& \frac{A^{OP}D_\Gamma^2N_B^{OP}}{4\hbar^4v_F^2\pi^4}\int_0^{2\pi}d\phi\int_0^{+\infty}\mathscr{E}d\mathscr{E}\int_0^{2\pi}\sin\phi\cos\phi d\theta''\{[f(\mathscr{E}-\hbar\omega,\mathbf{e}')(1-f(\mathscr{E},\mathbf{e}))(\mathscr{E}-\hbar\omega)H(\mathscr{E}-\hbar\omega) \\ &+e^{\beta\hbar\omega}f(\mathscr{E}+\hbar\omega,\mathbf{e}')(1-f(\mathscr{E},\mathbf{e}))(\mathscr{E}+\hbar\omega)\Big] \\ &-\Big[e^{\beta\hbar\omega}f(\mathscr{E},\mathbf{e})(1-f(\mathscr{E}-\hbar\omega,\mathbf{e}'))(\mathscr{E}-\hbar\omega)H(\mathscr{E}-\hbar\omega) \\ &+f(\mathscr{E},\mathbf{e})(1-f(\mathscr{E}+\hbar\omega,\mathbf{e}'))(\mathscr{E}+\hbar\omega)]\}. \end{aligned} \tag{D.17}$$

In the previous relations $\mathbf{e} = \cos\phi\,\mathbf{e_1} + \sin\phi\,\mathbf{e_2}$ while $\mathbf{e}' = \cos\psi\,\mathbf{e_1} + \sin\psi\,\mathbf{e_2}$.

The new productions arising from the scattering with K-phonons are

$$\begin{aligned} nC^{(K)}_{D_{11}} = & \frac{A^K D_K^2 N_B^K}{8\pi^4\hbar^4 v_F^2}\int_0^{2\pi} d\phi \int_0^{+\infty}\left\{\int_0^{2\pi} d\theta''(1-\cos\theta'')\left[(\mathscr{E}-\hbar\omega)f(\mathscr{E}-\hbar\omega,\mathbf{e}')(1-f(\mathscr{E},\mathbf{e}))H(\mathscr{E}-\hbar\omega)\right.\right. \\ & \left. + e^{\beta\hbar\omega}(\mathscr{E}+\hbar\omega)f(\mathscr{E}+\hbar\omega,\mathbf{e}')(1-f(\mathscr{E},\mathbf{e}))\right] \\ & \left. - \int_0^{2\pi} d\theta''(1-\cos\theta'')\left[e^{\beta\hbar\omega}f(\mathscr{E},\mathbf{e})(1-f(\mathscr{E}-\hbar\omega),\mathbf{e}')(\mathscr{E}-\hbar\omega)H(\mathscr{E}-\hbar\omega) + f(\mathscr{E},\mathbf{e})(1-f(\mathscr{E}+\hbar\omega,\mathbf{e}'))(\mathscr{E}+\hbar\omega)\right]\right\}\mathscr{E}\cos^2\phi\, d\mathscr{E}, \end{aligned} \tag{D.18}$$

$$\begin{aligned} nC^{(K)}_{D_{12}} = & \frac{A^K D_K^2 N_B^K}{8\pi^4\hbar^4 v_F^2}\int_0^{2\pi} d\phi \int_0^{+\infty}\left\{\int_0^{2\pi} d\theta''(1-\cos\theta'')\left[(\mathscr{E}-\hbar\omega)f(\mathscr{E}-\hbar\omega,\mathbf{e}')(1-f(\mathscr{E},\mathbf{e}))H(\mathscr{E}-\hbar\omega)\right.\right. \\ & \left. + e^{\beta\hbar\omega}(\mathscr{E}+\hbar\omega)f(\mathscr{E}+\hbar\omega,\mathbf{e}')(1-f(\mathscr{E},\mathbf{e}))\right] + \\ & \left. - \int_0^{2\pi} d\theta''(1-\cos\theta'')\left[e^{\beta\hbar\omega}f(\mathscr{E},\mathbf{e})(1-f(\mathscr{E}-\hbar\omega),\mathbf{e}')(\mathscr{E}-\hbar\omega)H(\mathscr{E}-\hbar\omega) + f(\mathscr{E},\mathbf{e})(1-f(\mathscr{E}+\hbar\omega,\mathbf{e}'))(\mathscr{E}+\hbar\omega)\right]\right\}\mathscr{E}\sin\phi\cos\phi\, d\mathscr{E}. \end{aligned} \tag{D.19}$$

D.2 Linear closure relations

By approximating the distribution function with the linearized MEP (4.80)[1], the relations between the field variables and the Lagrange multipliers are given by

$$n = \frac{1}{\pi\hbar^2 v_F^2}\int_0^{+\infty}\frac{\mathscr{E}}{1+e^{\lambda+\lambda_w\mathscr{E}}}\,d\mathscr{E}, \tag{D.20}$$

$$nW = \frac{1}{\pi\hbar^2 v_F^2}\int_0^{+\infty}\frac{\mathscr{E}^2}{1+e^{\lambda+\lambda_w\mathscr{E}}}\,d\mathscr{E}, \tag{D.21}$$

$$n\mathbf{V} = -\frac{1}{2\pi\hbar^2}\left\{\int_0^{+\infty}\frac{\mathscr{E}e^{\lambda+\lambda_w\mathscr{E}}}{(1+e^{\lambda+\lambda_w\mathscr{E}})^2}d\mathscr{E}\lambda_{\mathbf{V}} + \int_0^{+\infty}\frac{\mathscr{E}^2e^{\lambda+\lambda_w\mathscr{E}}}{(1+e^{\lambda+\lambda_w\mathscr{E}})^2}d\mathscr{E}\lambda_{\mathbf{S}}\right\}, \tag{D.22}$$

$$n\mathbf{S} = -\frac{1}{2\pi\hbar^2}\left\{\int_0^{+\infty}\frac{\mathscr{E}^2e^{\lambda+\lambda_w\mathscr{E}}}{(1+e^{\lambda+\lambda_w\mathscr{E}})^2}d\mathscr{E}\lambda_{\mathbf{V}} + \int_0^{+\infty}\frac{\mathscr{E}^3e^{\lambda+\lambda_w\mathscr{E}}}{(1+e^{\lambda+\lambda_w\mathscr{E}})^2}d\mathscr{E}\lambda_{\mathbf{S}}\right\}, \tag{D.23}$$

$$nD_{11} = -\frac{v_F^2}{8\pi\hbar^2}\lambda_D\int_0^{+\infty}\frac{\mathscr{E}e^{\lambda+\lambda_w\mathscr{E}}}{(1+e^{\lambda+\lambda_w\mathscr{E}})^2}d\mathscr{E}. \tag{D.24}$$

[1] We recall that the 1D case is considered

Regarding the relevant components of fluxes we have

$$\begin{aligned} nF_{11}^{(0)} &= \frac{2}{(2\pi)^2}\int_{\mathbb{R}^2} v_1 v_1 f_{MEP}(\mathbf{r},\mathbf{k},t)d^2\mathbf{k} = \frac{2v_F^2}{(2\pi\hbar v_F)^2}\int_0^{2\pi} d\phi \int_0^{+\infty} \mathscr{E}\, d\mathscr{E}\cos^2\phi f_{MEP}(\mathbf{r},\mathbf{k},t) \\ &\approx \frac{2\pi v_F^2}{(2\pi\hbar v_F)^2}\left\{\int_0^{+\infty}\frac{\mathscr{E}}{1+e^{\lambda+\lambda_w\mathscr{E}}}d\mathscr{E} - \frac{1}{4}v_F^2\lambda_D\int_0^{+\infty}\frac{\mathscr{E}e^{\lambda+\lambda_w\mathscr{E}}}{(1+e^{\lambda+\lambda_w\mathscr{E}})^2}d\mathscr{E}\right\}, \end{aligned} \tag{D.25}$$

$$\begin{aligned} nF_{11}^{(1)} &= \frac{2}{(2\pi)^2}\int_{\mathbb{R}^2} \mathscr{E} v_1 v_1 f_{MEP}(\mathbf{r},\mathbf{k},t)d^2\mathbf{k} = \frac{2v_F^2}{(2\pi\hbar v_F)^2}\int_0^{2\pi} d\phi \int_0^{+\infty} \mathscr{E}^2\, d\mathscr{E}\cos^2\phi f_{MEP}(\mathbf{r},\mathbf{k},t) \\ &\approx \frac{2\pi v_F^2}{(2\pi\hbar v_F)^2}\left\{\int_0^{+\infty}\frac{\mathscr{E}^2}{1+e^{\lambda+\lambda_w\mathscr{E}}}d\mathscr{E} - \frac{1}{4}v_F^2\lambda_D\int_0^{+\infty}\frac{\mathscr{E}^2e^{\lambda+\lambda_w\mathscr{E}}}{(1+e^{\lambda+\lambda_w\mathscr{E}})^2}d\mathscr{E}\right\}, \end{aligned} \tag{D.26}$$

$$\begin{aligned} nH_{111} &+ \frac{1}{2}nv_F^2V_1 = \frac{2}{(2\pi)^2}\int_{\mathbb{R}^2} v_1 v_1 v_1 f_{MEP}(\mathbf{r},\mathbf{k},t)d^2\mathbf{k} \\ &\approx -\frac{3v_F}{8\pi\hbar^2}\int_0^{+\infty}\frac{\mathscr{E}e^{\lambda+\lambda_w\mathscr{E}}}{(1+e^{\lambda+\lambda_w\mathscr{E}})^2}(\lambda_{\mathbf{V}}+\mathscr{E}\lambda_{\mathbf{S}})d\mathscr{E}. \end{aligned} \tag{D.27}$$

The drift terms are estimated as follows

$$n\mathbf{G}^{(0)}:E\mathbf{e_1} = nG_{11}^{(0)}E = \frac{E}{2\hbar^2\pi}\left\{\int_0^{+\infty}\frac{1}{1+e^{\lambda+\lambda_w\mathscr{E}}}d\mathscr{E} + \frac{\lambda_D}{4}\int_0^{+\infty}\frac{e^{\lambda+\lambda_w\mathscr{E}}}{(1+e^{\lambda+\lambda_w\mathscr{E}})^2}d\mathscr{E}\right\}, \tag{D.28}$$

$$n\mathbf{G}^{(1)}:E\mathbf{e_1} = nG_{11}^{(1)}E = \frac{E}{\hbar^2\pi}\int_0^{+\infty}\frac{\mathscr{E}}{1+e^{\lambda+\lambda_w\mathscr{E}}}d\mathscr{E}. \tag{D.29}$$

A bit more involved is the estimation of

$$n\mathbf{L}^{(0)}:\mathbf{E} := \frac{2}{\hbar(2\pi)^2}\sum_{h=1}^{2}\sum_{i=1}^{2}\sum_{j=1}^{2}E_h\left(\int_{\mathbb{R}^2} f(\mathbf{r},\mathbf{k},t)\left(\frac{\partial v_i}{\partial k_h}v_j + v_i\frac{\partial v_j}{\partial k_h}\right)d^2\mathbf{k}\right)\mathbf{e_i}\otimes\mathbf{e_j}. \tag{D.30}$$

Since

$$\frac{\partial}{\partial k_h}v_i = v_F\frac{\delta_{ih}}{|\mathbf{k}|} - \frac{v_F k_i k_h}{|\mathbf{k}|^3},$$

one gets

$$\begin{aligned} (nL^{(0)}:\mathbf{E})_{11} &= \frac{2E}{\hbar(2\pi)^2}\frac{1}{\hbar^2v_F^2}\int_0^{+\infty}d\mathscr{E}\int_0^{2\pi}d\phi\mathscr{E}f_{MEP}(\mathbf{r},\mathbf{k},t)\left[2\frac{v_F^2}{|\mathbf{k}|}\left(\cos\phi-\cos^3\phi\right)\right] \\ &\approx -\frac{Ev_F}{4\hbar^2\pi}\int_0^{+\infty}\frac{e^{\lambda+\lambda_w\mathscr{E}}}{(1+e^{\lambda+\lambda_w\mathscr{E}})^2}(\lambda_V+\mathscr{E}\lambda_S)d\mathscr{E}. \end{aligned} \tag{D.31}$$

D.2.0.1 Production terms

The production terms due to the scattering with the acoustic phonons are given by

$$nC_n^{(ac)} = 0, \tag{D.32}$$

$$nC_W^{(ac)} = 0, \tag{D.33}$$

$$nC_{\mathbf{V}}^{(ac)} = \frac{1}{8\pi^2\hbar^4 v_F^2} A^{(ac)} \left\{ \int_0^{+\infty} \frac{\mathscr{E}^2 e^{\lambda+\lambda_w\mathscr{E}}}{(1+e^{\lambda+\lambda_w\mathscr{E}})^2} (\lambda_{\mathbf{V}} + \mathscr{E}\lambda_{\mathbf{S}}) d\mathscr{E} \right\}, \tag{D.34}$$

$$nC_{\mathbf{S}}^{(ac)} = \frac{1}{8\pi^2\hbar^4 v_F^2} A^{(ac)} \left\{ \int_0^{+\infty} \frac{\mathscr{E}^3 e^{\lambda+\lambda_w\mathscr{E}}}{(1+e^{\lambda+\lambda_w\mathscr{E}})^2} (\lambda_{\mathbf{V}} + \mathscr{E}\lambda_{\mathbf{S}}) d\mathscr{E} \right\}, \tag{D.35}$$

$$nC_{D_{11}}^{(ac)} = \frac{A^{(ac)}}{16\pi^2\hbar^4} \lambda_D \left\{ \int_0^{+\infty} \frac{\mathscr{E}^2 e^{\lambda+\lambda_w\mathscr{E}}}{(1+e^{\lambda+\lambda_w\mathscr{E}})^2} d\mathscr{E} \right\}. \tag{D.36}$$

The production terms due to the scattering with the optical phonons read

$$nC_n^{(OP)} = 0, \tag{D.37}$$

$$nC_W^{(OP)} = \frac{A^{OP} D_\Gamma^2 N_B^{OP}}{\hbar^4 v_F^4 \pi^2} \hbar\omega (e^{\lambda_w\hbar\omega} - e^{\beta\hbar\omega}) \int_0^{+\infty} f^{(i)}(\mathscr{E}) \left(\frac{e^{\lambda+\lambda_w\mathscr{E}}}{1+e^{\lambda+\lambda_w(\mathscr{E}+\hbar\omega)}} \right) \mathscr{E}(\mathscr{E}+\hbar\omega) d\mathscr{E} \tag{D.38}$$

$$\begin{aligned} nC_{\mathbf{V}}^{(OP)} = {} & \frac{A^{OP} D_\Gamma^2 N_B^{OP}}{2\hbar^4 v_F^2 \pi^2} \left\{ \int_0^{+\infty} \left(\frac{e^{\lambda+\lambda_w(\mathscr{E}+\hbar\omega)}}{(1+e^{\lambda+\lambda_w(\mathscr{E}+\hbar\omega)})^2} (\lambda_{\mathbf{V}} + (\mathscr{E}+\hbar\omega)\lambda_{\mathbf{S}}) \right) \mathscr{E}(\mathscr{E}+\hbar\omega) \right. \\ & \times \left[f^{(i)}(\mathscr{E}) + \left(1 - f^{(i)}(\mathscr{E})\right) e^{\beta\hbar\omega} \right] d\mathscr{E} + \int_0^{+\infty} \left(\frac{e^{\lambda+\lambda_w\mathscr{E}}}{(1+e^{\lambda+\lambda_w\mathscr{E}})^2} (\lambda_{\mathbf{V}} + \mathscr{E}\lambda_{\mathbf{S}}) \right) \mathscr{E}(\mathscr{E}+\hbar\omega) \\ & \times \left. \left[e^{\beta\hbar\omega} f^{(i)}(\mathscr{E}+\hbar\omega) + \left(1 - f^{(i)}(\mathscr{E}+\hbar\omega)\right) \right] d\mathscr{E} \right\}, \end{aligned} \tag{D.39}$$

$$\begin{aligned} nC_{\mathbf{S}}^{(OP)} = {} & \frac{A^{OP} D_\Gamma^2 N_B^{OP}}{2\hbar^4 v_F^2 \pi^2} \left\{ \int_0^{+\infty} \left(\frac{e^{\lambda+\lambda_w(\mathscr{E}+\hbar\omega)}}{(1+e^{\lambda+\lambda_w(\mathscr{E}+\hbar\omega)})^2} (\lambda_{\mathbf{V}} + (\mathscr{E}+\hbar\omega)\lambda_{\mathbf{S}}) \right) \mathscr{E}(\mathscr{E}+\hbar\omega)^2 \right. \\ & \times \left[f^{(i)}(\mathscr{E}) + \left(1 - f^{(i)}(\mathscr{E})\right) e^{\beta\hbar\omega} \right] d\mathscr{E} + \int_0^{+\infty} \left(\frac{e^{\lambda+\lambda_w\mathscr{E}}}{(1+e^{\lambda+\lambda_w\mathscr{E}})^2} (\lambda_{\mathbf{V}} + \mathscr{E}\lambda_{\mathbf{S}}) \right) (\mathscr{E}+\hbar\omega)\mathscr{E}^2 \\ & \times \left. \left[e^{\beta\hbar\omega} f^{(i)}(\mathscr{E}+\hbar\omega) + \left(1 - f^{(i)}(\mathscr{E}+\hbar\omega)\right) \right] d\mathscr{E} \right\}, \end{aligned} \tag{D.40}$$

$$\begin{aligned} nC_{D_{11}}^{(OP)} = {} & \frac{A^{OP} D_\Gamma^2 N_B^{OP}}{16\hbar^4\pi^2} \lambda_D \left\{ \left(e^{\lambda_w\hbar\omega} - e^{\beta\hbar\omega} \right) \right. \\ & \times \int_0^{+\infty} f^{(i)}(\mathscr{E}) \left(\frac{e^{\lambda+\lambda_w\mathscr{E}}}{1+e^{\lambda+\lambda_w(\mathscr{E}+\hbar\omega)}} \right) \mathscr{E}(\mathscr{E}+\hbar\omega) \left[f^{(i)}(\mathscr{E}+\hbar\omega) - f^{(i)}(\mathscr{E}) \right] d\mathscr{E} \\ & + (e^{\beta\hbar\omega} + e^{\lambda_w\hbar\omega}) \left. \int_0^{+\infty} f^{(i)}(\mathscr{E}) \left(\frac{e^{\lambda+\lambda_w\mathscr{E}}}{1+e^{\lambda+\lambda_w(\mathscr{E}+\hbar\omega)}} \right) \mathscr{E}(\mathscr{E}+\hbar\omega) d\mathscr{E} \right\}. \end{aligned} \tag{D.41}$$

The production terms due to the scattering with the K-phonons are given by

$$nC_n^{(K)} = 0, \tag{D.42}$$

$$nC_W^{(K)} = \frac{A^K D_K^2 N_B^K}{2\hbar^4 v_F^4 \pi^2}(e^{\lambda_w \hbar\omega} - e^{\beta\hbar\omega})\hbar\omega \int_0^{+\infty} f^{(i)}(\mathscr{E})\left(\frac{e^{\lambda+\lambda_w\mathscr{E}}}{1+e^{\lambda+\lambda_w(\mathscr{E}+\hbar\omega)}}\right)\mathscr{E}(\mathscr{E}+\hbar\omega)d\mathscr{E}, \tag{D.43}$$

$$\begin{aligned} nC_{\mathbf{V}}^{(K)} &= \frac{3A^K D_K^2 N_B^K}{8\pi^2\hbar^4 v_F^2}\left\{\int_0^{+\infty}\left(\frac{e^{\lambda+\lambda_w(\mathscr{E}+\hbar\omega)}}{(1+e^{\lambda+\lambda_w(\mathscr{E}+\hbar\omega)})^2}(\lambda_{\mathbf{V}}+(\mathscr{E}+\hbar\omega)\lambda_{\mathbf{S}})\right)\mathscr{E}(\mathscr{E}+\hbar\omega)\right. \\ &\times \left[f^{(i)}(\mathscr{E})+(1-f^{(i)}(\mathscr{E}))e^{\beta\hbar\omega}\right]d\mathscr{E} + \int_0^{+\infty}\left(\frac{e^{\lambda+\lambda_w\mathscr{E}}}{(1+e^{\lambda+\lambda_w\mathscr{E}})^2}(\lambda_{\mathbf{V}}+\mathscr{E}\lambda_{\mathbf{S}})\right)\mathscr{E}(\mathscr{E}+\hbar\omega) \\ &\times \left.\left[1-f^{(i)}(\mathscr{E}+\hbar\omega)+f^{(i)}(\mathscr{E}+\hbar\omega)e^{\beta\hbar\omega}\right]d\mathscr{E}\right\}, \end{aligned} \tag{D.44}$$

$$\begin{aligned} nC_{\mathbf{S}}^{(K)} &= \frac{A^K D_K^2 N_B^K}{8\pi^2\hbar^4 v_F^2}\left\{\int_0^{+\infty}(3\mathscr{E}+2\hbar\omega)\left(\frac{e^{\lambda+\lambda_w(\mathscr{E}+\hbar\omega)}}{(1+e^{\lambda+\lambda_w(\mathscr{E}+\hbar\omega)})^2}(\lambda_{\mathbf{V}}+(\mathscr{E}+\hbar\omega)\lambda_{\mathbf{S}})\right)\mathscr{E}(\mathscr{E}+\hbar\omega)\right. \\ &\times \left[f^{(i)}(\mathscr{E})+(1-f^{(i)}(\mathscr{E}))e^{\beta\hbar\omega}\right]d\mathscr{E} + \int_0^{+\infty}(3\mathscr{E}+\hbar\omega)\left(\frac{e^{\lambda+\lambda_w\mathscr{E}}}{(1+e^{\lambda+\lambda_w\mathscr{E}})^2}(\lambda_{\mathbf{V}}+\mathscr{E}\lambda_{\mathbf{S}})\right)\mathscr{E}(\mathscr{E}+\hbar\omega) \\ &\times \left.\left[1-f^{(i)}(\mathscr{E}+\hbar\omega)+f^{(i)}(\mathscr{E}+\hbar\omega)e^{\beta\hbar\omega}\right]d\mathscr{E}\right\}, \end{aligned} \tag{D.45}$$

$$\begin{aligned} nC_{D_{11}}^{(K)} &= \frac{A^K D_K^2 N_B^K}{16\pi^2\hbar^4}\lambda_D\left\{(e^{\lambda_w\hbar\omega}-e^{\beta\hbar\omega})\right. \\ &\times \int_0^{+\infty} f^{(i)}(\mathscr{E}+\hbar\omega)\left(1-f^{(i)}(\mathscr{E})\right)\mathscr{E}(\mathscr{E}+\hbar\omega)[f^{(i)}(\mathscr{E}+\hbar\omega)-f^{(i)}(\mathscr{E})]d\mathscr{E} \\ &+(e^{\beta\hbar\omega}+e^{\lambda_w\hbar\omega})\left.\int_0^{+\infty} f^{(i)}(\mathscr{E}+\hbar\omega)\left(1-f^{(i)}(\mathscr{E})\right)\mathscr{E}(\mathscr{E}+\hbar\omega)\,d\mathscr{E}\right\}. \end{aligned} \tag{D.46}$$

APPENDIX E

CLOSURE RELATIONS FOR QUANTUM CORRECTED 6 MOMENT MODEL

Let us introduce[1]

$$X_{ij} = \frac{q\beta^2}{8}\frac{\partial^2\Phi(\mathbf{x})}{\partial x_i \partial x_j} + \frac{\beta^3 q^2}{24}\frac{\partial\Phi(\mathbf{x})}{\partial x_i}\frac{\partial\Phi(\mathbf{x})}{\partial x_j}, \quad Y_{ij} = \frac{q\beta^3}{24}\frac{\partial^2\Phi(\mathbf{x})}{\partial x_i \partial x_j}.$$

The field variables in terms of the Lagrange multipliers read

$$n \approx \frac{1}{2\pi\hbar^2}\left\{\int_0^{+\infty}\frac{2p}{1+e^{\lambda+\lambda_w\mathscr{E}(p)}}dp + v_F\hbar^2\exp(q\Phi(\mathbf{x})\beta)\int_0^{+\infty}\exp(-\beta(\mathscr{E}(p)-\varphi_F))\left[(X_{11}+X_{22})\left(-\frac{p^2}{(p^2+\alpha^2)^{3/2}}+\frac{2}{\sqrt{p^2+\alpha^2}}\right)+\right.\right. \tag{E.1}$$
$$\left.\left. -v_F\frac{p^2}{p^2+\alpha^2}(Y_{11}+Y_{22})\right]p\,dp\right\},$$

$$nW \approx \frac{v_F}{2\pi\hbar^2}\left\{\int_0^{+\infty}\frac{2p\sqrt{p^2+\alpha^2}}{1+e^{\lambda+\lambda_w\mathscr{E}(p)}}dp + v_F\hbar^2\exp(q\Phi(\mathbf{x})\beta)\int_0^{+\infty}\exp(-\beta(\mathscr{E}(p)-\varphi_F))\left[(X_{11}+X_{22})\left(-\frac{p^2}{p^2+\alpha^2}+2\right)+\right.\right. \tag{E.2}$$
$$\left.\left. -v_F\frac{p^2}{\sqrt{p^2+\alpha^2}}(Y_{11}+Y_{22})\right]p\,dp\right\},$$

$$n\mathbf{V} = -\frac{v_F^2}{2\pi\hbar^2}\left\{\int_0^{+\infty}\frac{p^3}{p^2+\alpha^2}\frac{e^{\lambda+\lambda_w\mathscr{E}}}{(1+e^{\lambda+\lambda_w\mathscr{E}})^2}dp\lambda_{\mathbf{V}} + \int_0^{+\infty}\frac{p^3}{p^2+\alpha^2}\frac{\mathscr{E}(p)e^{\lambda+\lambda_w\mathscr{E}}}{(1+e^{\lambda+\lambda_w\mathscr{E}})^2}dp\lambda_{\mathbf{S}}\right\}, \tag{E.3}$$

$$n\mathbf{S} = -\frac{v_F^3}{2\pi\hbar^2}\left\{\int_0^{+\infty}\frac{p^3}{\sqrt{p^2+\alpha^2}}\frac{e^{\lambda+\lambda_w\mathscr{E}}}{(1+e^{\lambda+\lambda_w\mathscr{E}})^2}dp\lambda_{\mathbf{V}} + \int_0^{+\infty}\frac{p^3}{\sqrt{p^2+\alpha^2}}\frac{\mathscr{E}(p)e^{\lambda+\lambda_w\mathscr{E}}}{(1+e^{\lambda+\lambda_w\mathscr{E}})^2}dp\lambda_{\mathbf{S}}\right\}. \tag{E.4}$$

Regarding the expression of the fluxes we have

$$nT^{(0)}_{ijk} = \frac{v_F^2}{2(\pi\hbar)^2}\int_{\mathbb{R}^2}\frac{e^{\lambda+\lambda_w\mathscr{E}(p)}}{(1+e^{\lambda+\lambda_w\mathscr{E}(p)})^2}(\lambda_{V_n}+\mathscr{E}(p)\lambda_{S_n})\left(\frac{p_n}{(p^2+\alpha^2)^2}(p_i\delta_{jk}+p_j\delta_{ik}+p_k\delta_{ij}) - 3\frac{p_n p_i p_j p_k}{(p^2+\alpha^2)^3}\right)d\mathbf{p}. \tag{E.5}$$

[1]Hereafter we don't use Einstein's summation convention.

We observe that the previous tensor is completey symmetric. Its only relevant components are given by

$$nT^{(0)}_{lrl} = \frac{v_F^2}{2\pi\hbar^2}\int_0^{+\infty} \frac{e^{\lambda+\lambda_w\mathscr{E}(p)}}{(1+e^{\lambda+\lambda_w\mathscr{E}(p)})^2}(\lambda_{V_r}+\mathscr{E}(p)\lambda_{S_r})\left(\frac{p^2}{(p^2+\alpha^2)^2}-\frac{3}{4}\frac{p^4}{(p^2+\alpha^2)^3}\right)p\,dp, r\neq l, \quad \text{(E.6)}$$

and $nT^{(0)}_{rrr} = 3nT^{(0)}_{lrl}$.

The same considerations are valid concerning the tensors $\mathbf{T}^{(1)}$, $\mathbf{G}^{(0)}$ and $\mathbf{G}^{(1)}$. Hence we have

$$nT^{(1)}_{ijk} = \frac{v_F^3}{2(\pi\hbar)^2}\int_{\mathbb{R}^2} \frac{e^{\lambda+\lambda_w\mathscr{E}(p)}}{(1+e^{\lambda+\lambda_w\mathscr{E}(p)})^2}(\lambda_{V_n}+\mathscr{E}(p)\lambda_{S_n})\left(\frac{p_n}{(p^2+\alpha^2)^{3/2}}(p_i\delta_{jk}+p_j\delta_{ik}+p_k\delta_{ij})-3\frac{p_np_ip_jp_k}{(p^2+\alpha^2)^{5/2}}\right)d\mathbf{p} \quad \text{(E.7)}$$

and the only relevant components are given by

$$nT^{(1)}_{lrl} = \frac{v_F^3}{2\pi\hbar^2}\int_0^{+\infty} \frac{e^{\lambda+\lambda_w\mathscr{E}(p)}}{(1+e^{\lambda+\lambda_w\mathscr{E}(p)})^2}(\lambda_{V_r}+\mathscr{E}(p)\lambda_{S_r})\left(\frac{p^2}{(p^2+\alpha^2)^{3/2}}-\frac{3}{4}\frac{p^4}{(p^2+\alpha^2)^{5/2}}\right)p\,dp \quad \text{(E.8)}$$

and $nT^{(i)}_{rrr} = 3nT^{(i)}_{lrl}$, for $i = 0, 1$;

$$nH^{(0)}_{ijkl} = \frac{v_F^2}{2(\pi\hbar)^2}\int_{\mathbb{R}^2} \frac{1}{1+e^{\lambda+\lambda_w\mathscr{E}(p)}}\left(-\frac{p_ip_l\delta_{jk}+p_jp_l\delta_{ik}+p_kp_l\delta_{ij}}{(p^2+\alpha^2)^2}+3\frac{p_ip_jp_kp_l}{(p^2+\alpha^2)^3}\right)d\mathbf{p}, \quad \text{(E.9)}$$

$$nH^{(1)}_{ijkl} = \frac{v_F^3}{2(\pi\hbar)^2}\int_{\mathbb{R}^2} \frac{1}{1+e^{\lambda+\lambda_w\mathscr{E}(p)}}\left(-\frac{p_ip_l\delta_{jk}+p_jp_l\delta_{ik}+p_kp_l\delta_{ij}}{(p^2+\alpha^2)^{3/2}}+3\frac{p_ip_jp_kp_l}{(p^2+\alpha^2)^{5/2}}\right)d\mathbf{p} \quad \text{(E.10)}$$

and only relevant components are given by

$$nH^{(0)}_{ppqq} = \frac{v_F^2}{2\pi\hbar^2}\int_0^{+\infty} \frac{p}{1+e^{\lambda+\lambda_w\mathscr{E}(p)}}\left(-\frac{p^2}{(p^2+\alpha^2)^2}+\frac{3}{4}\frac{p^4}{(p^2+\alpha^2)^3}\right)dp, \quad \text{(E.11)}$$

$$nH^{(1)}_{ppqq} = \frac{v_F^3}{2\pi\hbar^2}\int_0^{+\infty} \frac{p}{1+e^{\lambda+\lambda_w\mathscr{E}(p)}}\left(-\frac{p^2}{(p^2+\alpha^2)^{3/2}}+\frac{3}{4}\frac{p^4}{(p^2+\alpha^2)^{5/2}}\right)dp. \quad \text{(E.12)}$$

$$nH^{(i)}_{pppp} = 3nH^{(i)}_{ppqq} \quad \text{(E.13)}$$

for $i = 0, 1$.

The components of $\mathbf{G}^{(0)}$ and $\mathbf{G}^{(1)}$ read

$$\begin{aligned} nG^{(0)}_{ii} \approx \frac{2\pi v_F}{(2\pi\hbar)^2}\Bigg\{ &\int_0^{+\infty}\frac{1}{1+e^{\lambda+\lambda_w\mathscr{E}(p)}}\left(\frac{2p}{\sqrt{p^2+\alpha^2}}-\frac{p^3}{(p^2+\alpha^2)^{3/2}}\right)dp + v_F\hbar^2\frac{n(x,t)}{A_0(\beta)}\Bigg[\frac{1}{2}X_{ii}\int_0^{+\infty}\exp(-\beta(\mathscr{E}(p)-\varphi_F))\frac{p^5}{(p^2+\alpha^2)^3}dp + \\ &+\sum_{j=1}^{2}X_{jj}\int_0^{+\infty}\exp(-\beta(\mathscr{E}(p)-\varphi_F))\left(\frac{1}{4}\frac{p^5}{(p^2+\alpha^2)^3}-\frac{2p^3}{(p^2+\alpha^2)^2}+\frac{2p}{p^2+\alpha^2}+\frac{A(\beta)}{v_FA_0(\beta)}\left(\frac{p^3}{(p^2+\alpha^2)^{3/2}}-\frac{2p}{\sqrt{p^2+\alpha^2}}\right)\right)dp + \\ &+\frac{1}{2}v_FY_{ii}\int_0^{+\infty}\exp(-\beta(\mathscr{E}(p)-\varphi_F))\frac{p^5}{(p^2+\alpha^2)^{5/2}}dp + v_F\sum_{j=1}^{2}Y_{jj}\int_0^{+\infty}\exp(-\beta(\mathscr{E}(p)-\varphi_F))\left(\frac{1}{4}\frac{p^5}{(p^2+\alpha^2)^{5/2}}-\frac{p^3}{(p^2+\alpha^2)^{3/2}}-\right. \\ &\left.-\frac{B(\beta)}{v_F^2A_0(\beta)}\left(\frac{p^3}{(p^2+\alpha^2)^{3/2}}-\frac{2p}{\sqrt{p^2+\alpha^2}}\right)\right)dp\Bigg]\Bigg\}, \end{aligned} \quad \text{(E.14)}$$

$$nG^{(0)}_{12} = nG^{(0)}_{21} \approx \frac{\pi v_F^2}{(2\pi)^2}\frac{n(x,t)}{A_0(\beta)}\left(X_{12}\int_0^{+\infty}\exp(-\beta(\mathscr{E}(p)-\varphi_F))\frac{p^5}{(p^2+\alpha^2)^3}dp + v_FY_{12}\int_0^{+\infty}\exp(-\beta(\mathscr{E}(p)-\varphi_F))\frac{p^5}{(p^2+\alpha^2)^{5/2}}dp\right), \quad \text{(E.15)}$$

$$nG_{ii}^{(1)} \approx \frac{2\pi v_F^2}{(2\pi\hbar)^2}\left\{\int_0^{+\infty}\frac{p}{1+e^{\lambda+\lambda_w\mathscr{E}(p)}}\left(1+\frac{\alpha^2}{p^2+\alpha^2}\right)dp+v_F\hbar^2\frac{n(x,t)}{A_0(\beta)}\left[\frac{1}{2}X_{ii}\int_0^{+\infty}\exp(-\beta(\mathscr{E}(p)-\varphi_F))\frac{p^5}{(p^2+\alpha^2)^{5/2}}dp+\right.\right.$$
$$+\sum_{j=1}^{2}X_{jj}\int_0^{+\infty}\exp(-\beta(\mathscr{E}(p)-\varphi_F))\left(\frac{1}{4}\frac{p^5}{(p^2+\alpha^2)^{5/2}}-\frac{2p^3}{(p^2+\alpha^2)^{3/2}}+\frac{2p}{\sqrt{p^2+\alpha^2}}+\frac{A(\beta)}{v_FA_0(\beta)}\left(\frac{p^3}{p^2+\alpha^2}-2p\right)\right)dp+$$
$$+\frac{1}{2}v_FY_{ii}\int_0^{+\infty}\exp(-\beta(\mathscr{E}(p)-\varphi_F))\frac{p^5}{(p^2+\alpha^2)^2}dp+v_F\sum_{j=1}^{2}Y_{jj}\int_0^{+\infty}\exp(-\beta(\mathscr{E}(p)-\varphi_F))\left(\frac{1}{4}\frac{p^5}{(p^2+\alpha^2)^2}-\frac{p^3}{p^2+\alpha^2}-\right.$$
$$\left.\left.-\frac{B(\beta)}{v_F^2A_0(\beta)}\left(\frac{p^3}{p^2+\alpha^2}-2p\right)\right)dp\right]\right\}, \tag{E.16}$$

$$nG_{12}^{(1)}=nG_{21}^{(1)}\approx\frac{\pi v_F^2}{(2\pi)^2}\frac{n(x,t)}{A_0(\beta)}\left(X_{12}\int_0^{+\infty}\exp(-\beta(\mathscr{E}(p)-\varphi_F))\frac{p^5}{(p^2+\alpha^2)^{5/2}}dp+v_FY_{12}\int_0^{+\infty}\exp(-\beta(\mathscr{E}(p)-\varphi_F))\frac{p^5}{(p^2+\alpha^2)^2}dp\right). \tag{E.17}$$

and those of $\mathbf{F}^{(0)}$ and $\mathbf{F}^{(1)}$ read

$$nF_{ii}^{(0)}\approx\frac{v_F^2}{2\pi\hbar^2}\left\{\int_0^{+\infty}\frac{1}{1+e^{\lambda+\lambda_w\mathscr{E}}}\frac{p^3}{p^2+\alpha^2}dp+\hbar^2\frac{n(\mathbf{x},t)}{A_0(\beta)}\int_0^{+\infty}p\exp(-\beta(\mathscr{E}(p)-\varphi_F))\left(-\frac{1}{2}v_FX_{ii}\frac{p^4}{(p^2+\alpha^2)^{5/2}}+\right.\right.$$
$$+v_F\sum_{j=1}^{2}X_{jj}\left(-\frac{1}{4}\frac{p^4}{(p^2+\alpha^2)^{5/2}}+\frac{p^2}{(p^2+\alpha^2)^{3/2}}-\frac{A(\beta)}{v_FA_0(\beta)}\frac{p^2}{p^2+\alpha^2}\right)-\frac{1}{2}Y_{ii}\frac{v_F^2p^4}{(p^2+\alpha^2)^2}- \tag{E.18}$$
$$\left.\left.-\frac{1}{4}\sum_{j=1}^{2}Y_{jj}\left(v_F^2\frac{p^4}{(p^2+\alpha^2)^2}-\frac{B(\beta)}{A_0(\beta)}\frac{p^2}{p^2+\alpha^2}\right)\right\}\right)dp,$$

$$nF_{12}^{(0)}=nF_{21}^{(0)}\approx-\frac{v_F^2}{4\pi}\frac{n(x,t)}{A_0(\beta)}\int_0^{+\infty}\exp(-\beta(\mathscr{E}(p)-\varphi_F))\left[X_{12}\frac{v_Fp^4}{(p^2+\alpha^2)^{5/2}}+Y_{12}\frac{v_F^2p^4}{(p^2+\alpha^2)^2}\right]p\,dp, \tag{E.19}$$

$$nF_{ii}^{(1)}\approx\frac{v_F^3}{2\pi\hbar^2}\left\{\int_0^{+\infty}\frac{1}{1+e^{\lambda+\lambda_w\mathscr{E}}}\frac{p^3}{\sqrt{p^2+\alpha^2}}dp+\hbar^2\frac{n(\mathbf{x},t)}{A_0(\beta)}\int_0^{+\infty}p\exp(-\beta(\mathscr{E}(p)-\varphi_F))\left(-\frac{1}{2}v_FX_{ii}\frac{p^4}{(p^2+\alpha^2)^2}+\right.\right.$$
$$+v_F\sum_{j=1}^{2}X_{jj}\left(-\frac{1}{4}\frac{p^4}{p^2+\alpha^2}+\frac{p^2}{p^2+\alpha^2}-\frac{A(\beta)}{v_FA_0(\beta)}\frac{p^2}{\sqrt{p^2+\alpha^2}}\right)-\frac{1}{2}Y_{ii}\frac{v_F^2p^4}{(p^2+\alpha^2)^{3/2}}- \tag{E.20}$$
$$\left.\left.-\frac{1}{4}\sum_{j=1}^{2}Y_{jj}\left(v_F^2\frac{p^4}{(p^2+\alpha^2)^{3/2}}-\frac{B(\beta)}{A_0(\beta)}\frac{p^2}{\sqrt{p^2+\alpha^2}}\right)\right\}\right)dp,$$

$$nF_{12}^{(1)}=nF_{21}^{(1)}\approx-\frac{v_F^3}{4\pi}\frac{n(x,t)}{A_0(\beta)}\int_0^{+\infty}\exp(-\beta(\mathscr{E}(p)-\varphi_F))\left[X_{12}\frac{v_Fp^4}{(p^2+\alpha^2)^2}+Y_{12}\frac{v_F^2p^4}{(p^2+\alpha^2)^{3/2}}\right]p\,dp. \tag{E.21}$$

Finally the tensors $\mathbf{L}^{(0)}$ and $\mathbf{L}^{(1)}$ are given by

$$nL_{ijkl}^{(0)}\approx\frac{v_F}{2(\pi\hbar)^2}\int_{\mathbb{R}^2}\frac{1}{1+e^{\lambda+\lambda_w\mathscr{E}}}\left(\frac{3}{(\alpha^2+p^2)^{5/2}}(p_ip_l\delta_{jk}+p_jp_l\delta_{ik}+p_kp_l\delta_{ij}+\delta_{il}p_jp_k+\delta_{jl}p_ip_k+\delta_{kl}p_ip_j)-\right.$$
$$\left.-\frac{1}{(\alpha^2+p^2)^{3/2}}(\delta_{il}\delta_{jk}+\delta_{jl}\delta_{ik}+\delta_{lk}\delta_{ij})-15\frac{p_ip_jp_kp_l}{(\alpha^2+p^2)^{7/2}}\right)d\mathbf{p}, \tag{E.22}$$

$$nL_{ijkl}^{(0)}\approx\frac{v_F^2}{2(\pi\hbar)^2}\int_{\mathbb{R}^2}\frac{1}{1+e^{\lambda+\lambda_w\mathscr{E}}}\left(\frac{3}{(\alpha^2+p^2)^2}(p_ip_l\delta_{jk}+p_jp_l\delta_{ik}+p_kp_l\delta_{ij}+\delta_{il}p_jp_k+\delta_{jl}p_ip_k+\delta_{kl}p_ip_j)-\right.$$
$$\left.-\frac{1}{\alpha^2+p^2}(\delta_{il}\delta_{jk}+\delta_{jl}\delta_{ik}+\delta_{lk}\delta_{ij})-15\frac{p_ip_jp_kp_l}{(\alpha^2+p^2)^3}\right)d\mathbf{p}, \tag{E.23}$$

whose only non zero components are

$$nL_{rrrp}^{(0)}\approx\frac{v_F}{2\pi\hbar^2}\int_0^{+\infty}\frac{p}{1+e^{\lambda+\lambda_w\mathscr{E}}}\frac{9p^2}{(\alpha^2+p^2)^{5/2}}dp, \tag{E.24}$$

$$nL^{(0)}_{rrpp} \approx \frac{v_F}{2\pi\hbar^2}\int_0^{+\infty} \frac{p}{1+e^{\lambda+\lambda_w\mathscr{E}}}\left(\frac{6p^2}{(\alpha^2+p^2)^{5/2}} - \frac{2}{(\alpha^2+p^2)^{3/2}} - \frac{15}{4}\frac{p^4}{(\alpha^2+p^2)^{7/2}}\right)dp, \tag{E.25}$$

$$nL^{(1)}_{rrrp} \approx \frac{v_F^2}{2\pi\hbar^2}\int_0^{+\infty} \frac{p}{1+e^{\lambda+\lambda_w\mathscr{E}}}\frac{9p^2}{(\alpha^2+p^2)^2}dp, \tag{E.26}$$

$$nL^{(1)}_{rrpp} \approx \frac{v_F^2}{2\pi\hbar^2}\int_0^{+\infty} \frac{p}{1+e^{\lambda+\lambda_w\mathscr{E}}}\left(\frac{6p^2}{(\alpha^2+p^2)^2} - \frac{2}{\alpha^2+p^2} - \frac{15}{4}\frac{p^4}{(\alpha^2+p^2)^3}\right)dp, \tag{E.27}$$

$$nL^{(i)}_{pppp} = 3nL^{(i)}_{rrpp}$$

for $i = 0, 1$.

BIBLIOGRAPHY

[1] G. Alì, G. Mascali, V. Romano, C. R. Torcasio, *A Hydrodynamical Model for Covalent Semiconductors, with Applications to GaN and SiC*, Acta Appl. Math. **122** (1), 335 (2012).

[2] C.-G. Ambrozie, *Multivariate truncated moments problems and maximum entropy*, Anal. Math. Phys.,**3**(2): 145-161 (2013).

[3] L. Barletti, *Hydrodynamic equations for electrons in graphene obtained from the maximum entropy principle*, J. Math. Phys. **55**(8), 083303, (2014).

[4] L. Barletti. *Hydrodynamic equations for an electron gas in graphene*, J. of Math. in Industry, **6** 1-17 (2016).

[5] K. M. Borysenko, J. T. Mullen, E. A. Barry, S. Paul, Y. G. Semenov, J. M. Zavada, M. Buongiorno Nardelli, K. W. Kim, *First-principles analysis of electron-phonon interactions in graphene*, Phys. Rev. B **11**, 121412(R) (2010).

[6] J. M. Borwein, A.S. Lewis, *Convergence of Best Entropy Estimates*, SIAM J. Control Optim. **1**(2), 191-205 (1991).

[7] J. M. Borwein, A.S. Lewis, *Duality Relationships for entropy-like minimization problems*, SIAM J. of Control Theory and Optim. **29**(2), 325-328 (1991).

[8] J. M. Borwein, W. Huang, *Uniform convergence for moment problems with Fermi-Dirac type entropies* Math. Meth. of OR **40**(3): 239-252, 1994.

[9] V. D. Camiola, G. Mascali, V. Romano, *Numerical Simulation of a Double-Gate Mosfet with a Subband Model for Semiconductors Based on the Maximum Entropy Principle*, Continuum Mech. Therm. **24** (4-6), 417 (2012).

[10] V. D. Camiola, G. Mascali, V. Romano, *Simulation of a Double-Gate MOSFET by a Non-parabolic Hydrodynamical Subband Model for Semiconductors Based on the Maximum Entropy Principle*, Mathematical and Computer Modelling, **58**, 321 (2013).

[11] V. D. Camiola, G. Mascali, V. Romano, *Charge transport in low semiconductor structures*, Springer, In press.

[12] V.D. Camiola, and V. Romano, *Hydrodynamical model for charge transport in graphene*, Journal of Statistical Physics **157** 114-1137 (2014).

[13] A. H. Castro Neto, F. Guinea, N. M. R. Peres, K. S. Novoselov, A. K. Geim, *The electronic properties of graphene*, Rev. Modern Phys. **81**, 109 (2009).

[14] M. Coco, A. Majorana, G. Mascali, V. Romano, *Comparing kinetic and hydrodynamical models for electron transport in monolayer graphene*, Computational Methods for Coupled Problems in Science and Engineering p. 1003-1014, BARCELONA:CIMNE (Int. Center for Num. Meth. in Engineering), Venezia, 18-20 (2015).

[15] M. Coco, A. Majorana, V. Romano, *Cross validation of discontinuous Galerkin method and Monte Carlo simulations of charge transport in graphene on substrate*, Ricerche Mat. (2016).

[16] M. Coco, G. Mascali, V. Romano, *Monte Carlo analysis of thermal effects in monolayer graphene*, J. of Computational and Theoretical Transport, Vol. **45** (7): 540-553 (2016).

[17] M. Coco, V. Romano, *Simulation of electron-phonon coupling and heating dynamics in suspended monolayer graphene including all the phonon branches,*, J. Heat Transfer **45** (7): 540-553 (2016).

[18] W. Dreyer and H. Struchtrup, *Heat Pulse Experiments Revisited*, Cont. Mech. Thermodyn. **5**(1), 3-50 (1993).

[19] C. L. Gardner, *The quantum hydrodynamic model for semiconductor devices*, SIAM J. Appl. Math. **54 (2)**, 409–427 (1994).

[20] C. L Gardner, C. Ringhofer, *Approximation of thermal equilibrium for quantum gases with discontinuous potentials and application to semiconductor devices*, SIAM J. Appl. Math **58**, 780–805 (1998).

[21] A.K. Geim, K. S. Novoselov, *The Rise of Graphene*, Nature Materials, **6**, 183-191 (2007).

[22] H. Grad, *On the kinetic theory of rarefied gases*, Comm. Pure Appl. Math. **2** (4) 331-407 (1949).

[23] H. Grad, *The profile of a steady plane shock wave*, Comm. Pure Appl. Math. **5** (3) 257-300 (1952).

[24] M. N. Kogan, *Rarefied Gas Dynamics*, Plenum, New York, (1969).

[25] C. Jacoboni, *Theory of Electron Transport in Semiconductors*, Springer-Verlag Berlin Heidelberg, (2010).

[26] E. T. Jaynes, *Information Theory and Statistical Mechanics*, Phys. Rev. **106** 620 (1957).

[27] D. Jou, G. Lebon, J. Casas-Vázquez, *Extended Irreversible Thermodynamics*, Springer Berlin (1993).

[28] A. Jüngel, *Transport Equations for Semiconductors*, Springer-Verlag, Berlin Heidelberg (2009).

[29] M. Junk, V. Romano, *Maximum entropy moment system of the semiconductor Boltzmann equation using Kane's dispersion relation*, Cont. Mechanics Thermodynamics **17**, 247–267 (2005).

[30] S. La Rosa and V. Romano, *Maximum Entropy Principle Hydrodynamical Model for Holes in Silicon Semiconductors: the case of the warped bands*, J. Phys. A: Math. Theor. 41, 215103 (2008).

[31] S. La Rosa, G. Mascali and V. Romano, *Exact maximum entropy closure of the hydrodynamical model for Si semiconductors: the 8-moment case*, SIAM J. of Appl. Mathematics **70** (3)710–734 (2009).

[32] G. Lebon, D. Jou, J. Casas-Vázquez, *Understanding Non-equilibrium Thermodynamics: Foundations, Applications, Frontiers*, Springer-Verlag, Berlin,(2008).

[33] P. Lichtenberger, O. Morandi, F. Schürrer, *High-field transport and optical phonon scattering in graphene* Physical Review B **84**, 045406 (2011).

[34] L. Luca, V. Romano, *Hydrodynamical models for charge transport in graphene based on the Maximum Entropy Principle: The case of moments based on energy powers*, Atti della Accademia Peloritana dei Pericolanti, **96**, No. S1, A5 (2018).

[35] L. Luca, V. Romano, *Comparing linear and nonlinear hydrodynamical models for charge transport in graphene based on the Maximum Entropy Principle*, I. J. of Non-Linear Mech. **104**, 39–58 (2018).

[36] L. Luca, V. Romano, *Quantum corrected Hydrodynamic Models for Charge Transport in Graphene*, Submitted.

[37] A. Majorana, V. Romano, *Numerical solutions of the spatially homogeneous Boltzmann equation for electrons in n-doped graphene on a substrate*, J. Theoretical and Computational Transport **46**(3): 176-185,(2017).

[38] A. Majorana, G. Mascali, V. Romano, *Charge transport and mobility in monolayer graphene*, J. of Math. in Industry **7**(4): (2017).

[39] G. Mascali and V. Romano, *Maximum entropy principle in relativistic radiation hydrodynamics*, Ann. de l'Inst. H. Poincaré, Physique Thorique, **67** (2) 123-144 (1997).

[40] G. Mascali and V. Romano, *Si and GaAs mobility derived from a a hydrodynamical model for semiconductors based on the maximum entropy principle*, Physica A, **352** 459-476 (2005).

[41] G. Mascali, V. Romano, *A hydrodynamical model for holes in silicon semiconductors: The case of non-parabolic warped bands*, Math. and Comp. Modelling **55**, 1003–1020 (2012).

[42] G. Mascali, *A Hydrodynamic Model for Silicon Semiconductors Including Crystal Heating*, European J. of Appl. Math. **26**, 477 (2015).

[43] G. Mascali, *A New Formula for Thermal Conductivity Based on a Hierarchy of Hydrodynamical Models*, J Stat Phys **163** (5), 1268 (2016).

[44] G. Mascali, V. Romano, *Exploitation of the Maximum Entropy Principle in Mathematical Modeling of Charge Transport in Semiconductors*, Entropy 2017, **19**(1), 36;(open access article).

[45] G. Mascali, V. Romano, *Charge Transport in graphene including thermal effects*, SIAM J. Appl. Mathematics,**77**: 593-613,(2017) .

[46] O. Morandi, F. Schürrer, *Wigner model for quantum transport in graphene*, J. Phys. A: Math. Theor., **44**, 265301 (2011).

[47] O. Morandi, L. Barletti, *Particle dynamics in graphene: Collimated beam limit*, J. of Comp. and Theor. Transport, **43**(1-7), 418–432 (2015).

[48] I. Müller and T. Ruggeri, *Rational Extended Thermodynamics*, 2nd ed., Springer Tracts in Natural Philosophy 37, Springer-Verlag (New York), (1998).

[49] O. Muscato and V. Di Stefano, *Hydrodynamic simulation of a n+ - n - n+ silicon nanowire*, Contin. Mech. Thermodyn. **26**, 197-205, (2014).

[50] O. Muscato and W. Wagner, *A class of stochastic algorithms for the Wigner equation*, SIAM J. Sci. Comp., **38**(3), A1483-A1507, (2016).

[51] J. von Neumann,*Mathematical Foundation of Quantum Mechanics*, Princeton University Press (1995).

[52] D.L. Nika, A.A. Balandin, *Two-dimensional phonon transport in graphene*, J. Phys.: Condens. Matter, **24**: 233203 (2012).

[53] T. Ohta, A. Bostwick, T. Seyller, K. Horn, E. Rotenberg, *Controlling the electronic structure of bilayer graphene* Science 313(5789):951-4 (2006).

[54] A. Polkovnikov, *Microscopic diagonal entropy and its connection to basic thermodynamic relations*, Ann. Phys. **326**, 486 (2011) .

[55] E. Pop, V. Varshney, A.K. Roy, *Thermal properties of graphene: Fundamentals and applications*,MRS Bull, **37**: 1273, (2012).

[56] D. Querlioz, P. Dollfus, *The Wigner Monte Carlo Method for Nanoelectronic Devices*, ISTE Wiley (2010).

[57] V. Romano, *2D simulation of a silicon MESFET with a nonparabolic hydrodynamical model based on the maximum entropy principle*, J. of Comp. Physics **176**: 70-92 (2002).

[58] V. Romano, *Quantum corrections to the semiclassical hydrodynamical model of semiconductors based on the maximum entropy principle*, J. Math. Physics **48**, 123504 (2007).

[59] V. Romano, M. Zwierz, *Electron-phonon hydrodynamical model for semiconductors*, Z. Angew. Math. Phys. **61**, 1111–1131 (2010).

[60] V. Romano, *The Equilibrium Wigner Function in the Case of Nonparabolic Energy Bands*, in Progress in Industrial Mathematics at ECMI 2008, A. D. Fitt et al editors, series Math. in Industry 15, 135–140, Springer-Verlag Berlin, Heidelberg (2010).

[61] V. Romano, A. Majorana, M. Coco, *DSMC method consistent with the Pauli exclusion principle and comparison with deterministic solutions for charge transport in graphene*, J. Comp. Physics **302**, 267–284 (2015).

[62] D. L. Scharfetter, D. L. Gummel, *Large signal analysis of a Silicon Read diode oscillator*, IEEE Transaction on Electron Devices, Vol. ED-16, pp.64-77 (1969).

[63] A. Sellitto, V. A. Cimmelli, David Jou, *Mesoscopic Theories of Heat Transport in Nanosystems*, SEMA SIMAI Springer Series 2016.

[64] C. E. Shannon, *A Mathematical Theory of Communication*, Bell System Technical Journal. **27** (4), (1948).

[65] D.W. Snoke, Gangqing Liu S. M. Girvin, *The basis of the Second Law of thermodynamics in quantum field theory*, Annals of Physics **327**, 1825–1851 (2012).

[66] M. Teboulle, I. Vajda, *Convergence of best phi -entropy estimates* , IEEE Transactions on Information Theory, 297 - 301 (1993).

[67] P. R. Wallace, *The Band Theory of Graphite*, Phys. Rev. **71**, 622 (1947).

[68] E. Wigner, *On the quantum correction for thermodynamic equilibrium*, Phys. Rev. **40**, 749–749 (1932).

[69] Y. Zhang, TT. Tang, C. Girit, Z. Hao, MC. Martin, A. Zettl, MF Crommie, YR. Shen, F. Wang, *Direct observation of a widely tunable bandgap in bilayer graphene.* Nature 459 (7248):820-3 (2009)

[70] H. Zhao, Q. Guo, F. Xia, H. Wang, *Two-dimensional materials for nanophotonics application*, Nanophotonics **4**,28-142 (2015).