UNIVERSITÀ DEGLI STUDI DI FIRENZE

Facoltà di Scienze Matematiche, Fisiche e Naturali
Dipartimento di Matematica e Informatica "Ulisse Dini"
Dottorato di Ricerca in Matematica

Tesi di Dottorato

Quantum Fluid Models for Electron Transport in Graphene

Candidato:
Nicola Zamponi

Tutor:
Dott. Luigi Barletti

Coordinatore del Dottorato:
Prof. Alberto Gandolfi

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Contents

Introduction

Graphene is a single layer of carbon atoms disposed as an honeycomb lattice, that is, a single sheet of graphite [23] (see fig. 1). This new semiconductor material has attracted the attention of many physicists and engineers thanks to its remarkable electronic properties, which make it an ideal candidate for the construction of new electronic devices (see fig. 2) with strongly increased performances with respect to the usual silicon semiconductors [3, 9, 21, 32]. Potential applications include, for instance, spin field-effect transistors [27, 52], extremely sensitive gas sensors [46], one-electron graphene transistors [41], and graphene spin transistors [14]. The great interest around graphene is attested by the Nobel prize attributed in 2010 to Geim and Novoselov for its discovery.

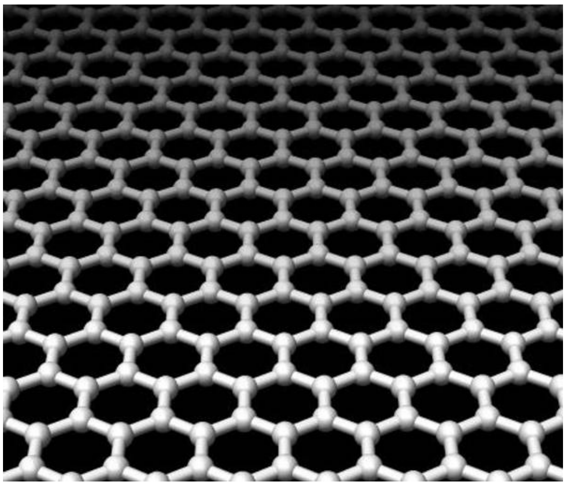

Figure 1: Graphene honeycomb cristal lattice.

Physically speaking, graphene is a zero-gap semiconductor: in the energy spectrum (shown in fig. 3) the valence band intersects the conduction band in some isolated points, named *Dirac points*; moreover, around such points the electron energy is approximately proportional to the modulus of pseudomomentum (or "cristal momentum"):

$$E = \pm v_F \, |p| = \pm v_F \hbar \, |k| \ , \tag{1}$$

where $p = (p_1, p_2)$ is the cristal momentum, $k = (k_1, k_2)$ is the Fermi wavevector,

$v_F \approx 10^6$ m/s is the zero-temperature Fermi velocity [38] and, as usual, $\hbar$ denotes the reduced Planck constant.

The dispersion relation (1) means that the electrons in graphene behave as massless relativistic particles [50], which means, like photons, with an "effective light speed" equal to v_F. This remarkable feature allows to test on graphene some of the predictions of relativistic quantum mechanics with experiments involving non-relativistic velocities; in particular, much attention has been devoted to the so-called *Klein paradox*, that is, unimpeded penetration of relativistic particles through high potential barriers (see e.g. [32] for details). Another interesting consequence of the Dirac-like dispersion relation (1) is that for positive energies the charge carriers are negatively charged and behave like electrons, while at negative energies, if the valence band is not full, its unoccupied electronic states behave as "holes", that is, as positively charged quasiparticles [32], which, in condensed matter physics, plays often the role of positrons [2]. However in condensed matter physics the electron and hole states are reciprocally independent, while in graphene they are interconnected, thanks to the particular structure of graphene cristal lattice, made up by two equivalent triangular sublattices (see fig. 4). This fact is actually at the origin of the linear (with respect to $|p|$) dispersion relation (1): the quantum-mechanical interactions between the two sublattices lead to the formation of two energy bands with sinusoidal shape, intersecting each other at the Dirac points and so yielding the locally conical energy spectrum. As a consequence, the charge carriers have an additional discrete degree of freedom, called "pseudospin", different from the real electron spin, indicating the contribution of each sublattice to the quasiparticles composition: for this reason graphene quasiparticles must be described by *spinors*, that is, two-component wavefunctions [32].

Recently, mathematical models of fluid-dynamic type has been developed in order to describe quantum transport in semiconductors [7, 8, 16, 17, 18, 28, 29, 31, 57]. Such models rely on a kinetic formulation of quantum mechanics (QM) by means of Wigner-type equations, and are derived by taking suitable moments of these latter; the resulting equations involve the chosen fluid-dynamic moments and usually additional expressions (referred to as *not closed* terms) which cannot be written as functions of the previous moments without further hypothesis. In order to solve the so-called *closure problem*, that is, to compute the not closed terms from the known moments, many techniques are employed, e.g. the pure-state hypothesis (which allows to obtain, for a scalar Hamiltonian of type $\hat{H} = -\frac{\hbar^2}{2m}\Delta + V(x)$, the so-called *Madelung equations* [34]; see also [11] for fluid-dynamic equations derived from a spinorial Hamiltonian of the form $\tilde{H} = -i\hbar c\,\vec{\sigma}\cdot\vec{\nabla}$), the ad-hoc ansatz (like the Gardner's equilibrium distribution, see [29]), and a strategy of entropy minimization[1] (which will be followed in this thesis, in analogy to the method employed in the closure of classical fluid-dynamic systems derived from the Boltzmann transport equation in the classical statistical mechanics, see [16, 17, 18, 33]).

In order to understand and describe the charge carrier transport in graphene,

[1] We adopt the reverse sign convention for entropy.

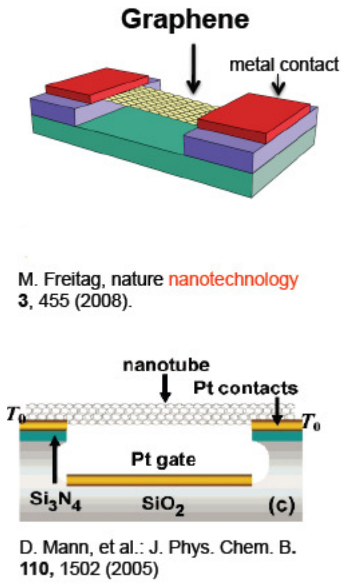

Figure 2: Schematics of a graphene-based device.

transport models, which incorporate the pseudospin degree of freedom, have to be devised. Theoretical models for spin-polarized transport involve fluid-type drift-diffusion equations, kinetic transport equations, and Monte-Carlo simulation schemes; see the references in [40]. A hierarchy of fluid-dynamic spin models was derived from a spinor Boltzmann transport equation in [10]. Suitable matrix collision operators were suggested and analyzed in [42]. Drift-diffusion models for spin transport were considered in several works; see, e.g., [8, 19, 45]. A mathematical analysis of spin drift-diffusion systems for the band densities is given in [25].

The main advantages of fluid-dynamic models with respect to "basic" tools like Schrödinger, Von Neumann, Wigner equations, are basically two. The first advantage is about physical interpretation: fluid-dynamic models contain already the most physically interesting quantities (like particle, momentum and spin densities), while other models usually involve more "abstract" objects (such as wavefunctions, density operators, Wigner functions), which do not have an immediate physical interpretation; in this latter case, further computations have to be made in order to obtain the quantities of real physical interest from the solution of the model. The second and most important advantage is about numerical computation: fluid-dynamic models for quantum systems with d degrees of freedom are sets of PDEs in d space variables and 1 time variable, while other models usually have more complicated structures (for example, Wigner equations are sets of PDEs in $2d$ space variables and 1 time variable); so fluid-dynamic models are usually more easily and quickly solvable via numerical computation than other models.

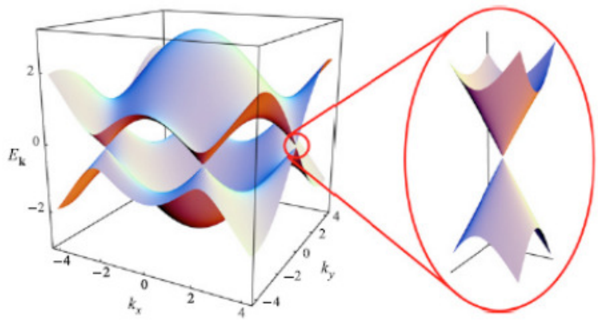

Figure 3: Graphene energy spectrum.

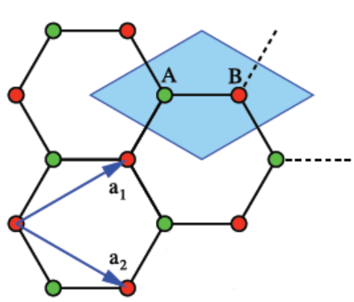

Figure 4: The two sublattices constituting graphene cristal lattice, denoted here with A, B.

We note that there are only very few articles concerned with kinetic or macroscopic transport models for graphene. In the physics literature, the focus is on transport properties such as the carrier mobility [26], charged impurity and phonon scattering [15], and Klein tunneling [39]. Wigner models were investigated in [37]. Starting from a Wigner equation, hydrodynamic spin models were derived in [57], and the work [55] is concerned with the derivation of drift-diffusion models for the band densities. In contrast, we will work in the present thesis with all components of the spin vector. Furthermore, we provide a mathematical analysis of one of the models and numerical simulations of both models.

Content of this Thesis

This Thesis can be divided into two main parts. In the first part several mathematical models of quantum transport of electrons in graphene are derived; in the second part an analytical study of a particular model (namely model QSDE1 (4.91), (4.92)) is carried out, and numerical results related to two of the derived models (more precisely, models QSDE1 (4.91), (4.92) and QSDE2 (4.107)) are presented.

The first part is organized as follows.
In Chapter 1 some mathematical tools for the study of statistical quantum systems, that is, systems composed by many quantum particles, will be exposed: the density matrices and Wigner formalism will be explained, and the Wigner equations for the system of interest, that is, electrons in graphene, will be presented. Finally a fluid model describing a pure state and based upon the fluid moments n_0 (charge density), $\vec{n}$ (spin vector), $\vec{J}$ (current density) will be derived, exploiting the closure relations that hold in this particular case.
In Chapter 2 the minimum entropy principle for quantum systems will be explained and a semiclassical expansion of the so-called "quantum exponential" $\mathcal{E}\mathrm{xp}(\cdot) \equiv \mathrm{Op}^{-1}\exp(\mathrm{Op}(\cdot))$[2] in the general spin case will be performed; such expansion will be exploited in the subsequent part of the Thesis in order to obtain explicit semiclassical approximations of the equilibrium distribution for many fluid models.
In Chapter 3 one hydrodynamic model and two drift-diffusion *two-band* models will be derived: the main feature of these models will reside in the choice of fluid-dynamic moments, namely the two band densities n_+, n_- and the two band currents J_+, J_-, that mirror the two-band structure of graphene energy spectrum.
In Chapter 4 two hydrodynamic models and two drift-diffusion *spinorial* models will be derived: differently from the two-band models exposed in the previous chapter, in these models all the Pauli components of the Wigner function will be taken into account separately in the definition of the fluid moments, which will be the charge density n_0, the spin vector $\vec{n}$, and the current density $\vec{J}$.

The second part is organized as follows.
In chapter 5 model QSDE1 (4.91), (4.92) will be studied from an analytical point of view. An initial value problem in a bounded domain for the system will be considered. The existence of a weak solution under suitable assumptions on the data, as long as the uniqueness of such solutions under further hypothesis, and strong regularity for the charge density n_0 and potential V, will be proved. An entropy inequality will be derived, and several results concerning the long-time behavior of the solutions, namely the convergence to zero of the spin vector $\vec{n}$ under suitable assumptions on the potential V, will be presented.
In chapter 6 several numerical results, related to models QSDE1 (4.91), (4.92) and QSDE2 (4.107) obtained with a Crank-Nicholson finite difference scheme in the 1-dimensional case, will be illustrated.

Almost all the results that will be presented in this Thesis have already been published by the author in [55, 57, 58].

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[2] In this Thesis Op denotes the Weyl quantization rule, given by Eq. (1.7).

Part I

Derivation of the models

Chapter 1

Kinetic models for quantum transport

1.1 The Von Neumann and Wigner equations

In this section we will briefly introduce some mathematical tools employed in the description of statistical quantum systems, i.e. systems composed of many quantum particles.

1.1.1 Statistical quantum mechanics and density operators

It is known that the state of a statistical quantum system, whose wavefunctions belong to a Hilbert space $\mathscr{H}$, can be described by a density operator S, which means, a linear self-adjoint operator on $\mathscr{H}$ such that:

- S is positive: $(\psi, S\psi) \geq 0 \quad \forall\, \psi \in \mathscr{H}$;
- S has unitary trace: $\mathrm{Tr}(S) = 1$.

It can be proven that, as a consequence, S is a Hilbert-Schmidt operator: $\mathrm{Tr}(S^2) < \infty$.

The evolution of the system is described by the Von Neumann equation:

$$i\hbar\partial_t S(t) = [H, S(t)] \equiv HS(t) - S(t)H\,, \tag{1.1}$$

with H the system hamiltonian.
The following results hold:

Proposition 1 *A linear operator S on $L^2(\mathbb{R}^d)$ is a* density operator *if and only* *if a function* $\rho \in L^2(\mathbb{R}^d \times \mathbb{R}^d, \mathbb{C})$ *exists such that:*

$$(S\psi)(x) = \int_{\mathbb{R}^d} \rho(x,y)\psi(y)\,dy \quad \forall \psi \in L^2(\mathbb{R}^d)\,,$$

$$\overline{\rho}(x,y) = \rho(y,x) \quad \forall (x,y) \in \mathbb{R}^d \times \mathbb{R}^d\,,$$

$$\iint_{\mathbb{R}^d\times\mathbb{R}^d} \rho(x,y)\overline{\psi}(x)\psi(y)\,dxdy \geq 0 \quad \forall \psi \in L^2(\mathbb{R}^d)\,,$$

$$\sum_{n\in\mathbb{N}} \iint_{\mathbb{R}^d\times\mathbb{R}^d} \rho(x,y)\overline{\psi_n}(x)\psi_n(y)\,dxdy = 1 \quad \forall (\psi_n)_{n\in\mathbb{N}} \text{ Hilbert basis of } L^2(\mathbb{R}^d, \mathbb{C})\,.$$

The function ρ *is called the* density matrix *associated to* S*, or simply the* kernel *of* S*.*

Proposition 2 *A linear operator* S *on a Hilbert space* $\mathscr{H}$ *is a* density operator *if and only if a complete orthonormal system* $(\psi_n)_{n\in\mathbb{N}}$ *of* $\mathscr{H}$ *and a sequence of real nonnegative numbers* $(\alpha_n)_{n\in\mathbb{N}}$ *exist such that:*

$$\sum_{n\in\mathbb{N}} \alpha_n = 1\,, \qquad S\varphi = \sum_{n\in\mathbb{N}} \alpha_n(\psi_n, \varphi)\psi_n \quad \forall \varphi \in \mathscr{H}\,;$$

moreover:

$$S\psi_k = \alpha_k\psi_k \quad \forall k \in \mathbb{N}\,, \qquad \mathrm{Tr}(S^2) = \sum_{n\in\mathbb{N}} \alpha_n^2 < \infty\,.$$

The system is said to be in a *pure state* if:

$$S = P_\psi \equiv (\psi, \cdot)\psi \tag{1.2}$$

for some (normalized) $\psi \in \mathscr{H}$, or equivalently, if:

$$\rho(x,y) = \psi(x)\overline{\psi(y)} \qquad \forall x, y \in \mathbb{R}^d\,; \tag{1.3}$$

in this case the Von Neumann equation (1.1) is equivalent to the Schrödinger equation:

$$i\hbar\partial_t\psi = H\psi\,; \tag{1.4}$$

if the system is not in a pure state it is said to be in a *mixed state*.

1.1.2 Wigner formalism for quantum mechanics

[1] The Wigner transform $\mathcal{W}_\hbar$ is a map which takes a mixed state in something like a phase-space distribution:

$$\mathcal{W}_\hbar :\ L^2(\mathbb{R}^d \times \mathbb{R}^d, \mathbb{C}) \to L^2(\mathbb{R}^d \times \mathbb{R}^d, \mathbb{C})\,,$$

$$(\mathcal{W}_\hbar\rho)(r,p) := (2\pi)^{-d} \int_{\mathbb{R}^d} \rho\Big(r + \frac{\hbar}{2}\xi, r - \frac{\hbar}{2}\xi\Big) e^{-ip\cdot\xi} d\xi \tag{1.5}$$

for all $\rho \in L^2(\mathbb{R}^d \times \mathbb{R}^d, \mathbb{C})$.
The most important properties of this map are:

[1] See [4, 5, 49] for details.

- given $\rho_1, \rho_2 \in L^2(\mathbb{R}^d \times \mathbb{R}^d, \mathbb{C})$,
$$(\mathcal{W}_\hbar \rho_1, \mathcal{W}_\hbar \rho_2) = (2\pi\hbar)^{-d}(\rho_1, \rho_2)\,;$$
in particular,
$$\mathcal{W}_\hbar :\ L^2(\mathbb{R}^d \times \mathbb{R}^d, \mathbb{C}) \to L^2(\mathbb{R}^d \times \mathbb{R}^d, \mathbb{C})$$
is continuous;
- The Wigner transform is invertible with bounded inverse given by:
$$(\mathcal{W}_\hbar^{-1} w)(x, y) = \int_{\mathbb{R}^d} w\Big(\frac{x+y}{2}, p\Big) e^{i(x-y)\cdot p/\hbar} dp \tag{1.6}$$
for all $w \in L^2(\mathbb{R}^d \times \mathbb{R}^d, \mathbb{C})$.

We remind that the Weyl quantization of a symbol γ is the functional $\mathrm{Op}_\hbar(\gamma)$ such that, for all $\psi \in L^2(\mathbb{R}^d, \mathbb{C})$:
$$(\mathrm{Op}_\hbar(\gamma)\psi)(x) = (2\pi\hbar)^{-2} \int_{\mathbb{R}^2 \times \mathbb{R}^2} \gamma\left(\frac{x+y}{2}, p\right) \psi(y) e^{i(x-y)\cdot p/\hbar}\, dydp \tag{1.7}$$
(for more details see Ref. [20]). So from property (1.6) we find immediately:
$$(\mathrm{Op}_\hbar(\gamma)\psi)(x) = (2\pi\hbar)^{-2} \int_{\mathbb{R}} (\mathcal{W}_\hbar^{-1} w)(x, y)\psi(y)\, dy\,,$$
which means that $\mathrm{Op}_\hbar$ and $\mathcal{W}_\hbar^{-1}$ can be identified, up to the identification of a density operator with its kernel.

The Wigner transform of a density matrix is called a Wigner function. The following results hold:

Proposition 3 *A function $w \in L^2(\mathbb{R}^d \times \mathbb{R}^d, \mathbb{C})$ is a Wigner function if and only if:*

(P1) w is real-valued;

(P2) $\int_{\mathbb{R}^d \times \mathbb{R}^d} w(x, p)\, dx\, dp = 1$;

(P3) $\int_{\mathbb{R}^d \times \mathbb{R}^d} w(x, p)(\mathcal{W}_\hbar P_\psi)(x, p)\, dx\, dp \geq 0\,, \quad \forall \psi \in \mathscr{H}$.

Proposition 4 *Let S a density operator and $w := \mathrm{Op}^{-1}(S)$. Let γ a classical symbol and $A_\gamma = \mathrm{Op}(\gamma)$. If $\mathrm{Tr}(SA_\gamma) < \infty$ then:*
$$\mathrm{Tr}(SA_\gamma) = \int_{\mathbb{R}^d \times \mathbb{R}^d} \gamma(x, p) w(x, p)\, dx\, dp\,. \tag{1.8}$$

Recalling that $\mathrm{Tr}(SA)$ is the expected value of the measurement of the observable A in the state S, from prop. 4 we deduce that w plays in the statistical quantum mechanics the role of weight in the computation of expected values of physical observables, like the Boltzmann distribution in the statistical classical mechanics; however, w is not almost everywhere nonnegative, so it is not really a phase-space distribution, unlike the Boltzmann distribution. Neverthless, it is possible to prove that the "marginal distributions" are nonnegative:
$$\int_{\mathbb{R}^d} w(x, p) dp = \rho(x, x) \geq 0\,, \qquad \int_{\mathbb{R}^d} w(x, p) dx = (\mathscr{F}\rho)(p, p) \geq 0\,.$$ [2]

[2] Here $\mathscr{F}$ is the Fourier transform with respect to $p \in \mathbb{R}^2$.

From the Von Neumann equation (1.1) it is possible to derive an evolution equation for the Wigner function w associated to the kernel ρ of the density operator S. The general procedure consists in writing (1.1) with respecto to ρ and then applying the Wigner transform to the resulting equation. For example, for a standard scalar Hamiltonian $H = -\frac{\hbar^2}{2m}\Delta + V$ this procedure leads to the Wigner equation in standard form:

$$\frac{\partial w}{\partial t} + \frac{\vec{p}}{m} \cdot \vec{\nabla}_x w + \Theta_\hbar(V) w = 0\,, \tag{1.9}$$

with the pseudo-differential operator $\Theta_\hbar(V)$ defined by Eq. (1.18).

1.1.3 The spinorial case

It is of particular interest, in this Thesis, the extension of the Wigner formalism to quantum systems with spin. This latter is a discrete degree of freedom of some quantum particles (namely a form of intrinsic magnetic moment) which has no classical counterpart, and leads to a more involved mathematical description of the system (see e.g. [53]). Indeed, the pure states of a system with spin are not represented by scalar wavefunctions, but rather by *spinors*, i.e. wavefunctions taking values in $\mathbb{C}^n$ for some $n > 1$. In this Thesis we will discuss the simplest case: $n = 2$.

The state of a spinorial quantum system is stil described by a density operator S, defined as in the scalar case; the evolution of the system is given again by the Von Neumann equation (1.1). Proposition 1 can be riformulated for a spinorial quantum system as:

Proposition 5 *A linear operator S on $L^2(\mathbb{R}^d)^2$ is a* density operator *if and only if a function $\rho \in L^2(\mathbb{R}^d \times \mathbb{R}^d, \mathbb{C}^{2\times 2})$ exists such that:*

$$(S\psi)(x) = \int_{\mathbb{R}^d} \rho(x,y)\psi(y)\,dy \quad \forall \psi \in L^2(\mathbb{R}^d, \mathbb{C}^2)\,,$$

$$\overline{\rho}_{ij}(x,y) = \rho_{ji}(y,x) \quad \forall (x,y) \in \mathbb{R}^d \times \mathbb{R}^d\,, \quad i,j = 1,2\,,$$

$$\iint_{\mathbb{R}^d \times \mathbb{R}^d} \sum_{i,j=1}^{2} \rho_{ij}(x,y)\overline{\psi}_i(x)\psi_j(y)\,dxdy \geq 0 \quad \forall \psi \in L^2(\mathbb{R}^d, \mathbb{C}^2)\,,$$

$$\sum_{n\in\mathbb{N}} \iint_{\mathbb{R}^d \times \mathbb{R}^d} \sum_{i,j=1}^{2} \rho_{ij}(x,y)\overline{\psi_{n,i}}(x)\psi_{n,j}(y)\,dxdy = 1 \quad \forall (\psi_n)_{n\in\mathbb{N}} \text{ Hilbert basis of } L^2(\mathbb{R}^d, \mathbb{C}^2)\,.$$

The function ρ is called the density matrix *associated to S, or simply the* kernel *of S.*

The analogue relations of eq. (1.3) for spinorial quantum systems is:

$$\rho_{ij}(x,y) = \psi_i(x)\overline{\psi_j(y)} \qquad \forall x,y \in \mathbb{R}^d\,, \quad i,j = 1,2\,. \tag{1.10}$$

The Wigner transform w of a density matrix $\rho = (\rho_{ij})_{i,j=1,2}$ and the Weyl quantization A of a classical symbol $\gamma = (\gamma_{ij})_{i,j=1,2}$ are defined componentwise:

$$w_{ij} = \mathcal{W}_\hbar \rho_{ij}\,, \qquad A_{ij} = \mathrm{Op}_\hbar(\gamma_{ij})\,, \qquad i,j = 1,2\,.$$

The following result extends Proposition (3) to the spinorial case:

Proposition 6 *A function $w \in L^2(\mathbb{R}^d \times \mathbb{R}^d, \mathbb{C}^{2\times 2})$ is a Wigner function if and only if:*

(P1) $w(x,p)$ *is a complex* 2×2 *hermitian matrix, for all* $x, p \in \mathbb{R}^d$*;*

(P2) $\mathrm{tr} \int_{\mathbb{R}^d \times \mathbb{R}^d} w(x,p)\, dx\, dp = 1$ *;* [3]

(P3) $\mathrm{tr} \int_{\mathbb{R}^d \times \mathbb{R}^d} w(x,p)(\mathcal{W}_\hbar P_\psi)(x,p)\, dx\, dp \geq 0\,, \quad \forall \psi \in \mathscr{H}$*.*

Let us introduce the *Pauli matrices*:

$$\sigma_0 = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}, \quad \sigma_1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \sigma_2 = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \quad \sigma_3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}. \tag{1.11}$$

The matrices in Eq. (1.11) form a basis of the space of the complex 2×2 hermitian matrices. Since the Wigner function $w(x,p)$ is a complex 2×2 hermitian matrix for all $x, p \in \mathbb{R}^d$, then it can be written in the Pauli basis:

$$w = w_0\sigma_0 + \sum_{s=1}^{3} w_s \sigma_s \equiv w_0\sigma_0 + \vec{w} \cdot \vec{\sigma}\,, \tag{1.12}$$

where the Pauli components $w_0 \dots w_3$ of w are *real-valued scalar* functions.

Proposition 7 *Let* S *a density operator and* $w := \mathrm{Op}_\hbar^{-1}(S)$*. Let* γ *a classical symbol and* $A_\gamma = \mathrm{Op}_\hbar(\gamma)$*. If* $\mathrm{Tr}(SA_\gamma) < \infty$ *then:*

$$\mathrm{Tr}(SA_\gamma) = \int_{\mathbb{R}^d \times \mathbb{R}^d} \mathrm{tr}(\gamma w)(x,p)\, dx\, dp = 2 \int_{\mathbb{R}^d \times \mathbb{R}^d} (\gamma_0 w_0 + \vec{\gamma} \cdot \vec{w})(x,p)\, dx\, dp\,. \tag{1.13}$$

1.2 Quantum transport in graphene

It is known (see e.g. [21], [32]) that the electron Hamiltonian in graphene can be approximated, for low energies and in absence of external potential, by the following Dirac-like operator:

$$H_0 = -i\hbar v_F \left(\sigma_1 \frac{\partial}{\partial x_1} + \sigma_2 \frac{\partial}{\partial x_2} \right), \tag{1.14}$$

where σ_1, σ_2 are given by Eq. (1.11).
The corresponding energy spectrum is:

$$E_\pm(p) = \pm v_F |p|\,. \tag{1.15}$$

However, in this Thesis we are not going to use (1.14) as the system Hamiltonian, because a rigorous discussion of a fluid-dynamic model involving (1.14) would require considering the Fermi-Dirac entropy instead of the Maxwell-Boltzmann,

[3] Here tr is the classical matrix trace.

due to the lower unboundedness of the energy spectrum of (1.14). Indeed, in the rest of the Thesis we will make the hypothesis that the system Hamiltonian is well approximated by the following operator:

$$H = \mathrm{Op}_\hbar\left(\frac{|p|^2}{2m}\sigma_0 + v_F\vec{\sigma}\cdot\vec{p}\right) = H_0 - \sigma_0\frac{\hbar^2}{2m}\Delta\,, \tag{1.16}$$

with $m > 0$ parameter (with the dimensions of a mass), whose energy spectrum is bounded from below:

$$E_\pm(p) = \frac{|p|^2}{2m} \pm v_F|p|\,.$$

Let $w = w(x, p, t)$ the system Wigner function, defined for $(x, p, t) \in \mathbb{R}^2 \times \mathbb{R}^2 \times (0, \infty)$. Notice that, due to the presence of the pseudospin, w is a complex hermitian matrix-valued function instead of a real scalar function; so we can write $w = \sum_{s=0}^{3} w_s\sigma_s$ with w_s Pauli components of w. [4] Moreover let:

$$\vec{w} = (w_1, w_2, w_3)\,,\ \ \partial_t = \frac{\partial}{\partial t}\,,\ \ \vec{\nabla} = \left(\frac{\partial}{\partial x_1}, \frac{\partial}{\partial x_2}, 0\right)\,,\ \ \vec{p} = (p_1, p_2, 0)\,,\ \ p = (p_1, p_2)\,.$$

The collisionless Wigner equations for quantum transport in graphene, associated with the one-particle Hamiltonian $H + V$, with H defined by (1.16), are:

$$\begin{aligned} \partial_t w_0 + \left[\frac{\vec{p}}{m}\cdot\vec{\nabla}\right] w_0 + v_F\vec{\nabla}\cdot\vec{w} + \Theta_\hbar(V)w_0 &= 0 \\ \partial_t\vec{w} + \left[\frac{\vec{p}}{m}\cdot\vec{\nabla}\right]\vec{w} + v_F\left[\vec{\nabla}w_0 + \frac{2}{\hbar}\vec{w}\wedge\vec{p}\right] + \Theta_\hbar(V)\vec{w} &= 0 \end{aligned} \tag{1.17}$$

with the pseudo-differential operator $\Theta_\hbar(V)$ defined by:

$$\begin{aligned} (\Theta_\hbar(V)w)(x, p) &= \frac{i}{\hbar}(2\pi)^{-2}\int_{\mathbb{R}^2\times\mathbb{R}^2}\delta V(x, \xi)w(x, p')e^{-i(p-p')\cdot\xi}d\xi dp'\,, \\ \delta V(x, \xi) &= V\left(x + \frac{\hbar}{2}\xi\right) - V\left(x - \frac{\hbar}{2}\xi\right)\,. \end{aligned} \tag{1.18}$$

We refer to [56, 57] for details about the derivation of (1.17) from the Von Neumann equation.

1.2.1 Non statistical closure: the pure state case

A first fluid-dynamic model for quantum electron transport in graphene can be derived from the Wigner equations under the hypothesis of pure state. We refer to [6] for further details.

Since we are considering the system in a pure state, we do not need to employ a statistical closure, based upon the minimum entropy principle, of the fluid

[4] Given a complex hermitian 2×2 matrix a, its Pauli components are real numbers given by:

$$a_s = \frac{1}{2}\mathrm{tr}(a\sigma_s) \qquad s = 0, 1, 2, 3\,.$$

equations derived from the Wigner equation: thus we can, for the sake of simplicity, use the operator H_0 defined in (1.14) instead of H (given by (1.16)) as the system Hamiltonian. As a consequence, the Wigner equation (1.17) take the simpler form:

$$\begin{aligned} \partial_t w_0 + v_F \vec{\nabla} \cdot \vec{w} + \Theta_\hbar(V) w_0 &= 0\,, \\ \partial_t \vec{w} + v_F \left[\vec{\nabla} w_0 + \frac{2}{\hbar} \vec{w} \wedge \vec{p} \right] + \Theta_\hbar(V) \vec{w} &= 0\,. \end{aligned} \tag{1.19}$$

Eqs. (1.19) will be exploited in order to obtain the pure state fluid model we are looking for.
Let us consider the following moments, for $k = 1, 2$, $s = 1, 2, 3$:

$$\begin{aligned} n_0 &= \int w_0 \, dp && \text{charge density,} \\ n_s &= \int w_s \, dp && \text{pseudospin density,} \\ J_k &= \int p_k w_0 \, dp && \text{pseudomomentum current,} \\ t_{sk} &= \int p_k w_s \, dp && \text{pseudospin currents.} \end{aligned} \tag{1.20}$$

By taking moments of eqs. (1.19) it is easy to find the following system of not-closed fluid equations:

$$\begin{aligned} &\partial_t n_0 + c \partial_j n_j = 0\,, \\ &\partial_t n_s + c \partial_s n_0 + \frac{2c}{\hbar} \eta_{sij} t_{ij} = 0\,, \\ &\partial_t J_k + c \partial_s t_{sk} + n_0 \partial_k V = 0\,. \end{aligned} \tag{1.21}$$

In order to find closure relations we exploit some identities that hold for pure states. The density matrix associated to such a state takes the form:

$$\rho_{ij}(x, y) = \psi_i(x) \overline{\psi_j(y)} \qquad (i, j = 1, 2); \tag{1.22}$$

so it is easy to prove that:

$$\rho \, \partial_{x_k} \rho = \mathrm{tr}(\partial_{x_k} \rho) \rho\,, \qquad \partial_{y_k} \rho \, \rho = \mathrm{tr}(\partial_{x_k} \rho) \rho \qquad (k = 1, 2)\,; \tag{1.23}$$

writing eqs. (1.23) in Pauli components[5] we obtain, for $k = 1, 2$:

$$\begin{aligned} \rho_0 \partial_{x_k} \rho_0 &= \vec{\rho} \cdot \partial_{x_k} \vec{\rho}\,, \\ \rho_0 \partial_{y_k} \rho_0 &= \vec{\rho} \cdot \partial_{y_k} \vec{\rho}\,, \\ i \vec{\rho} \wedge \partial_{x_k} \vec{\rho} &= \vec{\rho} \partial_{x_k} \rho_0 - \rho_0 \partial_{x_k} \vec{\rho}\,, \\ -i \vec{\rho} \wedge \partial_{y_k} \vec{\rho} &= \vec{\rho} \partial_{y_k} \rho_0 - \rho_0 \partial_{y_k} \vec{\rho}\,; \end{aligned} \tag{1.24}$$

[5] The matrices involved in the subsequent computations are not Hermitian; however, also generic complex 2×2 matrices can be written in the Pauli basis, provided that the components are complex numbers.

from eqs. (1.24) we immediately deduce:

$$\vec{\rho}\cdot(\partial_{x_k}-\partial_{y_k})\vec{\rho}=\rho_0(\partial_{x_k}-\partial_{y_k})\rho_0\,; \tag{1.25}$$

moreover, it is easy to prove, exploiting eqs. (1.5), (1.20), that (we omit the time dependence):

$$\begin{aligned} n_0(x)=&\rho_0(x,x)\,, \qquad \vec{n}(x)=\vec{\rho}(x,x)\,,\\ J_k(x)=&\frac{\hbar}{2i}(\partial_{x_k}\rho_0-\partial_{y_k}\rho_0)(x,x) \qquad (k=1,2)\,; \end{aligned} \tag{1.26}$$

so from eqs. (1.25), (1.26) it follows:

$$n_s t_{sk}=n_0 J_k \qquad (k=1,2,\ s=1,2,3)\,; \tag{1.27}$$

finally from eqs. (1.24) we find:

$$i\vec{\rho}\wedge(\partial_{x_k}-\partial_{y_k})\vec{\rho}=\vec{\rho}(\partial_{x_k}+\partial_{y_k})\rho_0-\rho_0(\partial_{x_k}+\partial_{y_k})\vec{\rho}\,, \tag{1.28}$$

and so, exploiting again eqs. (1.25), (1.26) we deduce:

$$\frac{2}{\hbar}\eta_{sij}n_i t_{jk}=n_0\partial_k n_s-n_s\partial_k n_0 \qquad (k=1,2,\ s=1,2,3)\,. \tag{1.29}$$

Notice now that from eqs. (1.22), (1.26) it is possible to find the known relation (see e.g. [6], [11]) between n_0 and $\vec{n}$ that holds for pure states:

$$n_0=|\vec{n}|=\sqrt{n_1^2+n_2^2+n_3^2}\,; \tag{1.30}$$

so defining $\vec{t_k}=(t_{1k},t_{2k},t_{3k})$ and exploiting eqs. (1.27), (1.29), (1.30) along with the easy relation:

$$(\vec{a}\wedge\vec{v})\wedge\vec{a}=(|\vec{a}|^2-\vec{a}\otimes\vec{a})\vec{v} \qquad \forall\vec{a},\ \vec{v}\in\mathbb{R}^3\,,$$

we conclude:

$$\begin{aligned} \vec{t_k}=&\left(\frac{\vec{n}}{|\vec{n}|}\cdot\vec{t_k}\right)\frac{\vec{n}}{|\vec{n}|}+\left(I-\frac{\vec{n}\otimes\vec{n}}{|\vec{n}|^2}\right)\vec{t_k}\\ =&\left(\frac{\vec{n}}{|\vec{n}|}\cdot\vec{t_k}\right)\frac{\vec{n}}{|\vec{n}|}+\left(\frac{2}{\hbar}\frac{\vec{n}}{|\vec{n}|}\wedge\vec{t_k}\right)\wedge\frac{\hbar}{2}\frac{\vec{n}}{|\vec{n}|}\\ =&J_k\frac{\vec{n}}{n_0}+\left(\partial_k\vec{n}-\frac{\vec{n}}{n_0}\partial_k n_0\right)\wedge\frac{\hbar}{2}\frac{\vec{n}}{n_0} \qquad (k=1,2)\,, \end{aligned}$$

which means:

$$n_0 t_{sk}=n_s J_k-\frac{\hbar}{2}\eta_{s\alpha\beta}n_\alpha\partial_k n_\beta \qquad (k=1,2,\ s=1,2,3)\,. \tag{1.31}$$

So eq. (1.21) along with the closure relation (1.31) allows us to obtain the following pure-state fluid model:

$$\begin{aligned} &\partial_t n_0+c\vec{\nabla}\cdot\vec{n}=0\,,\\ &\partial_t\vec{n}+c\vec{\nabla}n_0+\frac{2c}{\hbar}\frac{\vec{n}\wedge\vec{J}}{n_0}+\frac{c}{n_0}(\vec{\nabla}\cdot\vec{n}-\vec{n}\cdot\vec{\nabla})\vec{n}=0\,,\\ &\partial_t\vec{J}+c\vec{\nabla}\cdot\left(\frac{\vec{J}\otimes\vec{n}}{n_0}\right)-\frac{c\hbar}{2}\partial_s\left(\frac{1}{n_0}\eta_{sij}n_i\vec{\nabla}n_j\right)+n_0\vec{\nabla}V=0\,. \end{aligned} \tag{1.32}$$

Eqs. (1.32) can be regarded as the Madelung equations for a quantum particle described by the Hamiltonian (1.14). We remark that the first equation in (1.32) is redundant, since Eq. (1.30) holds.

1.2.2 Collisional Wigner equations

We will now derive two different kinetic models by adding a collisional term to the right side of eqs. (1.17) and performing two different scalings: a diffusive one and an hydrodynamic one. These models will be the starting point for the derivation of several fluid models in the subsequent part of this thesis.

The new set of Wigner equations we consider here is:

$$\begin{aligned} \partial_t w_0 + \left[\frac{\vec{p}}{m} \cdot \vec{\nabla}\right] w_0 + v_F \vec{\nabla} \cdot \vec{w} + \Theta_\hbar(V) w_0 &= \frac{g_0 - w_0}{\tau_c}\,, \\ \partial_t \vec{w} + \left[\frac{\vec{p}}{m} \cdot \vec{\nabla}\right] \vec{w} + v_F \left[\vec{\nabla} w_0 + \frac{2}{\hbar} \vec{w} \wedge \vec{p}\right] + \Theta_\hbar(V) \vec{w} &= \frac{\vec{g} - \vec{w}}{\tau_c}\,. \end{aligned} \tag{1.33}$$

The terms on the left hand side of (1.33) come from the Von Neumann equation (1.1) associated with the Hamiltonian (1.16). The terms on the right hand side of (1.33) are relaxation terms of BGK type, with g the local thermal equilibrium Wigner distribution, which will be defined later, and τ_c is the mean free time (the mean time interval between two subsequent collisions experienced by a particle).

We make the following diffusive scaling of the collisional Wigner equations (1.33):

$$x \mapsto \hat{x} x\,, \quad t \mapsto \hat{t} t\,, \quad p \mapsto \hat{p} p\,, \quad V \mapsto \hat{V} V\,, \tag{1.34}$$

with $\hat{x}$, $\hat{t}$, $\hat{p}$, $\hat{V}$ satisfying:

$$\frac{2 v_F \hat{p}}{\hbar} = \frac{\hat{V}}{\hat{x}\hat{p}}\,, \quad \frac{2\hat{p} v_F \tau_c}{\hbar} = \frac{\hbar}{2\hat{p} v_F \hat{t}}\,, \quad \hat{p} = \sqrt{m k_B T}\,; \tag{1.35}$$

T is the temperature of the phonon thermal bath [2]. Moreover let us define the *semiclassical parameter* ϵ, the *diffusive parameter* τ and the *scaled Fermi speed* c as:

$$\epsilon = \frac{\hbar}{\hat{x}\hat{p}}\,, \quad \tau = \frac{2\hat{p} v_F \tau_c}{\hbar}\,, \quad c = \sqrt{\frac{m v_F^2}{k_B T}}\,. \tag{1.36}$$

Notice that, if we choose as m the electron mass m_e, then $c^2 = \mathcal{E}_F/\mathcal{E}_{cl}$ is the ratio between the Fermi energy $\mathcal{E}_F = m_e v_F^2$ and the classical thermal energy $\mathcal{E}_{cl} = k_B T$ of the electrons.

We make two main approximations here: the well-known *semiclassical hypothesis* $\epsilon \ll 1$, and the following assumption, which we call *Low Scaled Fermi Speed* (LSFS):

$$c \sim \epsilon \qquad (\epsilon \to 0)\,. \tag{1.37}$$

By performing the scaling (1.34)–(1.36) on the equations (1.33) under the previous hypothesis, we obtain the following scaled Wigner system:

$$\begin{aligned} \tau\partial_t w_0 + T_0(w) =& \frac{g_0 - w_0}{\tau} \,, \\ \tau\partial_t w_s + T_s(w) =& \frac{g_s - w_s}{\tau} \,, \qquad s = 1,2,3 \end{aligned} \tag{1.38}$$

where:

$$\begin{aligned} T_0(w) =& \frac{\vec{p}\cdot\vec{\nabla}}{2\gamma} w_0 + \frac{\epsilon}{2}\vec{\nabla}\cdot\vec{w} + \Theta_\epsilon[V]w_0 \,, \\ T_s(w) =& \frac{\vec{p}\cdot\vec{\nabla}}{2\gamma} w_s + \frac{\epsilon}{2}\partial_s w_0 + \Theta_\epsilon[V]w_s + \eta_{sjk} w_j p_k \,, \qquad s = 1,2,3 \,, \end{aligned} \tag{1.39}$$

$$\begin{aligned} (\Theta_\epsilon(V)w)(x,p) =& \frac{i}{\epsilon}(2\pi)^{-2}\int_{\mathbb{R}^2\times\mathbb{R}^2} \delta\tilde{V}(x,\xi)w(x,p')e^{-i(p-p')\cdot\xi}d\xi dp' \,, \\ \delta\tilde{V}(x,\xi) =& V\left(x + \frac{\epsilon}{2}\xi\right) - V\left(x - \frac{\epsilon}{2}\xi\right) \,, \end{aligned} \tag{1.40}$$

and:

$$\gamma \equiv \frac{c}{\epsilon} = O(1) \quad (\epsilon \to 0) \tag{1.41}$$

for the hypothesis (1.37), $\partial_s = \frac{\partial}{\partial x_s}$ for $s = 1,2,3$, and η_{sjk} denotes the Levi-Civita tensor:

$$\eta_{sjk} a_j b_k = (\vec{a}\wedge\vec{b})_s \qquad (s = 1,2,3) \,, \quad \forall \vec{a},\, \vec{b} \in \mathbb{R}^3 \,.$$

Now we make a hydrodynamic scaling of the Wigner equations (1.33):

$$x \mapsto \hat{x}x \,, \quad t \mapsto \hat{t}t \,, \quad p \mapsto \hat{p}p \,, \quad V \mapsto \hat{V}V \,, \tag{1.42}$$

with $\hat{x}$, $\hat{t}$, $\hat{p}$, $\hat{V}$ satisfying:

$$\frac{1}{\hat{t}} = \frac{2v_F\hat{p}}{\hbar} = \frac{\hat{V}}{\hat{x}\hat{p}} \,, \quad \hat{p} = \sqrt{mk_BT} \,; \tag{1.43}$$

moreover, let us define the *hydrodynamic parameter* τ as:

$$\tau = \frac{\tau_c}{\hat{t}} \,. \tag{1.44}$$

Let c (scaled Fermi speed) be given again by (1.36). We make the same assumptions as in the first diffusive model, that is, the semiclassical hypothesis $\epsilon \ll 1$ and the LSFS hypothesis (1.37). Let γ be defined as in (1.41). If we perform the scaling (1.42) – (1.44) on (1.33) under the assumptions we have made, we obtain the following scaled Wigner system:

$$\begin{aligned} \partial_t w_0 + \frac{\vec{p}\cdot\vec{\nabla}}{2\gamma} w_0 + \frac{\epsilon}{2}\vec{\nabla}\cdot\vec{w} + \Theta_\epsilon[V]w_0 =& \frac{g_0 - w_0}{\tau} \,, \\ \partial_t \vec{w} + \frac{\vec{p}\cdot\vec{\nabla}}{2\gamma}\vec{w} + \frac{\epsilon}{2}\vec{\nabla}w_0 + \vec{w}\wedge\vec{p} + \Theta_\epsilon[V]\vec{w} =& \frac{\vec{g} - \vec{w}}{\tau} \,. \end{aligned} \tag{1.45}$$

Again, g is the quantum thermal equilibrium Wigner distribution.

Let us finish this chapter recalling some helpful formal properties of the operator Θ_ϵ defined in (1.40), already known in literature (see for example [56, pp. 29–30]):

$$\begin{aligned}
&\int \Theta_\epsilon[V]\, f\, dp = 0\,, \qquad \int p_i \Theta_\epsilon[V]\, f\, dp = \partial_i V \int f\, dp \quad (i = 1,2)\,, \\
&\Theta_\epsilon[V] f = -\vec{\nabla} V \cdot \vec{\nabla}_p f + O(\epsilon^2) \qquad \text{as } \epsilon \to 0\,, \\
&f \text{ even (resp. odd) w.r.t. } p \quad \Rightarrow \quad \Theta_\epsilon[V] f \text{ odd (resp. even) w.r.t. } p\,.
\end{aligned} \tag{1.46}$$

Chapter 2

Equilibrium distribution: definition and explicit construction

2.1 The minimum entropy principle

Given a quantum system, we define the local equilibrium distribution associated to the system as the minimizer of a suitable quantum entropy functional under the constraints of given macroscopic moments: this is, in short, the so-called Minimum Entropy Principle (MEP). Let us now describe the MEP in more details. Let $w = w_0\sigma_0 + w_s\sigma_s$ the (spinorial) system Wigner function, and let $S = \mathrm{Op}_\hbar(w)$ the Weyl quantization of w; moreover, let H the one-particle Hamiltonian of the system. We assume that the system temperature, T, is a positive constant, and we denote with k_B the Boltzmann constant.
We define following functional, which we call *Quantum Entropy* [17, 18]:

$$\mathscr{A}(S) = \mathrm{Tr}[S\log S - S + H/k_BT]\,, \tag{2.1}$$

defined for $S \in \mathcal{D}(\mathscr{A})$ suitable subset of the set of the density operators associated to the system. We notice that $\mathscr{A}$ is actually not the entropy, but rather a quantity proportional to the system *free energy*:

$$\begin{aligned} \mathscr{A}(S) =& \frac{1}{k_BT}\left(\mathrm{Tr}(HS) - T\mathscr{E}(S)\right)\,, \\ \mathscr{E}(S) =& -k_B\mathrm{Tr}[S\log S - S] \qquad \text{system entropy;} \end{aligned} \tag{2.2}$$

neverthless, we will refer from now on to the functional $\mathscr{A}$ as *quantum entropy functional* for conventional reasons.
We point out that the functional $\mathscr{A}$ in eq. (2.1) can be rewritten in terms of the Wigner distribution w associated to the density operator S:

$$\mathcal{A}(w) = \mathrm{tr}\iint [w\mathcal{L}\mathrm{og}_\hbar\, w - w + h/k_BT]\,dx\,dp\,, \tag{2.3}$$

where tr is the algebraic matrix trace, $\mathcal{L}\text{og}_\hbar\, w = \mathcal{W}_\hbar \log(\mathcal{W}_\hbar^{-1} w)$ is the so-called *Quantum Logarithm* of w, and $h = \mathcal{W}_\hbar H$ is the classical symbol of the Hamiltonian H.
Let now $\mu_0^{(k)}(p)$, $\mu_s^{(k)}(p)$ given real-valued functions of $p \in \mathbb{R}^2$, for $s = 1, 2, 3$, $k = 1 \dots N$, and let $\mu^{(k)}(p) \equiv \mu_0^{(k)}(p)\sigma_0 + \mu_s^{(k)}\sigma_s$ for $k = 1 \dots N$; moreover let $M^{(k)}(x)$ real-valued functions of $x \in \mathbb{R}^2$, for $k = 1 \dots N$.
We define the *distribution at thermal equilibrium* $g \equiv \mathcal{W}_\hbar G$ associated to the moments $\left(M^{(k)}\right)_{k=1\dots N}$ as the Wigner transform of the solution of the constrained minimization problem:

$$\begin{aligned} \mathscr{A}(G) = \min \Bigg\{ & \mathscr{A}(S) \ : \ S = \mathrm{Op}_\hbar w \in \mathcal{D}(\mathscr{A})\,, \\ & \mathrm{tr} \int \mu^{(k)}(p) w(x,p)\, dp = M^{(k)}(x)\,, \quad k = 1 \dots N\,,\ x \in \mathbb{R}^2 \Bigg\}\,. \end{aligned} \tag{2.4}$$

This problem can be solved formally by means of Lagrange multipliers; see [55, Section 3.2] (for scalar-valued Wigner functions, such problems are studied analytically in [36]). First, we notice that the constraints in (2.4) can be written as:

$$\mathrm{Tr}[S\mathrm{Op}_\hbar(\mu^{(k)}(p)\varphi^{(k)}(x))] = \int M^{(k)}\varphi^{(k)}\, dx \qquad \forall \varphi^{(1)} \dots \varphi^{(N)} \quad \text{test functions;} \tag{2.5}$$

now let us define, for $S \in \mathcal{D}(\mathscr{A})$ and $\left(\xi^{(k)}(x)\right)_{k=1\dots N}$ real functions (with suitable summation properties), the following Lagrangian functional:

$$\mathscr{L}(S, \xi^{(1)} \dots \xi^{(N)}) \equiv \mathscr{A}(S) - \mathrm{Tr}[S\mathrm{Op}_\hbar(\mu^{(k)}(p)\xi^{(k)}(x))] + \int M^{(k)}\xi^{(k)}\, dx\,; \tag{2.6}$$

according to the Lagrange multipliers theory, if G solves (2.4) then the Frechét derivative $\delta\mathscr{L}/\delta S$ of $\mathscr{L}$ with respect to S must vanish for $S = G$ and $\xi^{(k)} = \hat{\xi}^{(k)}$ ($k = 1 \dots N$), for suitable functions $(\hat{\xi}^{(k)})_{k=1\dots N}$ called *Lagrange multipliers*:

$$\frac{\delta\mathscr{L}}{\delta S}(G, \hat{\xi}^{(1)} \dots \hat{\xi}^{(N)}) = 0\,; \tag{2.7}$$

from (2.1), (2.6), (2.7) we deduce:

$$\mathrm{Tr}[(\log G + H - \mathrm{Op}_\hbar(\mu^{(k)}(p)\hat{\xi}^{(k)}(x)))\delta S] = 0 \qquad \forall \delta S\,, \tag{2.8}$$

and so, since the variation δS is arbitrary:

$$\log G + H - \mathrm{Op}_\hbar(\mu^{(k)}(p)\hat{\xi}^{(k)}(x)) = 0\,, \tag{2.9}$$

which means:

$$\begin{aligned} G &= \exp(-H + \mathrm{Op}_\hbar(\mu^{(k)}(p)\hat{\xi}^{(k)}(x)))\,, \\ g &= \mathcal{E}\mathrm{xp}_\hbar(-h[\hat{\xi}])\,, \quad h[\hat{\xi}] = \mathcal{W}_\hbar H - \mu^{(k)}(p)\hat{\xi}^{(k)}(x)\,, \end{aligned} \tag{2.10}$$

where $\mathcal{E}\mathrm{xp}$ is the so-called *quantum exponential*, defined by:

$$\mathcal{E}\mathrm{xp}_\hbar(w) \equiv \mathcal{W}_\hbar \exp(\mathcal{W}_\hbar^{-1} w)\,, \qquad \forall w \text{ Wigner function.} \tag{2.11}$$

We call $h[\hat{\xi}]$ the *modified hamiltonian* of the system. For more details concerning the quantum exponential see [20].
It is interesting to see that imposing that the variation of $\mathscr{L}$ with respect to $(\xi^{(k)})_{k=1\dots N}$ vanishes, we obtain the equations of the moments (2.5):

$$\delta_\xi \mathscr{L} = \frac{\delta \mathscr{L}}{\delta \xi^{(k)}} \delta \xi^{(k)} = -\mathrm{Tr}[S \mathrm{Op}_\hbar(\mu^{(k)}(p) \delta \xi^{(k)}(x))] + \int M^{(k)} \delta \xi^{(k)} \, dx = 0 \,,$$

for all $\delta\xi^{(k)} \dots \delta\xi^{(k)}$.
Let us now perform a generic scaling $x \mapsto \hat{x}x$, $p \mapsto \hat{p}p$. It is easy to see that the equilibrium distribution changes in this way:

$$g = \mathcal{E}\mathrm{xp}_\epsilon(-\hat{h}[\hat{\xi}]) = \mathcal{W}_\epsilon \exp(-\mathcal{W}_\epsilon^{-1}(\hat{h}[\hat{\xi}])) \,, \tag{2.12}$$

with $\hat{h}[\hat{\xi}]$ the scaled modified hamiltonian, and $\epsilon = \hbar/\hat{x}\hat{p}$.
The quantum exponential is a highly nonlinear and nonlocal operator: for this reason, we will derive in the next section an explicit approximation of it valid for small values of ϵ.

2.2 Semiclassical expansion of quantum exponential

In this section we find an explicit approximation of the quantum exponential of an arbitrary classical symbol with linear ϵ-dependence, which will be exploited in the rest of the thesis to find an explicit approximation of the equilibrium distribution for several fluid-dynamic models. Let:

$$\{f, g\} = \vec{\nabla}_x f \cdot \vec{\nabla}_p g - \vec{\nabla}_p f \cdot \vec{\nabla}_x g \,, \tag{2.13}$$

denote the Poisson brackets between $f(x,p)$, $g(x,p)$ scalar smooth functions. We apply here the general strategy for computing the semiclassical expansion of the quantum exponential adapted for the spinorial case (see [28, 29] for details). Let $a = a_0\sigma_0 + \vec{a} \cdot \vec{\sigma}$, $b = b_0\sigma_0 + \vec{b} \cdot \vec{\sigma}$ be arbitrary matrix hermitian-valued classical symbols, and let us consider the function:

$$g_\epsilon(\beta) = \mathcal{E}\mathrm{xp}_\epsilon(\beta(a + \epsilon b)) \,, \quad \beta \in \mathbb{R} \,. \tag{2.14}$$

Let us recall the definition of the so-called *Moyal product*:

$$f_1 \#_\epsilon f_2 = \mathrm{Op}_\epsilon^{-1}(\mathrm{Op}_\epsilon(f_1)\mathrm{Op}_\epsilon(f_2)) \tag{2.15}$$

between arbitrary classical symbols f_1, f_2. It is known [16] that the Moyal product has a semiclassical expansion:

$$\#_\epsilon = \sum_{n=0}^{\infty} \epsilon^n \#^{(n)} \,,$$

and the first three terms of this expansion (the only terms needed in this work) are:

$$\begin{aligned} f_1 \#^{(0)} f_2 &= f_1 f_2 \,, \\ f_1 \#^{(1)} f_2 &= \frac{i}{2} \left(\partial_{x_s} f_1 \partial_{p_s} f_2 - \partial_{p_s} f_1 \partial_{x_s} f_2\right) \,, \\ f_1 \#^{(2)} f_2 &= -\frac{1}{8} \left(\partial^2_{x_j x_s} f_1 \partial^2_{p_j p_s} f_2 - 2\partial^2_{x_j p_s} f_1 \partial^2_{p_j x_s} f_2 + \partial^2_{p_j p_s} f_1 \partial^2_{x_j x_s} f_2\right) \,. \end{aligned} \tag{2.16}$$

Now let us differentiate with respect to β the function $g_\epsilon(\beta)$ given by (2.14). By using the definition (2.15) of the Moyal product we obtain:

$$\partial_\beta g_\epsilon(\beta) = \frac{1}{2}((a+\epsilon b)\#_\epsilon g_\epsilon(\beta) + g_\epsilon(\beta)\#_\epsilon (a+\epsilon b)) \,, \tag{2.17}$$

and $g_\epsilon(0) = \sigma_0$. So by writing $g_\epsilon(\beta) = g^{(0)}(\beta) + \epsilon g^{(1)}(\beta) + \epsilon^2 g^{(2)}(\beta) + \dots$ and expanding the expressions in (2.17) in powers of ϵ we find:

$$\partial_\beta g^{(0)}(\beta) = \frac{1}{2}(g^{(0)}(\beta) a + a g^{(0)}(\beta)) \,, \tag{2.18}$$

$$\begin{aligned} \partial_\beta g^{(1)}(\beta) =& \frac{1}{2}(g^{(1)}(\beta) a + a g^{(1)}(\beta)) + \frac{1}{2}(g^{(0)}(\beta) b + b g^{(0)}(\beta)) \\ &+ \frac{1}{2}(g^{(0)}(\beta)\#^{(1)} a + a \#^{(1)} g^{(0)}(\beta)) \,, \end{aligned} \tag{2.19}$$

with the initial conditions:

$$g^{(0)}(0) = \sigma_0 \,, \qquad g^{(1)}(0) = 0 \,. \tag{2.20}$$

The equations (2.18), (2.19) with the initial conditions (2.20) can be explicitly solved in this order to obtain the $O(\epsilon^2)-$approximation of $\mathcal{E}\text{xp}_\epsilon(a) = g_\epsilon(1)$: in fact, each equation is, with respect to the variable β, a linear ODE with constant coefficients. It is easy to find the leading term in the expansion of $g_\epsilon(\beta)$:

$$g^{(0)}(\beta) = \exp(\beta a) = e^{\beta a_0} \left(\cosh(\beta|\vec{a}|)\sigma_0 + \sinh(\beta|\vec{a}|)\frac{\vec{a}}{|\vec{a}|} \cdot \vec{\sigma}\right) \,. \tag{2.21}$$

We now have to explicitly compute the first order correction of $g_\epsilon(\beta)$ from (2.19); to this aim, it is useful to employ some properties of the Pauli matrices. It is easy to verify that, for a, b arbitrary hermitian matrix-valued classical symbols, the following holds:

$$\begin{aligned} \frac{1}{2}(a\#^{(k)} b + b\#^{(k)} a) =& (a_0 \#^{(k)} b_0 + \vec{a} \cdot^{\#^{(k)}} \vec{b})\sigma_0 \\ & + (a_0 \#^{(k)} \vec{b} + b_0 \#^{(k)} \vec{a}) \cdot \vec{\sigma} \quad \text{for even } k, \\ \frac{1}{2}(a\#^{(k)} b + b\#^{(k)} a) =& i(\vec{a} \wedge^{\#^{(k)}} \vec{b}) \cdot \vec{\sigma} \quad \text{for odd } k, \end{aligned} \tag{2.22}$$

where we defined:

$$\vec{a} \cdot^{\#^{(k)}} \vec{b} = a_s \#^{(k)} b_s \,, \quad (\vec{a} \wedge^{\#^{(k)}} \vec{b})_j = \eta_{jst} a_s \#^{(k)} b_t \,.$$

The relations (2.22) allow us to reduce the calculus of the matrix $g^{(1)}(\beta)$ to that of its Pauli components; if fact, due to (2.22), (2.19) becomes:

$$\begin{aligned}\partial_\beta g_0^{(1)}(\beta) =& a_0 g_0^{(1)}(\beta) + \vec{a}\cdot\vec{g}^{(1)}(\beta) + b_0 g_0^{(0)}(\beta) + \vec{b}\cdot\vec{g}^{(0)}(\beta)\\ \partial_\beta \vec{g}^{(1)}(\beta) =& a_0\vec{g}^{(1)}(\beta) + \vec{a} g_0^{(1)}(\beta) + b_0\vec{g}^{(0)}(\beta) + \vec{b} g_0^{(0)}(\beta) + i\vec{a}\wedge^{\#^{(1)}}\vec{g}^{(0)}(\beta)\end{aligned} \tag{2.23}$$

In order to solve (2.23), let us consider the homogeneous problem:

$$\begin{aligned}\partial_\beta x_0(\beta) =& a_0 x_0(\beta) + \vec{a}\cdot\vec{x}(\beta) \qquad \beta > 0\,,\\ \partial_\beta \vec{x}(\beta) =& a_0\vec{x}(\beta) + \vec{a} x_0(\beta) \qquad \beta > 0\,.\end{aligned} \tag{2.24}$$

The problem (2.24) can be solved by elementary techniques, finding that the vector $X(\beta) = [x_0(\beta), \vec{x}(\beta)]$ is given by:

$$X(\beta) = S_a(\beta)X(0) \qquad \beta > 0\,,$$

with the semigroup operator $S_a(\beta)$ given by:

$$S_a(\beta) = e^{\beta a_0}\begin{pmatrix}\cosh(\beta|\vec{a}|) & \sinh(\beta|\vec{a}|)\vec{\alpha}^T\\ \sinh(\beta|\vec{a}|)\vec{\alpha} & (\cosh(\beta|\vec{a}|)-1)\vec{\alpha}\otimes\vec{\alpha} + I_{3\times 3}\end{pmatrix} \tag{2.25}$$

with $\vec{\alpha} \equiv \vec{a}/|\vec{a}|$, and $\vec{\alpha}^T$ denotes the transpose of the vector $\vec{\alpha}$. Now the semigroup theory allows us to write the solution of (2.23):

$$\begin{aligned}g_0^{(1)}(\beta) =& \int_0^\beta e^{(\beta-\lambda)a_0}\cosh((\beta-\lambda)|\vec{a}|)Y_0(\lambda)\,d\lambda\\ &+ \int_0^\beta e^{(\beta-\lambda)a_0}\sinh((\beta-\lambda)|\vec{a}|)\frac{\vec{a}}{|\vec{a}|}\cdot\vec{Y}(\lambda)\,d\lambda\,,\end{aligned} \tag{2.26}$$

$$\begin{aligned}\vec{g}^{(1)}(\beta) =& \int_0^\beta e^{(\beta-\lambda)a_0}\sinh((\beta-\lambda)|\vec{a}|)\frac{\vec{a}}{|\vec{a}|}Y_0(\lambda)\,d\lambda\\ &+ \int_0^\beta e^{(\beta-\lambda)a_0}\left([\cosh((\beta-\lambda)|\vec{a}|)-1]\frac{\vec{a}\otimes\vec{a}}{|\vec{a}|^2} + I_{3\times 3}\right)\vec{Y}(\lambda)\,d\lambda\,,\end{aligned} \tag{2.27}$$

$$\begin{aligned}Y_0(\lambda) =& b_0 g_0^{(0)}(\lambda) + \vec{b}\cdot\vec{g}^{(1)}(\lambda)\,,\\ \vec{Y}(\lambda) =& b_0\vec{g}^{(0)}(\lambda) + \vec{b} g_0^{(1)}(\lambda) + i\vec{a}\wedge^{\#^{(1)}}\vec{g}^{(0)}(\lambda)\,;\end{aligned} \tag{2.28}$$

finally, from (2.21), (2.26), (2.27), (2.28) we obtain:

$$\begin{aligned}&g_0^{(1)}(\beta)\\ =& \beta e^{\beta a_0}\left(\cosh(\beta|\vec{a}|)b_0 + \sinh(\beta|\vec{a}|)\frac{\vec{a}\cdot\vec{b}}{|\vec{a}|}\right)\\ &+ \beta e^{\beta a_0}\frac{\sinh(\beta|\vec{a}|) - \beta|\vec{a}|\cosh(\beta|\vec{a}|)}{4\beta|\vec{a}|^3}\eta_{jks}\{a_j, a_k\}a_s\,,\end{aligned} \tag{2.29}$$

$$
\begin{aligned}
&\vec{g}^{(1)}(\beta)\\
=&\beta e^{\beta a_0}\left(\sinh(\beta|\vec{a}|)b_0+\cosh(\beta|\vec{a}|)\frac{\vec{a}\cdot\vec{b}}{|\vec{a}|}-\frac{\sinh(\beta|\vec{a}|)}{4|\vec{a}|^2}\eta_{jks}\{a_j,a_k\}a_s\right)\frac{\vec{a}}{|\vec{a}|}\\
&+\beta e^{\beta a_0}\frac{\sinh(\beta|\vec{a}|)}{\beta|\vec{a}|}\left(\frac{\vec{a}\wedge\vec{b}}{|\vec{a}|}\right)\wedge\frac{\vec{a}}{|\vec{a}|}+\\
&+\beta e^{\beta a_0}\frac{\beta|\vec{a}|\sinh(\beta|\vec{a}|)-\cosh(\beta|\vec{a}|)+1}{2\beta|\vec{a}|^3}a_j\{a_j,\vec{a}\}\wedge\frac{\vec{a}}{|\vec{a}|}\\
&+\beta e^{\beta a_0}\frac{\beta|\vec{a}|\cosh(\beta|\vec{a}|)-\sinh(\beta|\vec{a}|)}{2\beta|\vec{a}|^2}\{a_0,\vec{a}\}\wedge\frac{\vec{a}}{|\vec{a}|}\,.
\end{aligned}
\tag{2.30}
$$

So we have explicitly computed the first-order semiclassical expansion of $g_\epsilon(\beta)=\mathcal{E}\mathrm{xp}_\epsilon(\beta(a+\epsilon b))$. We point out that in the scalar case the odd order terms in the semiclassical expansion of the quantum exponential are zero, while this does not happen in the spinorial case, due to the noncommutativity of the matrix product, which increases much the complexity in computation with respect to the scalar case.

We finish this section by considering a particular case, in which eqs. (2.29), (2.30) are simpler, that is:

$$
b_0\equiv 0\,,\quad \vec{a}(x,p)=q(x,p)\vec{p}\,,\quad \vec{b}(x,p)=r(x,p)\vec{p}\,,
\tag{2.31}
$$

for some suitable scalar functions $q(x,p)$, $r(x,p)$. In fact, in the case (2.31), the following relations hold:

$$
\begin{aligned}
\eta_{jks}\{a_j\,,\,a_k\}a_s=&0\,,\\
\vec{a}\wedge\vec{b}=&0\,,\\
a_j\{a_j,\vec{a}\}\wedge\frac{\vec{a}}{|\vec{a}|}=&\frac{|\vec{a}|^2}{|\vec{p}|^2}\vec{\nabla}_x|\vec{a}|\wedge\vec{p}\,,\\
\{a_0,\vec{a}\}\wedge\frac{\vec{a}}{|\vec{a}|}=&\frac{|\vec{a}|}{|p|^2}\vec{\nabla}_x a_0\wedge\vec{p}\,,\\
\frac{(\vec{a}\cdot\vec{b})\vec{a}}{|\vec{a}|^2}=&\frac{(\vec{p}\cdot\vec{b})\vec{p}}{|\vec{p}|^2}\,,
\end{aligned}
\tag{2.32}
$$

so from eqs. (2.29), (2.30), (2.32) it follows:

$$
\begin{aligned}
g_0^{(1)}(\beta)=&\beta e^{\beta a_0}\sinh(\beta|\vec{a}|)\frac{\vec{a}\cdot\vec{b}}{|\vec{a}|}\,,\\
\vec{g}^{(1)}(\beta)=&\beta e^{\beta a_0}\cosh(\beta|\vec{a}|)\frac{(\vec{p}\cdot\vec{b})\vec{p}}{|\vec{p}|^2}\\
&+\beta e^{\beta a_0}\frac{\beta|\vec{a}|\sinh(\beta|\vec{a}|)-\cosh(\beta|\vec{a}|)+1}{2\beta|\vec{a}|}\frac{\vec{\nabla}_x|\vec{a}|\wedge\vec{p}}{|\vec{p}|^2}\\
&+\beta e^{\beta a_0}\frac{\beta|\vec{a}|\cosh(\beta|\vec{a}|)-\sinh(\beta|\vec{a}|)}{2\beta|\vec{a}|}\frac{\vec{\nabla}_x a_0\wedge\vec{p}}{|p|^2}\,.
\end{aligned}
\tag{2.33}
$$

2.3 The weakly spinorial case

In this section we are going to derive the second order semiclassical expansion of the quantum exponential (2.14) in the case:

$$|\vec{a}| \equiv 0\,, \quad b_0 \equiv 0\,, \tag{2.34}$$

which we call *weakly spinorial*.
Clearly from eqs (2.21), (2.34) it follows:

$$g^{(0)}(\beta) = e^{\beta a_0}\sigma_0\,, \tag{2.35}$$

and, since $g^{(0)}(\beta)$ is scalar, (2.23) takes the form:

$$\partial_\beta g^{(1)}(\beta) = a_0 g^{(1)}(\beta) + g^{(0)}(\beta) b = a_0 g^{(1)}(\beta) + e^{\beta a_0} b \qquad \beta > 0\,;$$

with the condition $g^{(1)}(0) = 0$; then the solution is:

$$g^{(1)}(\beta) = \beta e^{\beta a_0} b \qquad \beta > 0\,. \tag{2.36}$$

Now we can compute also the second-order correction to $g_\epsilon(\beta)$, thanks to the approximations we have done. From (2.17), (2.34) we obtain:

$$\begin{aligned}
\partial_\beta g^{(2)}(\beta) =& a_0 g^{(2)}(\beta) + a_0 \#^{(2)} g^{(0)}(\beta) + \frac{1}{2}(b g^{(1)}(\beta) + g^{(1)}(\beta) b) \\
=& a_0 g^{(2)}(\beta) + a_0 \#^{(2)} g^{(0)}(\beta) + \beta e^{\beta a_0} b^2 \\
=& a_0 g^{(2)}(\beta) + a_0 \#^{(2)} g^{(0)}(\beta) + \beta e^{\beta a_0} |\vec{b}|^2 \sigma_0\,, \\
g^{(2)}(0) =& 0\,,
\end{aligned} \tag{2.37}$$

so we deduce that $g^{(2)}(\beta)$ is scalar: $|\vec{g}^{(2)}(\beta)| \equiv 0$.
Now let us consider the scalar quantity:

$$\tilde{g}_\epsilon(\beta) = g^{(0)}(\beta) + \epsilon^2 g^{(2)}(\beta) - \epsilon^2 \frac{\beta^2 |\vec{b}|^2}{2} e^{\beta a}\,; \tag{2.38}$$

from (2.35), (2.37), (2.38) it follows:

$$\begin{aligned}
\partial_\beta \tilde{g}^{(0)}(\beta) =& a_0 \tilde{g}^{(0)}(\beta)\,, \\
\partial_\beta \tilde{g}^{(2)}(\beta) =& a_0 \tilde{g}^{(2)}(\beta) + a_0 \#^{(2)} \tilde{g}^{(0)}(\beta)\,, \\
\tilde{g}^{(0)}(\beta) =& \sigma_0\,, \quad \tilde{g}^{(2)}(\beta) = 0\,;
\end{aligned} \tag{2.39}$$

so one finds that:

$$\mathcal{E}\mathrm{xp}_\epsilon(\beta a_0) = \tilde{g}_\epsilon(\beta) + O(\epsilon^4)\,, \tag{2.40}$$

which, along with (2.38), implies:

$$g_\epsilon(\beta) = e^{\beta a_0}\sigma_0 + \epsilon \beta e^{\beta a_0} \vec{b}\cdot\vec{\sigma} + \epsilon^2 \left[\mathcal{E}\mathrm{xp}^{(2)}(\beta a_0) + \frac{\beta^2}{2} |\vec{b}|^2 e^{\beta a_0} \right] \sigma_0 + O(\epsilon^3)\,, \tag{2.41}$$

where $\mathcal{E}\mathrm{xp}^{(2)}(\beta a_0)$ is the second order correction in the semiclassical expansion of the symbol $\mathcal{E}\mathrm{xp}_\epsilon(\beta a_0)$; since βa_0 is scalar, then $\mathcal{E}\mathrm{xp}^{(2)}(\beta a_0)$ is already known in literature [16].

Chapter 3

Two-band models

We are going to derive two diffusive models and two hydrodynamic models for quantum transport of electrons in graphene by taking moments of Eqs. (1.38)–(1.39), (1.45) and closing the resulting fluid-dynamic equations by writing the Wigner distribution w in terms of the equilibrium distribution g, constructed as in chapter 2. We will consider moments of this type:

$$m_k = \int \mu_k(p) \left(w_0(r,p) \pm \frac{\vec{p}}{|\vec{p}|} \cdot \vec{w}(r,p) \right) dp \qquad k = 0 \dots n\,, \tag{3.1}$$

with $\{\mu_k : \mathbb{R}^2 \to \mathbb{R} \mid k = 0 \dots n\}$ suitable monomials depending on p, and $n \in \mathbb{N}$ given.
The reason of such a choice is that the functions:

$$w_\pm(r,p) \equiv w_0(r,p) \pm \frac{\vec{p}}{|\vec{p}|} \cdot \vec{w}(r,p) \tag{3.2}$$

are the phase-space distribution functions of the two-bands (w_+ is relative to the conduction band, w_- is relative to the valence band). For this reasons we will refer to the models that are going to be presented in this chapter as “two-band models”.

The monomials $\mu_0(p) \dots \mu_n(p)$ appearing in Eq. (3.1) will be chosen among the set $\{1, p_1, p_2\}$, corresponding to the moments:

$$n_\pm(x) = \int w_\pm \, dp\,, \qquad J_\pm^{(k)}(x) = \int p_k w_\pm(x,p)\, dp \quad (k = 1, 2)\,. \tag{3.3}$$

The functions n_+, n_- in (3.3) are the so-called *band densities*, that is, the partial trace (w.r.t. p) of the quantum operators *band projections* $\Pi_\pm$:

$$\Pi_\pm = \mathrm{Op}(P_\pm)\,, \quad P_\pm(p) = \frac{1}{2}\left(\sigma_0 \pm \frac{\vec{p}}{|\vec{p}|} \cdot \vec{\sigma}\right)\,,$$
$$n_\pm(x) = \mathrm{Tr}(\Pi_\pm S|x) = \int \mathrm{tr}(P_\pm(p) w(x,p))\, dp\,;$$

here $S = \mathrm{Op}_\hbar(w)$ is the density operator which represents the state of the system, and the matrices $P_\pm(p)$ are the projection operators into the eigenspaces of the classical symbol h of the quantum Hamiltonian H, that is:

$$H = \mathrm{Op}_\hbar(h)\,, \quad h(p) = E_+(p)P_+(p) + E_-(p)P_-(p)\,,$$

and $E_\pm(p)$ are the eigenvalues of h, that is, the energy bands related to the Hamiltonian H:

$$E_\pm(p) = \frac{|p|^2}{2m} \pm v_F|p|\,.$$

The moments $\vec{J}_+ = (J_+^{(1)}, J_+^{(2)}, 0)$, $\vec{J}_- = (J_-^{(1)}, J_-^{(2)}, 0)$ in (3.3) are the *band currents*: they measure the contribution of each band to the total current, namely $\vec{J} = (J_+^{(1)} + J_-^{(1)}, J_+^{(2)} + J_-^{(2)}, 0) = \vec{J}_+ + \vec{J}_-$.

In the following part of this thesis, in order to compute moments of fluid equations, we will have to consider integrals in the sense of the principal value. For this reason we define the operator $\langle\cdot\rangle$ that generalizes the Lebesgue integral:

$$\langle f \rangle \equiv \lim_{r\to 0^+} \int_{|p|>r} f(p)\,dp\,, \tag{3.4}$$

for all scalar or vector functions f defined in $\mathbb{R}^2$ such that the limit in eq. (3.4) exists and is finite. If $f \in L^1(\mathbb{R}^2)$ clearly $\langle f \rangle$ exists, is finite and equals $\int_{\mathbb{R}^2} f(p)\,dp$.

In the remaining part of this thesis the following notations will be adopted:

$$a_\sigma \equiv \vec{a}\cdot\frac{\vec{p}}{|\vec{p}|}\,, \qquad a_\pm = a_0 \pm a_\sigma\,, \qquad \vec{a}^\perp \equiv \vec{a} - a_\sigma\frac{\vec{p}}{|\vec{p}|}\,, \tag{3.5}$$

for all a hermitian 2×2 matrices; moreover we define:

$$\begin{aligned} n_0 =& \frac{1}{2}(n_+ + n_-) \qquad \text{charge density,} \\ n_\sigma =& \frac{1}{2}(n_+ - n_-) \qquad \text{pseudo-spin polarization.} \end{aligned} \tag{3.6}$$

3.1 A first-order two-band hydrodynamic model

In this section we present a hydrodynamic model with a two-band structure, involving all the moments in Eq. (3.3).

The (scaled) equilibrium distribution has the following form:

$$\begin{aligned} g \equiv& g[n_+, n_-, J_+, J_-] = \mathcal{E}\mathrm{xp}_\epsilon(-h_\xi)\,, \\ h_\xi =& \left(\frac{|p|^2}{2} + A_0 + \vec{A}\cdot\vec{p}\right)\sigma_0 + (c|p| + B_0 + \vec{B}\cdot\vec{p})\frac{\vec{p}}{|p|}\cdot\vec{\sigma}\,, \end{aligned} \tag{3.7}$$

where the functions $A_0(x)$, $\vec{A}(x) \equiv (A_1(x), A_2(x), 0)$, $B_0(x)$, $\vec{B}(x) \equiv (B_1(x), B_2(x), 0)$ are such that the equilibrium distribution $g[n_+, n_-, J_+, J_-]$ satisfies the constraints (recall (3.2)):

$$\begin{aligned} \langle g_\pm[n_+, n_-, J_+, J_-]\rangle(x) =& n_\pm(x) \qquad x \in \mathbb{R}^2\,, \\ \langle p^k g_\pm[n_+, n_-, J_+, J_-]\rangle(x) =& J_\pm^k(x) \qquad x \in \mathbb{R}^2\,,\ k = 1, 2\,. \end{aligned} \tag{3.8}$$

We notice the following property. Since clearly $g^{(0)}[n_+,n_-,J_+,J_-]=\exp(-h_\xi)$, then:

$$g^{(0)}[n_+,n_-,J_+,J_-] = e^{-(\frac{|p|^2}{2}+A_0+A_1p_1+A_2p_2)}\Big[\cosh(c|p|+B_0+B_1p_1+B_2p_2)\sigma_0 + \frac{\sinh(c|p|+B_0+B_1p_1+B_2p_2)}{c|p|+B_0+B_1p_1+B_2p_2}\frac{\vec{p}}{|p|}\cdot\vec{\sigma}\Big]\,; \tag{3.9}$$

in particular:

$$\left(\vec{g}^{(0)}\right)^{\perp}=0\,. \tag{3.10}$$

3.1.1 Formal closure of the fluid equations

The following formal proposition provides a closed two-band fluid system.

Proposition 8 *Let $n^\tau_\pm$, $\vec{J}^\tau_\pm$ the moments of a solution w^τ of Eqs. (1.45) according to eq. (3.3). If $n^\tau_\pm\to n_\pm$, $\vec{J}^\tau_\pm\to\vec{J}$ as $\tau\to 0$ for suitable functions $n_\pm$, $\vec{J}_\pm$, then the limit moments $n_\pm$, $\vec{J}_\pm$ satisfy:*

$$\begin{aligned}
&\partial_t n_\pm+\partial_k\left\{\frac{1}{2\gamma}J^k_\pm+\frac{\epsilon}{2}\left\langle g_k\pm\frac{p_k}{|\vec{p}|}g_0\right\rangle\right\}\pm\left\langle\frac{p_k}{|\vec{p}|}\Theta_\epsilon g_k\right\rangle=0\,,\\
&\partial_t J^i_\pm+\partial_k\left\{\frac{1}{2\gamma}\langle p_ip_kg_\pm\rangle+\frac{\epsilon}{2}\left\langle p_i\left(g_k\pm\frac{p_k}{|\vec{p}|}g_0\right)\right\rangle\right\}\\
&\qquad+n_0\partial_iV\pm\left\langle\frac{p_ip_k}{|\vec{p}|}\Theta_\epsilon g_k\right\rangle=0\,,\qquad(i=1,2)\,.
\end{aligned} \tag{3.11}$$

Proof. Since w^τ satisfies eqs. (1.45) then the functions $w^\tau_\pm\equiv w_0\pm\vec{w}\cdot\vec{p}/|p|$ satisfy:

$$\partial_t w^\tau_\pm+\frac{p_k}{2\gamma}\partial_k w^\tau_\pm+\frac{\epsilon}{2}\left(\partial_k w^\tau_k\pm\frac{p_k}{|p|}\partial_k w^\tau_0\right)+\Theta_\epsilon w^\tau_0\pm\frac{p_k}{|p|}\Theta_\epsilon w^\tau_k=\frac{g_\pm-w^\tau_\pm}{\tau}\,; \tag{3.12}$$

then, since eqs. (3.3) hold, by integrating eqs. (3.12) against the weight functions 1, p_1, p_2 we find:

$$\begin{aligned}
&\partial_t n^\tau_\pm+\frac{\partial_k}{2\gamma}(J^\tau)^k_\pm+\frac{\epsilon}{2}\left\langle\partial_k w^\tau_k\pm\frac{p_k}{|\vec{p}|}\partial_k w^\tau_0\right\rangle+\left\langle\Theta_\epsilon w^\tau_0\pm\frac{p_k}{|\vec{p}|}\Theta_\epsilon w^\tau_k\right\rangle=0\,,\\
&\partial_t(J^\tau)^i_\pm+\frac{\partial_k}{2\gamma}\langle p_ip_kw^\tau_\pm\rangle+\frac{\epsilon}{2}\left\langle p_i\left(\partial_k w^\tau_k\pm\frac{p_k}{|\vec{p}|}\partial_k w^\tau_0\right)\right\rangle\\
&\qquad+\left\langle p_i\left(\Theta_\epsilon w^\tau_0\pm\frac{p_k}{|\vec{p}|}\Theta_\epsilon w^\tau_k\right)\right\rangle=0\,;
\end{aligned} \tag{3.13}$$

passing formally to the limit $\tau\to 0$ in eqs. (1.45) we deduce that $w^\tau\to g$ as $\tau\to 0$; so taking the same limit in eqs. (3.13) we obtain:

$$\begin{aligned}
&\partial_t n_\pm+\frac{1}{2\gamma}\partial_k J^k_\pm+\frac{\epsilon}{2}\left\langle\partial_k g_k\pm\frac{p_k}{|\vec{p}|}\partial_k g_0\right\rangle+\left\langle\Theta_\epsilon g_0\pm\frac{p_k}{|\vec{p}|}\Theta_\epsilon g_k\right\rangle=0\,,\\
&\partial_t J^i_\pm+\frac{1}{2\gamma}\partial_k\langle p_ip_kg_\pm\rangle+\frac{\epsilon}{2}\left\langle p_i\left(\partial_k g_k\pm\frac{p_k}{|\vec{p}|}\partial_k g_0\right)\right\rangle\\
&\qquad+\left\langle p_i\left(\Theta_\epsilon g_0\pm\frac{p_k}{|\vec{p}|}\Theta_\epsilon g_k\right)\right\rangle=0\,;
\end{aligned} \tag{3.14}$$

finally, recalling the properties (1.46) of the operator Θ_ϵ, we find eqs. (3.11).

□

Let us stress the fact that (3.11) is a formally closed system because g depends on $n_\pm$ and $\vec{J}_\pm$ through the constraints (3.8). Such dependance can be written explicitly in the semiclassical approximation that will be discussed in the next subsection.

3.1.2 Semiclassical computation of the moments

Now we solve the constraints (3.8) and find an explicit semiclassical expansion of the Lagrange multipliers $A_\pm$, $B^1_\pm$, $B^2_\pm$ in terms of the moments $n_\pm$, $J^1_\pm$, $J^2_\pm$.

From (3.9) we easily find:

$$g^{(0)}_\pm = e^{-\left(|\vec{p}|^2/2 + A_\pm + B^k_\pm p^k\right)} = e^{-A_\pm + |\vec{B}_\pm|^2/2} e^{-A_\pm + |\vec{B}_\pm|^2/2}\,, \tag{3.15}$$

with $\vec{B}_\pm = (B^1_\pm, B^2_\pm, 0)$. Let us impose the constraints (3.8). It follows:

$$\begin{aligned} n_\pm =& \left\langle g^{(0)} \right\rangle + O(\epsilon) = e^{-A_\pm + |\vec{B}_\pm|^2/2} \int e^{-A_\pm + |\vec{B}_\pm|^2/2}\, dp + O(\epsilon) \\ =& 2\pi e^{-A_\pm + |\vec{B}_\pm|^2/2} + O(\epsilon)\,, \\ J^k_\pm =& \left\langle p^k g^{(0)} \right\rangle + O(\epsilon) = e^{-A_\pm + |\vec{B}_\pm|^2/2} \int p^k e^{-A_\pm + |\vec{B}_\pm|^2/2}\, dp + O(\epsilon) \\ =& -2\pi B^k_\pm e^{-A_\pm + |\vec{B}_\pm|^2/2} + O(\epsilon)\,, \end{aligned} \tag{3.16}$$

and so:

$$\begin{aligned} B^k_\pm =& -u^k_\pm + O(\epsilon)\,, \quad u^k_\pm \equiv J^k_\pm / n_\pm\,, \qquad (k = 1, 2)\,, \\ A_\pm =& \frac{|\vec{B}_\pm|^2}{2} - \log\left(\frac{n_\pm}{2\pi}\right) + O(\epsilon) = \frac{1}{2}\sum_{k=1}^{2} |u^k_\pm|^2 - \log\left(\frac{n_\pm}{2\pi}\right) + O(\epsilon)\,, \\ g^{(0)}_\pm =& \frac{n_\pm}{2\pi} e^{-|\vec{p} - \vec{u}_\pm|^2/2}\,; \end{aligned} \tag{3.17}$$

since (3.10) holds, eq. (3.17) gives us the leading order term in the semiclassical expansion of g. In order to compute the first order correction to g we exploit eqs. (2.29), (2.30). In our case $\beta = 1$ and:

$$\begin{aligned} -a_0 =& \frac{|p|^2}{2} + \alpha_0 + \vec{\beta}_0 \cdot \vec{p}\,, \quad -\vec{a} = (\alpha_\sigma + \vec{\beta}_\sigma \cdot \vec{p}) \frac{\vec{p}}{|\vec{p}|}\,, \quad -b_0 = 0\,, \quad -\vec{b} = \vec{p}\,, \\ \alpha_0 =& \frac{A_+ + A_-}{2}\,, \quad \alpha_\sigma = \frac{A_+ - A_-}{2}\,, \quad \vec{\beta}_0 = \frac{\vec{B}_+ + \vec{B}_-}{2}\,, \quad \vec{\beta}_\sigma = \frac{\vec{B}_+ - \vec{B}_-}{2}\,. \end{aligned} \tag{3.18}$$

So from (3.18) follows:

$$\begin{aligned}\eta_{jks}\{a_j,a_k\}a_s =& -\eta_{jks}\left\{(\alpha_\sigma+\vec{\beta}_\sigma\cdot\vec{p})\frac{p_j}{|\vec{p}|}\,,\,(\alpha_\sigma+\vec{\beta}_\sigma\cdot\vec{p})\frac{p_k}{|\vec{p}|}\right\}(\alpha_\sigma+\vec{\beta}_\sigma\cdot\vec{p})\frac{p_s}{|\vec{p}|}=0\,,\\ a_j\,\{a_j\,,\,\vec{a}\}\wedge\frac{\vec{a}}{|\vec{a}|} =&(\alpha_\sigma+\vec{\beta}_\sigma\cdot\vec{p})|\alpha_\sigma+\vec{\beta}_\sigma\cdot\vec{p}|\vec{\nabla}_x(\alpha_\sigma+\vec{\beta}_\sigma\cdot\vec{p})\wedge\frac{\vec{p}}{|\vec{p}|^2}\,,\\ \{a_0\,,\,\vec{a}\}\wedge\frac{\vec{a}}{|\vec{a}|} =& -|\alpha_\sigma+\vec{\beta}_\sigma\cdot\vec{p}|\vec{\nabla}_x(\alpha_0+\vec{\beta}_0\cdot\vec{p})\wedge\frac{\vec{p}}{|\vec{p}|^2}\,;\end{aligned}\tag{3.19}$$

so from (3.19) we conclude:

$$\begin{aligned}g_\pm^{(1)} =& e^{a_0}\left[\frac{\sinh|\vec{a}|}{|\vec{a}|}\vec{a}\cdot\vec{b}\pm\frac{\cosh|\vec{a}|}{|\vec{a}|}(\vec{a}\cdot\vec{b})\frac{\vec{a}\cdot\vec{p}}{|\vec{a}||\vec{p}|}\right]\\ =& e^{a_0}\frac{\vec{a}\cdot\vec{b}}{|\vec{a}|}\left[\sinh|\alpha_\sigma+\vec{\beta}_\sigma\cdot\vec{p}|\mp\frac{\alpha_\sigma+\vec{\beta}_\sigma\cdot\vec{p}}{|\alpha_\sigma+\vec{\beta}_\sigma\cdot\vec{p}|}\cosh|\alpha_\sigma+\vec{\beta}_\sigma\cdot\vec{p}|\right]\\ =& \mp\, e^{a_0}\frac{\vec{a}\cdot\vec{b}}{|\vec{a}|}\frac{\alpha_\sigma+\vec{\beta}_\sigma\cdot\vec{p}}{|\alpha_\sigma+\vec{\beta}_\sigma\cdot\vec{p}|}e^{\mp(\alpha_\sigma+\vec{\beta}_\sigma\cdot\vec{p})}\\ =& \mp\,|\vec{p}|\,e^{-(|\vec{p}|^2/2+A_\pm+\vec{B}_\pm\cdot\vec{p})}\,;\end{aligned}\tag{3.20}$$

so by making a comparison between (3.15) and (3.20) we conclude:

$$g_\pm = e^{-\left(|\vec{p}|^2/2+A_\pm+B^k_\pm p^k\right)}[\,1\mp\epsilon|\vec{p}|\,]+O(\epsilon^2)\,.\tag{3.21}$$

Now we have to find the first-order correction to $A_\pm$, $\vec{B}_\pm$ by imposing that $g_\pm$ given by (3.21) satisfies (3.8). Let $C_\pm = e^{-A_\pm+|\vec{B}_\pm|^2/2}$. Then:

$$n_\pm = \left\langle g^{(0)}+\epsilon g^{(1)}\right\rangle+O(\epsilon^2)\,,\quad J^k_\pm = \left\langle p^k(g^{(0)}+\epsilon g^{(1)})\right\rangle+O(\epsilon^2)\,,$$

and so:

$$\begin{aligned}n_\pm =& 2\pi C_\pm\left(1\mp\epsilon\int|p|\frac{e^{-|B_\pm+p|^2/2}}{2\pi}\,dp\right)+O(\epsilon^2)\,,\\ J^k_\pm =& 2\pi C_\pm\left(-B^k\mp\epsilon\int p^k|p|\frac{e^{-|B_\pm+p|^2/2}}{2\pi}\,dp\right)+O(\epsilon^2)\,;\end{aligned}$$

if we define the function:

$$F:\mathbb{R}^2\to\mathbb{R}\,,\qquad F(u)=\int|p|e^{-|p-u|^2/2}\frac{dp}{2\pi}\qquad\forall u\in\mathbb{R}^2\,,\tag{3.22}$$

after straightforward computations it follows:

$$\begin{aligned}-B^k_\pm =& u^k_\pm\pm\epsilon\frac{\partial F}{\partial u_k}(u_\pm)+O(\epsilon^2)\,,\\ C_\pm =& \frac{n_\pm}{2\pi}(1\pm\epsilon F(u_\pm))+O(\epsilon^2)\,,\end{aligned}\tag{3.23}$$

and so we obtain the semiclassical expansion of the "equilibrium energy band distributions" $g_\pm$:

$$g_\pm = \frac{n_\pm}{2\pi}\left[1\pm\epsilon\left(F(u_\pm)-|p|+(p^k-u^k_\pm)\frac{\partial F}{\partial u_k}(u_\pm)\right)\right]e^{-|p-u_\pm|^2/2}+O(\epsilon^2)\,.\tag{3.24}$$

Now we have to compute $(\vec{g}^{(1)})^{\perp}$. From eq. (2.30) it follows:

$$\begin{aligned}(\vec{g}^{(1)})^{\perp} =& e^{a_0}\left[\frac{|\vec{a}|\sinh|\vec{a}|-\cosh|\vec{a}|+1}{2|\vec{a}|^3}a_j\{a_j,\vec{a}\}\wedge\frac{\vec{a}}{|\vec{a}|}\right.\\ &\left.+\frac{|\vec{a}|\cosh|\vec{a}|-\sinh|\vec{a}|}{2|\vec{a}|^2}\{a_0,\vec{a}\}\wedge\frac{\vec{a}}{|\vec{a}|}\right];\end{aligned} \tag{3.25}$$

recalling eq. (3.19) we get:

$$\begin{aligned}(\vec{g}^{(1)})^{\perp} =& \frac{e^{a_0}}{2}\left[\frac{|\vec{a}|\sinh|\vec{a}|-\cosh|\vec{a}|+1}{|\vec{a}|^2}(\alpha_\sigma+\vec{\beta}_\sigma\cdot\vec{p})\vec{\nabla}_x(\alpha_\sigma+\vec{\beta}_\sigma\cdot\vec{p})\right.\\ &\left.+\frac{\sinh|\vec{a}|-|\vec{a}|\cosh|\vec{a}|}{|\vec{a}|}\vec{\nabla}_x(\alpha_0+\vec{\beta}_0\cdot\vec{p})\right]\wedge\frac{\vec{p}}{|p|^2}\\ =&\frac{e^{a_0}}{2}\left[\left(\sinh(\alpha_\sigma+\vec{\beta}_\sigma\cdot\vec{p})+\frac{1-\cosh(\alpha_\sigma+\vec{\beta}_\sigma\cdot\vec{p})}{\alpha_\sigma+\vec{\beta}_\sigma\cdot\vec{p}}\right)\vec{\nabla}_x(\alpha_\sigma+\vec{\beta}_\sigma\cdot\vec{p})\right.\\ &\left.+\left(\frac{\sinh(\alpha_\sigma+\vec{\beta}_\sigma\cdot\vec{p})}{\alpha_\sigma+\vec{\beta}_\sigma\cdot\vec{p}}-\cosh(\alpha_\sigma+\vec{\beta}_\sigma\cdot\vec{p})\right)\vec{\nabla}_x(\alpha_0+\vec{\beta}_0\cdot\vec{p})\right]\wedge\frac{\vec{p}}{|p|^2};\end{aligned} \tag{3.26}$$

but from (3.18), (3.17) we immediately find:

$$\begin{aligned}\alpha_\sigma+\vec{\beta}_\sigma\cdot\vec{p} =& \frac{|\vec{u}_+|^2-|\vec{u}_-|^2}{4}-\frac{1}{2}\log\left(\frac{n_+}{n_-}\right)-\frac{\vec{u}_+-\vec{u}_-}{2}\cdot\vec{p}+O(\epsilon),\\ \alpha_0+\vec{\beta}_0\cdot\vec{p} =& \frac{|\vec{u}_+|^2+|\vec{u}_-|^2}{4}-\frac{1}{2}\log\left(\frac{n_+n_-}{4\pi^2}\right)-\frac{\vec{u}_++\vec{u}_-}{2}\cdot\vec{p}+O(\epsilon);\end{aligned} \tag{3.27}$$

moreover from (3.18), (3.17) we find that:

$$e^{a_0} = \frac{\sqrt{n_+n_-}}{2\pi}e^{-|\vec{u}_+-\vec{u}_-|^2/8}e^{-|p-(u_++u_-)/2|^2/2}+O(\epsilon); \tag{3.28}$$

so from (3.28), (3.27), (3.26) we conclude:

$$\begin{aligned}\vec{g}^{\perp} =& \epsilon|\vec{p}|^{-2}\,\vec{\Lambda}\wedge\vec{p}+O(\epsilon^2),\\ \vec{\Lambda}(x,p) \equiv& \frac{\sqrt{n_+n_-}}{2\pi}\exp\left[-\frac{1}{2}\left(\left|\frac{\vec{u}_+-\vec{u}_-}{2}\right|^2+\left|p-\frac{u_++u_-}{2}\right|^2\right)\right]\vec{\Psi}(x,p),\\ \vec{\Psi}(x,p) \equiv& \left[\sinh\Phi_\sigma+\frac{1-\cosh\Phi_\sigma}{\Phi_\sigma}\right]\vec{\nabla}_x\Phi_\sigma+\left[\frac{\sinh\Phi_\sigma}{\Phi_\sigma}-\cosh\Phi_\sigma\right]\vec{\nabla}_x\Phi_0,\\ \Phi_0(x,p) \equiv& \frac{|\vec{u}_+|^2+|\vec{u}_-|^2}{4}-\frac{1}{2}\log\left(\frac{n_+n_-}{4\pi^2}\right)-\frac{\vec{u}_++\vec{u}_-}{2}\cdot\vec{p},\\ \Phi_\sigma(x,p) \equiv& \frac{|\vec{u}_+|^2-|\vec{u}_-|^2}{4}-\frac{1}{2}\log\left(\frac{n_+}{n_-}\right)-\frac{\vec{u}_+-\vec{u}_-}{2}\cdot\vec{p}.\end{aligned} \tag{3.29}$$

Eqs. (3.22), (3.24), (3.29) constitute the semiclassical expansion of the equilibrium distribution that we were looking for.

Now we will compute a first-order approximation of (3.11) with respect to the semiclassical parameter ϵ exploiting the semiclassical expansion of the equilibrium distribution g given by eqs. (3.22), (3.24), (3.29). Recalling notation (3.5) and adopting Einstein summation convention we find:

$$\begin{aligned}\partial_k g_k \pm \frac{p_k}{|\vec p|}\partial_k g_0 &= \pm\frac{p_k}{|\vec p|}\partial_k g_\pm + \partial_k \left(\vec g^\perp\right)_k ,\\ \left\langle \Theta_\epsilon g_0 \pm \frac{p_k}{|\vec p|}\Theta_\epsilon g_k \right\rangle &= \mp \left\langle g_k \Theta_\epsilon\left(\frac{p_k}{|\vec p|}\right)\right\rangle ,\\ \left\langle p_i \left(\Theta_\epsilon g_0 \pm \frac{p_k}{|\vec p|}\Theta_\epsilon g_k\right)\right\rangle &= \frac{n_+ + n_-}{2}\partial_i V \mp \left\langle g_k \Theta_\epsilon\left(\frac{p_i p_k}{|\vec p|}\right)\right\rangle ;\end{aligned}$$

so (3.11) becomes:

$$\begin{aligned}&\partial_t n_\pm + \frac{1}{2\gamma}\partial_k J^k_\pm + \frac{\epsilon}{2}\partial_k\left[\pm\left\langle \frac{p_k}{|\vec p|}g_\pm\right\rangle + \left\langle \left(\vec g^\perp\right)_k\right\rangle\right] \mp \left\langle g_k\Theta_\epsilon\left(\frac{p_k}{|\vec p|}\right)\right\rangle = 0 ,\\ &\partial_t J^i_\pm + \frac{1}{2\gamma}\partial_k\left\langle p_i p_k g_\pm\right\rangle + \frac{\epsilon}{2}\partial_k\left[\pm\left\langle\frac{p_i p_k}{|\vec p|}g_\pm\right\rangle + \left\langle p_i\left(\vec g^\perp\right)_k\right\rangle\right]\\ &\qquad + \frac{n_+ + n_-}{2}\partial_i V \mp \left\langle g_k\Theta_\epsilon\left(\frac{p_i p_k}{|\vec p|}\right)\right\rangle = 0 .\end{aligned} \tag{3.30}$$

From eqs. (3.22), (3.24), (3.29) it follows:

$$\left\langle g_k\Theta_\epsilon\left(\frac{p_k}{|\vec p|}\right)\right\rangle = -\epsilon\partial_j V\left\langle g_k^{(1)}\frac{1}{|\vec p|}\left(\delta_{jk} - \frac{p_j p_k}{|\vec p|^2}\right)\right\rangle + O(\epsilon^2) ;$$

$$\begin{aligned}\left\langle g_k\Theta_\epsilon\left(\frac{p_i p_k}{|\vec p|}\right)\right\rangle &= -\,\partial_i V\left\langle (g_k^{(0)} + \epsilon g_k^{(1)})\frac{p_k}{|\vec p|}\right\rangle - \epsilon\partial_j V\left\langle\frac{p_i}{|\vec p|}g_k^{(1)}\left(\delta_{jk} - \frac{p_j p_k}{|\vec p|^2}\right)\right\rangle + O(\epsilon^2)\\ &\quad -\,\partial_i V\frac{n_+ - n_-}{2} - \epsilon\partial_j V\left\langle\frac{p_i}{|\vec p|}g_k^{(1)}\left(\delta_{jk} - \frac{p_j p_k}{|\vec p|^2}\right)\right\rangle + O(\epsilon^2) ;\end{aligned}$$

so we conclude:

$$\begin{aligned}&\partial_t n_\pm + \frac{1}{2\gamma}\partial_k J^k_\pm \pm \frac{\epsilon}{2}\partial_k\left\langle\frac{p_k}{|\vec p|}g_\pm^{(0)}\right\rangle \pm \epsilon\vec\nabla_x V\cdot\left\langle\frac{(\vec g^{(1)})^\perp}{|\vec p|}\right\rangle = 0 ,\\ &\partial_t J^i_\pm + \frac{1}{2\gamma}\partial_k\left\langle p_i p_k (g_\pm^{(0)} + \epsilon g_\pm^{(1)})\right\rangle \pm \frac{\epsilon}{2}\partial_k\left\langle\frac{p_i p_k}{|\vec p|}g_\pm^{(0)}\right\rangle\\ &\qquad + n_\pm\partial_i V \pm \epsilon\vec\nabla_x V\cdot\left\langle p^i\frac{(\vec g^{(1)})^\perp}{|\vec p|}\right\rangle = 0 \qquad (i = 1, 2) .\end{aligned} \tag{3.31}$$

Now let us compute the integrals involving $g^{(0)}$, $g^{(1)}$ in (3.31) exploiting eqs. (3.22), (3.24), (3.29). Let us begin with:

$$\begin{aligned}\left\langle\frac{p_k}{|\vec p|}g_\pm^{(0)}\right\rangle &= n_\pm\int\frac{p_k}{|\vec p|}e^{-|p-u_\pm|^2/2}\frac{dp}{2\pi} = n_\pm\int\partial_{p_k}|p|\cdot e^{-|p-u_\pm|^2/2}\frac{dp}{2\pi}\\ &= n_\pm\partial_{u_k}\left[\int|p|e^{-|p-u|^2/2}\frac{dp}{2\pi}\right]\Big|_{u\,=\,u_\pm} = n_\pm\frac{\partial F}{\partial u_k}(u_\pm) .\end{aligned} \tag{3.32}$$

Then let us consider:

$$\begin{aligned}\left\langle p_i p_k (g_{\pm}^{(0)} + \epsilon g_{\pm}^{(1)})\right\rangle =& n_{\pm}(1 \pm \epsilon F(u_{\pm})) \int p_i p_k e^{-|p-u_{\pm}|^2/2} \frac{dp}{2\pi} \\ & \pm \epsilon n_{\pm} \left[- \int |p| p_i p_k e^{-|p-u_{\pm}|^2/2} \frac{dp}{2\pi} \right. \\ & \left. + \int p_i p_k (p_s - u_{\pm}^s) e^{-|p-u_{\pm}|^2/2} \frac{dp}{2\pi} \frac{\partial F}{\partial u_s}(u_{\pm}) \right] ;\end{aligned} \tag{3.33}$$

but it holds:

$$\int p_i p_k e^{-|p-u|^2/2} \frac{dp}{2\pi} = \int (p_i + u_i)(p_k + u_k) e^{-|p|^2/2} \frac{dp}{2\pi} = \delta_{ik} + u_i u_k ; \tag{3.34}$$

moreover from the relations:

$$\begin{aligned}\frac{\partial F}{\partial u_i}(u) &= \int (u_i - p_i)|p| e^{-|p-u|^2/2} \frac{dp}{2\pi} = u_i F(u) - \int p_i |p| e^{-|p-u|^2/2} \frac{dp}{2\pi} , \\ \frac{\partial^2 F}{\partial u_i \partial u_k}(u) &= \int [\delta_{ik} + (u_i - p_i)(u_k - p_k)] |p| e^{-|p-u|^2/2} \frac{dp}{2\pi} \\ &= \delta_{ik} F(u) + \int (p_i - u_i)(p_k - u_k) |p| e^{-|p-u|^2/2} \frac{dp}{2\pi} ,\end{aligned} \tag{3.35}$$

we deduce:

$$\begin{aligned}- \int |p| p_i p_k e^{-|p-u|^2/2} \frac{dp}{2\pi} =& (\delta_{ik} - u_i u_k) F(u) + u_i \frac{\partial F}{\partial u_k}(u) \\ & + u_k \frac{\partial F}{\partial u_i}(u) - \frac{\partial^2 F}{\partial u_i \partial u_k}(u) ;\end{aligned} \tag{3.36}$$

finally from (3.34) it follows:

$$\begin{aligned}\int p_i p_k (p_s - u_s) e^{-|p-u|^2/2} \frac{dp}{2\pi} &= - \partial_{u_s} \int p_i p_k e^{-|p-u|^2/2} \frac{dp}{2\pi} \\ &= - \partial_{u_s} (\delta_{ik} + u_i u_k) = -\delta_{is} u_k - \delta_{ik} u_s ;\end{aligned} \tag{3.37}$$

so from eqs. (3.33), (3.34), (3.36), (3.37) we conclude:

$$\begin{aligned}\left\langle p_i p_k (g_{\pm}^{(0)} + \epsilon g_{\pm}^{(1)})\right\rangle =& n_{\pm}(1 \pm \epsilon F(u_{\pm}))(\delta_{ik} + u_{\pm}^i u_{\pm}^k) \\ & \pm \epsilon n_{\pm} \left[(\delta_{ik} - u_{\pm}^i u_{\pm}^k) F(u_{\pm}) + u_{\pm}^i \frac{\partial F}{\partial u_{\pm}^k}(u_{\pm}) \right. \\ & \left. - \frac{\partial^2 F}{\partial u_{\pm}^i \partial u_{\pm}^k}(u_{\pm}) - \delta_{ik} u_{\pm}^s \frac{\partial F}{\partial u_{\pm}^s}(u_{\pm}) \right] .\end{aligned} \tag{3.38}$$

Now let us consider the term:

$$
\begin{aligned}
\left\langle \frac{p_i p_k}{|\vec{p}|} g_\pm^{(0)} \right\rangle = \int \frac{p_i p_k}{|\vec{p}|} \frac{n_\pm}{2\pi} e^{-|p-u_\pm|^2/2}\, dp = n_\pm \int \partial_{p_i} |p| \cdot p_k e^{-|p-u_\pm|^2/2} \frac{dp}{2\pi} \\
= & n_\pm \left(-\delta_{ik} \int |p| e^{-|p-u_\pm|^2/2} \frac{dp}{2\pi} + \int |p| p_k (p_i - u_\pm^i) e^{-|p-u_\pm|^2/2} \frac{dp}{2\pi} \right) \\
= & n_\pm \Bigg[-\delta_{ik} F(u_\pm) - (\delta_{ik} - u_\pm^i u_\pm^k) F(u) - u_\pm^i \frac{\partial F}{\partial u_k}(u_\pm) \\
& - u_\pm^k \frac{\partial F}{\partial u_i}(u_\pm) + \frac{\partial^2 F}{\partial u_i \partial u_k}(u_\pm) + u_\pm^i \left(\frac{\partial F}{\partial u_k}(u_\pm) - u_\pm^k F(u_\pm) \right) \Bigg] ,
\end{aligned}
\tag{3.39}
$$

where in the last equality we applied eqs. (3.35), (3.36); so we find:

$$
\left\langle \frac{p_i p_k}{|\vec{p}|} g_\pm^{(0)} \right\rangle = n_\pm \left[\frac{\partial^2 F}{\partial u_i \partial u_k}(u_\pm) - u_\pm^k \frac{\partial F}{\partial u_i}(u_\pm) \right] . \tag{3.40}
$$

Now we consider the terms in (3.31) depending on $\vec{g}^\perp$. We start with the term:

$$
\left\langle \frac{(\vec{g}^{(1)})^\perp}{|\vec{p}|} \right\rangle = \epsilon \left\langle \frac{\vec{\Lambda} \wedge \vec{p}}{|\vec{p}|^3} \right\rangle + O(\epsilon^2) . \tag{3.41}
$$

We point out that the function $p \in \mathbb{R}^2 \mapsto \vec{\Lambda} \wedge \vec{p}/|p|^3$ is not L^1 due to a not integrable singularity at $p = 0$, so we must use the definition (3.4) of the operator $\langle \cdot \rangle$ as a principal value to deal with the term (3.41).

For the symmetry properties of the operator $\langle \cdot \rangle$ and the fact that the map $p \in \mathbb{R}^2 \mapsto \vec{\Lambda}(x,p) \in \mathbb{R}^3$ is C^∞ for all $x \in \mathbb{R}^2$, we obtain:

$$
\begin{aligned}
\left\langle \frac{(\vec{g}^{(1)})^\perp}{|\vec{p}|} \right\rangle = & \epsilon \left\langle \frac{[\vec{\Lambda}(\cdot\,,p) - \vec{\Lambda}(\cdot\,,-p)] \wedge \vec{p}}{2|\vec{p}|^3} \right\rangle + O(\epsilon^2) \\
= & \int \frac{[\vec{\Lambda}(\cdot\,,p) - \vec{\Lambda}(\cdot\,,-p)] \wedge \vec{p}}{2|p|^3} + O(\epsilon^2) ;
\end{aligned}
\tag{3.42}
$$

the other term in (3.31) depending on $\vec{g}^\perp$ is:

$$
\left\langle p^i \frac{(\vec{g}^{(1)})^\perp}{|\vec{p}|} \right\rangle = \int p^i \frac{(\vec{g}^{(1)})^\perp}{|\vec{p}|}\, dp = \int p^i \frac{\vec{\Lambda}(x,p) \wedge \vec{p}}{|\vec{p}|^3}\, dp . \tag{3.43}
$$

Since the structure of (3.29) is very involved, we will not attempt to write the integrals (3.42), (3.43) in a more explicit way.

Collecting eqs. (3.31), (3.22), (3.29), (3.32), (3.38), (3.40), (3.42), (3.43) we finally complete the proof of the following proposition, which yields the explicit first order model that we were looking for:

Proposition 9 *Eq. (3.11) is equivalent, up to $O(\epsilon^2)$ corrections, to the following two-band hydrodynamic system:*

$$
\begin{aligned}
& \partial_t n_\pm + \frac{1}{2\gamma} \partial_k \left(J_\pm^k \pm \epsilon \gamma n_\pm \frac{\partial F}{\partial u_k}(u_\pm) \right) \pm \epsilon Z_k \partial_k V = 0 , \\
& \partial_t J_\pm^i + \frac{1}{2\gamma} \partial_k \left(n_\pm U_\pm^{ik} \right) + (n_\pm \delta_{ik} \pm \epsilon R_{ik}) \partial_k V = 0 \qquad (i = 1, 2) ,
\end{aligned}
\tag{3.44}
$$

where F is given by (3.22),

$$
\begin{aligned}
Z_k =&\eta_{ks\ell}\int \frac{[\Lambda_s(\cdot\,,p)-\Lambda_s(\cdot\,,-p)]p_\ell}{2|p|^3}\,dp\,,\\
U^{ik}_\pm =&(1\pm\epsilon F(u_\pm))(\delta_{ik}+u^i_\pm u^k_\pm)\pm\epsilon\gamma\left(\frac{\partial^2 F}{\partial u_i\partial u_k}(u_\pm)-u^k_\pm\frac{\partial F}{\partial u_i}(u_\pm)\right)\\
&\pm\epsilon\left[(\delta_{ik}-u^i_\pm u^k_\pm)F(u_\pm)+u^i_\pm\frac{\partial F}{\partial u^k_\pm}(u_\pm)-\frac{\partial^2 F}{\partial u^i_\pm\partial u^k_\pm}(u_\pm)-\delta_{ik}u^s_\pm\frac{\partial F}{\partial u^s_\pm}(u_\pm)\right]\\
R_{ik} =&\eta_{ks\ell}\int p^i\frac{\Lambda_s(\cdot\,,p)p_\ell}{|\vec{p}|^3}\,dp\,,
\end{aligned}
$$

$\vec{\Lambda}(x,p)$ *is defined in* (3.29)*, and* $\eta_{ks\ell}$ *is again the Levi-Civita tensor.*

3.2 A first order two-band diffusive model

In this section we present a first order diffusive model with two-band structure and Hamiltonian given by (1.16). This model will be based on a Chapman-Enskog expansion of the Wigner distribution w and a semiclassical expansion of the equilibrium distribution g that appear in Eqs. (1.38)–(1.39).
The moments we choose are the *band densities* $n_\pm$ defined by (3.3).
The (scaled) equilibrium distribution has the following form:

$$
\begin{aligned}
g[n_+,n_-] =&\mathcal{E}\mathrm{xp}_\epsilon(-h_\xi)\,,\\
h_\xi =&\left(\frac{|p|^2}{2}+A\right)\sigma_0+(c|p|+B)\frac{\vec{p}}{|p|}\cdot\vec{\sigma}\,,
\end{aligned}
\tag{3.45}
$$

where $A=A(x)=(\xi^*_+(x)+\xi^*_-(x))/2$, $B=B(x)=(\xi^*_+(x)-\xi^*_-(x))/2$ are Lagrange multipliers such that:

$$
\langle g_\pm[n_+,n_-]\rangle(x)=n_\pm(x)\,,\qquad x\in\mathbb{R}^2\,. \tag{3.46}
$$

3.2.1 Formal closure of the diffusive equations

Let n^τ_+, n^τ_- the moments of a solution $w=w^\tau$ of (1.38) with g given by (3.45), (3.46), and let:

$$
Tw=\sigma_0 T_0(w)+\vec{\sigma}\cdot\vec{T}(w)\,. \tag{3.47}
$$

We claim that:

$$
\langle (Tg[n^\tau_+,n^\tau_-])_\pm\rangle=0\qquad\forall\tau>0\,. \tag{3.48}
$$

Indeed, it is immediate to verify that Eq. (3.48) is satisfied if $g_0[n^\tau_+,n^\tau_-]$ is an even function of p and $\vec{g}[n^\tau_+,n^\tau_-]$ is an odd function of p; as a matter of fact, $g[n^\tau_+,n^\tau_-]$ has this property, because of (3.45). The proof of this claim is quite similar to the proof of proposition 5.1 in [7]: one only has to consider the operator T given by (1.39), (3.47) instead of that one used in the paper and consider $\mathcal{C}$ as the set of all the $p-$dependent 2×2 matrices with the parity structure:

$$
(\mathrm{even},\mathrm{odd},\mathrm{odd},\mathrm{odd})
$$

instead of:

$$(\text{even}, \text{even}, \text{odd}, \text{even})\,.$$

The following (formal) result holds:

Theorem 1 *Let us suppose that:*

$$n_\pm^\tau \to n_\pm \qquad \text{as } \tau \to 0\,, \tag{3.49}$$

for suitable functions n_+, n_-*; then* n_+, n_- *satisfy:*

$$\partial_t n_\pm = \langle (TTg[n_+, n_-])_\pm \rangle\,. \tag{3.50}$$

Proof. The Wigner equation (1.38) can be rewritten, exploiting eq. (3.47):

$$\tau \partial_t w^\tau + T w^\tau = \frac{g[n_+^\tau, n_-^\tau] - w^\tau}{\tau}\,. \tag{3.51}$$

By performing the formal limit $\tau \to 0$ in eq. (3.51) we find $w^\tau \to g$; from this fact and eq. (3.51) we easily obtain the following Chapman-Enskog expansion of the Wigner distribution w^τ:

$$w^\tau = g[n_+^\tau, n_-^\tau] - \tau T g[n_+^\tau, n_-^\tau] + O(\tau^2)\,; \tag{3.52}$$

from eq. (3.51) we obtain immediately:

$$\tau \partial_t w_\pm^\tau + (T w^\tau)_\pm = \frac{g_\pm[n_+^\tau, n_-^\tau] - w_\pm^\tau}{\tau}\,; \tag{3.53}$$

integrating eq. (3.53), exploiting the constraints (3.46) and the Chapman-Enskog expansion (3.52) we get:

$$\tau \partial n_\pm + \left\langle (Tg[n_+^\tau, n_-^\tau])_\pm \right\rangle - \tau \left\langle (TTg[n_+^\tau, n_-^\tau])_\pm \right\rangle = O(\tau^2)\,; \tag{3.54}$$

since property (3.48) holds, then dividing (3.54) by τ, passing to the limit $\tau \to 0$ and exploiting hypothesis (3.49) we finally obtain eq. (3.50).

□

Let us write eqs. (3.50) in a more explicit way. Let $w = Tg[n_+, n_-]$. In the subsequent part we will often consider the moments n_0, n_σ defined in eq. (3.6). We have:

$$\langle (Tw)_0 \rangle = \frac{1}{2\gamma} \vec{\nabla} \cdot \langle \vec{p} w_0 \rangle + \frac{\epsilon}{2} \vec{\nabla} \cdot \langle \vec{w} \rangle\ , \tag{3.55}$$

$$\begin{aligned} \langle \vec{p} w_0 \rangle &= \langle \vec{p}\,(Tg[n_+, n_-])_0 \rangle \\ &= \left\langle \vec{p} \left[\frac{\vec{p} \cdot \vec{\nabla}}{2\gamma} g_0[n_+, n_-] + \frac{\epsilon}{2} \vec{\nabla} \cdot \vec{g}[n_+, n_-] + \Theta_\epsilon g_0[n_+, n_-] \right] \right\rangle \\ &= \vec{\nabla} \cdot \left\langle \frac{\vec{p} \otimes \vec{p}}{2\gamma} g_0[n_+, n_-] + \frac{\epsilon}{2} \vec{p} \otimes \vec{g}[n_+, n_-] \right\rangle + n_0 \vec{\nabla} V\,, \end{aligned} \tag{3.56}$$

$$\begin{aligned}\langle \vec{w}\rangle =&\left\langle \vec{T}g[n_+,n_-]\right\rangle\\ =&\left\langle \frac{\vec{p}\cdot\vec{\nabla}}{2\gamma}\vec{g}[n_+,n_-]+\frac{\epsilon}{2}\vec{\nabla}g_0[n_+,n_-]+\Theta_\epsilon\vec{g}[n_+,n_-]+\vec{g}[n_+,n_-]\wedge\vec{p}\right\rangle\\ =&\frac{1}{2\gamma}\vec{\nabla}\cdot\langle\vec{g}[n_+,n_-]\otimes\vec{p}\rangle+\frac{\epsilon}{2}\vec{\nabla}n_0+\langle\vec{g}[n_+,n_-]\wedge\vec{p}\rangle\ ;\end{aligned}\tag{3.57}$$

so from eqs. (3.55)–(3.57) it follows:

$$\begin{aligned}\langle (Tw)_0\rangle =&\frac{1}{2\gamma}\vec{\nabla}\otimes\vec{\nabla}:\left\langle\frac{\vec{p}\otimes\vec{p}}{2\gamma}g_0[n_+,n_-]+\frac{\epsilon}{2}\vec{p}\otimes\vec{g}[n_+,n_-]\right\rangle\\ &+\frac{1}{2\gamma}\vec{\nabla}\cdot\left(n_0\vec{\nabla}V\right)+\frac{\epsilon}{4\gamma}\vec{\nabla}\otimes\vec{\nabla}:\langle\vec{g}[n_+,n_-]\otimes\vec{p}\rangle\\ &+\frac{\epsilon}{2}\vec{\nabla}\cdot\langle\vec{g}[n_+,n_-]\wedge\vec{p}\rangle+\frac{\epsilon^2}{4}\Delta n_0\\ =&\frac{1}{2\gamma}\vec{\nabla}\otimes\vec{\nabla}:\left\langle\frac{\vec{p}\otimes\vec{p}}{2\gamma}g_0[n_+,n_-]+\epsilon\vec{p}\otimes\vec{g}[n_+,n_-]\right\rangle\\ &+\frac{1}{2\gamma}\vec{\nabla}\cdot\left(n_0\vec{\nabla}V\right)+\frac{\epsilon}{2}\vec{\nabla}\cdot\langle\vec{g}[n_+,n_-]\wedge\vec{p}\rangle+\frac{\epsilon^2}{4}\Delta n_0\,.\end{aligned}\tag{3.58}$$

Now let us consider the term:

$$\left\langle(\vec{T}w)\cdot\frac{\vec{p}}{|p|}\right\rangle=\frac{1}{2\gamma}\vec{\nabla}\cdot\left\langle\frac{\vec{p}\otimes\vec{p}}{|p|}\vec{w}\right\rangle+\frac{\epsilon}{2}\vec{\nabla}\cdot\left\langle\frac{\vec{p}}{|p|}w_0\right\rangle+\left\langle\frac{\vec{p}}{|p|}\cdot\Theta_\epsilon\vec{w}\right\rangle\ ;\tag{3.59}$$

$$\begin{aligned}\left\langle\frac{\vec{p}\otimes\vec{p}}{|p|}\vec{w}\right\rangle =&\left\langle\frac{\vec{p}\otimes\vec{p}}{|p|}\left[\frac{\vec{p}\cdot\vec{\nabla}}{2\gamma}\vec{g}[n_+,n_-]+\frac{\epsilon}{2}\vec{\nabla}g_0[n_+,n_-]\right]\right\rangle\\ &+\left\langle\frac{\vec{p}\otimes\vec{p}}{|p|}\left[\Theta_\epsilon\vec{g}[n_+,n_-]+\vec{g}[n_+,n_-]\wedge\vec{p}\right]\right\rangle\\ =&\vec{\nabla}\cdot\left\langle\frac{\vec{p}\otimes\vec{p}}{|p|}\left[\frac{1}{2\gamma}\vec{g}[n_+,n_-]\cdot\vec{p}+\frac{\epsilon}{2}g_0[n_+,n_-]\right]\right\rangle\\ &+\left\langle\frac{\vec{p}\otimes\vec{p}}{|p|}\Theta_\epsilon\vec{g}[n_+,n_-]\right\rangle\ ;\end{aligned}\tag{3.60}$$

$$\begin{aligned}\left\langle\frac{\vec{p}}{|p|}w_0\right\rangle =&\left\langle\frac{\vec{p}}{|p|}\left[\frac{\vec{p}\cdot\vec{\nabla}}{2\gamma}g_0[n_+,n_-]+\frac{\epsilon}{2}\vec{\nabla}\cdot\vec{g}[n_+,n_-]+\Theta_\epsilon g_0[n_+,n_-]\right]\right\rangle\\ =&\vec{\nabla}\cdot\left\langle\frac{1}{2\gamma}\frac{\vec{p}\otimes\vec{p}}{|p|}g_0[n_+,n_-]+\frac{\epsilon}{2}\frac{\vec{p}}{|p|}\otimes\vec{g}[n_+,n_-]\right\rangle\\ &+\left\langle\frac{\vec{p}}{|p|}\Theta_\epsilon g_0[n_+,n_-]\right\rangle\ ;\end{aligned}\tag{3.61}$$

$$\begin{aligned}\left\langle\frac{\vec{p}}{|p|}\cdot\Theta_\epsilon\vec{w}\right\rangle =&\left\langle\frac{\vec{p}}{|p|}\cdot\Theta_\epsilon\left[\frac{\vec{p}\cdot\vec{\nabla}}{2\gamma}\vec{g}[n_+,n_-]+\vec{g}[n_+,n_-]\wedge\vec{p}\right]\right\rangle\\ &+\left\langle\frac{\vec{p}}{|p|}\cdot\Theta_\epsilon\Theta_\epsilon\vec{g}[n_+,n_-]\right\rangle+\frac{\epsilon}{2}\left\langle\frac{\vec{p}}{|p|}\cdot\Theta_\epsilon\vec{\nabla}g_0[n_+,n_-]\right\rangle\ ;\end{aligned}\tag{3.62}$$

so from eqs. (3.59)–(3.62) we find:

$$\begin{aligned}
\left\langle (\vec{T}w)\cdot\frac{\vec{p}}{|p|}\right\rangle =&\frac{\vec{\nabla}\otimes\vec{\nabla}}{2\gamma}:\left\langle\frac{\vec{p}\otimes\vec{p}}{|p|}\left[\frac{1}{2\gamma}\vec{g}[n_+,n_-]\cdot\vec{p}+\frac{\epsilon}{2}g_0[n_+,n_-]\right]\right\rangle\\
&+\frac{1}{2\gamma}\vec{\nabla}\cdot\left\langle\frac{\vec{p}\otimes\vec{p}}{|p|}\Theta_\epsilon\vec{g}[n_+,n_-]\right\rangle\\
&+\frac{\epsilon}{2}\vec{\nabla}\otimes\vec{\nabla}:\left\langle\frac{1}{2\gamma}\frac{\vec{p}\otimes\vec{p}}{|p|}g_0[n_+,n_-]+\frac{\epsilon}{2}\frac{\vec{p}}{|p|}\otimes\vec{g}[n_+,n_-]\right\rangle\\
&+\frac{\epsilon}{2}\vec{\nabla}\cdot\left\langle\frac{\vec{p}}{|p|}\Theta_\epsilon g_0[n_+,n_-]\right\rangle\\
&+\left\langle\frac{\vec{p}}{|p|}\cdot\Theta_\epsilon\left[\frac{\vec{p}\cdot\vec{\nabla}}{2\gamma}\vec{g}[n_+,n_-]+\vec{g}[n_+,n_-]\wedge\vec{p}\right]\right\rangle\\
&+\left\langle\frac{\vec{p}}{|p|}\cdot\Theta_\epsilon\Theta_\epsilon\vec{g}[n_+,n_-]\right\rangle+\frac{\epsilon}{2}\left\langle\frac{\vec{p}}{|p|}\cdot\Theta_\epsilon\vec{\nabla}g_0[n_+,n_-]\right\rangle\\
=&\vec{\nabla}\otimes\vec{\nabla}:\left\{\frac{1}{2\gamma}\left\langle\frac{\vec{p}\otimes\vec{p}}{|p|}\left[\frac{1}{2\gamma}\vec{g}[n_+,n_-]\cdot\vec{p}+\epsilon g_0[n_+,n_-]\right]\right\rangle\right.\\
&\left.+\frac{\epsilon^2}{4}\left\langle\frac{\vec{p}}{|p|}\otimes\vec{g}[n_+,n_-]\right\rangle\right\}\\
&+\vec{\nabla}\cdot\left\{\frac{1}{2\gamma}\left\langle\frac{\vec{p}\otimes\vec{p}}{|p|}\Theta_\epsilon\vec{g}[n_+,n_-]\right\rangle+\frac{\epsilon}{2}\left\langle\frac{\vec{p}}{|p|}\Theta_\epsilon g_0[n_+,n_-]\right\rangle\right\}\\
&+\left\langle\frac{\vec{p}}{|p|}\cdot\Theta_\epsilon\left[\frac{\vec{p}\cdot\vec{\nabla}}{2\gamma}\vec{g}[n_+,n_-]+\vec{g}[n_+,n_-]\wedge\vec{p}\right]\right\rangle\\
&+\left\langle\frac{\vec{p}}{|p|}\cdot\Theta_\epsilon\Theta_\epsilon\vec{g}[n_+,n_-]\right\rangle+\frac{\epsilon}{2}\left\langle\frac{\vec{p}}{|p|}\cdot\Theta_\epsilon\vec{\nabla}g_0[n_+,n_-]\right\rangle .
\end{aligned} \tag{3.63}$$

Recall eq. (3.6), we can write system (3.50) in a more explicit form:

$$\begin{aligned}
\partial_t n_0 =&\frac{1}{2\gamma}\vec{\nabla}\otimes\vec{\nabla}:\left\langle\frac{\vec{p}\otimes\vec{p}}{2\gamma}g_0[n_+,n_-]+\epsilon\vec{p}\otimes\vec{g}[n_+,n_-]\right\rangle\\
&+\frac{1}{2\gamma}\vec{\nabla}\cdot\left(n_0\vec{\nabla}V\right)+\frac{\epsilon}{2}\vec{\nabla}\cdot\langle\vec{g}[n_+,n_-]\wedge\vec{p}\rangle+\frac{\epsilon^2}{4}\Delta n_0\,,\\
\partial_t n_\sigma =&\vec{\nabla}\otimes\vec{\nabla}:\left\{\frac{1}{2\gamma}\left\langle\frac{\vec{p}\otimes\vec{p}}{|p|}\left[\frac{1}{2\gamma}\vec{g}[n_+,n_-]\cdot\vec{p}+\epsilon g_0[n_+,n_-]\right]\right\rangle\right.\\
&\left.+\frac{\epsilon^2}{4}\left\langle\frac{\vec{p}}{|p|}\otimes\vec{g}[n_+,n_-]\right\rangle\right\}\\
&+\vec{\nabla}\cdot\left\{\frac{1}{2\gamma}\left\langle\frac{\vec{p}\otimes\vec{p}}{|p|}\Theta_\epsilon\vec{g}[n_+,n_-]\right\rangle+\frac{\epsilon}{2}\left\langle\frac{\vec{p}}{|p|}\Theta_\epsilon g_0[n_+,n_-]\right\rangle\right\}\\
&+\left\langle\frac{\vec{p}}{|p|}\cdot\Theta_\epsilon\left[\frac{\vec{p}\cdot\vec{\nabla}}{2\gamma}\vec{g}[n_+,n_-]+\vec{g}[n_+,n_-]\wedge\vec{p}\right]\right\rangle\\
&+\frac{\epsilon}{2}\left\langle\frac{\vec{p}}{|p|}\cdot\Theta_\epsilon\vec{\nabla}g_0[n_+,n_-]\right\rangle+\left\langle\frac{\vec{p}}{|p|}\cdot\Theta_\epsilon\Theta_\epsilon\vec{g}[n_+,n_-]\right\rangle .
\end{aligned} \tag{3.64}$$

System (3.64) is closed because we already defined (at least formally) the equilibrium distribution $g[n_+^\tau, n_-^\tau]$. Nevertheless it is very implicit, as the quantum exponential which appears in Eqs. (3.64) through Eq. (3.45) is very difficult to handle both analytically and numerically. As anticipated, in the following we will search for an approximated but more explicit version of Eqs. (3.64).

3.2.2 Semiclassical expansion of the equilibrium distribution

In order to obtain an explicit model from Eq. (3.50), we will exploit the approximations we have done, that is, the semiclassical one and the LSFS assumption (given by (1.37)). We will expand the equilibrium distribution $g[n_+, n_-]$ at the first order in ϵ, neglecting $O(\epsilon^2)$ terms; to do so, we exploit the approximation of the quantum exponential obtained in Chapter 2.
The equilibrium distribution $g[n_+, n_-]$ given by (3.45), (3.46), is written in the form (2.14) with $\beta = 1$ and

$$-a = \left(\frac{|p|^2}{2} + A\right)\sigma_0 + B\frac{\vec{p}}{|p|}\cdot\vec{\sigma}\,, \quad -b = \gamma\vec{p}\cdot\vec{\sigma}\,;$$

since (2.31) is satisfied, we can apply eqs. (2.21), (2.33) obtaining:

$$\begin{aligned}
g_0^{(0)}[n_+, n_-] =& e^{-(|p|^2/2+A)}\cosh B\,,\\
\vec{g}^{(0)}[n_+, n_-] =& -e^{-(|p|^2/2+A)}\sinh B\frac{\vec{p}}{|p|}\,,\\
g_0^{(1)}[n_+, n_-] =& \gamma|p|e^{-(|p|^2/2+A)}\sinh B\,,\\
\vec{g}^{(1)}[n_+, n_-] =& -\gamma\vec{p}e^{-(|p|^2/2+A)}\cosh B\\
&+ e^{-(|p|^2/2+A)}\frac{B\sinh B - \cosh B + 1}{2B}\frac{\vec{\nabla}_x B\wedge\vec{p}}{|\vec{p}|^2}\\
&- e^{-(|p|^2/2+A)}\frac{B\cosh B - \sinh B}{2B}\frac{\vec{\nabla}_x A\wedge\vec{p}}{|p|^2}\,.
\end{aligned} \tag{3.65}$$

Now we have to solve the constraints (3.46) with $g[n_+, n_-]$ given by (3.65) in order to write the Lagrange multipliers A, B as functions of $n_\pm$. We have:

$$\begin{aligned}
\left\langle g_0^{(0)}[n_+, n-] \pm \vec{g}^{(0)}[n_+, n_-]\cdot\frac{\vec{p}}{|p|}\right\rangle =& e^{-A}(\cosh B \mp \sinh B)\left\langle e^{-|p|^2/2}\right\rangle\\
=& 2\pi e^{-(A\pm B)}\,,\\
\left\langle g_0^{(1)}[n_+, n-] \pm \vec{g}^{(1)}[n_+, n_-]\cdot\frac{\vec{p}}{|p|}\right\rangle =& e^{-A}(\sinh B \mp \cosh B)\left\langle \gamma|p|e^{-|p|^2/2}\right\rangle\\
=& \mp 2\pi e^{-(A\pm B)}\gamma\sqrt{\frac{\pi}{2}}\,;
\end{aligned} \tag{3.66}$$

so from eqs. (3.46), (3.66) we deduce:

$$2\pi e^{-(A\pm B)}\left[1 \mp \epsilon\gamma\sqrt{\frac{\pi}{2}}\right] = n_\pm + O(\epsilon^2)\,,$$

and so:

$$A \pm B = -\log \frac{n_\pm}{2\pi} + \log \left[1 \mp \epsilon\gamma\sqrt{\frac{\pi}{2}}\right] + O(\epsilon^2) = -\log \frac{n_\pm}{2\pi} \mp \epsilon\gamma\sqrt{\frac{\pi}{2}} + O(\epsilon^2)\,,$$

which implies:

$$A = -\log \frac{\sqrt{n_+ n_-}}{2\pi} + O(\epsilon^2)\,, \quad B = -\log\sqrt{\frac{n_+}{n_-}} - \epsilon\gamma\sqrt{\frac{\pi}{2}} + O(\epsilon^2)\,. \tag{3.67}$$

From (3.67) it follows that:

$$\begin{aligned} e^{-A}\cosh B =& \frac{1}{2}\left[e^{-(A-B)} + e^{-(A+B)}\right] \\ =& \frac{1}{2}\left[\frac{n_-}{2\pi}\left(1 + \epsilon\gamma\sqrt{\frac{\pi}{2}}\right)^{-1} + \frac{n_+}{2\pi}\left(1 - \epsilon\gamma\sqrt{\frac{\pi}{2}}\right)^{-1}\right] + O(\epsilon^2) \\ =& \frac{1}{2\pi}\left[n_0 + n_\sigma\epsilon\gamma\sqrt{\frac{\pi}{2}}\right] + O(\epsilon^2)\,, \end{aligned} \tag{3.68}$$

$$\begin{aligned} e^{-A}\sinh B =& \frac{1}{2}\left[e^{-(A-B)} - e^{-(A+B)}\right] \\ =& \frac{1}{2}\left[\frac{n_-}{2\pi}\left(1 + \epsilon\gamma\sqrt{\frac{\pi}{2}}\right)^{-1} - \frac{n_+}{2\pi}\left(1 - \epsilon\gamma\sqrt{\frac{\pi}{2}}\right)^{-1}\right] + O(\epsilon^2) \\ =& -\frac{1}{2\pi}\left[n_\sigma + n_0\epsilon\gamma\sqrt{\frac{\pi}{2}}\right] + O(\epsilon^2)\,; \end{aligned} \tag{3.69}$$

moreover:

$$\begin{aligned} & e^{-A}\left[\frac{B\sinh B - \cosh B + 1}{2B}\vec{\nabla}_x B - \frac{B\cosh B - \sinh B}{2B}\vec{\nabla}_x A\right] \\ =& \frac{1}{4\pi B}\left[(Bn_\sigma + n_0 - \sqrt{n_0^2 - n_\sigma^2})\frac{1}{2}\left(\frac{\vec{\nabla}_x(n_0+n_\sigma)}{n_0+n_\sigma} - \frac{\vec{\nabla}_x(n_0-n_\sigma)}{n_0-n_\sigma}\right)\right. \\ & \left. + (Bn_0 + n_\sigma)\frac{1}{2}\left(\frac{\vec{\nabla}_x(n_0+n_\sigma)}{n_0+n_\sigma} + \frac{\vec{\nabla}_x(n_0-n_\sigma)}{n_0-n_\sigma}\right)\right] + O(\epsilon) \\ =& \frac{1}{8\pi}\left[\vec{\nabla}_x(n_0+n_\sigma) + \vec{\nabla}_x(n_0-n_\sigma)\right] \\ & + \frac{1}{8\pi B}\left[(n_0 - \sqrt{n_0^2 - n_\sigma^2})\left(\frac{\vec{\nabla}_x(n_0+n_\sigma)}{n_0+n_\sigma} - \frac{\vec{\nabla}_x(n_0-n_\sigma)}{n_0-n_\sigma}\right)\right. \\ & \left. + n_\sigma\left(\frac{\vec{\nabla}_x(n_0+n_\sigma)}{n_0+n_\sigma} + \frac{\vec{\nabla}_x(n_0-n_\sigma)}{n_0-n_\sigma}\right)\right] + O(\epsilon) \\ =& \frac{1}{4\pi}\vec{\nabla}_x n_0 + \frac{1}{8\pi B}\left[\vec{\nabla}_x(n_0+n_\sigma) - \vec{\nabla}_x(n_0-n_\sigma)\right. \\ & \left. - \sqrt{n_0^2 - n_\sigma^2}\,\frac{(n_0-n_\sigma)\vec{\nabla}_x(n_0+n_\sigma) - (n_0+n_\sigma)\vec{\nabla}_x(n_0-n_\sigma)}{n_0^2 - n_\sigma^2}\right] + O(\epsilon) \end{aligned}$$

$$
\begin{aligned}
=&\frac{1}{4\pi}\vec{\nabla}_x n_0 - \frac{1}{4\pi}\log^{-1}\sqrt{\frac{n_0+n_\sigma}{n_0-n_\sigma}}\left[\vec{\nabla}_x n_\sigma - \frac{1}{2}\sqrt{\frac{n_0-n_\sigma}{n_0+n_\sigma}}\vec{\nabla}_x(n_0+n_\sigma)\right.\\
&\left.+\frac{1}{2}\sqrt{\frac{n_0+n_\sigma}{n_0-n_\sigma}}\vec{\nabla}_x(n_0-n_\sigma)\,,\right] + O(\epsilon)
\end{aligned}
$$

and so:

$$
\begin{aligned}
&e^{-A}\left[\frac{B\sinh B - \cosh B + 1}{2B}\vec{\nabla}_x B - \frac{B\cosh B - \sinh B}{2B}\vec{\nabla}_x A\right]\\
=&\frac{1}{4\pi}\vec{\nabla}_x n_0 - \frac{1}{4\pi}\log^{-1}\sqrt{\frac{n_0+n_\sigma}{n_0-n_\sigma}}\left[\frac{n_\sigma}{\sqrt{n_0^2-n_\sigma^2}}\vec{\nabla}_x n_0\right.\\
&\left.+\left(1-\frac{n_0}{\sqrt{n_0^2-n_\sigma^2}}\right)\vec{\nabla}_x n_\sigma\right] + O(\epsilon)\,.
\end{aligned}
\tag{3.70}
$$

So from (3.65), (3.67), (3.68), (3.69), (3.70) we conclude:

$$
\begin{aligned}
g_0[n_+,n_-] =&\frac{e^{-|\vec{p}|^2/2}}{2\pi}\left\{n_0 + \epsilon\gamma\left(\sqrt{\frac{\pi}{2}} - |\vec{p}|\right)n_\sigma\right\} + O(\epsilon^2)\,,\\
\vec{g}[n_+,n_-] =&\frac{e^{-|\vec{p}|^2/2}}{2\pi}\left\{\left[n_\sigma + \epsilon\gamma\left(\sqrt{\frac{\pi}{2}} - |\vec{p}|\right)n_0\right]\frac{\vec{p}}{|\vec{p}|} + \epsilon\vec{F}\wedge\frac{\vec{p}}{|\vec{p}|^2}\right\} + O(\epsilon^2)\,,
\end{aligned}
\tag{3.71}
$$

with:

$$
\vec{F} \equiv \frac{1}{2}\vec{\nabla}_x n_0 - \frac{n_\sigma\vec{\nabla}_x n_0 + \left[\sqrt{n_0^2-n_\sigma^2} - n_0\right]\vec{\nabla}_x n_\sigma}{\left[\log(n_0+n_\sigma) - \log(n_0-n_\sigma)\right]\sqrt{n_0^2-n_\sigma^2}}
\tag{3.72}
$$

3.2.3 Computation of the moments

Now we will use eqs. (3.71), (3.72) to compute a $O(\epsilon^2)-$approximation of the implicit terms contained in eqs. (3.64). First we start computing several useful gaussian integrals: for $i, j = 1, 2$,

$$
\begin{aligned}
\int \frac{p_i p_j}{|p|^3} e^{-|p|^2/2}\frac{dp}{2\pi} &= \int \frac{1}{2|p|}\, e^{-|p|^2/2}\frac{dp}{2\pi}\delta_{ij} = \frac{1}{2}\sqrt{\frac{\pi}{2}}\delta_{ij}\,,\\
\int \frac{p_i p_j}{|p|^2} e^{-|p|^2/2}\frac{dp}{2\pi} &= \int \frac{1}{2}\, e^{-|p|^2/2}\frac{dp}{2\pi}\delta_{ij} = \frac{1}{2}\delta_{ij}\,,\\
\int \frac{p_i p_j}{|p|} e^{-|p|^2/2}\frac{dp}{2\pi} &= \int \frac{|p|}{2}\, e^{-|p|^2/2}\frac{dp}{2\pi}\delta_{ij} = \frac{1}{2}\sqrt{\frac{\pi}{2}}\delta_{ij}\,,\\
\int p_i p_j\, e^{-|p|^2/2}\frac{dp}{2\pi} &= \int \frac{|p|^2}{2}\, e^{-|p|^2/2}\frac{dp}{2\pi}\delta_{ij} = \delta_{ij}\,,\\
\int p_i p_j\, |p|\, e^{-|p|^2/2}\frac{dp}{2\pi} &= \int \frac{|p|^3}{2} e^{-|p|^2/2}\frac{dp}{2\pi}\delta_{ij} = \frac{3}{2}\sqrt{\frac{\pi}{2}}\delta_{ij}\,.
\end{aligned}
\tag{3.73}
$$

Now we can easily compute the moments in eqs. (3.64). We begin by considering the terms that do not contain the potential V: for $i, j = 1, 2$,

$$\begin{aligned}\langle p_i p_j\, g_0[n_+, n_-]\rangle &= \left(n_0 - \frac{\epsilon\gamma}{2}\sqrt{\frac{\pi}{2}} n_\sigma\right)\delta_{ij} + O(\epsilon^2)\,,\\ \langle \epsilon p_i g_j[n_+, n_-]\rangle &= \frac{\epsilon}{2}\sqrt{\frac{\pi}{2}} n_\sigma \delta_{ij} + O(\epsilon^2)\,,\\ \langle \epsilon p_i g_3[n_+, n_-]\rangle &= 0 + O(\epsilon^2)\,,\\ \frac{\epsilon}{2}\,\langle \vec{g}[n_+, n_-] \wedge \vec{p}\rangle &= 0 + O(\epsilon^2)\,,\\ \left\langle p_i p_j\, \vec{g}[n_+, n-] \cdot \frac{\vec{p}}{|p|}\right\rangle &= \left(n_\sigma - \frac{\epsilon\gamma}{2}\sqrt{\frac{\pi}{2}} n_0\right)\delta_{ij} + O(\epsilon^2)\,,\\ \left\langle \frac{p_i p_j}{|p|}\epsilon g_0[n_+, n_-]\right\rangle &= \frac{\epsilon}{2}\sqrt{\frac{\pi}{2}} n_0 \delta_{ij} + O(\epsilon^2)\,;\end{aligned} \tag{3.74}$$

then we have to compute the terms containing the potential:

$$\begin{aligned}\left\langle \frac{p_i p_k}{|p|}\Theta_\epsilon g_k[n_+, n_-]\right\rangle &= \partial_j V \int \partial_{p_j}\left(\frac{p_i p_k}{|p|}\right) g_k[n_+, n_-]\, dp + O(\epsilon^2)\\ &= \partial_j V \int \left[\frac{\delta_{ij} p_k + \delta_{kj} p_i}{|p|} - \frac{p_i p_j p_k}{|p|^3}\right] g_k[n_+, n_-]\, dp + O(\epsilon^2)\\ &= \partial_j V \int \left(\delta_{ij} - \frac{p_i p_j}{|p|^2}\right)\frac{\vec{p}\cdot\vec{g}[n_+, n_-]}{|p|}\, dp\\ &\quad + \partial_j V \int \frac{p_i}{|p|} g_j[n_+, n_-]\, dp + O(\epsilon^2)\,;\end{aligned} \tag{3.75}$$

since the mapping $\vec{p} \mapsto \vec{g}[n_+, n_-] \cdot \vec{p}/|p|$ depends only on $|p|$ up to $O(\epsilon^2)$, then:

$$\begin{aligned}\int \left(\delta_{ij} - \frac{p_i p_j}{|p|^2}\right)\frac{\vec{p}\cdot\vec{g}[n_+, n_-]}{|p|}\, dp &= \int \frac{\delta_{ij}}{2}\frac{\vec{p}\cdot\vec{g}[n_+, n_-]}{|p|}\, dp + O(\epsilon^2)\\ &= \frac{n_\sigma}{2}\delta_{ij} + O(\epsilon^2)\,;\end{aligned} \tag{3.76}$$

moreover since (remember (3.72)):

$$\vec{g}[n_+, n_-] = \left(\frac{\vec{p}}{|p|}\cdot\vec{g}[n_+, n_-]\right)\frac{\vec{p}}{|p|} + \epsilon\frac{e^{-|p|^2/2}}{2\pi}\vec{F} \wedge \frac{\vec{p}}{|p|^2} + O(\epsilon^2)\,,$$

then:

$$\begin{aligned}\int \frac{p_i}{|p|} g_j[n_+, n_-]\, dp &= \int \frac{p_i p_j}{|p|^2}\frac{\vec{p}}{|p|}\cdot\vec{g}[n_+, n_-]\, dp\\ &\quad + \epsilon\eta_{jks} F_k \int \frac{p_i p_s}{|p|^3} e^{-|p|^2/2}\frac{dp}{2\pi} + O(\epsilon^2)\\ &= \frac{n_\sigma}{2}\delta_{ij} + \frac{\epsilon}{2}\sqrt{\frac{\pi}{2}}\eta_{ijk} F_k + O(\epsilon^2)\,;\end{aligned} \tag{3.77}$$

so from eqs. (3.75)–(3.77) we deduce:

$$\left\langle \frac{\vec{p}\otimes\vec{p}}{|p|}\Theta_\epsilon\vec{g}[n_+, n_-]\right\rangle = n_\sigma\vec{\nabla}V + \frac{\epsilon}{2}\sqrt{\frac{\pi}{2}}\,\vec{\nabla}V \wedge \vec{F} + O(\epsilon^2)\,,$$

$$
\begin{aligned}
\frac{\epsilon}{2}\left\langle \frac{p_i}{|p|}\Theta_\epsilon g_0[n_+,n_-]\right\rangle =& \frac{\epsilon}{2}\partial_j V\left\langle \partial_{p_j}\left(\frac{p_i}{|p|}\right) g_0[n_+,n_-]\right\rangle + O(\epsilon^2)\\
=& \frac{\epsilon}{2} n_0 \partial_j V \int \frac{1}{|p|}\left(\delta_{ij}-\frac{p_ip_j}{|p|^2}\right) e^{-|p|^2/2}\frac{dp}{2\pi} + O(\epsilon^2)\\
=& \frac{\epsilon}{2}\left(\sqrt{\frac{\pi}{2}}\delta_{ij} - \frac{1}{2}\sqrt{\frac{\pi}{2}}\delta_{ij}\right) n_0\partial_j V + O(\epsilon^2)\\
=& \frac{\epsilon}{4}\sqrt{\frac{\pi}{2}}\, n_0 \partial_i V + O(\epsilon^2)\,;
\end{aligned}
$$

$$
\begin{aligned}
&\left\langle \frac{\vec p}{|p|}\cdot\Theta_\epsilon\left[\frac{\vec p\cdot\vec\nabla}{2\gamma}\vec g[n_+,n_-] + \vec g[n_+,n_-]\wedge\vec p\right]\right\rangle\\
&= \partial_i V\int\left(\delta_{ij}-\frac{p_ip_j}{|p|^2}\right)\left(\frac{p_k\partial_k}{2\gamma}g_j[n_+,n_-] + \eta_{jks}g_k[n_+,n_-]p_s\right)\frac{dp}{|p|} + O(\epsilon^2)\\
&= \partial_i V\left\{\frac{\partial_k}{2\gamma}\int\frac{p_k}{|p|}\left(\delta_{ij}-\frac{p_ip_j}{|p|^2}\right) g_j[n_+,n_-]\,dp + \eta_{iks}\int g_k[n_+,n_-]\frac{p_s}{|p|}\,dp\right\} + O(\epsilon^2)\\
&= \epsilon\partial_i V\left\{\frac{\partial_k}{2\gamma}\int\frac{p_k}{|p|}\eta_{ijs}F_j\frac{p_s}{|p|^2}e^{-|p|^2/2}\frac{dp}{2\pi} + \eta_{ksi}\int\eta_{kjl}F_j\frac{p_l}{|p|^2}\frac{p_s}{|p|}e^{-|p|^2/2}\frac{dp}{2\pi}\right\} + O(\epsilon^2)\\
&= \epsilon\partial_i V\left\{\frac{\partial_k F_j}{2\gamma}\eta_{ijs}\int\frac{p_kp_s}{|p|^3}e^{-|p|^2/2}\frac{dp}{2\pi} + F_j(\delta_{js}\delta_{il}-\delta_{ls}\delta_{ij})\int\frac{p_lp_s}{|p|^3}e^{-|p|^2/2}\frac{dp}{2\pi}\right\} + O(\epsilon^2)\\
&= \frac{\epsilon}{2}\sqrt{\frac{\pi}{2}}\partial_i V\left\{\frac{1}{2\gamma}\eta_{ijs}\partial_s F_j + F_j(\delta_{js}\delta_{il}-\delta_{ls}\delta_{ij})\delta_{ls}\right\} + O(\epsilon^2)\\
&= -\frac{\epsilon}{2}\sqrt{\frac{\pi}{2}}\vec\nabla V\cdot\left[\frac{1}{2\gamma}\vec\nabla\wedge\vec F + \vec F\right] + O(\epsilon^2)\,;
\end{aligned} \tag{3.78}
$$

$$
\begin{aligned}
\frac{\epsilon}{2}\left\langle \frac{\vec p}{|p|}\cdot\Theta_\epsilon\vec\nabla g_0[n_+,n_-]\right\rangle =& \frac{\epsilon}{2}\partial_j V\int\partial_{p_j}\left(\frac{p_i}{|p|}\right)\partial_i\left[\frac{n_0}{2\pi}e^{-|p|^2/2}\right]dp + O(\epsilon^2)\\
=& \frac{\epsilon}{2}\partial_j V\partial_i n_0\int\frac{1}{|p|}\left(\delta_{ij}-\frac{p_ip_j}{|p|^2}\right)e^{-|p|^2/2}\frac{dp}{2\pi} + O(\epsilon^2)\\
=& \frac{\epsilon}{2}\partial_j V\partial_i n_0\delta_{ij}\int\frac{e^{-|p|^2/2}}{2|p|}\frac{dp}{2\pi} + O(\epsilon^2)\\
=& \frac{\epsilon}{4}\sqrt{\frac{\pi}{2}}\vec\nabla n_0\cdot\vec\nabla V + O(\epsilon^2)\,;
\end{aligned} \tag{3.79}
$$

$$
\begin{aligned}
\left\langle \frac{\vec p}{|p|}\cdot\Theta_\epsilon\Theta_\epsilon\vec g[n_+,n_-]\right\rangle =& \left\langle \frac{\vec p}{|p|}\cdot\Theta_\epsilon\Theta_\epsilon\left(g_\sigma[n_+,n_-]\frac{\vec p}{|p|} + \vec g^\perp[n_+,n_-]\right)\right\rangle\\
=& \partial_j V\partial_k V\left\{\left\langle\frac{p_i}{|p|}\partial_{p_j}\partial_{p_k}\left(\vec g^\perp[n_+,n_-]\right)_i\right\rangle\right.\\
&\left. + \left\langle\frac{p_i}{|p|}\partial_{p_j}\partial_{p_k}\left(g_\sigma[n_+,n_-]\frac{p_i}{|p|}\right)\right\rangle\right\} + O(\epsilon^2)\,,
\end{aligned} \tag{3.80}
$$

where we have used notation (3.5).

Let us consider the first term in (3.80), exploiting the symmetry properties of the operator $\langle\cdot\rangle$:

$$\begin{aligned}
&\left\langle \frac{p_i}{|p|}\partial_j V \partial_k V \partial_{p_j}\partial_{p_k}\left(\vec{g}^{\perp}[n_+,n_-]\right)_i \right\rangle \\
&= \left\langle \frac{p_i}{|p|}\partial_j V \partial_k V \partial_{p_j}\partial_{p_k}\left(\frac{e^{-|p|^2/2}}{2\pi|p|^2}\epsilon\eta_{ils}F_l p_s\right)\right\rangle + O(\epsilon^2) \\
&= \left\langle \epsilon\eta_{ils}F_l\partial_j V\partial_k V\frac{p_i}{|p|}\left[\partial^2_{p_jp_k}\left(\frac{e^{-|p|^2/2}}{2\pi|p|^2}\right)p_s + 2\partial_{p_j}\left(\frac{e^{-|p|^2/2}}{2\pi|p|^2}\right)\delta_{ks}\right]\right\rangle + O(\epsilon^2) \\
&= -\left\langle \epsilon\eta_{ils}F_l\partial_j V\partial_s V\frac{p_i}{|p|}\frac{p_j}{|p|}\frac{e^{-|p|^2/2}}{\pi|p|^3}(|p|^2+2)\right\rangle + O(\epsilon^2) \\
&= -\left\langle \epsilon\eta_{ils}F_l\partial_j V\partial_s V\frac{\delta_{ij}}{2}\frac{e^{-|p|^2/2}}{\pi|p|^3}(|p|^2+2)\right\rangle + O(\epsilon^2) \\
&= -\left\langle \epsilon\eta_{ils}F_l\partial_i V\partial_s V\frac{e^{-|p|^2/2}}{2\pi|p|^3}(|p|^2+2)\right\rangle + O(\epsilon^2) = 0 + O(\epsilon^2)\,.
\end{aligned} \tag{3.81}$$

now we consider the other term in (3.80):

$$\begin{aligned}
&\left\langle \frac{p_i}{|p|}\partial_{p_j}\partial_{p_k}\left(g_\sigma[n_+,n_-]\frac{p_i}{|p|}\right)\right\rangle \\
&= \left\langle \frac{p_i}{|p|}\left[\frac{p_i}{|p|}\partial_{p_jp_k}g_\sigma[n_+,n_-] + g_\sigma[n_+,n_-]\partial_{p_jp_k}\left(\frac{p_i}{|p|}\right)\right]\right\rangle \\
&+ \left\langle \frac{p_i}{|p|}\left[\partial_{p_j}g_\sigma[n_+,n_-]\partial_{p_k}\left(\frac{p_i}{|p|}\right) + \partial_{p_k}g_\sigma[n_+,n_-]\partial_{p_j}\left(\frac{p_i}{|p|}\right)\right]\right\rangle \\
&= \left\langle g_\sigma[n_+,n_-]\frac{p_i}{|p|}\partial_{p_j}\partial_{p_k}\left(\frac{p_i}{|p|}\right)\right\rangle \\
&= -\left\langle \frac{1}{|p|^2}\left(\delta_{jk} - \frac{p_jp_k}{|p|^2}\right)g_\sigma[n_+,n_-]\right\rangle \\
&= -\left\langle \frac{1}{|p|^2}\left(\delta_{jk} - \frac{p_jp_k}{|p|^2}\right)\left[n_\sigma + \epsilon\gamma\sqrt{\frac{\pi}{2}}n_0\right]\frac{e^{-|p|^2/2}}{2\pi}\right\rangle \\
&+ \left\langle \frac{1}{|p|}\left(\delta_{jk} - \frac{p_jp_k}{|p|^2}\right)\epsilon\gamma n_0\frac{e^{-|p|^2/2}}{2\pi}\right\rangle \\
&= \frac{\delta_{jk}}{2}\left[n_\sigma + \epsilon\gamma\sqrt{\frac{\pi}{2}}n_0\right]\Gamma + \delta_{jk}\frac{\epsilon\gamma n_0}{2}\sqrt{\frac{\pi}{2}}\,,
\end{aligned} \tag{3.82}$$

with:

$$\Gamma \equiv -\left\langle \frac{e^{-|p|^2/2}}{2\pi|p|^2}\right\rangle\,. \tag{3.83}$$

Notice that, according to the definition of the operator $\langle\cdot\rangle$ given in eq. (3.4), Γ should be $-\infty$: this cannot be allowed for obvious both physical and analytical reasons, for the model we are deriving would be completely meaningless. So we are going to give to the expression (3.83) a different (heuristic) interpretation,

that will bring us to consider Γ as a real number.
We start considering the following Poisson equation in $\mathbb{R}^2$:

$$-\Delta u = \delta\,, \tag{3.84}$$

with δ the Dirac delta distribution. It is well known that a noteworthy distributional solution of (3.84) is the so-called *fundamental harmonic*:

$$u(x) = -\frac{1}{2\pi}\log|x| \qquad x \in \mathbb{R}^2\,; \tag{3.85}$$

let us now take the Fourier transform of eq. (3.84):

$$|k|^2\hat{u}(k) = \frac{1}{2\pi}\,; \tag{3.86}$$

so from a heuristic point of view:

$$\text{“}\ \frac{1}{2\pi|k|^2} = \hat{u}(k)\ \text{”}\,; \tag{3.87}$$

this suggests us to consider the expression in (3.83) as the duality product between the Fourier transform of the tempered regular distribution $u(x)$ and the Schwartz function $\varphi(p) \equiv e^{-|p|^2/2}$:

$$\begin{aligned}\Gamma &= -\left\langle \frac{e^{-|p|^2/2}}{2\pi|p|^2} \right\rangle = -\,\langle \hat{u}\,,\,\varphi\rangle_{(\mathcal{S}'(\mathbb{R}^2)\,,\,\mathcal{S}(\mathbb{R}^2))} = -\,\langle u\,,\,\hat{\varphi}\rangle_{(\mathcal{S}'(\mathbb{R}^2)\,,\,\mathcal{S}(\mathbb{R}^2))}\\ &= \int \log|p| e^{-|p|^2/2}\frac{dp}{2\pi} = \int_0^\infty e^{-\rho^2/2}\rho\log\rho\, d\rho\,,\end{aligned} \tag{3.88}$$

where $\mathcal{S}(\mathbb{R}^2)$ denotes the space of Schwartz functions. The latter integral can be numerically evaluated and yields:

$$\int_0^\infty e^{-\rho^2/2}\rho\log\rho\, d\rho \approx 5.79657\times 10^{-2}\,.$$

Notice that Γ is a real *positive* number: this testifies the nature of the expression in (3.83) as something different from the principal value of $-e^{-|p|^2/2}/(2\pi|p|^2)$.

The argument contained in eq. (3.88) that has lead us to define Γ as a real number is heuristic; however, making this argument rigorous seems quite a challenging task and goes beyond the purpose of this Thesis.

Collecting eqs. (3.64), (3.74)–(3.81) we finally obtain the following Quantum Two-Bands Drift-Diffusion model, which we call QDE model:

$$\begin{aligned}\partial_t n_0 =&\frac{1}{4\gamma^2}\Delta\left(n_0 + \frac{\epsilon\gamma}{2}\sqrt{\frac{\pi}{2}}n_\sigma\right) + \frac{1}{2\gamma}\vec{\nabla}\cdot\left(n_0\vec{\nabla}V\right) + O(\epsilon^2)\,,\\ \partial_t n_\sigma =&\frac{1}{4\gamma^2}\Delta\left(n_\sigma + \frac{\epsilon\gamma}{2}\sqrt{\frac{\pi}{2}}n_0\right) + \frac{1}{2\gamma}\vec{\nabla}\cdot\left[\left(n_\sigma + \frac{\epsilon\gamma}{2}\sqrt{\frac{\pi}{2}}\,n_0\right)\vec{\nabla}V\right]\\ &-\frac{\epsilon}{2\gamma}\sqrt{\frac{\pi}{2}}\vec{\nabla}V\cdot\left[\vec{\nabla}\wedge\vec{F} + \gamma\vec{F}\right] + \frac{\epsilon}{4}\sqrt{\frac{\pi}{2}}\vec{\nabla}n_0\cdot\vec{\nabla}V\\ &+\frac{|\vec{\nabla}V|^2}{2}\left[\left(n_\sigma + \epsilon\gamma\sqrt{\frac{\pi}{2}}n_0\right)\Gamma + \epsilon\gamma\sqrt{\frac{\pi}{2}}n_0\right] + O(\epsilon^2)\,,\end{aligned} \tag{3.89}$$

with F and Γ respectively given by (3.72), (3.88).

3.3 A second order two-band diffusive model

We are going to derive another diffusive model for quantum transport in graphene, starting again from the Wigner equations in diffusive scaling (1.38), considering the same fluid-dynamic moments $n_\pm$ of the Wigner distribution $w(r,p,t)$ and taking again as the equilibrium distribution the one given in (3.45), (3.46); however, we will now make stronger assumptions, which will allow us to consider also $O(\epsilon^2)-$terms in the fluid equations.

We make the semiclassical hypothesis $\epsilon \ll 1$ like in the previous model, and another hypothesis, stronger than (1.37), which we call *Strongly Mixed State* (SMS):

$$c = O(\epsilon)\,, \qquad B = O(\epsilon)\,. \tag{3.90}$$

(Recall the definitions (1.36), (3.45) of c and B, respectively). These further assumptions are necessary to overcome the computational difficulties arising from the spinorial nature of the problem: without these hypothesis, it would be hard to compute the second order expansion of the equilibrium distribution.

We will see that the two approximations will result in the fact:

$$\left|\frac{n_+ - n_-}{n_+ + n_-}\right| = \left|\frac{n_\sigma}{n_0}\right| = O(\epsilon)\,. \tag{3.91}$$

This means, from a physical point of view, that the charge carriers have approximately the same probability of being found in the conduction band or in the valence band of the energy spectrum, or equivalently, there is little difference (with respect to the total charge density) between the electron density and the hole density. From the analytical point of view, the main consequence of the SMS hypothesis (3.90) will be the decoupling of the modified Hamiltonian in a scalar part of order 1 and a spinorial perturbation of order ϵ; this fact will be very useful in computations.

3.3.1 Semiclassical expansion of the equilibrium distribution

For the sake of simplicity let us redefine $B \mapsto \epsilon B$ and consider $B = O(1)$.
Under our hypothesis, the classical symbol of the modified Hamiltonian becomes:

$$h_\xi = \left(\frac{|p|^2}{2} + A\right)\sigma_0 + \epsilon(\gamma|p| + B)\frac{\vec{p}}{|p|}\cdot\vec{\sigma}\,;$$

that is, as anticipated, the modified Hamiltonian h_ξ decouples in a *scalar* part of order $O(1)$ and a *spinorial* part of order $O(\epsilon)$, so that h_ξ can be seen as a small perturbation of a scalar Hamiltonian. We are going to see that this fact leads to remarkable simplifications in computations.

In order to explicitly compute the second order semiclassical expansion of the equilibrium distribution $g_\epsilon[n_+, n_-]$, let us write it in the form $g_\epsilon = \mathcal{E}\mathrm{xp}_\epsilon(a + \epsilon b)$, with:

$$-\,a = \left(\frac{|p|^2}{2} + A\right)\sigma_0\,, \qquad -b = (\gamma|p| + B)\frac{\vec{p}}{|p|}\cdot\vec{\sigma}\,; \tag{3.92}$$

we notice that condition (2.34) is satisfied. We can then exploit eq. (2.41) with $\beta = 1$:

$$\begin{aligned} g_\epsilon[n_+, n_-] =& e^{-\left(|p|^2/2+A\right)}\sigma_0 - \epsilon e^{-\left(|p|^2/2+A\right)}(\gamma|p| + B)\frac{\vec{p}}{|p|}\cdot\vec{\sigma} \\ &+ \epsilon^2 \mathcal{E}\mathrm{xp}^{(2)}\left(-\left(\frac{|p|^2}{2} + A\right)\right)\sigma_0 \\ &+ \frac{\epsilon^2}{2}(\gamma|p| + B)^2 e^{-\left(|p|^2/2+A\right)}\sigma_0 + O(\epsilon^3)\,, \end{aligned} \tag{3.93}$$

where the Lagrange multipliers A, B are such that (3.46) are satisfied at second order in ϵ by $g_\epsilon[n_+, n_-]$ given by (3.93).
Now let us define, for an arbitrary positive scalar function $n(x)$, the function $\mathcal{M}_\epsilon[n]$ as the $O(\epsilon^4)-$approximation of the scalar quantum Maxwellian with $\langle \mathcal{M}_\epsilon[n]\rangle = n$, that is:

$$\mathcal{M}_\epsilon[n] = \frac{n}{2\pi} e^{-|p|^2/2}\left[1 + \frac{\epsilon^2}{24}(\delta_{ij} - p_i p_j)\partial^2_{ij}\log n\right]\,; \tag{3.94}$$

this means that, if $\mathcal{M}^*[n] = \mathcal{E}\mathrm{xp}_\epsilon(-A^* - |p|^2/2)$ with $A^* = A^*(x)$ such that: $\int \mathcal{M}^*[n]\,dp = n$, then $\mathcal{M}^*[n] = \mathcal{M}_\epsilon[n] + O(\epsilon^4)$. See e.g. [16], [29] for details.
For convenience of calculus, we substitute the Lagrange multiplier A in (3.93) with a positive scalar function $\rho(x)$ in such a way that:

$$e^{-\left(|p|^2/2+A\right)} + \epsilon^2 \mathcal{E}\mathrm{xp}^{(2)}\left(-\left(\frac{|p|^2}{2} + A\right)\right) = \mathcal{M}_\epsilon[\rho]\,; \tag{3.95}$$

the relation between A and ρ can be written at first semiclassical order as:

$$\rho = 2\pi e^{-A} + O(\epsilon^2)\,; \tag{3.96}$$

so eq. (3.93) can be rewritten in terms of ρ, B:

$$\begin{aligned} g_\epsilon[n_+, n_-] =& \mathcal{M}_\epsilon[\rho] - \epsilon\frac{\rho}{2\pi}e^{-|p|^2/2}(\gamma|p| + B)\frac{\vec{p}}{|p|}\cdot\vec{\sigma} \\ &+ \frac{\epsilon^2}{2}(\gamma|p| + B)^2\frac{\rho}{2\pi}e^{-|p|^2/2}\sigma_0 + O(\epsilon^3)\,; \end{aligned} \tag{3.97}$$

but from (3.46), (3.97) it follows:

$$\begin{aligned} \frac{n_+ + n_-}{2} =& \langle g_\epsilon[n_+, n_-]_0\rangle \\ =& \rho - \frac{\epsilon^2}{2}\rho\int(\gamma^2|p|^2 + B^2 + 2\gamma B|p|)e^{-|p|^2/2}\frac{dp}{2\pi} + O(\epsilon^3) \\ =& \rho + \epsilon^2\rho\left(\gamma^2 + \frac{B^2}{2} + \gamma B\sqrt{\frac{\pi}{2}}\right) + O(\epsilon^3)\,, \\ \frac{n_+ - n_-}{2} =& \left\langle \vec{g}_\epsilon[n_+, n_-]\cdot\frac{\vec{p}}{|\vec{p}|}\right\rangle \\ =& -\epsilon\frac{\rho}{2\pi}\int e^{-|p|^2/2}(\gamma|p| + B)\,dp + O(\epsilon^3) \\ =& -\epsilon\rho\left(\gamma\sqrt{\frac{\pi}{2}} + B\right) + O(\epsilon^3)\,; \end{aligned} \tag{3.98}$$

if we recall definition (3.6) we obtain:

$$\begin{aligned} \rho =& n_0 \left[1 - \epsilon^2 \left(\gamma^2 + \frac{B^2}{2} + \gamma B \sqrt{\frac{\pi}{2}}\right)\right] + O(\epsilon^3)\,, \\ -B =& \frac{n_\sigma}{\epsilon n} + \gamma \sqrt{\frac{\pi}{2}} + O(\epsilon^2)\,, \end{aligned} \tag{3.99}$$

and so:

$$\begin{aligned} \rho =& n_0 - n_0 \epsilon^2 \left[\left(1 - \frac{\pi}{4}\right)\gamma^2 + \frac{1}{2}\left(\frac{n_\sigma}{\epsilon n_0}\right)^2\right] + O(\epsilon^3)\,, \\ -B =& \frac{n_\sigma}{\epsilon n_0} + \gamma \sqrt{\frac{\pi}{2}} + O(\epsilon^2)\,. \end{aligned} \tag{3.100}$$

Finally collecting eqs. (3.97), (3.100) we obtain the second order semiclassical expansion of the equilibrium distribution (3.45), (3.46):

$$\begin{aligned} g_\epsilon[n_+, n_-] =& \mathcal{M}_\epsilon \left[n_0 - n_0 \epsilon^2 \left(\left(1 - \frac{\pi}{4}\right)\gamma^2 + \frac{1}{2}\left(\frac{n_\sigma}{\epsilon n_0}\right)^2\right)\right] \sigma_0 \\ &+ \epsilon \frac{n_0}{2\pi} e^{-|p|^2/2} \left[\gamma\left(\sqrt{\frac{\pi}{2}} - |p|\right) + \frac{n_\sigma}{\epsilon n_0}\right] \frac{\vec{p}}{|p|} \cdot \vec{\sigma} \\ &+ \frac{\epsilon^2}{2} \left[\gamma\left(\sqrt{\frac{\pi}{2}} - |p|\right) + \frac{n_\sigma}{\epsilon n_0}\right]^2 \frac{n_0}{2\pi} e^{-|p|^2/2} \sigma_0 + O(\epsilon^3)\,; \end{aligned} \tag{3.101}$$

We point out that from eq. (3.100) it follows that the constraint (3.91) is satisfied.

3.3.2 Computation of the moments

Now we will exploit eqs. (3.94), (3.101) in order to compute a second order semiclassical approximation of the terms in eqs. (3.64).
Let us begin computing:

$$\begin{aligned} \langle p_i p_j \, g_0[n_+, n_-] \rangle =& \left\langle p_i p_j \, \mathcal{M}_\epsilon \left[n_0 - n_0 \epsilon^2 \left(\left(1 - \frac{\pi}{4}\right)\gamma^2 + \frac{1}{2}\left(\frac{n_\sigma}{\epsilon n_0}\right)^2\right)\right] \right\rangle \\ &+ \frac{\epsilon^2}{2} \left\langle p_i p_j \left[\gamma\left(|p| - \sqrt{\frac{\pi}{2}}\right) - \frac{n_\sigma}{\epsilon n_0}\right]^2 \frac{n_0}{2\pi} e^{-|p|^2/2} \right\rangle + O(\epsilon^3)\,; \end{aligned} \tag{3.102}$$

from eq. (3.94) we deduce (here n is an arbitrary positive scalar function):

$$\begin{aligned} \langle p_i p_j \, \mathcal{M}_\epsilon[n] \rangle =& \left\langle p_i p_j \frac{n}{2\pi} e^{-|p|^2/2} \left[1 + \frac{\epsilon^2}{24} \vec{\nabla} \cdot \left((\sigma_0 - \vec{p} \otimes \vec{p}) \vec{\nabla} \log n\right)\right] \right\rangle \\ =& n\delta_{ij} + \frac{\epsilon^2}{24} n \partial_{ks} \log n \cdot \int p_i p_j (\delta_{ks} - p_k p_s) e^{-|p|^2/2} \frac{dp}{2\pi}\,; \end{aligned} \tag{3.103}$$

since:

$$\begin{aligned}\int p_i p_j p_k p_s e^{-|p|^2/2}\frac{dp}{2\pi} &= -\int p_i p_j p_k \partial_{p_s}\left(e^{-|p|^2/2}\right)\frac{dp}{2\pi}\\ &= \int (\delta_{is}p_j p_k + \delta_{js}p_i p_k + \delta_{ks}p_i p_j)e^{-|p|^2/2}\frac{dp}{2\pi}\\ &= \delta_{is}\delta_{jk} + \delta_{js}\delta_{ik} + \delta_{ks}\delta_{ij}\,,\end{aligned} \tag{3.104}$$

then eq. (3.103) becomes:

$$\langle p_i p_j\, \mathcal{M}_\epsilon[n]\rangle = n\,\delta_{ij} - \frac{\epsilon^2}{12}n\,\partial_{ij}\log n\,; \tag{3.105}$$

so from eqs. (3.102), (3.105) we find:

$$\begin{aligned}\langle p_i p_j\, g_0[n_+,n_-]\rangle = &\left[n_0 - n_0\epsilon^2\left(\left(1-\frac{\pi}{4}\right)\gamma^2 + \frac{1}{2}\left(\frac{n_\sigma}{\epsilon n_0}\right)^2\right)\right]\delta_{ij} - \frac{\epsilon^2}{12}n_0\,\partial_{ij}\log n_0\\ &+ \frac{\epsilon^2}{2}\int p_i p_j\left[\gamma\left(|p| - \sqrt{\frac{\pi}{2}}\right) - \frac{n_\sigma}{\epsilon n_0}\right]^2\frac{n_0}{2\pi}e^{-|p|^2/2}\,dp + O(\epsilon^3)\,;\end{aligned} \tag{3.106}$$

let us now focus on the last term of (3.106):

$$\begin{aligned}&\int p_i p_j\left[\gamma\left(|p| - \sqrt{\frac{\pi}{2}}\right) - \frac{n_\sigma}{\epsilon n_0}\right]^2\frac{n_0}{2\pi}e^{-|p|^2/2}\,dp\\ &= \delta_{ij}\int\frac{|p|^2}{2}\left[\gamma|p| - \left(\gamma\sqrt{\frac{\pi}{2}} + \frac{n_\sigma}{\epsilon n_0}\right)\right]^2\frac{n_0}{2\pi}e^{-|p|^2/2}\,dp\\ &= \delta_{ij}\int\frac{|p|^2}{2}\left[\gamma^2|p|^2 - 2\gamma|p|\left(\gamma\sqrt{\frac{\pi}{2}} + \frac{n_\sigma}{\epsilon n_0}\right) + \left(\gamma\sqrt{\frac{\pi}{2}} + \frac{n_\sigma}{\epsilon n_0}\right)^2\right]\frac{n_0}{2\pi}e^{-|p|^2/2}\,dp\\ &= \delta_{ij}n_0\left\{\frac{\gamma^2}{2}\int|p|^4 e^{-|p|^2/2}\frac{dp}{2\pi} - \gamma\left(\gamma\sqrt{\frac{\pi}{2}} + \frac{n_\sigma}{\epsilon n_0}\right)\int|p|^3 e^{-|p|^2/2}\frac{dp}{2\pi}\right.\\ &\left.+\left(\gamma\sqrt{\frac{\pi}{2}} + \frac{n_\sigma}{\epsilon n_0}\right)^2\right\}\,;\end{aligned} \tag{3.107}$$

let us now compute:

$$\begin{aligned}\int|p|^3 e^{-|p|^2/2}\frac{dp}{2\pi} &= \int_0^\infty \rho^4 e^{-\rho^2/2}d\rho = 2\int_{\mathbb{R}}\frac{\rho^4}{4}e^{-\rho^2/2}d\rho\\ &= 2\frac{\partial^2}{\partial\beta^2}\left[\int_{\mathbb{R}}e^{-\beta\rho^2/2}d\rho\right]_{|_{\beta=1}} = 2\frac{\partial^2}{\partial\beta^2}\left[\frac{\sqrt{2\pi}}{\sqrt{\beta}}\right]_{|_{\beta=1}} = 3\sqrt{\frac{\pi}{2}}\,;\\ \int|p|^4 e^{-|p|^2/2}\frac{dp}{2\pi} &= 4\frac{\partial^2}{\partial\beta^2}\left[\int e^{-\beta|p|^2/2}\frac{dp}{2\pi}\right]_{|_{\beta=1}} = 4\frac{\partial^2}{\partial\beta^2}\left[\frac{1}{\beta}\right]_{|_{\beta=1}} = 8\,;\end{aligned} \tag{3.108}$$

so from eqs. (3.107), (3.108) it follows:

$$
\begin{aligned}
&\int p_i p_j \left[\gamma\left(|p| - \sqrt{\frac{\pi}{2}}\right) - \frac{n_\sigma}{\epsilon n_0}\right]^2 \frac{n_0}{2\pi} e^{-|p|^2/2}\, dp \\
&= \delta_{ij} n_0 \left\{4\gamma^2 - \frac{3}{2}\pi\gamma^2 - 3\sqrt{\frac{\pi}{2}}\gamma\frac{n_\sigma}{\epsilon n_0} + \frac{\pi}{2}\gamma^2 + 2\sqrt{\frac{\pi}{2}}\gamma\frac{n_\sigma}{\epsilon n_0} + \left(\frac{n_\sigma}{\epsilon n_0}\right)^2\right\} \\
&= \delta_{ij} n_0 \left\{(4-\pi)\gamma^2 - \gamma\sqrt{\frac{\pi}{2}}\frac{n_\sigma}{\epsilon n_0} + \left(\frac{n_\sigma}{\epsilon n_0}\right)^2\right\};
\end{aligned}
\tag{3.109}
$$

so from eqs. (3.106), (3.109) we deduce:

$$
\begin{aligned}
&\langle p_i p_j\, g_0[n_+, n_-]\rangle = n_0\delta_{ij} - n_0\delta_{ij}\epsilon^2\left(\left(1-\frac{\pi}{4}\right)\gamma^2 + \frac{1}{2}\left(\frac{n_\sigma}{\epsilon n_0}\right)^2\right) \\
&\quad - \frac{\epsilon^2}{12} n_0\, \partial_{ij}\log n_0 + \frac{\epsilon^2}{2}\delta_{ij} n_0 \left[(4-\pi)\gamma^2 - \gamma\sqrt{\frac{\pi}{2}}\frac{n_\sigma}{\epsilon n_0} + \left(\frac{n_\sigma}{\epsilon n_0}\right)^2\right] + O(\epsilon^3) \\
&\quad = n_0\delta_{ij} - \frac{\epsilon^2}{12} n_0\, \partial_{ij}\log n_0 + \epsilon\delta_{ij}\left[\left(1-\frac{\pi}{4}\right)\gamma^2\epsilon n_0 - \frac{\gamma}{2}\sqrt{\frac{\pi}{2}} n_\sigma\right] + O(\epsilon^3) \\
&\quad = \delta_{ij}\left[\left(1 + \epsilon^2\gamma^2\left(1-\frac{\pi}{4}\right)\right) n_0 - \frac{\epsilon\gamma}{2}\sqrt{\frac{\pi}{2}} n_\sigma\right] - \frac{\epsilon^2}{12} n_0\, \partial_{ij}\log n_0 + O(\epsilon^2).
\end{aligned}
\tag{3.110}
$$

Let us now consider the term:

$$
\begin{aligned}
&\langle 2\epsilon\gamma p_i g_j[n_+, n_-]\rangle \\
&= 2\gamma\epsilon^2 \int \frac{n_0}{2\pi} e^{-|p|^2/2}\left[\gamma\left(\sqrt{\frac{\pi}{2}} - |p|\right) + \frac{n_\sigma}{\epsilon n_0}\right]\frac{p_i p_j}{|p|}\, dp + O(\epsilon^3) \\
&= \gamma\epsilon^2\delta_{ij} \int \frac{n_0}{2\pi} e^{-|p|^2/2}\left[\gamma\left(\sqrt{\frac{\pi}{2}} - |p|\right) + \frac{n_\sigma}{\epsilon n_0}\right] |p|\, dp + O(\epsilon^3) \\
&= \gamma\epsilon^2\delta_{ij} n_0 \left[\left(\gamma\sqrt{\frac{\pi}{2}} + \frac{n_\sigma}{\epsilon n_0}\right)\sqrt{\frac{\pi}{2}} - 2\gamma\right] + O(\epsilon^3) \\
&= \delta_{ij}\left[-2\epsilon^2\gamma^2\left(1-\frac{\pi}{4}\right) n_0 + \epsilon\gamma\sqrt{\frac{\pi}{2}} n_\sigma\right] + O(\epsilon^3).
\end{aligned}
\tag{3.111}
$$

Putting eqs. (3.110), (3.111) together we find:

$$
\begin{aligned}
&\langle p_i p_j g_0[n_+, n_-] + 2\gamma\epsilon p_i g_j[n_+, n_-]\rangle \\
&= \delta_{ij}\left[\left(1 - \epsilon^2\gamma^2\left(1-\frac{\pi}{4}\right)\right) n_0 + \frac{\epsilon\gamma}{2}\sqrt{\frac{\pi}{2}} n_\sigma\right] - \frac{\epsilon^2}{12} n_0\, \partial_{ij}\log n_0 + O(\epsilon^2).
\end{aligned}
\tag{3.112}
$$

The last term to be computed in the equation for n_0 is:

$$
\langle \vec{g}[n_+, n_-] \wedge \vec{p}\rangle = 0 + O(\epsilon^3), \tag{3.113}
$$

since $\vec{g}[n_+, n_-]$ is parallel to $\vec{p}$ at this order.
Now we consider the terms in the equation for n_σ. Let us begin with:

$$\begin{aligned}
&\left\langle \frac{p_i p_j}{|p|} \left(\vec{g}[n_+, n_-] \cdot \vec{p} + 2\gamma\epsilon g_0[n_+, n_-]\right) \right\rangle \\
&= \int \frac{p_i p_j}{|p|} \left(\epsilon \frac{n_0}{2\pi} e^{-|p|^2/2} \left[\gamma \left(\sqrt{\frac{\pi}{2}} - |p| \right) + \frac{n_\sigma}{\epsilon n_0} \right] |p| + 2\gamma\epsilon \frac{n_0}{2\pi} e^{-|p|^2/2} \right) dp + O(\epsilon^3) \\
&= \epsilon n_0 \frac{\delta_{ij}}{2} \int |p| \left[2\gamma + \left(\gamma \sqrt{\frac{\pi}{2}} + \frac{n_\sigma}{\epsilon n_0} \right) |p| - \gamma |p|^2 \right] e^{-|p|^2/2} \frac{dp}{2\pi} + O(\epsilon^3) \\
&= \epsilon n_0 \frac{\delta_{ij}}{2} \left[2\gamma \sqrt{\frac{\pi}{2}} + 2 \left(\gamma \sqrt{\frac{\pi}{2}} + \frac{n_\sigma}{\epsilon n_0} \right) - 3\gamma \sqrt{\frac{\pi}{2}} \right] + O(\epsilon^3) \\
&= \delta_{ij} \left[\frac{\epsilon\gamma}{2} \sqrt{\frac{\pi}{2}} n_0 + n_\sigma \right] + O(\epsilon^3)\,.
\end{aligned} \tag{3.114}$$

Let us now compute the terms depending on the potential.

$$\begin{aligned}
&\left\langle \frac{p_i p_j}{|p|} \Theta_\epsilon g_j[n_+, n_-] \right\rangle = - \int \frac{p_i p_j}{|p|} \partial_k V \partial_{p_k} g_j[n_+, n_-]\, dp \\
&= \partial_k V \int \partial_{p_k} \left(\frac{p_i p_j}{|p|} \right) \left\{ \epsilon \frac{n_0}{2\pi} e^{-|p|^2/2} \left[\gamma \left(\sqrt{\frac{\pi}{2}} - |p| \right) + \frac{n_\sigma}{\epsilon n_0} \right] \frac{p_j}{|p|} \right\} dp + O(\epsilon^3) \\
&= \epsilon n_0 \partial_k V \int \left[\delta_{ik} \frac{p_j}{|p|} + p_i \partial_{p_k} \left(\frac{p_j}{|p|} \right) \right] \frac{p_j}{|p|} \left[\gamma \left(\sqrt{\frac{\pi}{2}} - |p| \right) + \frac{n_\sigma}{\epsilon n_0} \right] e^{-|p|^2/2} \frac{dp}{2\pi} + O(\epsilon^3) \\
&= \epsilon n_0 \partial_i V \int \left[\gamma \left(\sqrt{\frac{\pi}{2}} - |p| \right) + \frac{n_\sigma}{\epsilon n_0} \right] e^{-|p|^2/2} \frac{dp}{2\pi} + O(\epsilon^3) = n_\sigma \partial_i V + O(\epsilon^3)\,;
\end{aligned} \tag{3.115}$$

$$\begin{aligned}
&\epsilon\gamma \left\langle \frac{p_i}{|p|} \Theta_\epsilon g_0[n_+, n_-] \right\rangle = \epsilon\gamma \partial_k V \int \partial_{p_k} \left(\frac{p_i}{|p|} \right) \frac{n_0}{2\pi} e^{-|p|^2/2}\, dp + O(\epsilon^3) \\
&= \epsilon\gamma n_0 \partial_k V \int \frac{1}{|p|} \left(\delta_{ik} - \frac{p_i p_k}{|p|^2} \right) e^{-|p|^2/2} \frac{dp}{2\pi} + O(\epsilon^3) \\
&= \epsilon\gamma n_0 \partial_i V \int \frac{e^{-|p|^2/2}}{2|p|} \frac{dp}{2\pi} + O(\epsilon^3) = \frac{\epsilon\gamma}{2} \sqrt{\frac{\pi}{2}} n_0 \partial_i V + O(\epsilon^3)\,;
\end{aligned} \tag{3.116}$$

$$\begin{aligned}
&\left\langle \frac{\vec{p}}{|p|} \cdot \Theta_\epsilon \left[\frac{\vec{p} \cdot \vec{\nabla}}{2\gamma} \vec{g}[n_+, n_-] + \vec{g}[n_+, n_-] \wedge \vec{p} \right] \right\rangle \\
&= \partial_j V \left\{ \frac{\partial_k}{2\gamma} \int \partial_{p_j} \left(\frac{p_i}{|p|} \right) p_k g_i[n_+, n_-]\, dp + \int \partial_{p_j} \left(\frac{p_i}{|p|} \right) \eta_{iks} g_k[n_+, n_-] p_s\, dp \right\} \\
&= 0 + O(\epsilon^3)\,,
\end{aligned} \tag{3.117}$$

because $\vec{g}[n_+, n_-]$ is parallel to $\vec{p}$ at this order;

$$\begin{aligned}
&\frac{\epsilon}{2}\left\langle \frac{\vec{p}}{|p|}\cdot \Theta_\epsilon \vec{\nabla} g_0[n_+, n_-]\right\rangle = \frac{\epsilon}{2}\partial_j V \partial_i \int \partial_{p_j}\left(\frac{p_i}{|p|}\right)\frac{n_0}{2\pi}e^{-|p|^2/2}\,dp + O(\epsilon^3)\\
&= \frac{\epsilon}{2}\partial_i n_0\,\partial_j V\int \frac{1}{|p|}\left(\delta_{ij}-\frac{p_ip_j}{|p|^2}\right)e^{-|p|^2/2}\frac{dp}{2\pi} + O(\epsilon^3)\\
&= \frac{\epsilon}{2}\vec{\nabla} n_0\cdot\vec{\nabla} V\int \frac{e^{-|p|^2/2}}{2|p|}\frac{dp}{2\pi} + O(\epsilon^3) = \frac{\epsilon}{4}\sqrt{\frac{\pi}{2}}\,\vec{\nabla} n_0\cdot\vec{\nabla} V + O(\epsilon^3)\,;
\end{aligned} \tag{3.118}$$

$$\begin{aligned}
&\left\langle \frac{\vec{p}}{|p|}\cdot\Theta_\epsilon\Theta_\epsilon\vec{g}[n_+, n_-]\right\rangle\\
&= -\partial_i V\,\partial_j V\left\langle \partial_{p_i}\left(\frac{p_k}{|p|}\right)\partial_{p_j}\left\{\epsilon\frac{n_0}{2\pi}e^{-|p|^2/2}\left[\gamma\left(\sqrt{\frac{\pi}{2}}-|p|\right)+\frac{n_\sigma}{\epsilon n_0}\right]\frac{p_k}{|p|}\right\}\right\rangle + O(\epsilon^3)\\
&= -\partial_i V\,\partial_j V\left\langle \partial_{p_i}\left(\frac{p_k}{|p|}\right)\partial_{p_j}\left(\frac{p_k}{|p|}\right)\epsilon\frac{n_0}{2\pi}e^{-|p|^2/2}\left[\gamma\left(\sqrt{\frac{\pi}{2}}-|p|\right)+\frac{n_\sigma}{\epsilon n_0}\right]\right\rangle + O(\epsilon^3)\\
&= -\partial_i V\,\partial_j V\left\langle \frac{1}{|p|^2}\left(\delta_{ij}-\frac{p_ip_j}{|p|^2}\right)\epsilon\frac{n_0}{2\pi}e^{-|p|^2/2}\left[\gamma\sqrt{\frac{\pi}{2}}+\frac{n_\sigma}{\epsilon n_0}-\gamma|p|\right]\right\rangle + O(\epsilon^3)\\
&= -\epsilon n_0|\nabla V|^2\left\langle \frac{e^{-|p|^2/2}}{4\pi|p|^2}\left[\gamma\sqrt{\frac{\pi}{2}}+\frac{n_\sigma}{\epsilon n_0}-\gamma|p|\right]\right\rangle + O(\epsilon^3)\\
&= |\nabla V|^2\left\{\epsilon\gamma n_0\int\frac{e^{-|p|^2/2}}{4\pi|p|}dp - \left[\epsilon\gamma\sqrt{\frac{\pi}{2}}\,n_0+n_\sigma\right]\left\langle\frac{e^{-|p|^2/2}}{4\pi|p|^2}\right\rangle\right\} + O(\epsilon^3)\\
&= \frac{|\nabla V|^2}{2}\left\{\epsilon\gamma\sqrt{\frac{\pi}{2}}\,n_0 + \left[\epsilon\gamma\sqrt{\frac{\pi}{2}}\,n_0+n_\sigma\right]\Gamma\right\} + O(\epsilon^3)\,,
\end{aligned} \tag{3.119}$$

according to (3.88).
Let us collect eqs. (3.64), (3.112) – (3.119):

$$\begin{aligned}
\partial_t n_0 =& \frac{\Delta}{4\gamma^2}\left[\left(1-\epsilon^2\gamma^2\left(1-\frac{\pi}{4}\right)\right)n_0 + \frac{\epsilon\gamma}{2}\sqrt{\frac{\pi}{2}}n_\sigma\right] - \frac{\partial^2_{ij}}{4\gamma^2}\left(\frac{\epsilon^2}{12}n_0\,\partial^2_{ij}\log n_0\right)\\
&+\frac{1}{2\gamma}\vec{\nabla}\cdot\left(n_0\vec{\nabla} V\right)+\frac{\epsilon^2}{4}\Delta n_0\,,\\
\partial_t n_\sigma =& \frac{\Delta}{4\gamma^2}\left[\frac{\epsilon\gamma}{2}\sqrt{\frac{\pi}{2}}n_0+n_\sigma\right] + \frac{\vec{\nabla}}{2\gamma}\cdot\left\{n_\sigma\vec{\nabla} V+\frac{\epsilon\gamma}{2}\sqrt{\frac{\pi}{2}}\,n_0\vec{\nabla} V\right\}\\
&+\frac{\epsilon}{4}\sqrt{\frac{\pi}{2}}\,\vec{\nabla} n_0\cdot\vec{\nabla} V + \frac{|\nabla V|^2}{2}\left\{\epsilon\gamma\sqrt{\frac{\pi}{2}}\,n_0+\Gamma\left[\epsilon\gamma\sqrt{\frac{\pi}{2}}\,n_0+n_\sigma\right]\right\}\,;
\end{aligned} \tag{3.120}$$

we notice that:

$$-\frac{\partial^2_{ij}}{4\gamma^2}\left(\frac{\epsilon^2}{12}n_0\,\partial^2_{ij}\log n_0\right) = \frac{1}{2\gamma}\vec{\nabla}\cdot\left(n_0\vec{\nabla} V_B\right)\,, \tag{3.121}$$

where V_B is (up to a constant) the so-called *Bohm potential* (see e.g. [29]):

$$V_B = -\frac{1}{2\gamma}\frac{\epsilon^2}{6}\frac{\Delta\sqrt{n_0}}{\sqrt{n_0}}\,; \tag{3.122}$$

so we have finally proven the following:

Proposition 10 *Under the assumption* (3.90)*, eqs.* (3.50) *are equivalent, up to* $O(\epsilon^3)$*, to the* second order two-band drift-diffusion model*:*

$$\begin{aligned} \partial_t n_0 =& \frac{\Delta}{4\gamma^2}\left[\left(1+\epsilon^2\gamma^2\frac{\pi}{4}\right)n_0 + \frac{\epsilon\gamma}{2}\sqrt{\frac{\pi}{2}}n_\sigma\right] + \frac{\vec{\nabla}}{2\gamma}\cdot\left(n_0\vec{\nabla}(V+V_B)\right)\,, \\ \partial_t n_\sigma =& \frac{\Delta}{4\gamma^2}\left[\frac{\epsilon\gamma}{2}\sqrt{\frac{\pi}{2}}n_0 + n_\sigma\right] + \frac{\vec{\nabla}}{2\gamma}\cdot\left[\left(n_\sigma + \frac{\epsilon\gamma}{2}\sqrt{\frac{\pi}{2}}\,n_0\right)\vec{\nabla}V\right] \\ &+ \frac{\epsilon}{4}\sqrt{\frac{\pi}{2}}\,\vec{\nabla}n_0\cdot\vec{\nabla}V + \frac{|\nabla V|^2}{2}\left\{\epsilon\gamma\sqrt{\frac{\pi}{2}}\,(1+\Gamma)n_0 + \Gamma n_\sigma\right\}\,, \end{aligned} \tag{3.123}$$

with V_B *given by* (3.122) *and* Γ *defined in* (3.88)*.*

We notice that it would be possible to derive a second-order two-band hydrodynamic model based upon the Low Scaled Fermi Speed and Strongly Mixed State hypothesis:

$$c = O(\epsilon)\,, \quad \frac{|n_+ - n_-|}{n_+ + n_-} = O(\epsilon)\,, \quad \frac{|\vec{J}_+ - \vec{J}_-|}{n_+ + n_-} = O(\epsilon) \qquad \text{as } \epsilon \to 0\,, \tag{3.124}$$

with the moments $n_\pm$, $\vec{J}_\pm$ defined by eq. (3.3), in analogy with the second-order two-band diffusive model (3.123), (3.122); however, such an attempt would be computationally very difficult and cumbersome, therefore the afore mentioned hydrodynamic model will not be derived in this Thesis.

Chapter 4

Spinorial models

4.1 A first order spinorial hydrodynamic model

In this section we will derive a hydrodynamic model for quantum electron transport in graphene following a strategy similar to that one employed in the construction of the diffusive model (3.89).
The moments we choose are the following six:

$$n_s = \int w_s \, dp \qquad s = 0, 1, 2, 3 \,,$$
$$J_k = \int p_k w_0 \, dp \qquad k = 1, 2 \,.$$

n_0 is the *charge density*, $\vec{n} = (n_1, n_2, n_3)$ is the *spin vector*, $\vec{J} = (J_1, J_2, 0)$ is the *flow vector*. Note that the flow vector has only two components because graphene is a two-dimensional object.
According to the theory exposed in Chapter 2, the equilibrium distribution has the following form:

$$g[n_0, \vec{n}, \vec{J}] = \mathcal{E}\mathrm{xp}(-h_\xi) \,, \quad h_\xi = \left(\frac{|p|^2}{2} + p_k \Xi_k + \xi_0 \right) \sigma_0 + (\xi_s + c p_s) \sigma_s \,, \quad (4.1)$$

with $\xi_0(x)$, $(\xi_s(x))_{s=1,2,3}$, $(\Xi_k(x))_{k=1,2}$ Lagrange multipliers to be determined in such a way that:

$$\langle g_0[n_0, \vec{n}, \vec{J}] \rangle (x) = n_0(x) \,, \ \langle \vec{g}[n_0, \vec{n}, \vec{J}] \rangle (x) = \vec{n}(x) \,, \ \langle \vec{p} g_0[n_0, \vec{n}, \vec{J}] \rangle (x) = \vec{J}(x) \,, \quad (4.2)$$

for $x \in \mathbb{R}^2$.

4.1.1 Formal closure of fluid equations

The following formal theorem holds:

Theorem 2 *Let n_0^τ, $\vec{n}^\tau$, $\vec{J}^\tau$ the moments of a solution w^τ of Eqs. (1.45). If $n_0^\tau \to n_0$, $\vec{n}^\tau \to \vec{n}$, $\vec{J}^\tau \to \vec{J}$ as $\tau \to 0$, then the limit moments n_0, $\vec{n}$, $\vec{J}$ satisfy:*

$$\begin{aligned} \partial_t n_0 + \frac{\vec{\nabla}}{2\gamma} \cdot \vec{J} + \frac{\epsilon}{2} \vec{\nabla} \cdot \vec{n} &= 0 \\ \partial_t \vec{n} + \frac{\vec{\nabla}}{2\gamma} \cdot \langle \vec{g} \otimes \vec{p} \rangle + \frac{\epsilon}{2} \vec{\nabla} n_0 + \langle \vec{g} \wedge \vec{p} \rangle &= 0 \\ \partial_t \vec{J} + \frac{\vec{\nabla}}{2\gamma} \cdot \left(\frac{\vec{J} \otimes \vec{J}}{n_0} + \mathscr{P} \right) + \frac{\epsilon}{2} \vec{\nabla} \cdot \langle \vec{p} \otimes \vec{g} \rangle + n_0 \vec{\nabla} V &= 0 \end{aligned} \tag{4.3}$$

where:

$$\mathscr{P} = \left\langle (\vec{p} - \vec{J}/n_0) \otimes (\vec{p} - \vec{J}/n_0) g_0 \right\rangle \tag{4.4}$$

is the so-called quantum stress tensor.

The proof of Theorem 2 is analogue to the proof of Theorem 4.2 in [29]: one must consider (1.45) as Wigner equations and use the weight functions $k(p) = \{1, \vec{p}\}$ for the first equation in (1.45) and $k(p) = 1$ for the second equation.

Eqs. (4.3) are a closed system of hydrodynamic equations, indeed $g[n_0, \vec{n}, \vec{J}]$ is a function of the moments n_0, $\vec{n}$, $\vec{J}$ only; however, the system (4.3) is a very implicit model; in the next subsection we will derive an approximated but more explicit version of (4.3) by exploiting the hypothesis we have done (the semiclassical and Low Scaled Fermi Speed (1.37)).

4.1.2 Semiclassical expansion of the equilibrium distribution

It is possible to write the first-order approximation of $g[n_0, \vec{n}, \vec{J}]$ given by (4.1) by following a strategy similar to that one employed to compute the approximation of the equilibrium distribution for the first diffusive model. More precisely, we consider (2.21), (2.29), (2.30) with:

$$-a = \left(\frac{|p|^2}{2} + p_k \Xi_k + \xi_0 \right) \sigma_0 + \xi_s \sigma_s \,, \qquad -b = \gamma \vec{p} \cdot \vec{\sigma} \,;$$

then we impose the constraints (4.2). We recall the definition (2.13) of the Poisson brackets. Since $\vec{a}$ does not depend from p then $\{a_j \,,\, a_k\} = 0$ for $j, k = 1, 2, 3$; so eqs. (2.21), (2.29), (2.30) becomes:

$$\begin{aligned} g_0^{(0)}[n_0, \vec{n}, \vec{J}] &= e^{-(|p|^2/2 + \vec{p}\cdot\vec{\Xi} + \xi_0)} \cosh |\vec{\xi}| \,, \\ \vec{g}^{(0)}[n_0, \vec{n}, \vec{J}] &= -\, e^{-(|p|^2/2 + \vec{p}\cdot\vec{\Xi} + \xi_0)} \frac{\sinh |\vec{\xi}|}{|\vec{\xi}|} \vec{\xi} \,, \end{aligned} \tag{4.5}$$

$$\begin{aligned}
g_0^{(1)}[n_0,\vec{n},\vec{J}] =&\gamma e^{-(|p|^2/2+\vec{p}\cdot\vec{\Xi}+\xi_0)}\frac{\sinh|\vec{\xi}|}{|\vec{\xi}|}\vec{\xi}\cdot\vec{p},\\
\vec{g}^{(1)}[n_0,\vec{n},\vec{J}] =&-\gamma e^{-(|p|^2/2+\vec{p}\cdot\vec{\Xi}+\xi_0)}\cosh|\vec{\xi}|\frac{\vec{\xi}\otimes\vec{\xi}}{|\vec{\xi}|^2}\vec{p}\\
&-\gamma e^{-(|p|^2/2+\vec{p}\cdot\vec{\Xi}+\xi_0)}\frac{\sinh|\vec{\xi}|}{|\vec{\xi}|}\left(\frac{\vec{\xi}\wedge\vec{p}}{|\vec{\xi}|}\right)\wedge\frac{\vec{\xi}}{|\vec{\xi}|}\\
&-e^{-(|p|^2/2+\vec{p}\cdot\vec{\Xi}+\xi_0)}\frac{|\vec{\xi}|\cosh|\vec{\xi}|-\sinh|\vec{\xi}|}{2|\vec{\xi}|^3}\left\{\left(\frac{|p|^2}{2}+p_k\Xi_k+\xi_0\right),\vec{\xi}\right\}\wedge\vec{\xi};
\end{aligned} \tag{4.6}$$

moreover, clearly:

$$\begin{aligned}
\left[\left\{\left(\frac{|p|^2}{2}+p_k\Xi_k+\xi_0\right),\vec{\xi}\right\}\wedge\vec{\xi}\right]_i =&\eta_{ijk}\,\partial_{p_s}\left(\frac{|p|^2}{2}+p_l\Xi_l+\xi_0\right)\cdot\partial_{x_s}\xi_j\cdot\xi_k\\
=&\eta_{ijk}\,(p_s+\Xi_s)\cdot\partial_{x_s}\xi_j\cdot\xi_k\\
=&\left[((\vec{p}+\vec{\Xi})\cdot\vec{\nabla})\vec{\xi}\wedge\vec{\xi}\right]_i \qquad (i=1,2,3),
\end{aligned} \tag{4.7}$$

$$\left(\frac{\vec{\xi}\wedge\vec{p}}{|\vec{\xi}|}\right)\wedge\frac{\vec{\xi}}{|\vec{\xi}|}=\left(I-\frac{\vec{\xi}\otimes\vec{\xi}}{|\vec{\xi}|^2}\right)\vec{p}, \tag{4.8}$$

so we obtain:

$$\begin{aligned}
g_0^{(0)}[n_0,\vec{n},\vec{J}] =&Ke^{-|p+\Xi|^2/2}\cosh|\vec{\xi}|,\\
\vec{g}^{(0)}[n_0,\vec{n},\vec{J}] =&-Ke^{-|p+\Xi|^2/2}\frac{\sinh|\vec{\xi}|}{|\vec{\xi}|}\vec{\xi},\\
g_0^{(1)}[n_0,\vec{n},\vec{J}] =&\gamma Ke^{-|p+\Xi|^2/2}\frac{\sinh|\vec{\xi}|}{|\vec{\xi}|}\vec{\xi}\cdot\vec{p},\\
\vec{g}^{(1)}[n_0,\vec{n},\vec{J}] =&-\gamma Ke^{-|p+\Xi|^2/2}\left(\mathscr{A}[\vec{\xi}](\vec{p}+\vec{\Xi})-\mathscr{B}[\vec{\xi}]\vec{\Xi}\right),
\end{aligned} \tag{4.9}$$

where:

$$\begin{aligned}
K \equiv& \exp([(\Xi_1)^2+(\Xi_2)^2]/2-\xi_0),\\
\mathscr{A}_{ij}[\vec{\xi}] \equiv& \cosh|\vec{\xi}|\frac{\xi_i\xi_j}{|\xi|^2}+\frac{\sinh|\vec{\xi}|}{|\vec{\xi}|}\left(\delta_{ij}-\frac{\xi_i\xi_j}{|\xi|^2}\right)\\
&+\frac{|\vec{\xi}|\cosh|\vec{\xi}|-\sinh|\vec{\xi}|}{2\gamma|\vec{\xi}|^3}\eta_{iks}\partial_j\xi_k\cdot\xi_s,\\
\mathscr{B}_{ij}[\vec{\xi}] \equiv& \cosh|\vec{\xi}|\frac{\xi_i\xi_j}{|\xi|^2}+\frac{\sinh|\vec{\xi}|}{|\vec{\xi}|}\left(\delta_{ij}-\frac{\xi_i\xi_j}{|\xi|^2}\right).
\end{aligned} \tag{4.10}$$

Now we exploit eqs. (4.2), (4.9) to find an explicit semiclassical expansion of the Lagrange multipliers ξ_0, $\vec{\xi}$, $\vec{\Xi}$ depending on the moments n_0, $\vec{n}$, $\vec{J}$:

$$\begin{aligned}
n_0 =& \int\left[Ke^{-|p+\Xi|^2/2}\cosh|\vec{\xi}|+\epsilon\gamma Ke^{-|p+\Xi|^2/2}\frac{\sinh|\vec{\xi}|}{|\vec{\xi}|}\vec{\xi}\cdot\vec{p}\right]dp+O(\epsilon^2)\\
=&2\pi K\cosh|\vec{\xi}|-2\pi\epsilon\gamma K\frac{\sinh|\vec{\xi}|}{|\vec{\xi}|}\vec{\xi}\cdot\vec{\Xi}+O(\epsilon^2);
\end{aligned} \tag{4.11}$$

$$\vec{n} = \int \left[-Ke^{-|p+\Xi|^2/2} \frac{\sinh|\vec{\xi}|}{|\vec{\xi}|}\vec{\xi} - \epsilon\gamma K e^{-|p+\Xi|^2/2} \left(\mathscr{A}(\vec{p}+\vec{\Xi}) - \mathscr{B}\vec{\Xi} \right) \right] dp + O(\epsilon^2)$$
$$= -\,2\pi K \frac{\sinh|\vec{\xi}|}{|\vec{\xi}|}\vec{\xi} + 2\pi\epsilon\gamma K \mathscr{B}[\vec{\xi}]\vec{\Xi} + O(\epsilon^2)\,; \tag{4.12}$$

$$\vec{J} = \int \vec{p} \left[Ke^{-|p+\Xi|^2/2} \cosh|\vec{\xi}| + \epsilon\gamma K e^{-|p+\Xi|^2/2} \frac{\sinh|\vec{\xi}|}{|\vec{\xi}|} \vec{\xi}\cdot\vec{p} \right] dp + O(\epsilon^2)$$
$$= -\,2\pi K \cosh|\vec{\xi}|\,\vec{\Xi} + 2\pi\epsilon\gamma K \frac{\sinh|\vec{\xi}|}{|\vec{\xi}|} \left(I + \vec{\Xi}\otimes\vec{\Xi} \right) \vec{\xi} + O(\epsilon^2)\,; \tag{4.13}$$

to solve eqs. (4.11)–(4.13) we first consider them at leading order:

$$\begin{aligned} n_0 =& 2\pi K \cosh|\vec{\xi}| + O(\epsilon)\,, \\ \vec{n} =& -\,2\pi K \frac{\sinh|\vec{\xi}|}{|\vec{\xi}|}\vec{\xi} + O(\epsilon)\,, \\ \vec{J} =& -\,2\pi K \cosh|\vec{\xi}|\,\vec{\Xi} + O(\epsilon)\,; \end{aligned} \tag{4.14}$$

if we define:

$$\vec{u} \equiv \frac{\vec{J}}{n_0} = \left(\frac{J_1}{n_0}, \frac{J_2}{n_0}, 0 \right)\,, \qquad \vec{s} \equiv \frac{\vec{n}}{n_0}\,, \tag{4.15}$$

it follows:

$$-\vec{\Xi} = \vec{u} + O(\epsilon)\,, \quad |\vec{s}| = \tanh|\vec{\xi}| + O(\epsilon)\,, \quad \frac{\vec{s}}{|\vec{s}|} = -\frac{\vec{\xi}}{|\vec{\xi}|} + O(\epsilon)\,, \tag{4.16}$$

and so:

$$\vec{\Xi} = -\vec{u} + O(\epsilon)\,, \qquad \vec{\xi} = -\frac{\vec{s}}{|\vec{s}|} \log\sqrt{\frac{1+|\vec{s}|}{1-|\vec{s}|}} + O(\epsilon)\,; \tag{4.17}$$

again from eq. (4.14) we find:

$$K = \frac{1}{2\pi}\sqrt{n_0^2 - |\vec{n}|^2} + O(\epsilon) = \frac{n_0}{2\pi}\sqrt{1-|\vec{s}|^2} + O(\epsilon)\,. \tag{4.18}$$

Let us observe the following fact. From eqs. (4.9), (4.17), (4.18) we easily conclude that:

$$g_0[n_0,\vec{n},\vec{J}] = \frac{n_0}{2\pi} e^{-|\vec{p}-\vec{u}|^2/2} \left(\alpha_0^\epsilon(x) + p_1\alpha_1^\epsilon(x) + p_2\alpha_2^\epsilon(x) \right) + O(\epsilon^2)\,, \tag{4.19}$$

for some scalar ($\epsilon-$dependent) fuctions $\alpha_j^\epsilon(x)$, $j = 0,1,2$; but eq. (4.2) provides, for a generic fixed $x \in \mathbb{R}^2$, three scalar constraints for $g_0[n_0,\vec{n},\vec{J}]$, which translate into a linear 3×3 system for the vector $(\alpha_0^\epsilon(x), \alpha_1^\epsilon(x), \alpha_2^\epsilon(x))$ with matrix:

$$\mathscr{M} = \begin{pmatrix} 1 & u_1 & u_2 \\ u_1 & 1+u_1^2 & u_1u_2 \\ u_2 & u_1u_2 & 1+u_2^2 \end{pmatrix}\;;$$

since $\det \mathscr{M} = 1$, then for the uniqueness of the solution of a linear system with nonsingular matrix we deduce that:

$$g_0[n_0, \vec{n}, \vec{J}] = \frac{n_0}{2\pi} e^{-|\vec{p}-\vec{u}|^2/2} + O(\epsilon^2)\,. \tag{4.20}$$

In a similar way, from eqs. (4.9), (4.17), (4.18) we deduce:

$$\vec{g}[n_0, \vec{n}, \vec{J}] = \frac{n_0}{2\pi} e^{-|\vec{p}-\vec{u}|^2/2} \left[\vec{\mu}(x) + \mathcal{M}^\epsilon(x)(\vec{p}-\vec{u})\right] + O(\epsilon^2)\,, \tag{4.21}$$

for a suitable vector-valued function $\vec{\mu}(x)$ and a suitable 3×3 matrix-valued function $\mathcal{M}(x)$; but since eqs. (4.2) must hold then $\vec{\mu} \equiv \vec{s}$:

$$\vec{g}[n_0, \vec{n}, \vec{J}] = \frac{n_0}{2\pi} e^{-|\vec{p}-\vec{u}|^2/2} \left[\vec{s} + \mathcal{M}^\epsilon(x)(\vec{p}-\vec{u})\right] + O(\epsilon^2)\,; \tag{4.22}$$

moreover from eqs. (4.9), (4.14) it follows immediately that $\mathcal{M}^\epsilon = O(\epsilon)$; so we can define $\mathcal{M}^\epsilon = -\epsilon\gamma\mathcal{Z}$ with $\mathcal{Z}$ independent from ϵ:

$$\vec{g}[n_0, \vec{n}, \vec{J}] = \frac{n_0}{2\pi} e^{-|\vec{p}-\vec{u}|^2/2} \left[\vec{s} - \epsilon\gamma\mathcal{Z}(\vec{p}-\vec{u})\right] + O(\epsilon^2)\,. \tag{4.23}$$

From a comparison between eqs. (4.9) and (4.23) we easily deduce:

$$\mathcal{Z}(\vec{p}-\vec{u}) = \frac{2\pi}{n_0} K^{(0)} \mathscr{A}[\vec{\xi}^{(0)}](\vec{p}-\vec{u})\,, \tag{4.24}$$

with $K^{(0)}$ and $\vec{\xi}^{(0)}$ the leading order terms in the expansion of K and $\vec{\xi}$, respectively; so from eqs. (4.14), (4.17) and (4.24) we conclude:

$$\begin{aligned}
\mathcal{Z}_{ij} &= \frac{2\pi}{n_0} K^{(0)} \mathscr{A}_{ij}[\vec{\xi}^{(0)}] \\
&= \frac{2\pi}{n_0} K^{(0)} \left\{ \cosh|\vec{\xi}^{(0)}| \frac{n_i n_j}{|\vec{n}|^2} + \frac{\sinh|\vec{\xi}^{(0)}|}{|\vec{\xi}^{(0)}|}\left(\delta_{ij} - \frac{n_i n_j}{|\vec{n}|^2}\right) \right. \\
&\quad \left. + \frac{|\vec{\xi}^{(0)}|\cosh|\vec{\xi}^{(0)}| - \sinh|\vec{\xi}^{(0)}|}{2\gamma|\vec{\xi}^{(0)}|^3} \eta_{iks}\partial_j \xi_k^{(0)} \cdot \xi_s^{(0)} \right\} + O(\epsilon^2) \\
&= \frac{1}{n_0} \left\{ n_0 \frac{n_i n_j}{|\vec{n}|^2} + \frac{|\vec{n}|}{\log\sqrt{\frac{n_0+|\vec{n}|}{n_0-|\vec{n}|}}} \left(\delta_{ij} - \frac{n_i n_j}{|\vec{n}|^2}\right) \right. \\
&\quad \left. + \frac{1}{2\gamma}\left[n_0 - \frac{|\vec{n}|}{\log\sqrt{\frac{n_0+|\vec{n}|}{n_0-|\vec{n}|}}} \right] \eta_{iks}\partial_j s_k \cdot s_s \right\} + O(\epsilon^2)\,;
\end{aligned} \tag{4.25}$$

finally, by collecting eqs. (4.20), (4.23), (4.24) we find the first-order semiclassical expansion of the equilibrium distribution that we were seeking:

$$\begin{aligned}
g_0[n_0, \vec{n}, \vec{J}] &= \frac{n_0}{2\pi} e^{-|\vec{p}-\vec{u}|^2/2} + O(\epsilon^2)\,, \\
\vec{g}[n_0, \vec{n}, \vec{J}] &= \frac{n_0}{2\pi} e^{-|\vec{p}-\vec{u}|^2/2} \left(\frac{\vec{n}}{n_0} - \epsilon\gamma\mathcal{Z}(\vec{p}-\vec{u})\right) + O(\epsilon^2)\,,
\end{aligned} \tag{4.26}$$

$$\begin{aligned}
\mathcal{Z}_{ij} &\equiv \frac{n_i n_j}{|\vec{n}|^2} + \omega\left(\delta_{ij} - \frac{n_i n_j}{|\vec{n}|^2}\right) + \frac{1-\omega}{2\gamma} \eta_{iks} \frac{n_k}{|\vec{n}|} \partial_j \left(\frac{n_s}{|\vec{n}|}\right)\,, \\
\omega &\equiv \frac{|\vec{n}|/n_0}{\log\sqrt{\frac{n_0+|\vec{n}|}{n_0-|\vec{n}|}}}\,.
\end{aligned} \tag{4.27}$$

4.1.3 Computation of the moments

Now we will exploit eq. (4.26) in order to compute a first-order expansion of the implicit terms in eq. (4.3).
Let us begin with the quantum stress tensor, which coincides, at this semiclassical order, with the classical stress tensor:

$$\begin{aligned}\mathscr{P} &= \left\langle (\vec{p}-\vec{u})\otimes(\vec{p}-\vec{u})g_0[n_0,\vec{n},\vec{J}]\right\rangle \\ &= \int (\vec{p}-\vec{u})\otimes(\vec{p}-\vec{u})\frac{n_0}{2\pi}e^{-|\vec{p}-\vec{u}|^2/2}\,dp + O(\epsilon^2) = n_0\, I + O(\epsilon^2)\,;\end{aligned} \tag{4.28}$$

now let us consider the terms depending on $\vec{g}[n_0,\vec{n},\vec{J}]$:

$$\begin{aligned}&\left\langle \vec{p}\otimes\vec{g}[n_0,\vec{n},\vec{J}]\right\rangle = \int \vec{p}\otimes\frac{n_0}{2\pi}e^{-|\vec{p}-\vec{u}|^2/2}\left(\frac{\vec{n}}{n_0}-\epsilon\gamma\mathcal{Z}(\vec{p}-\vec{u})\right)dp + O(\epsilon^2)\\ &= \vec{u}\otimes\vec{n} - \epsilon\gamma n_0\int \vec{p}\otimes[\mathcal{Z}(\vec{p}-\vec{u})]\,e^{-|\vec{p}-\vec{u}|^2/2}\frac{dp}{2\pi} + O(\epsilon^2)\\ &= \vec{u}\otimes\vec{n} - \epsilon\gamma n_0\int \vec{p}\otimes[\mathcal{Z}\vec{p}]\,e^{-|\vec{p}|^2/2}\frac{dp}{2\pi} + O(\epsilon^2)\,;\end{aligned} \tag{4.29}$$

but it holds:

$$\int p_i\mathcal{Z}_{jk}p_k e^{-|\vec{p}|^2/2}\frac{dp}{2\pi} = \mathcal{Z}_{jk}\delta_{ik} = \mathcal{Z}_{ji}\,; \tag{4.30}$$

so from eqs. (4.29), (4.30) it follows:

$$\left\langle \vec{p}\otimes\vec{g}[n_0,\vec{n},\vec{J}]\right\rangle = \vec{u}\otimes\vec{n} - \epsilon\gamma n_0\mathcal{Z}^T + O(\epsilon^2)\,, \tag{4.31}$$

where the superscript T denotes transpose.
From eq. (4.31) it is immediate to find:

$$\begin{aligned}\left\langle \vec{g}[n_0,\vec{n},\vec{J}]\wedge\vec{p}\right\rangle_i =&\eta_{ijk}\left\langle p_k g_j[n_0,\vec{n},\vec{J}]\right\rangle\\ =&\eta_{ijk}\left[u_k n_j - \epsilon\gamma n_0\mathcal{Z}_{jk}\right] + O(\epsilon^2)\,;\end{aligned} \tag{4.32}$$

let us put our attention on the term:

$$\begin{aligned}\eta_{ijk}\mathcal{Z}_{jk} =&\eta_{ijk}\frac{1-\omega}{2\gamma}\eta_{jsl}\frac{n_s}{|\vec{n}|}\partial_k\left(\frac{n_l}{|\vec{n}|}\right)\\ =&(\delta_{ks}\delta_{il}-\delta_{kl}\delta_{is})\frac{1-\omega}{2\gamma}\frac{n_s}{|\vec{n}|}\partial_k\left(\frac{n_l}{|\vec{n}|}\right)\\ =&\frac{1-\omega}{2\gamma}[\vec{s}\cdot\vec{\nabla}-\vec{\nabla}\cdot\vec{s}]s_i\,;\end{aligned} \tag{4.33}$$

so from eqs. (4.32), (4.33) we deduce:

$$\left\langle \vec{g}[n_0,\vec{n},\vec{J}]\wedge\vec{p}\right\rangle = \vec{n}\wedge\vec{u} + \frac{\epsilon}{2}n_0(1-\omega)[\vec{\nabla}\cdot\vec{s}-\vec{s}\cdot\vec{\nabla}]\vec{s}; \tag{4.34}$$

finally by collecting eqs. (4.3), (4.28), (4.31), (4.34) we have proven the following:

Proposition 11 *Under the LSFS hypothesis* (1.37)*, Eqs.* (4.3) *are equivalent, up to* $O(\epsilon^2)$*, to the* first-order spinorial hydrodynamic model*:*

$$\partial_t n_0 + \frac{\vec{\nabla}}{2\gamma} \cdot \left(\vec{J} + \epsilon\gamma\vec{n} \right) = 0 \,,$$
$$\partial_t \vec{n} + \frac{\vec{\nabla}}{2\gamma} \cdot (\vec{n} \otimes \vec{u} - \epsilon\gamma n_0 \mathcal{Z} + \epsilon\gamma n_0 \, I) + \vec{n} \wedge \vec{u} + \frac{\epsilon}{2} n_0 (1-\omega)[\vec{\nabla} \cdot \vec{s} - \vec{s} \cdot \vec{\nabla}]\vec{s} = 0 \,,$$
$$\partial_t \vec{J} + \frac{\vec{\nabla}}{2\gamma} \cdot \left[n_0 (I + \vec{u} \otimes \vec{u}) + \epsilon\gamma \left(\vec{u} \otimes \vec{n} - \epsilon\gamma n_0 \mathcal{Z}^T \right) \right] + n_0 \vec{\nabla} V = 0 \,, \tag{4.35}$$

where the functions $\vec{u}$*,* $\vec{s}$*,* $\mathcal{Z}$ *are defined by eqs.* (4.15)*,* (4.27)*.*

4.2 A second order spinorial hydrodynamic model

We are going to deduce another spinorial hydrodynamic model, which is analogue to model (3.123). We will start again from the Wigner equations in hydrodynamic scaling (1.45), we will consider the same fluid-dynamic moments n_0, $\vec{n}$, $\vec{J}$ of the Wigner distribution $w(r,p,t)$ and we will take again as the equilibrium distribution the one given in (4.1), (4.2); however, we will make stronger assumptions than (1.37), which will allow us to consider also $O(\epsilon^2)-$terms in the fluid equations.

We make the semiclassical assumption $\epsilon \ll 1$ and the SMS hypothesis, that is we suppose:

$$c = O(\epsilon) \,, \qquad |\vec{\xi}^{\,0}| = O(\epsilon) \,, \tag{4.36}$$

where $\vec{\xi}^{\,0} = (\xi_1^0, \xi_2^0, \xi_3^0)$ are the Lagrange multipliers appearing in (4.1). We will see that from the hypothesis (4.36) will follow that:

$$\frac{|\vec{n}|}{n_0} = O(\epsilon) \tag{4.37}$$

which is the hydrodynamic analogue of the relation (3.91) valid for the diffusive model (3.123).

Moreover, for the sake of simplicity we make the *irrotational hypothesis* $|\mathrm{curl}\, \vec{u}| = O(\epsilon^2)$, which means:

$$\partial_i u_j - \partial_j u_i = O(\epsilon^2) \qquad i,j = 1,2 \,. \tag{4.38}$$

4.2.1 Semiclassical expansion of the equilibrium distribution

For the sake of simplicity, let us redefine: $\vec{\xi}^{\,0} \mapsto \epsilon\vec{\xi}^{\,0}$ and consider $|\vec{\xi}^{\,0}| = O(1)$. Under our hypothesis, the classical symbol of the modified Hamiltonian becomes:

$$-h_\xi = a + \epsilon b \,, \quad -a = \left(\frac{|p|^2}{2} + \Xi_k p_k + \xi_0 \right) \sigma_0 \,, \quad -b = (\gamma p_s + \xi_s)\sigma_s \,, \tag{4.39}$$

where $\gamma = c/\epsilon$ as in (1.41); that is, the modified Hamiltonian decouples in a *scalar* part of order $O(1)$ and a *spinorial* part of order $O(\epsilon)$: again, this fact leads to remarkable simplifications in computations.

We can compute the second order expansion of the equilibrium distribution (4.1), (4.2) under the hypothesis (4.36) through a strategy similar to that one employed to compute the second order expansion of the equilibrium distribution for the second diffusive model: first we substitute (4.39) in (2.41), then we impose the constraints (4.2).

$$\begin{aligned} g_0[n_0, \vec{n}, \vec{J}] =& e^{-(|p|^2/2 + \vec{\Xi}\cdot\vec{p} + \xi_0)}\left(1 + \frac{\epsilon^2}{2}|\gamma\vec{p} + \vec{\xi}|^2\right) \\ &+ \epsilon^2 \mathcal{E}\mathrm{xp}^{(2)}(-(|p|^2/2 + \vec{\Xi}\cdot\vec{p} + \xi_0)) + O(\epsilon^3)\,, \\ \vec{g}[n_0, \vec{n}, \vec{J}] =& -\epsilon e^{-(|p|^2/2 + \vec{\Xi}\cdot\vec{p} + \xi_0)}(\gamma\vec{p} + \vec{\xi}) + O(\epsilon^3)\,. \end{aligned} \tag{4.40}$$

Let us now consider the constraints (4.2) for charge density n_0 and current $\vec{J}$ up to $O(\epsilon^2)$:

$$\begin{aligned} n_0 &= \int e^{-(|p|^2/2 + \vec{\Xi}\cdot\vec{p} + \xi_0)}\, dp + O(\epsilon^2)\,, \\ J_i &= \int p_i e^{-(|p|^2/2 + \vec{\Xi}\cdot\vec{p} + \xi_0)}\, dp + O(\epsilon^2) \qquad i = 1, 2\,; \end{aligned} \tag{4.41}$$

it follows easily that:

$$e^{-(|p|^2/2 + \vec{\Xi}\cdot\vec{p} + \xi_0)} = \frac{n_0}{2\pi} e^{-|\vec{p} - \vec{u}|^2/2} + O(\epsilon^2)\,, \tag{4.42}$$

with $\vec{u}$ given again by (4.15); so from eqs. (4.2), (4.42) it follows:

$$\begin{aligned} \vec{n} &= -\epsilon \int e^{-(|p|^2/2 + \vec{\Xi}\cdot\vec{p} + \xi_0)}(\gamma\vec{p} + \vec{\xi})\, dp + O(\epsilon^3) \\ &= -\epsilon \int \frac{n_0}{2\pi} e^{-|\vec{p} - \vec{u}|^2/2}(\gamma\vec{p} + \vec{\xi})\, dp + O(\epsilon^3) \\ &= -\epsilon n_0(\gamma\vec{u} + \vec{\xi}) + O(\epsilon^3)\,, \end{aligned}$$

and so:

$$-\epsilon\vec{\xi} = \frac{\vec{n}}{n_0} + \epsilon\gamma\vec{u} + O(\epsilon^3)\,; \tag{4.43}$$

then from eqs. (4.40), (4.43) we deduce:

$$\vec{g}[n_0, \vec{n}, \vec{J}] = \frac{n_0}{2\pi} e^{-|\vec{p} - \vec{u}|^2/2}\left[\frac{\vec{n}}{n_0} - \epsilon\gamma(\vec{p} - \vec{u})\right] + O(\epsilon^3)\,. \tag{4.44}$$

Now let us put our attention on $g_0[n_0, \vec{n}, \vec{J}]$, which can be rewritten, exploiting Eqs. (4.40), (4.42), (4.43), in the form:

$$\begin{aligned} g_0[n_0, \vec{n}, \vec{J}] =& e^{-(|p|^2/2 + \vec{\Xi}\cdot\vec{p} + \xi_0)} + \epsilon^2 \mathcal{E}\mathrm{xp}^{(2)}(-(|p|^2/2 + \vec{\Xi}\cdot\vec{p} + \xi_0)) \\ &+ \frac{n_0}{4\pi} e^{-|\vec{p} - \vec{u}|^2/2}\left|\frac{\vec{n}}{n_0} - \epsilon\gamma(\vec{p} - \vec{u})\right|^2 + O(\epsilon^3)\,. \end{aligned} \tag{4.45}$$

Let us define, for an arbitrary positive function $\mathcal{N}(x)$ and an arbitrary vector function $\vec{\mathcal{J}}(x) = (\mathcal{J}_1(x), \mathcal{J}_2(x), 0)$:

$$\mathcal{M}_\epsilon[\mathcal{N}, \vec{\mathcal{J}}] = \frac{\mathcal{N}}{2\pi} e^{-|\vec{p}-\vec{\mathcal{U}}|^2/2} \left[1 - \frac{\epsilon^2}{24} \left(2\Delta \log \mathcal{N} + \frac{|\nabla \mathcal{N}|^2}{\mathcal{N}^2} - \mathcal{Q}(\mathcal{N}, \vec{\mathcal{J}}) \right) \right], \tag{4.46}$$

where:

$$\begin{aligned} \mathcal{Q}(\mathcal{N}, \vec{\mathcal{J}}) =& 3(\Delta \mathcal{A} + p_k \Delta \mathcal{U}_k + \partial_i \mathcal{U}_j \, \partial_j \mathcal{U}_i) - 2\partial_i \mathcal{U}_j (p_i - \mathcal{U}_i)(\partial_j \mathcal{A} + p_k \partial_j \mathcal{U}_k) \\ & - (\partial^2_{ij} \mathcal{A} + p_k \partial^2_{ij} \mathcal{U}_k)(p_i - \mathcal{U}_i)(p_j - \mathcal{U}_j) + |\nabla(\mathcal{A} + p_k \mathcal{U}_k)|^2 , \\ \vec{\mathcal{U}} =& \vec{\mathcal{J}}/\mathcal{N} , \qquad \mathcal{A} = \log\left(\frac{\mathcal{N}}{2\pi}\right) - \frac{|\vec{\mathcal{U}}|^2}{2} . \end{aligned} \tag{4.47}$$

The function $\mathcal{M}_\epsilon[n, \vec{\mathcal{J}}](x, p)$ is actually the $O(\epsilon^4)-$semiclassical expansion of the scalar quantum Maxwellian with moments $\left\langle \mathcal{M}_\epsilon[\mathcal{N}, \vec{\mathcal{J}}] \right\rangle = \mathcal{N}$, $\left\langle \vec{p}\mathcal{M}_\epsilon[\mathcal{N}, \vec{\mathcal{J}}] \right\rangle = \vec{\mathcal{J}}$ in the "irrotational case", which means, under the hypothesis:

$$\partial_i \mathcal{U}_j - \partial_j \mathcal{U}_i = O(\epsilon^2) \qquad i, j = 1, 2 ; \tag{4.48}$$

see e.g. [30] for details.

Since the first two terms of (4.45) constitute the $O(\epsilon^4)-$semiclassical expansion of a scalar quantum Maxwellian, and since we assumed (4.38), we have:

$$\mathcal{M}_\epsilon[\mathcal{N}, \vec{\mathcal{J}}] = e^{-(|p|^2/2 + \vec{\Xi}\cdot\vec{p} + \xi_0)} + \epsilon^2 \mathcal{E}\mathrm{xp}^{(2)}(-(|p|^2/2 + \vec{\Xi}\cdot\vec{p} + \xi_0)) , \tag{4.49}$$

for a suitable choice of the moments $\mathcal{N}$, $\vec{\mathcal{J}}$; so we can rewrite $g_0[n_0, \vec{n}, \vec{J}]$ as:

$$g_0[n_0, \vec{n}, \vec{J}] = \mathcal{M}_\epsilon[\mathcal{N}, \vec{\mathcal{J}}] + \frac{n_0}{4\pi} e^{-|\vec{p}-\vec{u}|^2/2} \left| \frac{\vec{n}}{n_0} - \epsilon\gamma(\vec{p} - \vec{u}) \right|^2 + O(\epsilon^3) , \tag{4.50}$$

with $\mathcal{N}(x)$, $\vec{\mathcal{J}}(x)$ such that the right-hand side of eq. (4.50) satisfies the constraints for n_0, $\vec{J}$ contained in eq. (4.2):

$$\begin{aligned} n_0 =& \mathcal{N} + \int \frac{n_0}{4\pi} e^{-|\vec{p}-\vec{u}|^2/2} \left| \frac{\vec{n}}{n_0} - \epsilon\gamma(\vec{p} - \vec{u}) \right|^2 dp + O(\epsilon^3) , \\ \vec{J} =& \vec{\mathcal{J}} + \int \vec{p} \, \frac{n_0}{4\pi} e^{-|\vec{p}-\vec{u}|^2/2} \left| \frac{\vec{n}}{n_0} - \epsilon\gamma(\vec{p} - \vec{u}) \right|^2 dp + O(\epsilon^3) ; \end{aligned} \tag{4.51}$$

so from (4.51) it follows:

$$\mathcal{N} = n_0 - n_0 \left(\frac{1}{2} \left| \frac{\vec{n}}{n_0} \right|^2 + \epsilon^2\gamma^2 \right) + O(\epsilon^3) , \tag{4.52}$$

$$\begin{aligned} \vec{\mathcal{J}} =& \vec{J} - n_0 \vec{u} \left(\frac{1}{2} \left| \frac{\vec{n}}{n_0} \right|^2 + \epsilon^2\gamma^2 \right) \\ & - \int (\vec{p} - \vec{u}) \, \frac{n_0}{4\pi} e^{-|\vec{p}-\vec{u}|^2/2} \left| \frac{\vec{n}}{n_0} - \epsilon\gamma(\vec{p} - \vec{u}) \right|^2 dp + O(\epsilon^3) \\ & = \vec{J} - n_0 \vec{u} \left(\frac{1}{2} \left| \frac{\vec{n}}{n_0} \right|^2 + \epsilon^2\gamma^2 \right) + \epsilon\gamma\vec{n} + O(\epsilon^3) . \end{aligned} \tag{4.53}$$

We remark that, since $n_0 = \mathcal{N}$ and $\vec{J} = \vec{\mathcal{J}}$ up to $O(\epsilon^2)$, then Eq. (4.38) is equivalent to Eq. (4.48).

By collecting Eqs. (4.50), (4.52), (4.53) we obtain the explicit second-order semiclassical expansion of the equilibrium distribution $g[n_0, \vec{n}, \vec{J}]$:

$$\begin{aligned} g_0[n_0,\vec{n},\vec{J}] =& \mathcal{M}\left[n_0 - n_0\left(\frac{|\vec{n}|^2}{2n_0^2}+\epsilon^2\gamma^2\right), \vec{J}+\epsilon\gamma\vec{n} - \left(\frac{|\vec{n}|^2}{2n_0^2}+\epsilon^2\gamma^2\right)\vec{J}\right] \\ &+ \frac{n_0}{4\pi}e^{-|\vec{p}-\vec{J}/n_0|^2/2}\left|\frac{\vec{n}}{n_0} - \epsilon\gamma\left(\vec{p}-\frac{\vec{J}}{n_0}\right)\right|^2 + O(\epsilon^3), \\ \vec{g}[n_0,\vec{n},\vec{J}] =& \frac{n_0}{2\pi}e^{-|\vec{p}-\vec{J}/n_0|^2/2}\left(\frac{\vec{n}}{n_0} - \epsilon\gamma\left(\vec{p}-\frac{\vec{J}}{n_0}\right)\right) + O(\epsilon^3). \end{aligned} \tag{4.54}$$

Let us just stress that eq. (4.43) shows that the SMS approximation leads to (4.37), as anticipated.

4.2.2 Computation of the moments

Now let us exploit eq. (4.54) in order to compute a second-order semiclassical expansion of the implicit terms in eq. (4.3).
Let us begin by recalling a known property of $\mathcal{M}_\epsilon[n_0, \vec{J}]$ defined by (4.46) (see [30] for details):

$$\left\langle \left(\vec{p}-\frac{\vec{\mathcal{J}}}{\mathcal{N}}\right)\otimes\left(\vec{p}-\frac{\vec{\mathcal{J}}}{\mathcal{N}}\right)\mathcal{M}_\epsilon[\mathcal{N},\vec{\mathcal{J}}]\right\rangle = \mathcal{N} - \frac{\epsilon^2}{12}\mathcal{N}\,\vec{\nabla}\otimes\vec{\nabla}\log\mathcal{N}, \tag{4.55}$$

valid for arbitrary functions $\mathcal{N}(x) > 0$, $\vec{\mathcal{J}}(x)$.
Let us consider now $\mathcal{N}(x)$, $\vec{\mathcal{J}}(x)$ given by eq. (4.53). We have:

$$\begin{aligned} \frac{\vec{\mathcal{J}}}{\mathcal{N}} =& \frac{\vec{J} - n_0\vec{u}\left(\frac{1}{2}\left|\frac{\vec{n}}{n_0}\right|^2+\epsilon^2\gamma^2\right)+\epsilon\gamma\vec{n}}{n_0 - n_0\left(\frac{1}{2}\left|\frac{\vec{n}}{n_0}\right|^2+\epsilon^2\gamma^2\right)} + O(\epsilon^3) \\ =& \left[\vec{u} - \vec{u}\left(\frac{1}{2}\left|\frac{\vec{n}}{n_0}\right|^2+\epsilon^2\gamma^2\right)+\epsilon\gamma\frac{\vec{n}}{n_0}\right]\left[1+\frac{1}{2}\left|\frac{\vec{n}}{n_0}\right|^2+\epsilon^2\gamma^2\right] + O(\epsilon^3) \\ =& \vec{u} - \vec{u}\left(\frac{1}{2}\left|\frac{\vec{n}}{n_0}\right|^2+\epsilon^2\gamma^2\right)+\epsilon\gamma\frac{\vec{n}}{n_0} + \vec{u}\left(\frac{1}{2}\left|\frac{\vec{n}}{n_0}\right|^2+\epsilon^2\gamma^2\right) + O(\epsilon^3) \\ =& \vec{u} + \epsilon\gamma\frac{\vec{n}}{n_0} + O(\epsilon^3); \end{aligned} \tag{4.56}$$

so from eqs. (4.4), (4.54), (4.55), (4.56) we deduce:

$$\begin{aligned}
\mathscr{P} =& \left\langle (\vec{p} - \vec{J}/n_0) \otimes (\vec{p} - \vec{J}/n_0)\, g_0[n_0, \vec{n}, \vec{J}] \right\rangle \\
=& \left\langle \left(\vec{p} - \frac{\vec{\mathcal{J}}}{\mathcal{N}} + \epsilon\gamma \frac{\vec{n}}{n_0} \right) \otimes \left(\vec{p} - \frac{\vec{\mathcal{J}}}{\mathcal{N}} + \epsilon\gamma \frac{\vec{n}}{n_0} \right) \mathcal{M}_\epsilon[\mathcal{N}, \vec{\mathcal{J}}] \right\rangle \\
&+ \left\langle (\vec{p} - \vec{J}/n_0) \otimes (\vec{p} - \vec{J}/n_0) \frac{n_0}{4\pi} e^{-|\vec{p} - \vec{J}/n_0|^2/2} \left| \frac{\vec{n}}{n_0} - \epsilon\gamma \left(\vec{p} - \frac{\vec{J}}{n_0} \right) \right|^2 \right\rangle + O(\epsilon^3) \\
=& \mathcal{N} - \frac{\epsilon^2}{12} \mathcal{N}\, \vec{\nabla} \otimes \vec{\nabla} \log \mathcal{N} + \int \frac{|\vec{p}|^2}{2} \frac{n_0}{4\pi} e^{-|\vec{p}|^2/2} \left| \frac{\vec{n}}{n_0} - \epsilon\gamma\vec{p} \right|^2 dp + O(\epsilon^3) \\
=& n_0 - n_0 \left(\frac{1}{2} \left| \frac{\vec{n}}{n_0} \right|^2 + \epsilon^2\gamma^2 \right) - \frac{\epsilon^2}{12} n_0\, \vec{\nabla} \otimes \vec{\nabla} \log n_0 \\
&+ \frac{n_0}{2} \left[\left| \frac{\vec{n}}{n_0} \right|^2 + 4\epsilon^2\gamma^2 \right] + O(\epsilon^3) \\
=& (1 + \epsilon^2\gamma^2) n_0 - \frac{\epsilon^2}{12} n_0\, \vec{\nabla} \otimes \vec{\nabla} \log n_0 + O(\epsilon^3)\,.
\end{aligned} \tag{4.57}$$

Now let us consider the term:

$$\begin{aligned}
\left\langle \vec{p} \otimes \vec{g}[n_0, \vec{n}, \vec{J}] \right\rangle =& \int \vec{p} \otimes \left[\frac{n_0}{2\pi} e^{-|\vec{p} - \vec{J}/n_0|^2/2} \left(\frac{\vec{n}}{n_0} - \epsilon\gamma \left(\vec{p} - \frac{\vec{J}}{n_0} \right) \right) \right] dp + O(\epsilon^3) \\
=& \frac{\vec{J} \otimes \vec{n}}{n_0} - \epsilon\gamma n_0 \int \vec{p} \otimes \vec{p}\, e^{-|p|^2/2} \frac{dp}{2\pi} + O(\epsilon^3) \\
=& \frac{\vec{J} \otimes \vec{n}}{n_0} - \epsilon\gamma n_0\, I + O(\epsilon^3)\,.
\end{aligned} \tag{4.58}$$

Finally, by collecting Eqs. (4.3), (4.57), (4.58) and by recalling Eq. (3.121), we obtain the proof of the following:

Proposition 12 *Under the SMS assumption (4.36) and the irrotational hypothesis (4.38), Eq. (4.3) is equivalent, up to $O(\epsilon^3)$, to the* second-order spinorial hydrodynamic model*:*

$$\begin{aligned}
\partial_t n_0 + \frac{\vec{\nabla}}{2\gamma} \cdot (\vec{J} + \epsilon\gamma\vec{n}) =& 0\,, \\
\partial_t \vec{n} + \frac{\vec{\nabla}}{2\gamma} \cdot \left(\frac{\vec{n} \otimes \vec{J}}{n_0} \right) + \frac{\vec{n} \wedge \vec{J}}{n_0} =& 0\,, \\
\partial_t \vec{J} + \frac{\vec{\nabla}}{2\gamma} \cdot \left(\frac{\vec{J} \otimes (\vec{J} + \epsilon\gamma\vec{n})}{n_0} \right) + \frac{\vec{\nabla} n_0}{2\gamma} + n_0 \vec{\nabla}(V + V_B) =& 0\,,
\end{aligned} \tag{4.59}$$

where V_B is again the Bohm potential, defined by (3.122).

4.3 A first order spinorial diffusive model

In this section we will derive a first order spinorial drift-diffusion model for quantum transport of electrons in graphene, with a proceduce very similar to the one adopted in the derivation of the first order diffusive model (3.89). In fact, we will start from the Wigner equation in diffusive scaling (1.38), (1.39), we will compute a Chapman-Enskog expansion of the Wigner distribution w and a first order semiclassical expansion of the equilibrium distribution g, and we will exploit these expansions to obtain a closed explicit fluid model.

The fluid-dynamic moments we will use to deduce the drift-diffusion model of interest are the following, already considered in the derivation of the spinorial hydrodynamic models:

$$\begin{aligned} n_0(x,t) =& \langle w_0(x,p,t)\rangle \qquad \text{charge density,} \\ \vec{n}(x,t) =& \langle \vec{w}(x,p,t)\rangle \qquad \text{spin vector.} \end{aligned} \tag{4.60}$$

The equilibrium distribution can be written as (we have already applied the scaling (1.34)–(1.36)):

$$g[n_0,\vec{n}] = \mathcal{E}\mathrm{xp}_\epsilon(-h_{A,\vec{B}})\,, \qquad h_{A,\vec{B}} = \left(\frac{|p|^2}{2} + A\right)\sigma_0 + (c\vec{p} + \vec{B})\cdot\vec{\sigma}\,, \tag{4.61}$$

where $A(x,t)$, $\vec{B}(x,t) = (B_1(x,t), B_2(x,t), B_3(x,t))$ are Lagrange multipliers to de determined in such a way that:

$$\langle g_0[n_0,\vec{n}]\rangle(x,t) = n_0(x,t)\,,\ \langle \vec{g}[n_0,\vec{n}]\rangle(x,t) = \vec{n}(x,t) \quad \forall (x,t) \in \mathbb{R}^2 \times (0,\infty)\,. \tag{4.62}$$

4.3.1 Derivation of the model

Let us consider again the scaled Wigner equations for the system (1.38), (1.39). We assume that the semiclassical parameter ϵ and the diffusive parameter τ are of the same order and small, so we will take the limit $\tau \to 0$ in the Wigner equations:

$$\lambda \equiv \frac{c}{\tau} = \frac{\epsilon\gamma}{\tau} = O(1) \qquad (\tau \to 0)\,. \tag{4.63}$$

Under the assumption (4.63), we perform a Chapman-Enskog expansion (see section 3.2) of the Wigner function $w = w_0 + \vec{w}\cdot\vec{\sigma}$:

$$\begin{aligned} w_0 =& g_0 - \tau\left(\frac{\vec{p}\cdot\vec{\nabla}}{2\gamma} + \Theta_0\right) g_0 + O(\tau^2)\,, \\ \vec{w} =& \vec{g} - \tau\left[\left(\frac{\vec{p}\cdot\vec{\nabla}}{2\gamma} + \Theta_0\right)\vec{g} + \vec{g}\wedge\vec{p}\right] + O(\tau^2)\,, \end{aligned} \tag{4.64}$$

where $\Theta_0 = -\vec{\nabla}V\cdot\vec{\nabla}_p$ is the leading order term in the semiclassical expansion of the operator $\Theta_\epsilon[V]$ given by (1.40). Now we take moments of eqs. (1.38) obtaining:

$$\begin{aligned}\tau\partial_t n_0 + \frac{\vec{\nabla}}{2\gamma}\cdot\langle\vec{p}w_0\rangle + \frac{\epsilon}{2}\vec{\nabla}\cdot\vec{n} &=0\,,\\ \tau\partial_t\vec{n} + \frac{\vec{\nabla}}{2\gamma}\cdot\langle\vec{w}\otimes\vec{p}\rangle + \frac{\epsilon}{2}\vec{\nabla}n_0 + \langle\vec{w}\wedge\vec{p}\rangle &=0\,.\end{aligned} \tag{4.65}$$

4.3.2 Semiclassical expansion of the equilibrium distribution

Now we will derive a first-order semiclassical expansion of the equilibrium distribution (4.61), (4.62), which will be exploited in the subsequent sections to compute up to $O(\epsilon^2)$ the implicit terms in the fluid equations.
We start by considering eqs. (2.21), (2.29), (2.30) with:

$$\beta = 1\,,\quad -a = \left(\frac{|p|^2}{2} + A\right)\sigma_0 + \vec{B}\cdot\vec{\sigma}\,,\quad -b = \gamma\vec{p}\cdot\vec{\sigma}\,. \tag{4.66}$$

Since $\vec{a} = -B$ depends only on x, then clearly:

$$\{a_j, a_k\} = 0 \qquad j,k\;=\;1,2,3\,; \tag{4.67}$$

moreover:

$$\eta_{ijk}\{a_0,a_j\}a_k = \eta_{ijk}\left[\partial_{p_s}\left(\frac{|p|^2}{2}\right)\partial_{x_s}B_j\right]B_k = \eta_{ijk}\left[(\vec{p}\cdot\vec{\nabla})B_j\right]B_k \qquad (i=1,2,3)\,,$$

which means:

$$\{a_0,\vec{a}\}\wedge\vec{a} = \left[(\vec{p}\cdot\vec{\nabla}_x)\vec{B}\right]\wedge\vec{B}\,; \tag{4.68}$$

so from eqs. (2.21), (2.29), (2.30), (4.66)–(4.68) we deduce:

$$\begin{aligned} g[n_0,\vec{n}] =& g^{(0)}[n_0,\vec{n}] + \epsilon g^{(1)}[n_0,\vec{n}] + O(\epsilon^2)\,,\\ g^{(0)}[n_0,\vec{n}] =& e^{-(A+|p|^2/2)}\left[\cosh|\vec{B}|\,\sigma_0 - \frac{\sinh|\vec{B}|}{|\vec{B}|}\vec{B}\cdot\vec{\sigma}\right]\,,\\ g^{(1)}[n_0,\vec{n}] =& \gamma e^{-(A+|p|^2/2)}\Bigg\{\frac{\sinh|\vec{B}|}{|\vec{B}|}\vec{B}\cdot\vec{p}\sigma_0\\ &+\Bigg[-\left(\left(\cosh|\vec{B}| - \frac{\sinh|\vec{B}|}{|\vec{B}|}\right)\frac{\vec{B}\otimes\vec{B}}{|\vec{B}|^2} + \frac{\sinh|\vec{B}|}{|\vec{B}|}I\right)\vec{p}\\ &+\left(\cosh|\vec{B}| - \frac{\sinh|\vec{B}|}{|\vec{B}|}\right)\frac{[(\vec{p}\cdot\vec{\nabla}_x)\vec{B}]\wedge\vec{B}}{2\gamma|\vec{B}|^2}\Bigg]\cdot\vec{\sigma}\Bigg\}\,. \end{aligned} \tag{4.69}$$

Now we impose that the right-hand side of (4.69) satisfies the constraints (4.62) up to $O(\epsilon^2)$. We notice that $g^1[n_0,\vec{n}]$ is odd with respect to p, and so gives no contribution to the computation of $\langle g_0[n_0,\vec{n}]\rangle$, $\langle \vec{g}[n_0,\vec{n}]\rangle$:

$$\begin{aligned} n_0\sigma_0 + \vec{n}\cdot\vec{\sigma} =& \left\langle g_0^{(0)}[n_0,\vec{n}]\right\rangle + 0 + O(\epsilon^2) \\ =& \int e^{-(A+|p|^2/2)}\left[\cosh|\vec{B}|\,\sigma_0 - \frac{\sinh|\vec{B}|}{|\vec{B}|}\vec{B}\cdot\vec{\sigma}\right]dp + O(\epsilon^2) \\ =& 2\pi e^{-A}\left[\cosh|\vec{B}|\,\sigma_0 - \frac{\sinh|\vec{B}|}{|\vec{B}|}\vec{B}\cdot\vec{\sigma}\right] + O(\epsilon^2)\,; \end{aligned} \tag{4.70}$$

it follows:

$$\begin{aligned} 2\pi e^{-A} =& \sqrt{n_0^2 - |\vec{n}|^2} + O(\epsilon^2)\,, \\ \tanh|\vec{B}| =& \frac{|\vec{n}|}{n_0} + O(\epsilon^2)\,, \qquad \frac{\vec{B}}{|\vec{B}|} = -\frac{\vec{n}}{|\vec{n}|} + O(\epsilon^2)\,; \end{aligned} \tag{4.71}$$

in particular:

$$\cosh|\vec{B}| = \frac{n_0}{\sqrt{n_0^2 - |\vec{n}|^2}} + O(\epsilon^2)\,, \qquad \sinh|\vec{B}| = \frac{|\vec{n}|}{\sqrt{n_0^2 - |\vec{n}|^2}} + O(\epsilon^2)\,; \tag{4.72}$$

so from eqs. (4.69), (4.71), (4.72) we find:

$$\begin{aligned} g_0^{(0)}[n_0,\vec{n}] =& \frac{e^{-|p|^2/2}}{2\pi} n_0\,, \\ \vec{g}^{(0)}[n_0,\vec{n}] =& \frac{e^{-|p|^2/2}}{2\pi}\vec{n}\,, \\ g_0^{(1)}[n_0,\vec{n}] =& -\gamma\frac{e^{-|p|^2/2}}{2\pi}\vec{n}\cdot\vec{p}\,, \\ \vec{g}^{(1)}[n_0,\vec{n}] =& -\gamma\frac{e^{-|p|^2/2}}{2\pi}n_0\left[\left((1-\omega)\frac{\vec{n}\otimes\vec{n}}{|\vec{n}|^2} + \omega\,I\right)\vec{p} - (1-\omega)\frac{[(\vec{p}\cdot\vec{\nabla}_x)\vec{n}]\wedge\vec{n}}{2\gamma|\vec{n}|^2}\right]\,, \end{aligned} \tag{4.73}$$

where the function ω, already introduced in eq. (4.27), is given by:

$$\omega = \frac{|\vec{n}|/n_0}{\log\sqrt{\frac{n_0+|\vec{n}|}{n_0-|\vec{n}|}}}\,. \tag{4.74}$$

Eqs. (4.73) provide an explicit approximation of the equilibrium distribution $g[n_0,\vec{n}]$: in the next sections they will be exploited in order to derive a first-order spinorial drift-diffusion model for the system.

4.3.3 Computation of the moments

Now we will exploit eqs. (4.73) in order to compute the implicit terms of eq. (4.65). From eqs. (4.63)–(4.65), it follows:

$$\begin{aligned}
&\tau\partial_t n_0+\frac{\vec{\nabla}}{2\gamma}\cdot\left\langle\vec{p}\left[g_0-\tau\left(\frac{\vec{p}\cdot\vec{\nabla}}{2\gamma}+\Theta_0\right)g_0\right]\right\rangle+\frac{\epsilon}{2}\vec{\nabla}\cdot\vec{n}=O(\epsilon^2)=O(\tau^2)\,,\\
&\tau\partial_t\vec{n}+\frac{\vec{\nabla}}{2\gamma}\cdot\left\langle\left\{\vec{g}-\tau\left[\left(\frac{\vec{p}\cdot\vec{\nabla}}{2\gamma}+\Theta_0\right)\vec{g}+\vec{g}\wedge\vec{p}\right]\right\}\otimes\vec{p}\right\rangle+\frac{\epsilon}{2}\vec{\nabla}n_0\\
&\qquad+\left\langle\left\{\vec{g}-\tau\left[\left(\frac{\vec{p}\cdot\vec{\nabla}}{2\gamma}+\Theta_0\right)\vec{g}+\vec{g}\wedge\vec{p}\right]\right\}\wedge\vec{p}\right\rangle=O(\epsilon^2)=O(\tau^2)\,;
\end{aligned}\tag{4.75}$$

from eq. (4.73) we deduce that $g^{(0)}[n_0,\vec{n}]$ (respectively $g^{(1)}[n_0,\vec{n}]$) is even (respectively odd) with respect to p; so we can rewrite (4.75):

$$\begin{aligned}
&\tau\partial_t n_0+\frac{\vec{\nabla}}{2\gamma}\cdot\left\langle\vec{p}\left[\epsilon g_0^{(1)}-\tau\left(\frac{\vec{p}\cdot\vec{\nabla}}{2\gamma}+\Theta_0\right)g_0^{(0)}\right]\right\rangle+\frac{\epsilon}{2}\vec{\nabla}\cdot\vec{n}=O(\epsilon^2)=O(\tau^2)\,,\\
&\tau\partial_t\vec{n}+\frac{\vec{\nabla}}{2\gamma}\cdot\left\langle\left\{\epsilon\vec{g}^{(1)}-\tau\left[\left(\frac{\vec{p}\cdot\vec{\nabla}}{2\gamma}+\Theta_0\right)\vec{g}^{(0)}+\vec{g}^{(0)}\wedge\vec{p}\right]\right\}\otimes\vec{p}\right\rangle+\frac{\epsilon}{2}\vec{\nabla}n_0\\
&\qquad+\left\langle\left\{\epsilon\vec{g}^{(1)}-\tau\left[\left(\frac{\vec{p}\cdot\vec{\nabla}}{2\gamma}+\Theta_0\right)\vec{g}^{(0)}+\vec{g}^{(0)}\wedge\vec{p}\right]\right\}\wedge\vec{p}\right\rangle=O(\epsilon^2)=O(\tau^2)\,;
\end{aligned}\tag{4.76}$$

dividing eq. (4.76) by τ and passing (formally) to the limit $\epsilon\to 0$ ($\tau\to 0$) it is immediate to obtain:

$$\begin{aligned}
&\partial_t n_0+\partial_s\left(\frac{1}{2\gamma}F_{0s}+\frac{\lambda}{2}n_s\right)=0\,,\\
&\partial_t n_j+\partial_s\left(\frac{1}{2\gamma}F_{js}+\frac{\lambda}{2}\delta_{js}n_0\right)+\eta_{jks}F_{ks}=0\qquad(j=1,2,3)\,,
\end{aligned}\tag{4.77}$$

with $(F_{0s})_{s=1,2,3}$, $(F_{js})_{j,s=1,2,3}$ given by:

$$\begin{aligned}
F_{0s}=&\lambda\left\langle p_s g_0^{(1)}[n_0,\vec{n}]\right\rangle-\left\{\frac{1}{2\gamma}\partial_k\left\langle p_k p_s g_0^{(0)}[n_0,\vec{n}]\right\rangle+n_0\partial_s V\right\}\qquad(s=1,2,3)\,,\\
F_{js}=&\lambda\left\langle p_s g_j^{(1)}[n_0,\vec{n}]\right\rangle-\left\{\frac{1}{2\gamma}\partial_k\left\langle p_k p_s g_j^{(0)}[n_0,\vec{n}]\right\rangle+n_j\partial_s V\right.\\
&\left.+\eta_{jkl}\left\langle p_s p_l g_k^{(0)}[n_0,\vec{n}]\right\rangle\right\}\qquad(j,s=1,2,3)\,.
\end{aligned}\tag{4.78}$$

Before computing the terms in Eq. (4.78), we notice the following fact. The first order two-band diffusive model (3.89) is derived (see section 3.2) from a closed set of fluid equations, namely Eq. (3.50), having a different structure from Eqs. (4.77), (4.78): in fact, the ratio $\lambda=c/\tau$, present in Eqs. (4.77), (4.78), does not appear in Eq. (3.50). Actually, due to the particular choice of the moments (4.60) used to derive Eqs. (4.77), (4.78), the equivalent of property (3.48) for the spinorial case, namely:

$$\langle Tg[n_0^\tau, \vec{n}^\tau]\rangle = 0 \qquad \forall \tau > 0\,, \tag{4.79}$$

does not hold; instead we have:

$$\langle Tg[n_0, \vec{n}]\rangle = O(\epsilon) \qquad \text{as } \epsilon \to 0\,. \tag{4.80}$$

Because of property (4.80) we were forced to assume (4.63): otherwise the terms containing the first order term in the semiclassical expansion of the equilibrium distribution $g[n_0, \vec{n}]$ would have been divergent for $\tau \to 0$.

Let us now compute the terms in eq. (4.78) by exploiting eqs. (4.73).

$$\left\langle p_s g_0^{(1)}[n_0, \vec{n}]\right\rangle = -\,\gamma \int p_s \frac{e^{-|p|^2/2}}{2\pi} \vec{n}\cdot\vec{p}\, dp = -\gamma n_s\,; \tag{4.81}$$

$$\left\langle p_k p_s g_0^{(0)}[n_0, \vec{n}]\right\rangle = \int p_k p_s \frac{e^{-|p|^2/2}}{2\pi} n_0\, dp = n_0 \delta_{ks}\,; \tag{4.82}$$

let us define, for the sake of brevity:

$$\mathscr{N}_{jk} = (1-\omega)\frac{n_j n_k}{|\vec{n}|^2} + \omega\delta_{jk} - (1-\omega)\eta_{jsl}\frac{\partial_k n_s \cdot n_l}{2\gamma|\vec{n}|^2} \qquad (j,k = 1,2,3)\,, \tag{4.83}$$

so that from eqs. (4.73), (4.83) it follows:

$$\vec{g}^{(1)}[n_0, \vec{n}] = -\gamma n_0 \frac{e^{-|p|^2/2}}{2\pi} \mathscr{N}\vec{p}; \tag{4.84}$$

but from eq. (4.84) we deduce:

$$\left\langle p_s g_j^{(1)}[n_0, \vec{n}]\right\rangle = -\gamma n_0 \mathscr{N}_{jk} \int p_s p_k \frac{e^{-|p|^2/2}}{2\pi}\, dp = -\gamma n_0 \mathscr{N}_{js}\,; \tag{4.85}$$

$$\left\langle p_k p_s g_j^{(0)}[n_0, \vec{n}]\right\rangle = n_j \int p_k p_s \frac{e^{-|p|^2/2}}{2\pi}\, dp = n_j \delta_{ks}\,; \tag{4.86}$$

then collecting eqs. (4.78)–(4.86) we find:

$$\begin{aligned} F_{0s} &= -\,\lambda\gamma n_s - \left\{ \frac{1}{2\gamma}\partial_s n_0 + n_0 \partial_s V \right\}\,, \\ F_{js} &= -\,\lambda\gamma n_0 \mathscr{N}_{js} - \left\{ \frac{1}{2\gamma}\partial_s n_j + n_j \partial_s V + \eta_{jks} n_k \right\}\,, \end{aligned} \tag{4.87}$$

implying that:

$$\begin{aligned} \eta_{jks} F_{ks} &= -\,\eta_{jks}\left[\lambda\gamma n_0 \mathscr{N}_{ks} + \frac{1}{2\gamma}\partial_s n_k + n_k \partial_s V + \eta_{kls} n_l \right] \\ &= -\,\lambda\gamma n_0 \eta_{jks}\mathscr{N}_{ks} + \frac{1}{2\gamma}(\vec{\nabla}\wedge\vec{n})_j - (\vec{n}\wedge\vec{\nabla}V)_j + \eta_{jks}\eta_{lks} n_l\,; \end{aligned} \tag{4.88}$$

but clearly:

$$
\begin{aligned}
\eta_{jks}\eta_{lks} =& 2\delta_{jl}\,, \\
-\eta_{jks}\mathscr{N}_{ks} =& -\eta_{jks}\left[(1-\omega)\frac{n_k n_s}{|\vec{n}|^2}+\omega\delta_{ks}-(1-\omega)\eta_{k\alpha l}\frac{\partial_s n_\alpha\cdot n_l}{2\gamma|\vec{n}|^2}\right] \\
=&(1-\omega)\eta_{ksj}\eta_{k\alpha l}\frac{\partial_s n_\alpha\cdot n_l}{2\gamma|\vec{n}|^2} \\
=&(1-\omega)(\delta_{s\alpha}\delta_{jl}-\delta_{sl}\delta_{j\alpha})\frac{\partial_s n_\alpha\cdot n_l}{2\gamma|\vec{n}|^2} \\
=&\frac{1-\omega}{2\gamma|\vec{n}|^2}\left[\vec{\nabla}\cdot\vec{n}-\vec{n}\cdot\vec{\nabla}\right]n_j\,;
\end{aligned}
\tag{4.89}
$$

so from eqs. (4.88), (4.89) we deduce:

$$
\eta_{jks}F_{ks}=\left[\lambda n_0\frac{1-\omega}{2|\vec{n}|^2}\left(\vec{\nabla}\cdot\vec{n}-\vec{n}\cdot\vec{\nabla}\right)\vec{n}+\frac{1}{2\gamma}\vec{\nabla}\wedge\vec{n}-\vec{n}\wedge\vec{\nabla}V+2\vec{n}\right]_j\,;
\tag{4.90}
$$

by collecting eqs. (4.74), (4.77), (4.83), (4.87), (4.90) we obtain the proof of the following formal:

Proposition 13 *Under the assumption* (4.63)*, Eqs.* (4.77)*,* (4.78) *are equivalent to the* first order spinorial drift-diffusion model*:*

$$
\begin{aligned}
\partial_t n_0 =& \partial_s J_s\,, \\
J_s =& \partial_s n_0 + n_0\partial_s V\,,
\end{aligned}
\tag{4.91}
$$

$$
\begin{aligned}
\partial_t n_j =& \partial_s A_{js} + F_j\,, && (j=1,2,3) \\
A_{js} =& \left(\delta_{jl}+b_k\left[\frac{\vec{n}}{n_0}\right]\eta_{jkl}\right)\partial_s n_l + n_j\partial_s V \\
& -2\eta_{jsl}n_l + b_k\left[\frac{\vec{n}}{n_0}\right](\delta_{jk}n_s-\delta_{js}n_k)\,, && (j,s=1,2,3) \\
F_j =& \eta_{jkl}n_k\partial_l V - 2n_j + b_s\left[\frac{\vec{n}}{n_0}\right]\partial_s n_j - b_j\left[\frac{\vec{n}}{n_0}\right]\partial_s n_s\,, && (j=1,2,3)\,,
\end{aligned}
\tag{4.92}
$$

where we defined, for all $\vec{u}$, $\vec{v}\in\mathbb{R}^3$, $0<|v|<1$*:*

$$
b_k[\vec{v}] = \lambda v_k|\vec{v}|^{-2}\left(1-\frac{2|\vec{v}|}{\log(1+|\vec{v}|)-\log(1-|\vec{v}|)}\right)\,,\qquad (k=1,2,3)\,.
\tag{4.93}
$$

We refer to model (4.91)–(4.93) *as* Quantum Spin Diffusion Equations (QSDE1)*.*

We notice that:

$$
\begin{aligned}
&|b_k[\vec{v}]|<\lambda \qquad \text{for } 0<|v|<1,\ k=1,2,3\,, \\
&b_k[\vec{v}]=\frac{\lambda}{3}v_k+O(|\vec{v}|^3) \qquad \text{as } |\vec{v}|\to 0\,, \\
&b_k[\vec{v}]\to\lambda v_k \qquad \text{as } |\vec{v}|\to 1\,.
\end{aligned}
\tag{4.94}
$$

The model (4.91)–(4.93) will be studied from an analytical point of view in chapter 6.

4.4 A first order spinorial diffusive model with pseudomagnetic field

In the model QSDE1 (4.91), (4.92) the charge density n_0 evolves independently of the spin vector $\vec{n}$: we are going to modify the QSDE1 model in order to obtain a fully coupled system by adding a "pseudomagnetic" field able to interact with the charge carriers pseudospin. The idea of such a field has already been proposed in [24]: the Authors suggest that by breaking graphene sublattices symmetry (see the Introduction to this thesis) through strain, it is possible to generate a pseudomagnetic field and therefore obtain Landau levels and quantum Hall phases without breaking time reversal symmetry (see e.g. [47] about this topics).

Negulescu and Possanner, in their paper [42], consider a semiconductor subject to a magnetic field interacting with the electron spin, and derive a purely semiclassical (without quantum corrections) diffusive model for the charge density n_0 and the spin vector $\vec{n}$ throught a Chapman-Enskog espansion of the Boltzmann distribution. We will follow a similar procedure to obtain our new model.

4.4.1 Derivation of the model

We define two quantities:

$$\begin{aligned} \zeta =& \zeta(x,t) \qquad \text{pseudo-spin polarization of scattering rate;} \\ \vec{\omega} =& \vec{\omega}(x,t) \qquad \text{direction of local pseudo-magnetization.} \end{aligned} \tag{4.95}$$

The quantity $\zeta(x,t)$ satisfies:

$$s_\uparrow = \frac{1+|\zeta(x,t)|}{1-|\zeta(x,t)|} s_\downarrow \,,$$

where $s_{\uparrow\downarrow}$ are the scattering rates of electrons in the upper band and in the lower band; it is bounded between 0 and 1. The vector $\vec{\omega}$, being a direction, has modulus equal to 1.

We modify the scaled Wigner equations (1.38) in this way:

$$\begin{aligned} \tau\partial_t w_0 + \frac{\vec{p}\cdot\vec{\nabla}}{2\gamma} w_0 + \frac{\epsilon}{2}\vec{\nabla}\cdot\vec{w} + \Theta_\epsilon[V]w_0 =& \frac{Q_0(w)}{\tau} \,, \\ \tau\partial_t \vec{w} + \frac{\vec{p}\cdot\vec{\nabla}}{2\gamma}\vec{w} + \frac{\epsilon}{2}\vec{\nabla} w_0 + \vec{w}\wedge\vec{p} + \Theta_\epsilon[V]\vec{w} + \tau\vec{\omega}\wedge\vec{w} =& \frac{\vec{Q}(w)}{\tau} \,, \end{aligned} \tag{4.96}$$

with the collision operator $Q(w)$ defined by:

$$Q(w) = \mathcal{P}^{1/2}(g-w)\mathcal{P}^{1/2} \,, \qquad \mathcal{P} = \sigma_0 + \zeta\vec{\omega}\cdot\vec{\sigma} \,. \tag{4.97}$$

The hermitian matrix $\mathcal{P}$ is the so-called *polarization matrix*. Note that its eigenvalues:

$$\lambda_\pm(\mathcal{P}) = 1 \pm |\zeta\vec{\omega}|^2 = 1 \pm \zeta^2$$

are positive since $0 \le \zeta < 1$, so $\mathcal{P}$ is positive definite and $\mathcal{P}^{1/2}$ makes sense.

We assume again (4.63) and we perform a Chapman-Enskog expansion of the Wigner distribution $w = w_0\sigma_0 + \vec{w}\cdot\vec{\sigma}$:

$$w = g - \tau\mathcal{P}^{-1/2}\left(\mathcal{T}_0[g]\sigma_0 + \vec{\mathcal{T}}[g]\cdot\vec{\sigma}\right)\mathcal{P}^{-1/2} + O(\tau^2)\,, \tag{4.98}$$

where the action of the operators $\mathcal{T}_0$, $\vec{\mathcal{T}}$ on an arbitrary (smooth enough) function $f = f_0\sigma_0 + \vec{f}\cdot\vec{\sigma}$ is defined by:

$$\mathcal{T}_0[f] = \frac{\vec{p}\cdot\vec{\nabla}}{2\gamma}f_0 + \Theta_0 f_0\,, \qquad \vec{\mathcal{T}}[f] = \frac{\vec{p}\cdot\vec{\nabla}}{2\gamma}\vec{f} + \Theta_0\vec{f} + \vec{f}\wedge\vec{p}; \tag{4.99}$$

it is straightforward to prove that for all hermitian matrices $a = a_0\sigma_0 + \vec{a}\cdot\vec{\sigma}$ the following relation holds:

$$\begin{aligned}\mathcal{P}^{-1/2}a\mathcal{P}^{-1/2} =& (1-\zeta^2)^{-1}\{(a_0 - \zeta\vec{\omega}\cdot\vec{a})\sigma_0 \\ &+ [\zeta\vec{\omega}a_0 + (\vec{\omega}\otimes\vec{\omega} + \sqrt{1-\zeta^2}(I - \vec{\omega}\otimes\vec{\omega}))\vec{a}]\cdot\vec{\sigma}\}\,;\end{aligned} \tag{4.100}$$

so from eqs. (4.98), (4.100) we find:

$$\begin{aligned} w_0 =& g_0 - \tau(1-\zeta^2)^{-1}(\mathcal{T}_0[g] - \zeta\vec{\omega}\cdot\vec{\mathcal{T}}[g]) + O(\tau^2)\,, \\ \vec{w} =& \vec{g} - \tau\left[\zeta\vec{\omega}\mathcal{T}_0[g] + (\vec{\omega}\otimes\vec{\omega} + \sqrt{1-\zeta^2}(I-\vec{\omega}\otimes\vec{\omega}))\vec{\mathcal{T}}[g]\right] + O(\tau^2)\,;\end{aligned} \tag{4.101}$$

now let us we take the moments of eqs. (4.96) obtaining:

$$\begin{aligned} \tau\partial_t n_0 + \frac{\vec{\nabla}}{2\gamma}\cdot\langle\vec{p}w_0\rangle + \frac{\epsilon}{2}\vec{\nabla}\cdot\vec{n} =& 0\,, \\ \tau\partial_t\vec{n} + \frac{\vec{\nabla}}{2\gamma}\cdot\langle\vec{w}\otimes\vec{p}\rangle + \frac{\epsilon}{2}\vec{\nabla}n_0 + \langle\vec{w}\wedge\vec{p}\rangle + \tau\vec{\omega}\wedge\vec{n} =& 0\,;\end{aligned} \tag{4.102}$$

So from eqs. (4.101), (4.102) we deduce:

$$\begin{aligned} &\tau\partial_t n_0 + \frac{\vec{\nabla}}{2\gamma}\cdot\left\langle\vec{p}\left\{g_0 - \tau(1-\zeta^2)^{-1}(\mathcal{T}_0[g] - \zeta\vec{\omega}\cdot\vec{\mathcal{T}}[g])\right\}\right\rangle + \frac{\epsilon}{2}\vec{\nabla}\cdot\vec{n} = O(\tau^2)\,, \\ &\tau\partial_t\vec{n} + \frac{\vec{\nabla}}{2\gamma}\cdot\left\langle\left\{\vec{g} - \tau\left[\zeta\vec{\omega}\mathcal{T}_0[g] + (\vec{\omega}\otimes\vec{\omega} + \sqrt{1-\zeta^2}(I-\vec{\omega}\otimes\vec{\omega}))\vec{\mathcal{T}}[g]\right]\right\}\otimes\vec{p}\right\rangle \\ &\quad + \left\langle\left\{\vec{g} - \tau\left[\zeta\vec{\omega}\mathcal{T}_0[g] + (\vec{\omega}\otimes\vec{\omega} + \sqrt{1-\zeta^2}(I-\vec{\omega}\otimes\vec{\omega}))\vec{\mathcal{T}}[g]\right]\right\}\wedge\vec{p}\right\rangle \\ &\quad + \frac{\epsilon}{2}\vec{\nabla}n_0 + \tau\vec{\omega}\wedge\vec{n} = O(\tau^2)\,;\end{aligned} \tag{4.103}$$

again, from eq. (4.73) we deduce that $g^{(0)}[n_0,\vec{n}]$ (respectively $g^{(1)}[n_0,\vec{n}]$) is even (respectively odd) with respect to p; moreover, $\mathcal{T}_0$, $\vec{\mathcal{T}}$ are odd operators, in the sense that, for an arbitrary function $f = f_0\sigma_0 + \vec{f}\cdot\vec{\sigma}$:

$$\begin{aligned} f \text{ even with respect to } p \quad &\Rightarrow \quad \mathcal{T}_0[f],\ \vec{\mathcal{T}}[f] \text{ odd with respect to } p\,; \\ f \text{ odd with respect to } p \quad &\Rightarrow \quad \mathcal{T}_0[f],\ \vec{\mathcal{T}}[f] \text{ even with respect to } p\,;\end{aligned} \tag{4.104}$$

so we can rewrite (4.103)in this form:

$$\begin{aligned}
&\tau\partial_t n_0 + \frac{\vec{\nabla}}{2\gamma}\cdot\left\langle \vec{p}\left\{\epsilon g_0^{(1)} - \tau(1-\zeta^2)^{-1}(\mathcal{T}_0[g^{(0)}] - \zeta\vec{\omega}\cdot\vec{\mathcal{T}}[g^{(0)}])\right\}\right\rangle + \frac{\epsilon}{2}\vec{\nabla}\cdot\vec{n} = O(\tau^2)\,,\\
&\tau\partial_t\vec{n} + \frac{\vec{\nabla}}{2\gamma}\cdot\left\langle\left\{\epsilon\vec{g}^{(1)} - \tau\left[\zeta\vec{\omega}\mathcal{T}_0[g^{(0)}] + (\vec{\omega}\otimes\vec{\omega} + \sqrt{1-\zeta^2}(I-\vec{\omega}\otimes\vec{\omega}))\vec{\mathcal{T}}[g^{(0)}]\right]\right\}\otimes\vec{p}\right\rangle\\
&\quad + \left\langle\left\{\epsilon\vec{g}^{(1)} - \tau\left[\zeta\vec{\omega}\mathcal{T}_0[g^{(0)}] + (\vec{\omega}\otimes\vec{\omega} + \sqrt{1-\zeta^2}(I-\vec{\omega}\otimes\vec{\omega}))\vec{\mathcal{T}}[g^{(0)}]\right]\right\}\wedge\vec{p}\right\rangle\\
&\quad + \frac{\epsilon}{2}\vec{\nabla}n_0 + \tau\vec{\omega}\wedge\vec{n} = O(\tau^2)\,;
\end{aligned} \tag{4.105}$$

now we divide eqs. (4.105) for τ and, recalling eq. (4.63), we pass to the limit $\tau\to 0$, obtaining:

$$\begin{aligned}
&\partial_t n_0 + \frac{\vec{\nabla}}{2\gamma}\cdot\left\langle \vec{p}\left\{\lambda g_0^{(1)} - (1-\zeta^2)^{-1}(\mathcal{T}_0[g^{(0)}] - \zeta\vec{\omega}\cdot\vec{\mathcal{T}}[g^{(0)}])\right\}\right\rangle + \frac{\lambda}{2}\vec{\nabla}\cdot\vec{n} = 0\,,\\
&\partial_t\vec{n} + \frac{\vec{\nabla}}{2\gamma}\cdot\left\langle\left\{\lambda\vec{g}^{(1)} - \left[\zeta\vec{\omega}\mathcal{T}_0[g^{(0)}] + (\vec{\omega}\otimes\vec{\omega} + \sqrt{1-\zeta^2}(I-\vec{\omega}\otimes\vec{\omega}))\vec{\mathcal{T}}[g^{(0)}]\right]\right\}\otimes\vec{p}\right\rangle\\
&\quad + \left\langle\left\{\lambda\vec{g}^{(1)} - \left[\zeta\vec{\omega}\mathcal{T}_0[g^{(0)}] + (\vec{\omega}\otimes\vec{\omega} + \sqrt{1-\zeta^2}(I-\vec{\omega}\otimes\vec{\omega}))\vec{\mathcal{T}}[g^{(0)}]\right]\right\}\wedge\vec{p}\right\rangle\\
&\quad + \frac{\lambda}{2}\vec{\nabla}n_0 + \vec{\omega}\wedge\vec{n} = 0\,;
\end{aligned} \tag{4.106}$$

finally, exploiting eqs. (4.81), (4.82), (4.83), (4.85), (4.86), (4.99) to compute the integrals in (4.106) we can prove the following formal:

Proposition 14 *Under the assumption* (4.63)*, Eqs.* (4.106) *are equivalent to the* first-order spinorial drift-diffusion model with pseudomagnetic field*:*

$$\begin{aligned}
\partial_t n_0 =& \partial_s M_{0s}\,,\\
\partial_t n_j =& \partial_s M_{js} + \eta_{jks}(M_{ks} + n_k\omega_s)\\
&+ \partial_s\left\{b_k\left[\frac{\vec{n}}{n_0}\right](\eta_{jkl}\partial_s n_l + \delta_{jk}n_s - \delta_{js}n_k)\right\}\\
&+ b_s\left[\frac{\vec{n}}{n_0}\right]\partial_s n_j - b_j\left[\frac{\vec{n}}{n_0}\right]\partial_s n_s \qquad (j=1,2,3)\,,\\
M_{0s} =& \phi^{-2}\{(\partial_s n_0 + n_0\partial_s V) - \zeta\omega_k(\partial_s n_k + n_k\partial_s V + \eta_{kls}n_l)\}\,,\\
M_{js} =& \phi^{-2}\{-\zeta\omega_j(\partial_s n_0 + n_0\partial_s V)\\
&+ [\omega_j\omega_k + \phi(\delta_{jk} - \omega_j\omega_k)](\partial_s n_k + n_k\partial_s V + \eta_{kls}n_l)\}\,,\\
\phi =& \sqrt{1-\zeta^2}\,,
\end{aligned} \tag{4.107}$$

with $b_k[\vec{n}/n_0]$ *still given by* (4.93)*.*
We call model (4.107) Quantum Spin Diffusion Equation 2 (QSDE2)*.*

We remark that in the model QSDE2 (4.107) the charge density n_0 depends on the spin vector $\vec{n}$ through the pseudomagnetic field; such dependence takes the form of cross-diffusion terms proportional to $\zeta\vec{\omega}$.
Model QSDE2 (4.107) will be studied in Chapter 6 from the numerical point of view.

Part II

Analytical results and numerical simulations

Chapter 5

Analytical results

5.1 Introduction

In this section we will present some analytical results concerning the model (4.91), (4.92). We will prove existence of (weak) solutions satisfying suitable L^∞ bounds, prove uniqueness of solutions under stronger assumptions, find an entropy inequality, and study the long-time behaviour of the solutions.
The model (4.107) will not be studied from an analytical point of view in this Thesis. Differently from model (4.91), (4.92), it is a completely coupled system of PDE: the equation for n_0 depends on $\vec{n}$, and conversely. Moreover, it is possible to prove that the system (4.107) is uniformly parabolic if $\sup_{\Omega_T} \zeta(x,t) < 1$. However, the presence of cross-diffusion terms makes hard proving L^∞ bounds for the moments; for this reason, an analytical study of model (4.107) goes beyond the purpose of this Thesis.
From now on we will consider the potential V which appear in eqs. (4.91), (4.92) as self-consistently given by the Poisson equation:

$$- \lambda_D^2 \Delta V = n_0 - C\,. \tag{5.1}$$

The constant $\lambda_D > 0$ is the so-called *scaled Debye length* and $C : \Omega \to \mathbb{R}$ is the so-called *doping profile*, which is an assigned function.
We consider in this chapter the following two boundary value problems for the model QSDE1 (4.91), (4.92):

$$\begin{aligned}
\partial_t n_0 =& \text{div } (\nabla n_0 + n_0 \nabla V) && x \in \Omega\,,\ t \in [0,T]\,,\\
-\lambda_D^2 \Delta V =& n_0 - C(x) && x \in \Omega\,,\ t \in [0,T]\,,\\
n_0(x,t) =& n_\Gamma(x,t) && x \in \partial\Omega\,,\ t \in [0,T]\,,\\
V(x,t) =& \mathcal{U}(x,t) && x \in \partial\Omega\,,\ t \in [0,T]\,,\\
n_0(x,0) =& n_{0I}(x) && x \in \Omega\,,
\end{aligned} \tag{5.2}$$

$$
\begin{aligned}
\partial_t \vec{n} =& \text{div } J + \vec{F} \qquad x \in \Omega\,, \quad t \in [0,T]\,,\\
\vec{n}(x,t) =& 0 \qquad x \in \partial\Omega\,,\ t \in [0,T]\,,\\
\vec{n}(x,0) =& \vec{n}_I(x) \qquad x \in \Omega\,,\\
F_j =& \eta_{jk\ell} n_k \partial_\ell V - 2n_j + b_k[\vec{n}/n_0]\partial_k n_j - b_j[\vec{n}/n_0]\vec{\nabla}\cdot\vec{n},\\
J_{js} =& \big(\delta_{j\ell} + b_k[\vec{n}/n_0]\eta_{jk\ell}\big)\partial_s n_\ell + n_j \partial_s V\\
& - 2\eta_{js\ell} n_\ell + b_k[\vec{n}/n_0](\delta_{jk} n_s - \delta_{js} n_k) \qquad (j,s = 1,2,3)\,,\\
\vec{b}[\vec{v}] =& \lambda \frac{\vec{v}}{|\vec{v}|^2}\left[1 - \frac{2|\vec{v}|}{\log\left(\frac{1+|\vec{v}|}{1-|\vec{v}|}\right)}\right] \qquad \vec{v} \in \mathbb{R}^3,\ 0 < |\vec{v}| < 1\,.
\end{aligned}
\tag{5.3}
$$

Here $\Omega \subset \mathbb{R}^2$ is a bounded domain, $n_\Gamma : \partial\Omega \times [0,T] \to \mathbb{R}$, $n_I : \Omega \to \mathbb{R}$, $\mathcal{U} : \partial\Omega \times [0,T] \to \mathbb{R}$ (scaled applied voltage), $\vec{n}_I = (n_{1I}, n_{2I}, n_{3I}) : \Omega \to \mathbb{R}^3$ are given functions, whose properties will be specified later.
Since problem (5.2) is decoupled from problem (5.3), we will first solve (5.2) and then we will solve (5.3) considering n_0 and V as given function with suitable properties. Moreover, we notice that problem (5.2) is already known in literature, since it is the classical drift-diffusion model coupled with the Poisson equation [22, 35].
We define $\Omega_T \equiv \Omega \times [0,T]$; moreover, for an arbitrary $A \subset \mathbb{R}^2$, we denote with $\mathbf{1}_A$ the characteristic function of A:

$$\mathbf{1}_A(x) = 1 \quad \text{if } x \in A\,, \qquad \mathbf{1}_A(x) = 0 \quad \text{if } x \notin A\,;$$

finally for an arbitrary function $u : \mathbb{R}^2 \to \mathbb{R}$ we indicate with u_+ the positive part of u:

$$u_+(x) = u(x) \quad \text{if } u(x) > 0\,, \qquad u_+(x) = 0 \quad \text{if } u(x) \leq 0\,.$$

To prove the subsequent theorems, we will need the following:

Lemma 1 *Let $u \in H^1(\Omega)$, $u \leq 0$ a.e. on $\partial\Omega$,*[1] *$\Omega_+ \equiv \{x \in \Omega : u(x) > 0\}$. Then $u_+ \in H_0^1(\Omega)$ and $\partial_i u_+ = \mathbf{1}_{\Omega_+}\partial_i u$ for $i = 1, 2$.*

Proof. Let us preliminarily consider the case $u \in C^1(\mathbb{R}^2)$. Let $\phi \in H^1(\Omega)$ arbitrary, and $D \in \{\partial_1, \partial_2\}$. It follows:

$$\int_\Omega u_+ D\phi = \int_{\Omega_+} uD\phi = \int_{\partial\Omega_+} u\phi - \int_{\Omega_+} \phi Du = \int_{\partial\Omega_+} u\phi - \int_\Omega \phi \mathbf{1}_{\Omega_+} Du\,. \tag{5.4}$$

Clearly $\partial\Omega_+ = (\partial\Omega \cap \overline{A}_+) \cup (\overline{\Omega} \cap \partial A_+)$ with $A_+ = \{x \in \mathbb{R}^2 : u(x) > 0\}$. Since u is continuous on $\mathbb{R}^2$ it vanishes on ∂A_+ and a fortiori on $\overline{\Omega} \cap \partial A_+$; but $u \equiv 0$ also on $\partial\Omega \cap \overline{A}_+$ because $u \leq 0$ on $\partial\Omega$; so the boundary integral in Eq. (5.4) is equal to zero. It follows:

$$\int_\Omega u_+ D\phi = -\int_\Omega \phi \mathbf{1}_{\Omega_+} Du\,,$$

[1] It means that the set of points where the trace of u on $\partial\Omega$ is positive has zero measure with respect to the one-dimensional Lebesgue measure on $\partial\Omega$; see [12] for details.

which proves the thesis for the case $u \in C^1(\mathbb{R}^2)$.

Let us now consider the general case $u \in H^1(\Omega)$. From standard results on Sobolev spaces (see [12] for details), a sequence $(u_n)_n \in C_c^\infty(\mathbb{R}^2)$ exists such that $(u_n)_{|\Omega} \to u$ in $H^1(\Omega)$. Again let $\phi \in H^1(\Omega)$ arbitrary. From the previous discussion we already know:

$$\int_\Omega (u_n)_+ D\phi = -\int_\Omega \phi \mathbf{1}_{\Omega_{+,n}} Du_n \,, \tag{5.5}$$

where $\Omega_{+,n} = \{x \in \Omega \,:\, u_n(x) > 0\}$. Let us consider the first member of Eq. (5.5):

$$\int_\Omega (u_n)_+ D\phi = \int_\Omega \mathbf{1}_{\Omega_{+,n}} u_n D\phi = \int_\Omega (\mathbf{1}_{\Omega_{+,n}} - \mathbf{1}_{\Omega_+}) u_n D\phi + \int_\Omega \mathbf{1}_{\Omega_+} u_n D\phi \,. \tag{5.6}$$

We have:

$$\left| \int (\mathbf{1}_{\Omega_{+,n}} - \mathbf{1}_{\Omega_+}) u_n D\phi \right| \leq \|\mathbf{1}_{\Omega_{+,n}} - \mathbf{1}_{\Omega_+}\|_{L^4(\Omega)} \|u_n\|_{L^4(\Omega)} \|\phi\|_{L^2(\Omega)} \,. \tag{5.7}$$

From Sobolev embedding theorem it follows that $H^1(\Omega) \subset L^4(\Omega)$; since $(u_n)_{|\Omega} \to u$ on $H^1(\Omega)$, this means that $\|u_n\|_{L^4(\Omega)}$ is uniformely bounded with respect to n. Moreover $u_n \to u$ a.e. on Ω, which implies $\mathbf{1}_{\Omega_{+,n}} \to \mathbf{1}_{\Omega_+}$ a.e. on Ω; so from dominated convergence theorem we obtain $\|\mathbf{1}_{\Omega_{+,n}} - \mathbf{1}_{\Omega_+}\|_{L^4(\Omega)} \to 0$. Thus the left-hand side of Eq. (5.7) vanishes as $n \to \infty$:

$$\int (\mathbf{1}_{\Omega_{+,n}} - \mathbf{1}_{\Omega_+}) u_n D\phi \to 0 \,. \tag{5.8}$$

Taking the limit $n \to \infty$ in Eq. (5.6), exploiting Eq. (5.8) and recalling the fact that $(u_n)_{|\Omega} \to u$ in $H^1(\Omega)$ we find:

$$\int_\Omega (u_n)_+ D\phi \to \int_\Omega \mathbf{1}_{\Omega_+} u D\phi = \int_\Omega u_+ D\phi \,. \tag{5.9}$$

In a similar way it can be proven that:

$$\int_\Omega \phi \mathbf{1}_{\Omega_{+,n}} Du_n \to \int_\Omega \phi \mathbf{1}_{\Omega_+} Du \,. \tag{5.10}$$

Taking the limit $n \to \infty$ in Eq. (5.5) and exploiting Eqs. (5.9), (5.10) we obtain:

$$\int_\Omega u_+ D\phi = -\int_\Omega \phi \mathbf{1}_{\Omega_+} Du \,,$$

which yields the thesis.

□

In the next section we will also make use of the following Gagliardo-Niremberg inequality (see e.g. [12]). Given $1 \leq q \leq p < \infty$, a constant $k > 0$ exists such that:

$$\|v\|_{L^p(\Omega)} \leq k \|v\|_{L^q(\Omega)}^{q/p} \|v\|_{H^1(\Omega)}^{1-q/p} \qquad \forall v \in H^1(\Omega) \,. \tag{5.11}$$

5.2 Existence of solutions for first problem

Now we will study the existence and regularity of solutions (n_0, V) of Problem (5.2).
We impose the following conditions on the data:

$$n_\Gamma \in H^1(0,T;H^2(\Omega)) \cap H^2(0,T;L^2(\Omega)) \cap L^\infty(0,T;L^\infty(\Omega)), \tag{5.12}$$

$$n_{0I} \in H^1(\Omega), \quad \inf_\Omega n_{0I} > 0, \quad n_{0I} = n_\Gamma(0) \quad \text{on } \partial\Omega, \quad \inf_{\partial\Omega\times(0,T)} n_\Gamma > 0, \tag{5.13}$$

$$\mathcal{U} \in L^\infty(0,T;W^{2,p}(\Omega)) \cap H^1(0,T;H^1(\Omega)), \quad C \in L^\infty(\Omega),\ C \geq 0 \text{ in } \Omega, \tag{5.14}$$

for some $p > 2$. Under these assumptions, we are able to prove the existence of strong solutions (n_0, V) to the drift-diffusion model (5.2). We remark that results of existence and uniqueness of weak solutions to (5.2), as long as nonnegativity of the charge density, under weaker assumptions on the data, are already known in literature (see e.g. [22]); however, here we are going to prove a result of improved regularity for the solution and uniform positivity for the charge density, which will be exploited further on during the proof of the existence theorem for Problem (5.3).

Theorem 3 *Let $T > 0$ arbitrary and assume (5.12)-(5.14). Then there exists a unique solution (n_0, V) to Problem (5.2) satisfying:*

$$n_0 \in L^\infty([0,T],H^2(\Omega)) \cap H^1([0,T],H^1(\Omega)) \cap H^2([0,T],(H^1(\Omega))'), \tag{5.15a}$$

$$V \in L^\infty([0,T],W^{1,\infty}(\Omega)) \cap H^1([0,T],H^2(\Omega)), \tag{5.15b}$$

$$0 < me^{-\mu t} \leq n_0 \leq M \quad \text{in } \Omega,\ t > 0, \tag{5.15c}$$

where:

$$\begin{aligned} \mu &= \lambda_D^{-2} m\,, \\ M &= \max\left\{ \sup_{\partial\Omega\times(0,T)} n_\Gamma,\ \sup_\Omega n_{0I},\ \sup_\Omega C \right\}, \\ m &= \min\left\{ \inf_{\partial\Omega\times(0,T)} n_\Gamma,\ \inf_\Omega n_{0I} \right\} > 0\,. \end{aligned} \tag{5.16}$$

Proof. The existence and uniqueness of a weak solution (n_0, V) to problem (5.2) satisfying:

$$n_0 \geq 0, \quad n_0 \in L^2(0,T;H^1(\Omega)) \cap H^1(0,T;(H^1(\Omega))'), \quad V \in L^2(0,T;H^1(\Omega)),$$

is shown in [22] (also see Section 3.9 in [35]), for less regular boundary data. To prove the L^∞ bounds and the strong regularity properties for n_0 we will first prove that $n_0 \in L^\infty(\Omega_T)$.

Let $v \equiv (n_0 - M)_+$. From the definition (5.16) of M and Lemma 1 it follows that $v \in H_0^1(\Omega)$ and $\nabla v = \mathbf{1}_{\{n_0 > M\}} \nabla n_0$. By multiplying the first equation in (5.2) by v and integrating in Ω we find, with simple manipulations:

$$\frac{d}{dt}\int \frac{v^2}{2} = -\int |\nabla v|^2 + \int \Delta V \left[\frac{v^2}{2} + Mv\right]\,; \tag{5.17}$$

the last integral in (5.17) can be rewritten using (5.1) as:

$$\int \Delta V \left[\frac{v^2}{2} + Mv\right] = \lambda_D^{-2} \int (C - M - v) \left[\frac{v^2}{2} + Mv\right] \leq 0\,; \tag{5.18}$$

so from eqs. (5.17), (5.18) we find:

$$\frac{d}{dt} \int \frac{v(t)^2}{2} \leq 0\,, \qquad \int \frac{v(0)^2}{2} = 0\,,$$

which implies $v = (n_0 - M)_+ \equiv 0$ in Ω_T, meaning that $n_0 \leq M$ on Ω_T. So the upper bound for n_0 in Eq. (5.15c) has been proved. Along with the nonnegativity of n_0, this implies that:

$$n_0 \in L^\infty(\Omega_T)\,. \tag{5.19}$$

Eq. (5.19) shows that the right-hand side of the Poisson equation is an element of $L^\infty([0,T], L^\infty(\Omega))$. Then, by elliptic regularity (see e.g. [12] for details), $V \in L^\infty([0,T], W^{2,p}(\Omega))$, where $p > 2$ is the same as in (5.14); in particular $V \in L^2([0,T], H^2(\Omega))$ because Ω is bounded. Since $W^{2,p}(\Omega) \hookrightarrow W^{1,\infty}(\Omega)$ (we recall that $\Omega \subset \mathbb{R}^2$), it follows that:

$$\nabla V \in L^\infty(\Omega_T)\,. \tag{5.20}$$

Now we prove the lower bound for n_0 in Eq. (5.15c). Let:

$$\tilde{n}_0 = e^{\mu t} n_0\,, \qquad \mu \equiv \lambda_D^{-2}\,, \tilde{v} = (\tilde{n}_0 - m)_-\,. \tag{5.21}$$

From eqs. (4.91), (5.21) it follows:

$$\partial_t \tilde{n}_0 = \operatorname{div}(\nabla \tilde{n}_0 + \tilde{n}_0 \nabla V) + \mu \tilde{n}_0\,. \tag{5.22}$$

Notice that $\tilde{v} = (\tilde{n}_0 - m)_- = -(-\tilde{n}_0 + m)_+ \in H_0^1(\Omega)$ from the definition (5.16) of m and from Lemma 1; so we can multiply eq. (5.22) by $\tilde{v}$ and integrate on Ω:

$$\begin{aligned} \partial_t \int \frac{\tilde{v}^2}{2} &= -\int |\nabla \tilde{v}|^2 - \int \tilde{n}_0 \nabla \tilde{v} \cdot \nabla V + \mu \int \tilde{n}_0 \tilde{v} \\ &= -\int |\nabla \tilde{v}|^2 - \int \tilde{v} \nabla \tilde{v} \cdot \nabla V \\ &\quad - m \int \nabla \tilde{v} \cdot \nabla V + \mu \int \tilde{v}^2 + \mu m \int \tilde{v} \\ &= -\int |\nabla \tilde{v}|^2 - \int \tilde{v} \nabla \tilde{v} \cdot \nabla V \\ &\quad + \mu \int \tilde{v}^2 + m \int \tilde{v} \left[\Delta V + \mu\right]\,. \end{aligned} \tag{5.23}$$

Let us consider the last integral in Eq. (5.23):

$$\begin{aligned} &\int \tilde{v} \left[\Delta V + \mu\right] = \int \tilde{v} \left[\lambda_D^{-2}(C - e^{-\mu t}\tilde{n}_0) + \mu\right] \\ &= \int \tilde{v} \left[\lambda_D^{-2} C - e^{-\mu t} \lambda_D^{-2} \tilde{v} - e^{-\mu t} \lambda_D^{-2} m + \mu\right] \\ &\leq \int \tilde{v} \left[\mu - e^{-\mu t} \lambda_D^{-2} m\right]\,; \end{aligned} \tag{5.24}$$

from the definition (5.16) of μ and Eq. (5.24) we conclude:

$$\int \tilde{v}\,[\Delta V + \mu] \leq 0\,,$$

whcih implies, along with Eq. (5.23):

$$\partial_t \int \frac{\tilde{v}^2}{2} \leq -\int |\nabla \tilde{v}|^2 - \int \tilde{v}\nabla\tilde{v}\cdot\nabla V + \mu \int \tilde{v}^2\,. \tag{5.25}$$

Exploiting the boundedness of ∇V and applying Young inequality we can estimate the second integral on the right-hand side of Eq. (5.25) finding:

$$\left|\int \tilde{v}\nabla\tilde{v}\cdot\nabla V\right| \leq \|\nabla V\|_{L^\infty(\Omega_T)} \left[\frac{\varepsilon}{2}\int |\nabla\tilde{v}|^2 + \frac{1}{2\varepsilon}\int \tilde{v}^2\right], \tag{5.26}$$

with $\varepsilon = 2/\|\nabla V\|_{L^\infty(\Omega_T)}$. By collecting Eqs. (5.16), (5.21), (5.25) and (5.26) we obtain:

$$\begin{aligned}\partial_t \int \tilde{v}(t)^2 \leq & \left[\frac{1}{2}\|\nabla V\|^2_{L^\infty(\Omega_T)} + 2\mu\right] \int \tilde{v}(t)^2 \qquad t\in[0,T]\,,\\ \int \tilde{v}(0)^2 =& 0\,,\end{aligned}$$

so from Gronwall's lemma we conclude that $\tilde{v} = (\tilde{n}_0 - m)_- \equiv 0$ and then the lower bound for n_0 in (5.15c) has been proved.

Now we exploit the full regularity of n_Γ in (5.12) in order to show that n_0 has the regularity stated in (5.15a).
Since Eq. (5.12) holds, from standard results about the theory of traces in Sobolev spaces (see e.g. [12]), a function $N_\Gamma : \Omega_T \to \mathbb{R}$ exists with the properties:

$$\begin{aligned} N_\Gamma,\, \partial_t N_\Gamma \in & L^2([0,T], H^2(\Omega))\,, \quad \partial^2_{tt} N_\Gamma \in L^2(\Omega_T)\,,\\ N_\Gamma =& n_\Gamma \qquad \text{on } \partial\Omega\times[0,T]\,;\end{aligned} \tag{5.27}$$

note in particular that, since $N_\Gamma,\, \partial_t N_\Gamma \in L^2([0,T], H^2(\Omega))$, then:

$$N_\Gamma \in C([0,T], H^2(\Omega))\,. \tag{5.28}$$

We define $\tilde{n} = n_0 - N_\Gamma$ which is the solution of:

$$\begin{aligned} \partial_t \tilde{n} =& \operatorname{div}(\nabla\tilde{n} + \tilde{n}\nabla V) + f \qquad \text{on } \Omega_T\,,\\ f =& -\partial_t N_\Gamma + \operatorname{div}(\nabla N_\Gamma + N_\Gamma \nabla V)\,,\\ \tilde{n} =& 0 \qquad \text{on } \partial\Omega\times[0,T]\,,\\ \tilde{n}(x,0) =& n_{0I}(x) - N_\Gamma(x,0) \qquad x\in\Omega\,.\end{aligned} \tag{5.29}$$

Let us rewrite f exploiting eq. (5.1):

$$\begin{aligned} f =& -\partial_t N_\Gamma + \Delta N_\Gamma + \nabla N_\Gamma\cdot\nabla V + N_\Gamma \Delta V\\ =& -\partial_t N_\Gamma + \Delta N_\Gamma + \nabla N_\Gamma\cdot\nabla V - \lambda_D^{-2}(n_0 - C)N_\Gamma\,;\end{aligned} \tag{5.30}$$

from eqs. (5.19), (5.20), (5.27), (5.28), (5.30) we can easily deduce that $f \in L^2(\Omega_T)$; so from standard results on parabolic PDE theory we obtain that:

$$\partial_t n_0,\, \partial_t \tilde{n} \in L^2(\Omega_T)\,. \tag{5.31}$$

Now let us consider the time derivative of f, which can be immediately computed from eqs. (5.2), (5.30):

$$\begin{aligned} \partial_t f = &- \partial^2_{tt} N_\Gamma + \Delta \partial_t N_\Gamma + \nabla \partial_t N_\Gamma \cdot \nabla V + \nabla N_\Gamma \cdot \nabla \partial_t V \\ &- \lambda_D^{-2} N_\Gamma \partial_t n_0 - \lambda_D^{-2}(n_0 - C)\partial_t N_\Gamma\,. \end{aligned} \tag{5.32}$$

From (5.1) we find:

$$- \lambda_D^2 \Delta \partial_t V = \partial_t n_0 \quad \text{in } \Omega_T\,, \qquad \partial_t V = \partial_t \mathcal{U} \quad \text{in } \partial\Omega \times [0,T]\,, \tag{5.33}$$

and so:

$$\partial_t V \in L^2([0,T], H^2(\Omega))\,. \tag{5.34}$$

Let us then estimate the term, appearing in (5.32):

$$\begin{aligned} \int_0^T ||\nabla N_\Gamma \cdot \nabla \partial_t V||^2_{L^2(\Omega)}\, dt \le & \int_0^T ||\nabla N_\Gamma||^2_{L^4(\Omega)} ||\nabla \partial_t V||^2_{L^4(\Omega)}\, dt \\ & \le \sup_{[0,T]} ||\nabla N_\Gamma||^2_{L^4(\Omega)} \int_0^T ||\nabla \partial_t V||^2_{L^4(\Omega)}\, dt\,; \end{aligned}$$

from (5.28) it follows that $\sup_{[0,T]} ||\nabla N_\Gamma||^2_{L^4(\Omega)} < \infty$; moreover, applying (5.11) with $p = 4$, $q = 2$ and recalling (5.34) we find:

$$\begin{aligned} \int_0^T ||\nabla \partial_t V||^2_{L^4(\Omega)}\, dt \le & c \int_0^T ||\nabla \partial_t V||_{L^2(\Omega)} ||\nabla \partial_t V||_{H^1(\Omega)}\, dt \\ \le & \frac{c}{2} \int_0^T \left(||\nabla \partial_t V||^2_{L^2(\Omega)} + ||\nabla \partial_t V||^2_{H^1(\Omega)} \right) dt < \infty\,; \end{aligned}$$

so we conclude that:

$$\int_0^T ||\nabla N_\Gamma \cdot \nabla \partial_t V||^2_{L^2(\Omega)}\, dt < \infty\,. \tag{5.35}$$

By collecting (5.19), (5.20), (5.27), (5.31), (5.32), (5.34) and (5.35) we can easily deduce that $\partial_t f \in L^2(\Omega_T)$; moreover from (5.27) we have $n_{0I} - N_\Gamma(\cdot, 0) \in H^2(\Omega) \cap H^1_0(\Omega)$; so from [59, Theorem 1.3.1] the regularity statements on $n_0 = \tilde{n} + N_\Gamma$ finally follows.

□

5.3 Existence of solution for second problem

Now we are going to study Problem (5.3) considering n_0 and V as given by Theorem 3. We will prove the following:

Theorem 4 *Let (n_0, V) be the solution to Problem (5.2) according to Theorem 3 and let $\vec{n}^0 \in H_0^1(\Omega)^3$ such that:*

$$\sup_{x\in\Omega} \frac{|\vec{n}^0(x)|}{n_{0I}(x)} < 1\,; \tag{5.36}$$

then Problem (5.3) has a solution $\vec{n}$ such that:

$$\vec{n} \in L^2([0,T], H_0^1(\Omega))^3 \cap H^1([0,T], H^{-1}(\Omega))^3\,, \quad \sup_{\Omega_T} \frac{|\vec{n}|}{n_0} < 1\,; \tag{5.37}$$

furthermore, there exists at most one weak solution satisfying (5.37) and $\vec{n} \in L^\infty([0,T], W^{1,4}(\Omega))^3$.

In order to prove Theorem 4, we will first truncate the differential equations in (5.3) and prove existence of solutions for the truncated problem by applying Leray-Schauder fixed-point theorem; then we will find an L^∞ bound for the solution of the truncated problem which will imply that this latter is also a solution of (5.3).
For the sake of brevity we define:

$$X \equiv L^2([0,T], H_0^1(\Omega)) \cap H^1([0,T], H^{-1}(\Omega)) \subset L^2(\Omega_T)\,. \tag{5.38}$$

The compact embedding $X \subset\subset C([0,T], L^2(\Omega))$ follows from Aubin's lemma.
Let $0 < \chi < 1$ a fixed parameter, $\phi_\chi : \mathbb{R} \to \mathbb{R}$ a continuous nonincreasing function such that: $\phi_\chi(y) = 1$ for $y \le 1-\chi$, $\phi_\chi(y) = 0$ for $y \ge 1$, and let:

$$\vec{b}^\chi[\vec{v}] = \phi_\chi(|\vec{v}|)\,\vec{b}[\vec{v}] \qquad \forall \vec{v} \in \mathbb{R}^3\,. \tag{5.39}$$

Notice in particular that, from eqs. (5.3), (5.39) it follows:

$$|\vec{b}^\chi[\vec{v}]| \le \lambda \qquad \forall \vec{v} \in \mathbb{R}^3\,. \tag{5.40}$$

We split the proof of Theorem 4 in several lemmas.

Lemma 2 (Application of the fixed-point theorem) *The truncated problem:*

$$\begin{aligned}
\partial_t \vec{n} =& \operatorname{div} J^\chi + \vec{F}^\chi \qquad \text{in } \Omega_T\,,\\
F_j^\chi =& \eta_{jk\ell} n_k \partial_\ell V - 2n_j + b_k^\chi[\vec{n}/n_0]\partial_k n_j - b_j^\chi[\vec{n}/n_0]\vec{\nabla}\cdot\vec{n},\\
J_{js}^\chi =& \big(\delta_{j\ell} + b_k^\chi[\vec{n}/n_0]\eta_{jk\ell}\big)\partial_s n_\ell + n_j \partial_s V\\
&- 2\eta_{js\ell} n_\ell + b_k^\chi[\vec{n}/n_0](\delta_{jk} n_s - \delta_{js} n_k) \qquad (j,s = 1,2,3)\,,
\end{aligned} \tag{5.41}$$

with $\vec{b}^\chi$ given by (5.39), has at least one weak solution $\vec{n} \in X^3$.

Proof. In order to define a fixed point operator, let $\vec{n}' \in L^2(\Omega_T)$ and $\sigma \in [0,1]$. We wish to solve the linear problem, which is the weak form of linearized (5.3):

$$\begin{aligned}
\langle \partial_t n_j\,,\, z_j \rangle_{(H^{-1}(\Omega), H_0^1(\Omega))} + a_\sigma(\vec{n}, \vec{z}; t) =& 0 \qquad \vec{z} \in H_0^1(\Omega)^3\,,\ \text{a.e. } t \in [0,T]\,,\\
\vec{n}(t=0) =& \vec{n}^0\,,
\end{aligned} \tag{5.42}$$

where, for a.e. $t \in [0,T]$, $a_\sigma(\cdot,\cdot;t)$ is the bilinear form on $H_0^1(\Omega)^3$ defined by:

$$\begin{aligned} a_\sigma(\vec{n},\vec{z};t) = &\int \partial_s z_j \left\{ \left(\delta_{jl} + \sigma b_k^\chi \left[\frac{\vec{n}'(t)}{n_0(t)}\right] \eta_{jkl} \right) \partial_s n_l \right. \\ &\left. + n_j \partial_s V(t) - 2\eta_{jsl} n_l + \sigma b_k^\chi \left[\frac{\vec{n}'(t)}{n_0(t)}\right] (\delta_{jk} n_s - \delta_{js} n_k) \right\} \\ &- \int z_j \left\{ \eta_{jkl} n_k \partial_l V(t) - 2n_j + \sigma b_s^\chi \left[\frac{\vec{n}'(t)}{n_0(t)}\right] \partial_s n_j \right. \\ &\left. - \sigma b_j^\chi \left[\frac{\vec{n}'(t)}{n_0(t)}\right] \partial_s n_s \right\} \qquad \forall \vec{n},\, \vec{z} \in H_0^1(\Omega)^3 \,, \end{aligned} \tag{5.43}$$

and $\langle \cdot\,,\,\cdot \rangle_{(H^{-1}(\Omega),H_0^1(\Omega))}$ is the duality product between $H^{-1}(\Omega)$ and $H_0^1(\Omega)$. Due to the bounds (5.20), (5.40) on $\vec{\nabla} V$ and $\vec{b}^\chi\,[\vec{n}'/n_0]$, we deduce that a constant $C > 0$ independent of t and σ exists such that:

$$|a_\sigma(\vec{n},\vec{z};t)| \le C \|\vec{n}\|_{H_0^1(\Omega)} \|\vec{z}\|_{H_0^1(\Omega)} \qquad \forall \vec{n},\vec{z} \in H_0^1(\Omega)\,, \quad \text{a.e. } t \in [0,T]\,; \tag{5.44}$$

moreover, since η_{jkl} is antisymmetric, for arbitrary $\vec{n} \in H_0^1(\Omega)$ we have [2]:

$$\begin{aligned} a_\sigma(\vec{n},\vec{n};t) = \int \Bigg\{ &|\vec{\nabla}\vec{n}|^2 + 2|\vec{n}|^2 + n_j \partial_k V(t) \partial_k n_j \\ &+ \sigma b_k^\chi \left[\frac{\vec{n}'(t)}{n_0(t)}\right] (\delta_{jk} n_s - \delta_{js} n_k) \partial_s n_j \\ &- n_j \left(\sigma b_s^\chi \left[\frac{\vec{n}'(t)}{n_0(t)}\right] \partial_s n_j - \sigma b_j^\chi \left[\frac{\vec{n}'(t)}{n_0(t)}\right] \partial_s n_s \right) \Bigg\} \,. \end{aligned} \tag{5.45}$$

All the terms on the right-hand side can be written as a product of n_j, $\partial_k n_l$, and possibly an L^∞ function. Note that the only term in $a_\sigma(\vec{n},\vec{n};t)$, which does not have this structure, $b_k^\chi \eta_{jkl} \partial_s n_l \partial_s n_j$, vanishes because of the antisymmetry of $\eta_{jk\ell}$. Therefore, the Hölder and Cauchy-Schwarz inequalities yield

$$a_\sigma(\vec{n},\vec{n};t) \ge c_1 \|\vec{n}\|^2_{H_0^1(\Omega)} - c_2 \|\vec{n}\|^2_{L^2(\Omega)} \,, \tag{5.46}$$

for some positive constants c_1, c_2, independent of t, σ. Finally, $t \mapsto a_\sigma(\vec{n},\vec{z};t)$ is measurable in $[0,T]$, for all $\vec{n}$, $\vec{z} \in H_0^1$. So from standard results of linear parabolic equations theory (see e.g. [54, Corollary 23.26]) it follows that Eq. (5.42) has exactly one solution $\vec{n} \in X^3$; moreover (5.42) is equivalent to the following operator equation:

$$\begin{aligned} \partial_t \vec{n}(t) + A(t)\vec{n}(t) &= 0 \qquad \text{a.e. } t \in [0,T]\,, \\ \vec{n}(0) &= \vec{n}^0\,, \end{aligned} \tag{5.47}$$

where $A(t) : H_0^1(\Omega) \to H^{-1}(\Omega)$ is defined by:

$$\langle A(t)u\,,\,v \rangle_{(H^{-1}(\Omega),H_0^1(\Omega))} = a(u,v;t) \qquad \forall u,v \in H_0^1(\Omega)\,, \quad \text{a.e. } t \in [0,T]\,.$$

Notice that the test functions $\vec{z}$ in (5.42) are independent from t. However,

[2] here $|\vec{\nabla}\vec{n}|^2 = \sum_{s,k} (\partial_s n_k)^2$.

in the subsequent part of this thesis we will often choose time-dependent test functions in (5.42); this is possible because (5.42) is equivalent to (5.47), and the operator $A(t)$ in (5.47) extends in a natural way to an operator $\tilde{A}: L^2([0,T], H_0^1(\Omega)) \to L^2([0,T], H^{-1}(\Omega))$ defined by:

$$\langle \tilde{A}u\,,\, v\rangle_{(L^2([0,T],H^{-1}(\Omega)),L^2([0,T],H_0^1(\Omega)))} = \int_0^T a(u(t), v(t); t)\,,$$

for all $u, v \in L^2([0,T], H_0^1(\Omega))$. This fact allows us to choose $\vec{z} \in L^2([0,T], H_0^1(\Omega))$ in (5.42).

We seek now an estimate of $\|\vec{n}\|_X$ in terms of $\|\vec{n}^0\|_{L^2(\Omega)}$, which will be used later. Using $\vec{n} \in L^2([0,T], H_0^1(\Omega))$ as a test function in (5.42) and exploiting (5.46) we get:

$$\frac{1}{2}\partial_t\|\vec{n}\|_{L^2(\Omega)} = -a(\vec{n}, \vec{n}; t) \le -c_1\|\vec{n}\|^2_{H_0^1(\Omega)} + c_2\|\vec{n}\|_{L^2(\Omega)}\,, \tag{5.48}$$

so from Gronwall's Lemma we find:

$$\|\vec{n}\|_{L^\infty([0,T],L^2(\Omega))} \le e^{2c_2T}\|\vec{n}^0\|_{L^2(\Omega)}\,; \tag{5.49}$$

integrating in time (5.48) and exploiting (5.49) we obtain:

$$\begin{aligned} c_1\int_0^T \|\vec{n}\|^2_{H_0^1(\Omega)} \le& c_2\int_0^T \|\vec{n}\|^2_{L^2(\Omega)} + \frac{1}{2}\left(\|\vec{n}^0\|^2_{L^2(\Omega)} - \|\vec{n}(T)\|^2_{L^2(\Omega)}\right) \\ \le& \left(c_2Te^{2c_2T} + \frac{1}{2}\right)\|\vec{n}^0\|^2_{L^2(\Omega)}\,. \end{aligned} \tag{5.50}$$

Let us consider again (5.42). Making use of (5.44) we get:

$$\langle \partial_t\vec{n}\,,\, \vec{z}\rangle_{(H^{-1}(\Omega),H_0^1(\Omega))} \le C\|\vec{n}\|_{H_0^1(\Omega)}\|\vec{z}\|_{H_0^1(\Omega)} \qquad \forall z \in H_0^1(\Omega)\,,$$

so:

$$\|\partial_t\vec{n}\|_{H^{-1}(\Omega)} \le C\|\vec{n}\|_{H_0^1(\Omega)} \qquad \text{a.e. } t \in [0,T]\,,$$

which, together with (5.50), implies:

$$c_1\int_0^T \|\partial_t\vec{n}\|^2_{H^{-1}(\Omega)} \le C^2\left(c_2Te^{2c_2T} + \frac{1}{2}\right)\|\vec{n}^0\|^2_{L^2(\Omega)}\,. \tag{5.51}$$

From eqs. (5.50), (5.51) it follows that a constant $D > 0$ independent of σ exists such that:

$$\|\vec{n}\|_X \le D\|\vec{n}^0\|_{L^2(\Omega)}\,. \tag{5.52}$$

We define now the operator $F : [0,1] \times L^2(\Omega_T) \to L^2(\Omega_T)$ such that: for all $(\sigma, \vec{n}') \in [0,1] \times L^2(\Omega_T)$, $\vec{n} = F(\sigma, \vec{n}') \in X^3$ is the solution of eq. (5.42). We note that $F(0, \vec{n}') = 0$.

From the compact embedding $X \subset\subset C([0,T], L^2(\Omega))$ and (5.52) it follows that F is compact. Let us show that F is also continuous.

Let $\left(\vec{n}'^{(k)}\right)_{k\in\mathbb{N}} \subset L^2(\Omega_T)$ a sequence converging in $L^2(\Omega_T)$ to a function $\vec{n}' \in L^2(\Omega_T)$, and $(\sigma^{(k)})_{k\in\mathbb{N}} \subset [0,1]$ a sequence converging to σ. Let $\vec{n}^{(k)} = F(\vec{n}'^{(k)}, \sigma^{(k)}) \in$

X^3 and $\vec{b}^{\chi,k} = \vec{b}^{\chi}\left[\vec{n}'^{(k)}/n_0\right]$ for all $k \in \mathbb{N}$. The following relations hold for all $k \in \mathbb{N}$:

$$
\begin{aligned}
&\langle \partial_t n_j^{(k)}\,,\, z_j \rangle_{(H^{-1}(\Omega), H_0^1(\Omega))} = -\int \partial_s z_j \Big\{ \left(\delta_{jl} + \sigma b_r^{\chi,k} \eta_{jrl}\right) \partial_s n_l^{(k)} \\
&+ n_j^{(k)} \partial_s V - 2\eta_{jsl} n_l^{(k)} + \sigma b_r^{\chi,k} \left(\delta_{jr} n_s^{(k)} - \delta_{js} n_r^{(k)}\right) \Big\} \\
&+ \int z_j \Big\{ \eta_{jrl} n_r^{(k)} \partial_l V - 2n_j^{(k)} + \sigma b_s^{\chi,k} \partial_s n_j^{(k)} \\
&- \sigma b_j^{\chi,k} \partial_s n_s^{(k)} \Big\} \qquad \forall \vec{z} \in C_c^{\infty}(\Omega)^3\,, \\
&\vec{n}^{(k)}(t=0) = \vec{n}^0\,.
\end{aligned}
\tag{5.53}
$$

Since X is relatively compact in $L^2(\Omega_T)$ and F is compact, it follows that, up to a subsequence:

$$
\begin{aligned}
\vec{n}^{(k)} &\to \vec{n} && \text{in } L^2(\Omega_T)\,, \\
\vec{n}^{(k)} &\rightharpoonup \vec{n} && \text{in } X^3\,, \\
\partial_t \vec{n}^{(k)} &\to \partial_t \vec{n} && \text{in } H^{-1}(\Omega)\,, \\
\vec{n}'^{(k)} &\to \vec{n}' && \text{a.e. in } \Omega\,;
\end{aligned}
\tag{5.54}
$$

from Lebesgue's dominated convergence theorem and bound (5.40) follows that:

$$
b_s^{\chi}\left[\frac{\vec{n}'^{(k)}}{n_0}\right] \to b_s^{\chi}\left[\frac{\vec{n}'}{n_0}\right] \qquad \text{in } L^2(\Omega_T) \quad (s = 1, 2, 3)\,;
$$

so in the limit $k \to \infty$ from (5.53) follows:

$$
\begin{aligned}
&\langle \partial_t n_j\,,\, z_j \rangle_{(H^{-1}(\Omega), H_0^1(\Omega))} = -\int \partial_s z_j \Big\{ \left(\delta_{jl} + \sigma b_k^{\chi}\left[\frac{\vec{n}'}{n_0}\right] \eta_{jkl}\right) \partial_s n_l \\
&+ n_j \partial_s V - 2\eta_{jsl} n_l + \sigma b_k^{\chi}\left[\frac{\vec{n}'}{n_0}\right] (\delta_{jk} n_s - \delta_{js} n_k) \Big\} \\
&+ \int z_j \Big\{ \eta_{jkl} n_k \partial_l V - 2n_j + \sigma b_s^{\chi}\left[\frac{\vec{n}'}{n_0}\right] \partial_s n_j \\
&- \sigma b_j^{\chi}\left[\frac{\vec{n}'}{n_0}\right] \partial_s n_s \Big\} \qquad \forall \vec{z} \in C_c^{\infty}(\Omega)^3\,, \\
&\vec{n}(t=0) = \vec{n}^0\,;
\end{aligned}
\tag{5.55}
$$

by a density argument we conclude that $\vec{n} = F(\vec{n}', \sigma)$, which proves the continuity.

Let now assume that $\vec{n}$ is a fixed point of $F(\cdot\,, \sigma)$ for all $\sigma \in [0,1]$:

$$
F(\vec{n}, \sigma) = \vec{n} \qquad \sigma \in [0,1]\,;
\tag{5.56}
$$

from eq. (5.52) follows that a constant $K > 0$ independent from σ exists such that:

$$
\|\vec{n}\|_{L^2(\Omega_T)} \leq K \qquad \forall \sigma \in [0,1]\,.
\tag{5.57}
$$

Finally, $F(\vec{n}', 0)$ is easily shown to be independent from $\vec{n}' \in L^2(\Omega_T)$ since all the terms in (5.42) containing $\vec{n}'$ disappear when $\sigma = 0$.

So we can apply Leray-Schauder fixed point theorem [54] and find that the operator $F(\cdot\,,1) : L^2(\Omega_T) \to L^2(\Omega_T)$ has a fixed point $\vec{n} \in L^2(\Omega_T)$, that is, $\vec{n} \in X^3$ and satisfies:

$$\begin{aligned}
&\langle \partial_t n_j \,,\, z_j \rangle_{(H^{-1}(\Omega),H_0^1(\Omega))} = -\int \partial_s z_j \Bigg\{ \left(\delta_{jl} + \sigma b_k^\chi \left[\frac{\vec{n}'}{n_0}\right] \eta_{jkl} \right) \partial_s n_l \\
&+ n_j \partial_s V - 2\eta_{jsl} n_l + \sigma b_k^\chi \left[\frac{\vec{n}'}{n_0}\right] (\delta_{jk} n_s - \delta_{js} n_k) \Bigg\} \\
&+ \int z_j \Bigg\{ \eta_{jkl} n_k \partial_l V - 2n_j + \sigma b_s^\chi \left[\frac{\vec{n}'}{n_0}\right] \partial_s n_j \\
&- \sigma b_j^\chi \left[\frac{\vec{n}'}{n_0}\right] \partial_s n_s \Bigg\} \qquad \forall \vec{z} \in H_0^1(\Omega)^3 \,, \\
&\vec{n}(t=0) = \vec{n}^0 \,;
\end{aligned} \tag{5.58}$$

which means that $\vec{n} \in X^3$ is a weak solution of Problem (5.41).

□

Lemma 3 (L^∞ bound for $\vec{n}$) *The solution $\vec{n}$ of the truncated problem (5.41) belongs to $L^\infty(\Omega_T)^3$.*

Proof. Now we will prove that the solution $\vec{n}$ of (5.58) is bounded in Ω_T. To this purpose, we define the function:

$$\psi \equiv \sqrt{1 + |\vec{n}|^2} \,; \tag{5.59}$$

clearly we have: $\psi \in H_0^1(\Omega)$, $\partial_t \psi \in H^{-1}(\Omega)$. Let us scalarly multiply (5.41) by $\vec{n}/\sqrt{1+|\vec{n}|^2} \in H_0^1(\Omega)$; exploiting the antisymmetry of the tensor η_{jks}, we obtain (in the sense of distributions):

$$\begin{aligned}
\psi \partial_t \psi =& \vec{n} \cdot \partial_t \vec{n} = n_j \partial_s \Bigg[\left(\delta_{jl} + b_k^\chi \left[\frac{\vec{n}}{n_0}\right] \eta_{jkl} \right) \partial_s n_l + n_j \partial_s V \\
&- 2\eta_{jsl} n_l + b_k^\chi \left[\frac{\vec{n}}{n_0}\right] (\delta_{jk} n_s - \delta_{js} n_k) \Bigg] \\
&+ n_j \Bigg[\eta_{jkl} n_k \partial_l V - 2n_j + b_s^\chi \left[\frac{\vec{n}}{n_0}\right] \partial_s n_j - b_j^\chi \left[\frac{\vec{n}}{n_0}\right] \partial_s n_s \Bigg] \\
=& \partial_s \left[\partial_s \frac{|\vec{n}|^2}{2} + |\vec{n}|^2 \partial_s V \right] - \Bigg[\sum_{j,k} (\partial_j n_k)^2 + \frac{1}{2} \nabla |\vec{n}|^2 \cdot \nabla V \\
&+ 2\vec{n} \cdot \vec{\nabla} \wedge \vec{n} + b_k^\chi \left[\frac{\vec{n}}{n_0}\right] (\delta_{jk} n_s - \delta_{js} n_k) \partial_s n_j \Bigg] \\
&- 2|\vec{n}|^2 + n_j b_s^\chi \left[\frac{\vec{n}}{n_0}\right] \partial_s n_j - n_j b_j^\chi \left[\frac{\vec{n}}{n_0}\right] \partial_s n_s \,;
\end{aligned} \tag{5.60}$$

since from the definition of b_k (see Eq. (5.3)) it follows that $\vec{b}[\vec{v}]$ is parallel to $\vec{v}$ for all $\vec{v} \in \mathbb{R}^3$, then the terms containing $\vec{b}^\chi$ in eq. (5.60) cancel out and we obtain:

$$\partial_t \psi = \frac{1}{2\psi}\left(\Delta(|\vec{n}|^2) + 2\mathrm{div}(|\vec{n}|^2\nabla V) - \nabla V\cdot\nabla|\vec{n}|^2 - 2\mathscr{G}[\vec{n}]\right)\,, \tag{5.61}$$

where $\mathscr{G}$ is defined by:

$$\mathscr{G}[\vec{v}] \equiv \sum_{j,k}(\partial_j v_k)^2 + 2\vec{v}\cdot\mathrm{curl}\ \vec{v} + 2|\vec{v}|^2 \qquad \forall\vec{v}\in H^1(\Omega)^3\,. \tag{5.62}$$

Let us find some relations that will be helpful for our argument. We have:

$$\begin{aligned}\Delta\psi =&\partial_j\left(\frac{n_s}{\psi}\partial_j n_s\right) = \psi^{-1}\left[\partial_j(n_s\partial_j n_s) - n_s\partial_j n_s\frac{\partial_j\psi}{\psi}\right]\\ =&\psi^{-1}\left[\Delta\left(\frac{|\vec{n}|^2}{2}\right) - |\nabla\psi|^2\right]\,,\end{aligned} \tag{5.63}$$

and so:

$$\frac{1}{2\psi}\Delta(|\vec{n}|^2) = \Delta\psi + \frac{1}{\psi}|\nabla\psi|^2\,; \tag{5.64}$$

moreover it is immediate to see that:

$$\frac{1}{2\psi}\nabla V\cdot\nabla|\vec{n}|^2 = \nabla V\cdot\nabla\psi\,; \tag{5.65}$$

finally exploiting eq. (5.65) we obtain:

$$\begin{aligned}\mathrm{div}\ (\psi\nabla V) =&\nabla\psi\cdot\nabla V + \psi\Delta V = \frac{\nabla|\vec{n}|^2}{2\psi}\cdot\nabla V + \psi\Delta V\\ =&\frac{1}{2\psi}\mathrm{div}\,(|\vec{n}|^2\nabla V) - \frac{|\vec{n}|^2}{2\psi}\Delta V + \psi\Delta V\\ =&\frac{1}{2\psi}\mathrm{div}\,(|\vec{n}|^2\nabla V) + \frac{2+|\vec{n}|^2}{2\psi}\Delta V\\ =&\frac{1}{\psi}\mathrm{div}\,(|\vec{n}|^2\nabla V) + \frac{1}{\psi}\Delta V + \frac{|\vec{n}|^2}{2\psi}\Delta V - \frac{1}{2\psi}\mathrm{div}\,(|\vec{n}|^2\nabla V)\\ =&\frac{1}{\psi}\mathrm{div}\,(|\vec{n}|^2\nabla V) + \frac{1}{\psi}\Delta V - \frac{\nabla|\vec{n}|^2}{2\psi}\cdot\nabla V\\ =&\frac{1}{\psi}\mathrm{div}\,(|\vec{n}|^2\nabla V) + \frac{1}{\psi}\Delta V - \nabla\psi\cdot\nabla V\,,\end{aligned} \tag{5.66}$$

and so:

$$\frac{1}{\psi}\mathrm{div}(|\vec{n}|^2\nabla V) = \mathrm{div}(\psi\nabla V) + \nabla V\cdot\nabla\psi - \frac{1}{\psi}\Delta V\,; \tag{5.67}$$

so from eqs. (5.61), (5.64), (5.65), (5.67) we deduce:

$$\partial_t\psi = \Delta\psi + \mathrm{div}(\psi\nabla V) - \psi^{-1}\Delta V - \psi^{-1}(\mathscr{G}[\vec{n}] - |\nabla\psi|^2)\,; \tag{5.68}$$

in order to estimate the term $2\vec{v}\cdot\mathrm{curl}\ \vec{v}$ contained into $\mathscr{G}[\vec{n}]$ let us consider the expression ($\vec{v}\,:\,\Omega\to\mathbb{R}^3$ arbitrarily smooth):

$$\begin{aligned}|\mathrm{curl}\ \vec{v}|^2 =&\eta_{ijk}\partial_j v_k\,\eta_{isl}\partial_s v_l = (\delta_{js}\delta_{kl} - \delta_{jl}\delta_{ks})\,\partial_j v_k\,\partial_s v_l\\ =&\partial_j v_k\,(\partial_j v_k - \partial_k v_j) = -\partial_k v_j\,(\partial_j v_k - \partial_k v_j)\\ =&\frac{1}{2}\sum_{j,k}(\partial_j v_k - \partial_k v_j)^2 \leq \sum_{j,k}\left[(\partial_j v_k)^2 + (\partial_k v_j)^2\right]\,,\end{aligned} \tag{5.69}$$

so we have proven the following inequality:

$$|\text{curl } \vec{v}|^2 \leq 2 \sum_{j,k} (\partial_j v_k)^2 \; ; \tag{5.70}$$

then, exploiting (5.70) and applying Young inequality, from eq. (5.62) we obtain:

$$\begin{aligned} \mathscr{G}[\vec{v}] &\geq \sum_{j,k} (\partial_j v_k)^2 - 2|\vec{v}||\text{curl } \vec{v}| + 2|\vec{v}|^2 \\ &\geq \sum_{j,k} (\partial_j v_k)^2 - \alpha|\vec{v}|^2 - \frac{1}{\alpha}|\text{curl } \vec{v}|^2 + 2|\vec{v}|^2 \\ &\geq \left(1 - \frac{2}{\alpha}\right) \sum_{j,k} (\partial_j v_k)^2 + (2-\alpha)|\vec{v}|^2 \, , \end{aligned} \tag{5.71}$$

with $\alpha > 0$ arbitrary; so, for all $\vec{v} : \Omega \to \mathbb{R}^3$ smooth enough, the following estimate holds:

$$\mathscr{G}[\vec{v}] \geq \sup_{\alpha > 0} \left[\left(1 - \frac{2}{\alpha}\right) \sum_{j,k} (\partial_j v_k)^2 + (2-\alpha)|\vec{v}|^2 \right] \geq 0 \, ; \tag{5.72}$$

moreover from eq. (5.59) it follows:

$$\begin{aligned} \psi^2 \sum_{j,k} \left[\partial_j \left(\frac{n_k}{\psi} \right) \right]^2 &= \sum_{j,k} \psi^{-2} \left[\psi \partial_j n_k - n_k \partial_j \psi \right]^2 \\ &= \sum_{j,k} (\partial_j n_k)^2 - 2 \sum_{j,k} \frac{n_k}{\psi} \partial_j n_k \partial_j \psi + \frac{|\vec{n}|^2}{\psi^2} |\nabla \psi|^2 \\ &= \sum_{j,k} (\partial_j n_k)^2 + \left(\frac{|\vec{n}|^2}{\psi^2} - 2 \right) |\nabla \psi|^2 \\ &= \sum_{j,k} (\partial_j n_k)^2 - (1 + \psi^{-2}) |\nabla \psi|^2 \, ; \end{aligned} \tag{5.73}$$

so from eqs. (5.62), (5.72), (5.73) we deduce:

$$\mathscr{G}[\vec{n}] - |\nabla \psi|^2 = \psi^2 \mathscr{G}\left[\frac{\vec{n}}{\psi}\right] + \frac{|\nabla \psi|^2}{\psi^2} \geq 0 \, . \tag{5.74}$$

Now we are going to exploit eqs. (5.68), (5.74) and the boundedness of ΔV, ∇V to prove, with the Stampacchia truncations method (see e.g. [12] for details), that:

$$\psi = \sqrt{1 + |\vec{n}|^2} \in L^\infty(\Omega_T) \, , \tag{5.75}$$

and so $\vec{n} \in L^\infty(\Omega_T)^3$.
Let:

$$\begin{aligned} \tilde{M} &\equiv \sup_{\Omega} \sqrt{1 + |\vec{n}^{\,0}|^2} \, , \qquad \mu \equiv -(1 + \tilde{M}^{-1}) \sup_{\Omega_T} |\Delta V| \, , \\ \tilde{\psi} &\equiv e^{\mu t} \psi \, , \qquad \Psi \equiv (\tilde{\psi} - \tilde{M})_+ \, . \end{aligned} \tag{5.76}$$

Notice that $\Psi \in H_0^1(\Omega)$ from Lemma 1.
From eq. (5.68) we immediately find the following equation for $\tilde{\psi}$:

$$\partial_t \tilde{\psi} = \Delta\tilde{\psi} + \mathrm{div}(\tilde{\psi}\nabla V) - e^{\mu t}\psi^{-1}\Delta V - e^{\mu t}\psi^{-1}(\mathscr{G}[\vec{n}] - |\nabla\psi|^2) + \mu\tilde{\psi} . \quad (5.77)$$

By multiplying eq. (5.77) by Ψ and integrating over Ω we find:

$$\begin{aligned}\partial_t \int \frac{\Psi^2}{2} = &- \int |\nabla\Psi|^2 - \int \Psi\nabla\Psi\cdot\nabla V + \tilde{M}\int \Psi\Delta V \\ &- \int \Psi e^{\mu t}\psi^{-1}\Delta V - \int \Psi e^{\mu t}\psi^{-1}(\mathscr{G}[\vec{n}] - |\nabla\psi|^2) \\ &- \mu\int \Psi^2 + \mu\tilde{M}\int\Psi ;\end{aligned} \quad (5.78)$$

but recalling the inequality (5.74) eq. (5.78) implies:

$$\begin{aligned}\partial_t \int \frac{\Psi^2}{2} \leq &- \int |\nabla\Psi|^2 - \int \Psi\nabla\Psi\cdot\nabla V - \int\Psi^2 \\ &+ \int \Psi\left[\tilde{M}\Delta V - e^{\mu t}\psi^{-1}\Delta V + \mu\tilde{M}\right] ;\end{aligned} \quad (5.79)$$

the last integral in eq. (5.79) is nonpositive because of eq. (5.76); so applying Young inequality we find:

$$\partial_t \int \Psi^2 \leq -\int |\nabla\Psi|^2 + \left(\sup_{\Omega_T}|\nabla V| - 2\right)\int\Psi^2 ; \quad (5.80)$$

finally, recalling that $\Psi(t=0)=0$, from eq. (5.80) and Gronwall's lemma we conclude:

$$\int \Psi^2 = \int (\tilde{\psi} - M)_+^2 = \int (e^{\mu t}\psi - M)_+^2 \equiv 0$$

and so $\psi = \sqrt{1+|\vec{n}|^2} \leq Me^{-\mu t}$, which implies that $\vec{n} \in L^\infty(\Omega_T)^3$.

□

Lemma 4 (L^∞ bound for $|\vec{n}|/n_0$) *A number $\varepsilon = \varepsilon(T)$ independent from χ exists such that:*

$$|\vec{n}| \leq (1-\varepsilon)n_0 \qquad (x,t)\in\Omega_T ; \quad (5.81)$$

in particular, we can choose $\chi < \varepsilon$ so that $\vec{b}^\chi[\vec{n}/n_0] = \vec{b}[\vec{n}/n_0]$, implying that the solution $\vec{n}$ of the truncated problem (5.41) satisfies (5.3).

Proof. Let us define

$$u \equiv 1 - \frac{|\vec{n}|^2}{n_0^2} ; \quad (5.82)$$

from the fact that $\vec{n} \in \left(X^3 \cap L^\infty(\Omega_T)\right)^3$ follows that $u \in H^1(\Omega)$, $\partial_t u \in H^{-1}(\Omega)$; we will show that $\inf_{\Omega_T} u > 0$.
From eqs. (5.59), (5.61) we deduce:

$$\vec{n}\cdot\partial_t\vec{n} = \psi\partial_t\psi = \Delta(|\vec{n}|^2) + 2\mathrm{div}(|\vec{n}|^2\nabla V) - \nabla V\cdot\nabla|\vec{n}|^2 - 2\mathscr{G}[\vec{n}] ; \quad (5.83)$$

so from eqs. (5.3), (5.82), (5.83) it follows:

$$\begin{aligned}\partial_t u =& -\frac{2}{n_0^2}\vec{n}\cdot\partial_t\vec{n} + \frac{2|\vec{n}|^2}{n_0^3}\partial_t n_0\\ =& -\frac{1}{n_0^2}\left\{\Delta(|\vec{n}|^2) + 2\mathrm{div}(|\vec{n}|^2\nabla V) - \nabla V\cdot\nabla|\vec{n}|^2 - 2\mathscr{G}[\vec{n}]\right\}\\ &+\frac{2|\vec{n}|^2}{n_0^3}\left\{\Delta n_0 + \mathrm{div}\,(n_0\nabla V)\right\}.\end{aligned} \tag{5.84}$$

Let us consider the terms containing the potential:

$$\begin{aligned}&-\frac{2}{n_0^2}\mathrm{div}\,(|\vec{n}|^2\nabla V) + \frac{1}{n_0^2}\nabla V\cdot\nabla|\vec{n}|^2 + \frac{2|\vec{n}|^2}{n_0^3}\mathrm{div}\,(n_0\nabla V)\\ &=\left[-\frac{2}{n_0^2}\nabla(|\vec{n}|^2) + \frac{\nabla(|\vec{n}|^2)}{n_0^2} + \frac{2|\vec{n}|^2}{n_0^3}\nabla n_0\right]\cdot\nabla V\\ &=\left[-\frac{\nabla(|\vec{n}|^2)}{n_0^2} - |\vec{n}|^2\nabla\left(\frac{1}{n_0^2}\right)\right]\cdot\nabla V = \nabla u\cdot\nabla V\,;\end{aligned} \tag{5.85}$$

moreover from eq. (5.62) it follows:

$$\begin{aligned}\mathscr{G}\left[\frac{\vec{n}}{n_0}\right] =& \sum_{j,k}\left[\partial_j\left(\frac{n_k}{n_0}\right)\right]^2 + 2\frac{\vec{n}}{n_0}\cdot\mathrm{curl}\,\frac{\vec{n}}{n_0} + 2\left|\frac{\vec{n}}{n_0}\right|^2\\ =& \sum_{j,k}\left[\frac{\partial_j n_k}{n_0} - \frac{n_k}{n_0^2}\partial_j n_0\right]^2 + n_0^{-2}\left(2\vec{n}\cdot\mathrm{curl}\,\vec{n} + 2\,|\vec{n}|^2\right)\\ =& n_0^{-2}\mathscr{G}[\vec{n}] - 2n_0^{-3}n_k\partial_j n_k\,\partial_j n_0 + n_0^{-4}|\vec{n}|^2|\nabla n_0|^2\,;\end{aligned} \tag{5.86}$$

so from eqs. (5.84)–(5.86) we deduce:

$$\begin{aligned}\partial_t u =& \nabla u\cdot\nabla V + 2\mathscr{G}\left[\frac{\vec{n}}{n_0}\right] + 4n_0^{-3}n_k\partial_j n_k\,\partial_j n_0\\ &- 2n_0^{-4}|\vec{n}|^2|\nabla n_0|^2 - \frac{\Delta(|\vec{n}|^2)}{n_0^2} + \frac{2|\vec{n}|^2}{n_0^3}\Delta n_0\,;\end{aligned} \tag{5.87}$$

but it holds:

$$\begin{aligned}\nabla\log n_0\cdot\nabla u =& \frac{\nabla n_0}{n_0}\cdot\nabla\left(1 - \frac{|\vec{n}|^2}{n_0^2}\right)\\ =& -\frac{\partial_j n_0}{n_0}\left(\frac{2n_k\partial_j n_k}{n_0^2} - \frac{2|\vec{n}|^2}{n_0^3}\partial_j n_0\right)\\ =& \frac{2|\vec{n}|^2}{n_0^4}|\nabla n_0|^2 - \frac{2n_k\partial_j n_k\,\partial_j n_0}{n_0^3}\,;\end{aligned} \tag{5.88}$$

so we can rewrite eq. (5.87) exploiting eq. (5.88):

$$\begin{aligned}\partial_t u =& \nabla(2\log n_0 + V)\cdot\nabla u + 2\mathscr{G}\left[\frac{\vec{n}}{n_0}\right] + \mathscr{C}\,,\\ \mathscr{C} =& 8n_0^{-3}n_k\partial_j n_k\,\partial_j n_0 - 6n_0^{-4}|\vec{n}|^2|\nabla n_0|^2 - \frac{\Delta(|\vec{n}|^2)}{n_0^2} + \frac{2|\vec{n}|^2}{n_0^3}\Delta n_0\,.\end{aligned} \tag{5.89}$$

Now we find show that $\mathscr{C} = \Delta u$, in fact:

$$\begin{aligned}\Delta u = &- \Delta\left(\frac{|\vec{n}|^2}{n_0^2}\right) = -\frac{\Delta(|\vec{n}|^2)}{n_0^2} - 2\nabla(|\vec{n}|^2)\cdot\nabla(n_0^{-2}) - |\vec{n}|^2\Delta(n_0^{-2}) \\ = &- \frac{\Delta(|\vec{n}|^2)}{n_0^2} + 8n_0^{-3}n_k\partial_j n_k\,\partial_j n_0 - |\vec{n}|^2\mathrm{div}\left(-2n_0^{-3}\nabla n_0\right) \\ = &- \frac{\Delta(|\vec{n}|^2)}{n_0^2} + 8n_0^{-3}n_k\partial_j n_k\,\partial_j n_0 + 2|\vec{n}|^2\left(-3n_0^{-4}|\nabla n_0|^2 + n_0^{-3}\Delta n_0\right) \\ =&\mathscr{C}\,;\end{aligned} \tag{5.90}$$

so from eqs. (5.89), (5.90) we conclude:

$$\partial_t u = \Delta u + \nabla(2\log n_0 + V)\cdot\nabla u + 2\mathscr{G}[\vec{n}/n_0]\,. \tag{5.91}$$

We are going to prove the lower bound for u by means of the Stampacchia truncations method (see e.g. [12] for details). Let:

$$m \equiv \min\left\{\inf_{\partial\Omega\times[0,T]} u,\ \inf_{\Omega\times\{0\}} u\right\}\,, \quad U \equiv (u-m)_-\,. \tag{5.92}$$

Notice that $U \in L^2([0,T], H_0^1(\Omega))$ from Lemma 1. if we use U as a test function in the weak formulation of (5.91), after an integration by parts we find:

$$\partial_t\int\frac{U^2}{2} = -\int|\nabla U|^2 + \int U\nabla(2\log n_0 + V)\cdot\nabla U + 2\int U\mathscr{G}[\vec{n}/n_0]\,; \tag{5.93}$$

let us estimate the term:

$$\left|\int U\nabla\log n_0\cdot\nabla U\right| \le \left(\inf_{\Omega_T} n_0\right)^{-1}\int|U||\nabla n_0||\nabla U|\,; \tag{5.94}$$

applying the Young and Cauchy-Schwartz inequalities with an arbitrary $\varepsilon > 0$:

$$\begin{aligned}\int|U||\nabla n_0||\nabla U| \le&\frac{1}{2\varepsilon}\int|U|^2|\nabla n_0|^2 + \frac{\varepsilon}{2}\int|\nabla U|^2 \\ \le&\frac{1}{2\varepsilon}||\nabla n_0||^2_{L^4(\Omega)}||U||^2_{L^4(\Omega)} + \frac{\varepsilon}{2}\int|\nabla U|^2\,;\end{aligned} \tag{5.95}$$

applying Gagliardo-Nirenberg (5.11) and Young inequalities we deduce:

$$||U||^2_{L^4(\Omega)} \le c||U||_{L^2(\Omega)}||U||_{H^1(\Omega)} \le \frac{c}{2}\left(\varepsilon^{-2}||U||^2_{L^2(\Omega)} + \varepsilon^2||U||^2_{H^1(\Omega)}\right)\,; \tag{5.96}$$

from the regularity properties of n_0 we find:

$$||\nabla n_0||_{L^4(\Omega)} \le c\sup_{[0,T]}||n_0||_{H^2(\Omega)} < \infty\,; \tag{5.97}$$

so from (5.94)–(5.97) and Poincaré inequality we conclude:

$$\left|\int U\nabla\log n_0\cdot\nabla U\right| \le k(\varepsilon)\int|U|^2 + \varepsilon\tilde{k}\int|\nabla U|^2\,, \tag{5.98}$$

for some positive constants $k(\varepsilon)$, $\tilde{k}$, with $\tilde{k}$ independent from ε.
So we rewrite eq. (5.98) exploiting eqs. (5.72), (5.93):

$$\begin{aligned}\partial_t \int \frac{U^2}{2} \leq & -\int |\nabla U|^2 + \frac{1}{2\varepsilon} \sup_{\Omega\times[0,T]} |\nabla V|^2 \int U^2 + \frac{\varepsilon}{2}\int |\nabla U|^2 \\ & + k(\varepsilon)\int U^2 + \varepsilon\tilde{k}\int |\nabla U|^2 \,;\end{aligned} \tag{5.99}$$

if $\varepsilon < (\tilde{k}+1/2)^{-1}$ then:

$$\partial_t \int \frac{U^2}{2} \leq \left[k(\varepsilon) + \frac{1}{2\varepsilon} \sup_{\Omega\times[0,T]} |\nabla V|^2 \right] \int \frac{U^2}{2} \,; \tag{5.100}$$

so, since $U(t=0) \equiv 0$ in Ω from eq. (5.36), we conclude from Gronwall's lemma that $U = (u-m)_- \equiv 0$ in $\Omega \times [0,T]$ and so $u \geq m$, which means $|\vec{n}| < Cn_0$ in Ω_T for some constant $0 < C < 1$ which is clearly independent from χ.

□

Lemma 5 (Uniqueness of solutions) *If $\vec{u}$, $\vec{v}$ are solutions of (5.3) satisfying (5.37) and $\vec{u}$, $\vec{v} \in L^\infty([0,T], W^{1,4}(\Omega))^3$, then $\vec{u} = \vec{v}$ a.e. on Ω_T.*

Proof. Let $\vec{w} = \vec{u} - \vec{v}$. Taking the difference of the equations satisfied by $\vec{u}$ and $\vec{v}$, respectively, and employing $\vec{w} \in L^2([0,T], H^1_0(\Omega))$ as a test function, we find that:

$$\begin{aligned}&\frac{1}{2}\frac{d}{dt}\int |\vec{w}|^2 + \int \|\nabla \vec{w}\|^2 \leq \int \big\{ -w_j \partial_k w_j \partial_k V + 2\eta_{jk\ell} w_\ell \partial_k w_j \\ &- (b_k[\vec{u}] - b_k[\vec{v}])(\eta_{jk\ell}\partial_s u_\ell + \delta_{jk} u_s - \delta_{js} u_k)\partial_s w_j - b_k[\vec{v}](\delta_{jk} w_s - \delta_{js} w_k)\partial_s w_j \big\} \\ &+ \int \big\{ (\eta_{jk\ell} w_k \partial_\ell V - 2w_j) w_j + [(b_s[\vec{u}] - b_s[\vec{v}])\partial_s u_j + b_s[\vec{v}]\partial_s w_j] w_j \\ &- [(b_j[\vec{u}] - b_j[\vec{v}])\partial_s u_s + b_j[\vec{v}]\partial_s w_s] w_j \big\} \,.\end{aligned}$$

Thanks to the L^∞ bounds on ∇V, $\vec{u}$, and $\vec{v}$, we can estimate as follows:

$$\begin{aligned}\frac{1}{2}\frac{d}{dt}\int |\vec{w}|^2 &\leq -\int \|\nabla \vec{w}\|^2 + c\int \big(|\vec{w}|\,\|\nabla \vec{w}\| + \|\nabla \vec{u}\|\,|\vec{w}|^2 + \|\nabla \vec{u}\|\,|\vec{w}|\,|\nabla \vec{w}\| \big) \\ &\leq -\frac{1}{2}\int \|\nabla \vec{w}\|^2 + c\|\nabla \vec{u}\|_{L^4(\Omega_T)}(1 + \|\nabla \vec{u}\|_{L^4(\Omega_T)})\int |\vec{w}|^2 \,,\end{aligned}$$

where $c > 0$ is some generic constant.
Let us estimate now the following integral by exploiting the $W^{1,4}$ regularity for $\vec{u}$:

$$\begin{aligned}\int |\nabla u||w||\nabla w| \leq& \frac{1}{2\varepsilon}\int |\nabla u|^2 |w|^2 + \frac{\varepsilon}{2}\int |\nabla w|^2 \\ \leq& \frac{1}{2\varepsilon}\left[\sup_{[0,T]} ||\nabla u||^2_{L^4(\Omega)} \right] ||w||^2_{L^4(\Omega)} + \frac{\varepsilon}{2}\int |\nabla w|^2 \\ \leq& \frac{K}{2\varepsilon} ||w||_{L^2(\Omega)} ||w||_{H^1(\Omega)} + \frac{\varepsilon}{2}\int |\nabla w|^2 \\ \leq& \frac{K}{4\varepsilon^2}\int |w|^2 + \varepsilon K' \int |\nabla w|^2 \,,\end{aligned}$$

with $\varepsilon > 0$ arbitrary constant and K, $K' > 0$ suitable constants independent from ε. So, choosing $\varepsilon > 0$ small enough, we obtain:

$$\frac{d}{dt}\int |w|^2 \leq K'' \int |\vec{w}|^2 \,, \qquad \vec{w}(t=0) = \vec{u}(t=0) - \vec{v}(t=0) = 0 \,,$$

for $K'' > 0$ suitable constant. By applying Gronwall's inequality we conclude that $\vec{w} \equiv 0$ a.e. on Ω_T.

□

The proof of Theorem 4 is now concluded.

In the next section we shall prove an entropy dissipation relation for model QSDE1 (5.2), (5.3).

5.4 Entropicity of the system

Let $(n_0, \vec{n}, V)$ be a solution to eqs. (5.2), (5.3) according to Theorems 3 and 4. We assume boundary data of global thermal equilibrium for the charge density n_0 and vanishing spin vector $\vec{n}$, i.e.

$$n_\Gamma = e^{-\mathcal{U}}, \quad V = \mathcal{U}, \quad \vec{n} = 0 \quad \text{on } \partial\Omega, \tag{5.101}$$

where $\mathcal{U} = \mathcal{U}(x)$ is time-independent. We remark that the first equation in (5.101) makes sense because we are working with dimensionless variables. In this subsection, we will show that the macroscopic entropy

$$S(t) = \int_\Omega \Big(\frac{1}{2}(n_0 + |\vec{n}|)\big(\log(n_0 + |\vec{n}|) - 1\big) + \frac{1}{2}(n_0 - |\vec{n}|)\big(\log(n_0 - |\vec{n}|) - 1\big) \\ + (n_0 - C(x))V - \frac{\lambda_D^2}{2}|\nabla V|^2 \Big)\, dx \tag{5.102}$$

is nonincreasing in time. Note that $n_0 < |\vec{n}|$ by Theorem 3 and then $\log(n_0 - |\vec{n}|)$ is well defined.

The functional $S(t)$ can be derived as follows. Inserting the thermal equilibrium distribution $g[n_0, \vec{n}]$ in the quantum entropy $A[w]$ defined by eq. (2.3) and taking into account the electric energy contribution, it follows that the total macroscopic free energy reads as

$$\widetilde{S}(t) = A[g[n_0, \vec{n}]] - \int_\Omega \Big(C(x)V + \frac{\lambda_D^2}{2}|\nabla V|^2 \Big)\, dx.$$

Then the semiclassical expansion of $g[n_0, \vec{n}]$ yields the above formula for $\widetilde{S}(t) = S(t) + O(\epsilon)$.

In fact, from eqs. (2.3), (4.61) we find immediately:

$$\begin{aligned} \mathcal{A}[g[n_0, \vec{n}]] &= \operatorname{tr} \iint g[n_0, \vec{n}] \left(-A\sigma_0 - \vec{B}\cdot\vec{\sigma} - I \right) dx dp \\ &= -\int \left((A+1)n_0 + \vec{B}\cdot\vec{n} \right) dx \,. \end{aligned} \tag{5.103}$$

Notice that from eqs. (5.2), (5.101) it follows that $\int \partial_t n_0 \, dx = 0$, so the total charge $\int n_0 \, dx$ is constant in time; since we are interested in an estimate for $\partial_t S$, we can neglect terms proportional to $\int n_0 \, dx$ in the expression for $\widetilde{S}$. From eqs. (4.71) we obtain:

$$\begin{aligned} -A &= -\log(2\pi) + \log\sqrt{n_0^2 - |\vec{n}|^2} + O(\epsilon^2)\,, \\ -\vec{B} &= \frac{\vec{n}}{|\vec{n}|}\log\sqrt{\frac{n_0 + |\vec{n}|}{n_0 - |\vec{n}|}} + O(\epsilon^2)\,, \end{aligned} \tag{5.104}$$

so eq. (5.103) becomes:

$$\mathcal{A}[g[n_0, \vec{n}]] = \int \left(n_0 \log\sqrt{n_0^2 - |\vec{n}|^2} + |\vec{n}| \log\sqrt{\frac{n_0 + |\vec{n}|}{n_0 - |\vec{n}|}} \right) + O(\epsilon^2)\,; \tag{5.105}$$

then we conclude that the total macroscopic free energy $\widetilde{S}$ can be approximated up to $O(\epsilon^2)$ terms by the entropy S.

Proposition 15 *The entropy dissipation dS/dt can be written as:*

$$\begin{aligned} \frac{dS}{dt} =& -\frac{1}{2}\int (n_0 + |\vec{n}|)\,|\nabla(\log(n_0 + |\vec{n}|) + V)|^2 \\ & -\frac{1}{2}\int (n_0 - |\vec{n}|)\,|\nabla(\log(n_0 - |\vec{n}|) + V)|^2 \\ & -\frac{1}{2}\int |\vec{n}| \log\left(\frac{n_0 + |\vec{n}|}{n_0 - |\vec{n}|}\right) \mathscr{G}\left[\frac{\vec{n}}{|\vec{n}|}\right] \le 0\,, \end{aligned} \tag{5.106}$$

with $\mathscr{G}$ given by (5.62).

Proof. In order to compute the time derivative of S, let us first consider the function inside the first integral in (5.102). Putting:

$$\rho = \frac{1}{2}\sum_{\zeta=\pm} (n_0 + \zeta|\vec{n}|)\left[\log(n_0 + \zeta|\vec{n}|) - 1 + V\right]\,; \tag{5.107}$$

from elementary computations follows:

$$\begin{aligned} \partial_t \rho =& \rho_1 \partial_t n_0 + \vec{\rho}_2 \cdot \partial_t \vec{n}\,, \\ \rho_1 =& \log\sqrt{n_0^2 - |\vec{n}|^2} + V\,, \qquad \vec{\rho}_2 = \frac{\vec{n}}{|\vec{n}|}\log\sqrt{\frac{n_0 + |\vec{n}|}{n_0 - |\vec{n}|}}\,; \end{aligned} \tag{5.108}$$

from the regularity results contained in Theorems 3, 4 we can easily prove that $\rho_1 \in L^2(\Omega_T)$, $\rho_2 \in L^2([0,T], H_0^1(\Omega))$, so we can exchange integration and time derivation and write:

$$\begin{aligned} \frac{dS}{dt} =& \int \left[\left(\log\sqrt{n_0^2 - |\vec{n}|^2} + V \right) \partial_t n_0 + \frac{1}{|\vec{n}|}\log\sqrt{\frac{n_0 + |\vec{n}|}{n_0 - |\vec{n}|}}\,\vec{n} \cdot \partial_t \vec{n} \right] \\ & + \int n_0 \partial_t V - \partial_t \int \left(CV + \frac{\lambda_D^2}{2}|\nabla V|^2 \right)\,, \end{aligned} \tag{5.109}$$

where the second term in the first integral of eq. (5.109) makes sense since $\partial\vec{n} \in L^2([0,T], H^{-1}(\Omega))^3$ and $\frac{\vec{n}}{|\vec{n}|}\log\sqrt{\frac{n_0+|\vec{n}|}{n_0-|\vec{n}|}} \in L^2([0,T], H_0^1(\Omega))^3$. from (5.1), (5.101) (in particular from the fact that $\partial_t V$ vanishes in $\partial\Omega$) we find:

$$\int n_0 \partial_t V = \int (C - \lambda_D^2 \Delta V)\partial_t V = \partial_t \int \left(CV + \frac{\lambda_D^2}{2}|\nabla V|^2 \right) ; \tag{5.110}$$

moreover from (5.3) we deduce:

$$\vec{n}\cdot\partial_t\vec{n} = \Delta\left(\frac{|\vec{n}|^2}{2}\right) + \operatorname{div}\left(|\vec{n}|^2\nabla V\right) - \nabla\left(\frac{|\vec{n}|^2}{2}\right)\cdot\nabla V - \mathscr{G}[\vec{n}] ; \tag{5.111}$$

so from (5.2), (5.109), (5.110), (5.111) we find:

$$\begin{aligned} \frac{dS}{dt} = \int \Bigg\{ & \left(\log\sqrt{n_0^2 - |\vec{n}|^2} + V\right)\operatorname{div}(\nabla n_0 + n_0\nabla V) \\ & + \frac{1}{|\vec{n}|}\log\sqrt{\frac{n_0+|\vec{n}|}{n_0-|\vec{n}|}}\left[\Delta\left(\frac{|\vec{n}|^2}{2}\right) + \operatorname{div}\left(|\vec{n}|^2\nabla V\right)\right. \\ & \left. - \nabla\left(\frac{|\vec{n}|^2}{2}\right)\cdot\nabla V - \mathscr{G}[\vec{n}]\right]\Bigg\} ; \end{aligned} \tag{5.112}$$

from (5.112) follows integrating by parts:

$$\begin{aligned} \frac{dS}{dt} = -\int \Bigg\{ & \nabla\left(\log\sqrt{n_0^2 - |\vec{n}|^2} + V\right)\cdot(\nabla n_0 + n_0\nabla V) \\ & + \nabla\left(\frac{1}{|\vec{n}|}\log\sqrt{\frac{n_0+|\vec{n}|}{n_0-|\vec{n}|}}\right)\cdot\left[\nabla\left(\frac{|\vec{n}|^2}{2}\right) + |\vec{n}|^2\nabla V\right] \\ & + \frac{1}{|\vec{n}|}\log\sqrt{\frac{n_0+|\vec{n}|}{n_0-|\vec{n}|}}\left[\nabla\left(\frac{|\vec{n}|^2}{2}\right)\cdot\nabla V + \mathscr{G}[\vec{n}]\right]\Bigg\} , \end{aligned} \tag{5.113}$$

and so:

$$\begin{aligned} \frac{dS}{dt} = -\int \Bigg\{ & \nabla\left(\log\sqrt{n_0^2 - |\vec{n}|^2} + V\right)\cdot(\nabla n_0 + n_0\nabla V) \\ & + \frac{1}{|\vec{n}|}\nabla\left(\log\sqrt{\frac{n_0+|\vec{n}|}{n_0-|\vec{n}|}}\right)\cdot\left[\nabla\left(\frac{|\vec{n}|^2}{2}\right) + |\vec{n}|^2\nabla V\right]\Bigg\} \\ & - \int \log\sqrt{\frac{n_0+|\vec{n}|}{n_0-|\vec{n}|}}\Bigg\{\nabla\left(\frac{1}{|\vec{n}|}\right)\cdot\left[\nabla\left(\frac{|\vec{n}|^2}{2}\right) + |\vec{n}|^2\nabla V\right] \\ & + \frac{1}{|\vec{n}|}\left[\nabla\left(\frac{|\vec{n}|^2}{2}\right)\cdot\nabla V + \mathscr{G}[\vec{n}]\right]\Bigg\} ; \end{aligned} \tag{5.114}$$

from a computation very similar to the one shown in eq. (5.86) we obtain:

$$\begin{aligned} \mathscr{G}\left[\frac{\vec{n}}{|\vec{n}|}\right] & = |\vec{n}|^{-2}\mathscr{G}[\vec{n}] - 2|\vec{n}|^{-3} n_k \partial_j n_k\, \partial_j|\vec{n}| + |\vec{n}|^{-2}|\nabla|\vec{n}|\,|^2 \\ & = |\vec{n}|^{-2}\mathscr{G}[\vec{n}] - |\vec{n}|^{-2}|\nabla|\vec{n}|\,|^2 \\ & = |\vec{n}|^{-2}\mathscr{G}[\vec{n}] + |\vec{n}|^{-1}\nabla\left(\frac{1}{|\vec{n}|}\right)\cdot\nabla\left(\frac{|\vec{n}|^2}{2}\right) , \end{aligned} \tag{5.115}$$

which leads to:

$$\begin{aligned}|\vec{n}|\mathscr{G}\left[\frac{\vec{n}}{|\vec{n}|}\right] =&\nabla\left(\frac{1}{|\vec{n}|}\right)\cdot\left[\nabla\left(\frac{|\vec{n}|^2}{2}\right)+|\vec{n}|^2\nabla V\right]\\ &+\frac{1}{|\vec{n}|}\left[\nabla\left(\frac{|\vec{n}|^2}{2}\right)\cdot\nabla V+\mathscr{G}[\vec{n}]\right];\end{aligned} \tag{5.116}$$

so rearranging the terms in the first integral in (5.114) and applying (5.116) in the second one, we find:

$$\begin{aligned}\frac{dS}{dt} =&-\frac{1}{2}\int\Big\{\nabla(\log(n_0+|\vec{n}|)+V)\cdot(\nabla(n_0+|\vec{n}|)+(n_0+|\vec{n}|)\nabla V)\\ &+\nabla(\log(n_0-|\vec{n}|)+V)\cdot(\nabla(n_0-|\vec{n}|)+(n_0-|\vec{n}|)\nabla V)\Big\}\\ &-\int|\vec{n}|\log\sqrt{\frac{n_0+|\vec{n}|}{n_0-|\vec{n}|}}\mathscr{G}\left[\frac{\vec{n}}{|\vec{n}|}\right].\end{aligned} \tag{5.117}$$

We observe that the expression

$$|\vec{n}|\log\left(\frac{n_0+|\vec{n}|}{n_0-|\vec{n}|}\right)\mathscr{G}\left[\frac{\vec{n}}{|\vec{n}|}\right]=\frac{1}{n_0}\frac{1}{|\vec{n}|/n_0}\log\left(\frac{1+|\vec{n}|/n_0}{1-|\vec{n}|/n_0}\right)|\vec{n}|^2\mathscr{G}\left[\frac{\vec{n}}{|\vec{n}|}\right]$$

is integrable because $\inf_{\Omega_T} n_0>0$, $\sup_{\Omega_T}|\vec{n}|/n_0<1$, the map

$$(0,1-\varepsilon)\to\mathbb{R},\quad x\mapsto\frac{1}{x}\log\left(\frac{1+x}{1-x}\right)$$

is bounded for all $\varepsilon>0$ and $|\vec{n}|^2\mathscr{G}[\vec{n}/|\vec{n}|]\in L^1(\Omega_T)$ (see eqs. (5.62), (5.115)). Since

$$\nabla(n_0\pm|\vec{n}|)+(n_0\pm|\vec{n}|)\nabla V=(n_0\pm|\vec{n}|)\nabla\big(\log(n_0\pm|\vec{n}|)+V\big),$$

from eq. (5.117) we immediately obtain eq. (5.106).

□

5.5 Long-time decay of the solutions

Let $(n_0,\vec{n},V)$ be a solution to (5.2), (5.3), according to Theorems 3 and 4. We will show that, under suitable assumptions on the electric potential, the spin vector converges to zero as $t\to\infty$.
We start by proving the following:

Lemma 6 *Let $\mathscr{G}$ given by eq. (5.62). A constant $\mathcal{K}_\Omega>0$ exists, depending only on Ω, such that:*

$$\int\mathscr{G}[\vec{u}]\geq\mathcal{K}_\Omega\int|\vec{u}|^2,\quad\forall\vec{u}\in H^1(\Omega)^3. \tag{5.118}$$

Proof. Let $\mu > 0$, and let $B_\mu(\vec{u}, \vec{v})$ the following bilinear form on $H_0^1(\Omega)^3$:

$$B_\mu(\vec{u}, \vec{v}) = \int \left[\sum_{j,k} \partial_j u_k \, \partial_j v_k + \vec{u} \cdot \text{curl } \vec{v} + \vec{v} \cdot \text{curl } \vec{u} + (2 + \mu) \vec{u} \cdot \vec{v} \right] . \quad (5.119)$$

We point out that from eqs. (5.62), (5.119) follows:

$$B_\mu(\vec{u}, \vec{u}) = \int_\Omega \mathscr{G}[\vec{u}] + \mu \int_\Omega |\vec{u}|^2 dx \qquad \forall \vec{u} \in H_0^1(\Omega)^3 . \quad (5.120)$$

The bilinear form B is symmetric, continuous, and coercive on $H_0^1(\Omega)^3$; in fact, exploiting eq. (5.71) with $\alpha = 2 + \mu$, eq. (5.120) and the Poincaré inequality:

$$\begin{aligned} B_\mu(\vec{u}, \vec{u}) &\geq \int_\Omega \left(1 - \frac{2}{\alpha} \right) \sum_{j,k} (\partial_j u_k)^2 + \int_\Omega (2 - \alpha) |\vec{u}|^2 + \mu \int_\Omega |\vec{u}|^2 dx \\ &= \int_\Omega \left(1 - \frac{2}{2 + \mu} \right) \sum_{j,k} (\partial_j u_k)^2 \geq c \left(1 - \frac{2}{2 + \mu} \right) \|\vec{u}\|^2_{H_0^1(\Omega)} . \end{aligned} \quad (5.121)$$

Hence by the Lax-Milgram lemma for all $\vec{f} \in L^2(\Omega)^3$ there exist a unique solution $\vec{u} \in H_0^1(\Omega)$ to:

$$B(\vec{u}, \vec{v}) = \int \vec{f} \cdot \vec{v} \qquad \forall \vec{v} \in H_0^1(\Omega)^3 . \quad (5.122)$$

This defines a linear operator $\mathcal{T}_\mu : L^2(\Omega)^3 \to L^2(\Omega)^3$, $\mathcal{T}_\mu(\vec{f}) = \vec{u}$. Moreover, $\mathcal{T}_\mu(L^2(\Omega)^3) \subset H_0^1(\Omega)^3$, $\mathcal{T}_\mu$ is compact (since B is coercive and the embedding $H_0^1(\Omega) \subset L^2(\Omega)$ is compact), symmetric (since B is symmetric), and positive, that is: $\int \vec{f} \cdot \mathcal{T}_\mu(\vec{f}) > 0$ for all $\vec{f} \in L^2(\Omega)$ (since B is coercive). By the Hilbert-Schmidt theorem for symmetric compact operators (see, e.g., [44, Theorem VI.16]), there exists a complete orthonormal system $(\vec{u}^{(k)})$ of $L^2(\Omega)$ of eigenfunctions of the operator $\mathcal{T}_\mu$:

$$\mathcal{T}_\mu(\vec{u}^{(k)}) = \lambda_k \vec{u}^{(k)} , \quad 0 < \lambda_k \searrow 0 , \quad \int \vec{u}^{(j)} \cdot \vec{u}^{(k)} = \delta_{jk} \qquad \forall j, k \in \mathbb{N} . \quad (5.123)$$

Note that, since $\mathcal{T}_\mu(L^2(\Omega)^3) \subset H_0^1(\Omega)^3$, $(\vec{u}^{(k)})_{k \in \mathbb{N}} \subset H_0^1(\Omega)^3$.
From (5.122), (5.123) it follows:

$$B_\mu(\vec{u}^{(k)}, \vec{v}) = \lambda_k^{-1} \int \vec{u}^{(k)} \cdot \vec{v} \qquad \forall k \in \mathbb{N} , \; \forall \vec{v} \in H_0^1(\Omega) . \quad (5.124)$$

We want to prove that $\lambda_1^{-1} > \mu$. Let us suppose $\lambda_1^{-1} \leq \mu$; then from eqs. (5.119), (5.120), (5.124) we deduce:

$$\int_\Omega \mathscr{G}[\vec{u}^{(1)}] = B_\mu(\vec{u}^{(1)}, \vec{u}^{(1)}) - \mu \int_\Omega |\vec{u}^{(1)}|^2 = (\lambda_1^{-1} - \mu) \int_\Omega |\vec{u}^{(1)}|^2 \leq 0 ,$$

and so, since $\mathscr{G}[\vec{u}] \geq 0$ (see eq. (5.72)), from the definition (5.62) of $\mathscr{G}$ we obtain:

$$\mathscr{G}[\vec{u}^{(1)}] = \sum_{j,k} \left(\partial_j u_k^{(1)} \right)^2 + 2 \vec{u}^{(1)} \cdot \text{curl } \vec{u}^{(1)} + 2 |\vec{u}^{(1)}|^2 \equiv 0 . \quad (5.125)$$

From eq. (5.70), (5.125) it follows:

$$|\text{curl } \vec{u}^{(1)}|^2 + 4\vec{u}^{(1)} \cdot \text{curl } \vec{u}^{(1)} + 4|\vec{u}^{(1)}|^2 \leq 0\,, \tag{5.126}$$

and so:

$$|\text{curl } \vec{u}^{(1)} + 2\vec{u}^{(1)}|^2 \leq 0\,; \tag{5.127}$$

moreover, since in eq. (5.127) the equal sign must hold almost everywhere (a.e.), then it has to hold a.e. also in eq. (5.70); this means that the Young inequality in eq. (5.69) must hold a.e. with the equal sign and so:

$$\partial_j u_k^{(1)} = -\partial_k u_j^{(1)} \qquad (j,k = 1,2,3)\,; \tag{5.128}$$

so collecting eqs. (5.127), (5.128) we obtain:

$$\text{curl } \vec{u}^{(1)} = -2\vec{u}^{(1)}\,, \quad \partial_j u_k^{(1)} = -\partial_k u_j^{(1)} \quad (j,k = 1,2,3)\,; \tag{5.129}$$

but since $\Omega \subset \mathbb{R}^2$ then from eq. (5.129) it follows:

$$\begin{aligned} -2u_1^{(1)} =& \partial_2 u_3^{(1)} - \partial_3 u_2^{(1)} = -2\partial_3 u_2^{(1)} \equiv 0\,, \\ -2u_2^{(1)} =& \partial_3 u_1^{(1)} - \partial_1 u_3^{(1)} = 2\partial_3 u_1^{(1)} \equiv 0\,, \\ -2u_3^{(1)} =& \partial_1 u_2^{(1)} - \partial_2 u_1^{(1)} \equiv 0\,. \end{aligned} \tag{5.130}$$

We have concluded that $\vec{u}^{(1)} \equiv 0$ in Ω, and this is absurd. Then $\lambda_1^{-1} > \mu$.
Now let $\vec{u} \in H_0^1(\Omega)^3 \cap H^2(\Omega)^3$. We can write: $\vec{u} = \sum_{k \in \mathbb{N}} \alpha_k \vec{u}^{(k)}$, with the series converging in $L^2(\Omega)$. By an easy integration by parts we find that:

$$\int_\Omega \vec{v} \cdot \text{curl } \vec{w} = \int_\Omega \vec{w} \cdot \text{curl } \vec{v} \qquad \forall \vec{v},\, \vec{w} \in H_0^1(\Omega)\,; \tag{5.131}$$

so from eqs. (5.119), (5.131) we obtain, again integrating by parts:

$$\begin{aligned} B_\mu(\vec{u},\vec{u}) &= \int_\Omega \vec{u} \cdot \{-\Delta\vec{u} + 2\text{curl } \vec{u} + (2+\mu)\vec{u}\} \\ &= \int_\Omega \sum_{j\in\mathbb{N}} \alpha_j \vec{u}^{(j)} \cdot \{-\Delta\vec{u} + 2\text{curl } \vec{u} + (2+\mu)\vec{u}\} \\ &= \sum_{j\in\mathbb{N}} \alpha_j \int_\Omega \vec{u}^{(j)} \cdot \{-\Delta\vec{u} + 2\text{curl } \vec{u} + (2+\mu)\vec{u}\} \\ &= \sum_{j\in\mathbb{N}} \alpha_j \int_\Omega \vec{u} \cdot \{-\Delta\vec{u}^{(j)} + 2\text{curl } \vec{u}^{(j)} + (2+\mu)\vec{u}^{(j)}\} \\ &= \sum_{j,k\in\mathbb{N}} \alpha_j\alpha_k \int_\Omega \vec{u}^{(k)} \cdot \{-\Delta\vec{u}^{(j)} + 2\text{curl } \vec{u}^{(j)} + (2+\mu)\vec{u}^{(j)}\} \\ &= \sum_{j,k\in\mathbb{N}} \alpha_j\alpha_k B_\mu(\vec{u}^{(j)},\vec{u}^{(k)})\,. \end{aligned} \tag{5.132}$$

We point out that (5.132) is not trivial, since B_μ is countinuous on $H_0^1(\Omega)^3$, while the series $\vec{u} = \sum_{k\in\mathbb{N}} \alpha_k \vec{u}^{(k)}$ is only convergent in $L^2(\Omega)^3$. Collecting eqs. (5.132), (5.123), (5.124) we find:

$$\begin{aligned}B_\mu(\vec{u},\vec{u}) =& \sum_{j,k\in\mathbb{N}} \alpha_j\alpha_k\lambda_j^{-1}\int_\Omega \vec{u}^{(j)}\cdot\vec{u}^{(k)} = \sum_{j\in\mathbb{N}}\alpha_j^2\lambda_j^{-1}\int_\Omega |\vec{u}^{(j)}|^2 \\ \geq& \lambda_1^{-1}||\vec{u}||^2_{L^2(\Omega)}\,;\end{aligned} \tag{5.133}$$

by a density argument we deduce that eq. (5.133) holds for all $\vec{u}\in H_0^1(\Omega)$. From the fact that $\lambda_1^{-1}>\mu$ and eq. (5.120) we conclude that (5.118) holds with $\mathcal{K}_\Omega=\lambda_1^{-1}-\mu>0$.

□

We are now able to prove the following:

Theorem 5 *Let $\mathcal{K}_\Omega$ as in (5.118), and let $2<p<\infty$ arbitrary.*

1 *A positive constant $c=c(p,\Omega)$ exists such that: if $\sup_{\Omega_T}|\nabla V|<c$ then:*

$$\|\vec{n}\|_{L^p(\Omega)}(t)\leq\|\vec{n}_I\|_{L^p(\Omega)}e^{-kt}\qquad\forall t>0\,, \tag{5.134}$$

for a suitable number $k=k(p,\Omega,\sup_{\Omega_T}|\nabla V|)>0$.

2 *If $\sup_{\Omega_T}\Delta V<\mathcal{K}_\Omega$ then:*

$$\|\vec{n}\|_{L^2(\Omega)}(t)\leq\|\vec{n}_I\|_{L^2(\Omega)}e^{-k't}\qquad\forall t>0\,, \tag{5.135}$$

with $k'=2\mathcal{K}_\Omega-\sup_{\Omega_T}\Delta V>0$.

3 *If $\sup_{\Omega_T}\Delta V<0$ then:*

$$\|\vec{n}\|_{L^\infty(\Omega)}(t)\leq\|\vec{n}_I\|_{L^\infty(\Omega)}e^{-k''t}\qquad\forall t>0\,, \tag{5.136}$$

with $k''=-\sup_{\Omega_T}\Delta V>0$.

Proof. Let us prove the first point. Since $p>2$, from the smoothness properties of $\vec{n}$, n_0 and the bound (5.37) on $\vec{n}$ it follows that $|\vec{n}|^{p-2}\vec{n}\in H_0^1(\Omega)$. So integrating the differential equation in (5.3) against the test function $p|\vec{n}|^{p-2}\vec{n}$ and recalling eq. (5.111) we find:

$$\begin{aligned}\partial_t\int|\vec{n}|^p =& \langle\partial_t\vec{n},\,p|\vec{n}|^{p-2}\vec{n}\rangle_{(H^{-1},\,H_0^1)} = \int p|\vec{n}|^{p-2}\Bigg\{\Delta\left(\frac{|\vec{n}|^2}{2}\right) \\ &+\operatorname{div}\left(|\vec{n}|^2\nabla V\right)-\nabla\left(\frac{|\vec{n}|^2}{2}\right)\cdot\nabla V-\mathscr{G}[\vec{n}]\Bigg\}\,;\end{aligned} \tag{5.137}$$

let us consider first:

$$\begin{aligned}\int p|\vec{n}|^{p-2}\Delta\left(\frac{|\vec{n}|^2}{2}\right) &= -\int\frac{p}{2}\nabla(|\vec{n}|^{p-2})\cdot\nabla(|\vec{n}|^2) \\ &= -\int\frac{p(p-2)}{4}(|\vec{n}|^2)^{p/2-2}|\nabla(|\vec{n}|^2)|^2 \\ &= -\int\frac{p(p-2)}{4}\left|(|\vec{n}|^2)^{p/4-1}\nabla(|\vec{n}|^2)\right|^2 \\ &= -\int\frac{p(p-2)}{4}\left|\frac{4}{p}\nabla(|\vec{n}|^2)^{p/4}\right|^2 \\ &= -\frac{4(p-2)}{p}\int|\nabla|\vec{n}|^{p/2}|^2\,;\end{aligned} \tag{5.138}$$

now let us compute:

$$\begin{aligned}
&\int p|\vec{n}|^{p-2}\left\{\operatorname{div}\left(|\vec{n}|^2\nabla V\right) - \nabla\left(\frac{|\vec{n}|^2}{2}\right)\cdot\nabla V\right\} \\
&= -\int\left\{p\nabla(|\vec{n}|^{p-2})\cdot|\vec{n}|^2\nabla V + p|\vec{n}|^{p-2}\nabla\left(\frac{|\vec{n}|^2}{2}\right)\cdot\nabla V\right\} \\
&= -\int p\nabla(|\vec{n}|^p)\cdot\nabla V + \int\frac{p}{2}|\vec{n}|^{p-2}\nabla(|\vec{n}|^2)\cdot\nabla V \\
&= -\int p\nabla(|\vec{n}|^p)\cdot\nabla V + \int\nabla(|\vec{n}|^p)\cdot\nabla V \\
&= -\int(p-1)\nabla(|\vec{n}|^p)\cdot\nabla V\,;
\end{aligned} \tag{5.139}$$

so from eqs. (5.137)–(5.139) we deduce:

$$\begin{aligned}
\partial_t\int|\vec{n}|^p = &-\frac{4(p-2)}{p}\int|\nabla|\vec{n}|^{p/2}|^2 - (p-1)\int\nabla V\cdot\nabla|\vec{n}|^p \\
&-p\int|\vec{n}|^{p-2}\mathscr{G}[\vec{n}]\,.
\end{aligned} \tag{5.140}$$

Let us exploit the fact that $\mathscr{G}[\vec{n}]\geq 0$ (see eq. (5.72)):

$$\partial_t\int|\vec{n}|^p \leq -\frac{4(p-2)}{p}\int|\nabla|\vec{n}|^{p/2}|^2 - (p-1)\int\nabla V\cdot\nabla|\vec{n}|^p\,; \tag{5.141}$$

now, since $\vec{n}\in H_0^1(\Omega)^3$, from Poincaré inequality we deduce that a constant $C>0$ exists such that:

$$\int|\nabla|\vec{n}|^{p/2}|^2 \geq C\int|\vec{n}|^p\,; \tag{5.142}$$

moreover from Cauchy-Schwartz and Young inequalities we get:

$$\left|\int\nabla V\cdot\nabla|\vec{n}|^p\right| \leq \frac{1}{\alpha}\sup_{\Omega_T}|\nabla V|^2\int|\vec{n}|^p + \alpha\int|\nabla|\vec{n}|^{p/2}|^2\,,\quad\forall\alpha>0\,; \tag{5.143}$$

so from (5.142), (5.143) we conclude, choosing $\alpha>0$ small enough:

$$\partial_t\int|\vec{n}|^p \leq \left(k_1\sup_{\Omega_T}|\nabla V|^2 - k_2\right)\int|\vec{n}|^p\,, \tag{5.144}$$

with k_1, $k_2>0$ suitable constants, depending only on Ω, p. So by applying Gronwall's Lemma the estimate (5.134) is proved.

Now let us prove the second point. Writing (5.140) for $p=2$, integrating by parts and using (5.118) we find:

$$\partial_t\int|\vec{n}|^2 \leq \sup_{\Omega_T}\Delta V\int|\vec{n}|^2 - 2\int\mathscr{G}[\vec{n}] \leq \left(\sup_{\Omega_T}\Delta V - 2\mathcal{K}_\Omega\right)\int|\vec{n}|^2\,, \tag{5.145}$$

which immediately implies (5.135).

Finally let us prove the third point. From (5.141) we easily deduce, by an integration by parts:

$$\partial_t \int |\vec{n}|^p \leq (p-1) \sup_{\Omega_T} \Delta V \int |\vec{n}|^p \,,$$

and so

$$||\vec{n}||_{L^p(\Omega)}(t) \leq e^{(1-1/p)(\sup_{\Omega_T} \Delta V)t} ||\vec{n}||_{L^p(\Omega)}(0) \quad \forall t > 0\,; \tag{5.146}$$

passing to the limit $p \to \infty$ in (5.146) yields (5.136).

□

We observe that it is not possible to prove eq. (5.134) for $p = 2$ with the strategy followed in Theorem 5. In fact, the first integral on the right-hand side of (5.141) vanishes in this case, so we cannot control the term $\int \nabla V \cdot \nabla |\vec{n}|^p$ in (5.141), unless we integrate it by parts and we bound it with the $\sup_{\Omega_T} \Delta V$. We also point out that (5.136) holds even if $\sup_{\Omega_T} \Delta V$ is nonnegative (it can be easily seen from the proof of the third point of Theorem 5); it is clear, however, that (5.136) is not trivial only if $\sup_{\Omega_T} \Delta V < 0$, since $\vec{n}$ is bounded.

Chapter 6

Numerical simulations

6.1 Introduction

In this chapter we present some numerical results related to some of the models derived in part 1. More precisely, we solved the spinorial diffusive model without pseudomagnetic field QSDE1, and the spinorial diffusive model with pseudo magnetic field QSDE2, both coupled with the Poisson equation, in one space dimension.
Recall model QSDE1:

$$\begin{aligned} \partial_t n_0 =& \text{div } (\nabla n_0 + n_0 \nabla V) && (x,t) \in \Omega_T \,, \\ \partial_t n_j =& \partial_s J_{js} + F_j \quad (j=1,2,3) && (x,t) \in \Omega_T \,, \\ \Delta V =& \lambda_D^{-2}(C - n_0) && (x,t) \in \Omega_T \,, \end{aligned} \tag{6.1}$$

$$\begin{aligned} F_j =& \eta_{jk\ell} n_k \partial_\ell V - 2n_j + b_k[\vec{n}/n_0]\partial_k n_j - b_j[\vec{n}/n_0]\vec{\nabla} \cdot \vec{n}, \\ J_{js} =& \big(\delta_{j\ell} + b_k[\vec{n}/n_0]\eta_{jk\ell}\big)\partial_s n_\ell + n_j \partial_s V \\ & - 2\eta_{js\ell} n_\ell + b_k[\vec{n}/n_0](\delta_{jk} n_s - \delta_{js} n_k) \qquad (j,s = 1,2,3)\,, \\ \vec{b}[\vec{v}] =& \lambda \frac{\vec{v}}{|\vec{v}|^2}\left(1 - \frac{2|\vec{v}|}{\log(1+|\vec{v}|) - \log(1-|\vec{v}|)}\right) \qquad \forall \vec{v} \in \mathbb{R}^3 \,, \end{aligned} \tag{6.2}$$

and model QSDE2:

$$\begin{aligned} \partial_t n_0 =& \partial_x M_{01} && (x,t) \in \Omega_T \,, \\ \partial_t n_j =& \partial_x M_{j1} + \eta_{jks}(M_{ks} + n_k \omega_s) \\ & + \partial_x \left\{ b_k \left[\frac{\vec{n}}{n_0}\right] (\eta_{jkl}\partial_x n_l + \delta_{jk} n_1 - \delta_{j1} n_k) \right\} \\ & + b_1 \left[\frac{\vec{n}}{n_0}\right] \partial_x n_j - b_j \left[\frac{\vec{n}}{n_0}\right] \partial_x n_1 \quad (j=1,2,3) && (x,t) \in \Omega_T \,, \\ \Delta V =& \lambda_D^{-2}(C - n_0) && (x,t) \in \Omega_T \,, \end{aligned} \tag{6.3}$$

$$
\begin{aligned}
M_{0s} =& \phi^{-2}\{(\partial_s n_0 + n_0 \partial_s V) - \zeta\omega_k(\partial_s n_k + n_k \partial_s V + \eta_{kls} n_l)\}\,, \\
M_{js} =& \phi^{-2}\{-\zeta\omega_j(\partial_s n_0 + n_0\partial_s V) \\
& + [\omega_j\omega_k + \phi(\delta_{jk} - \omega_j\omega_k)](\partial_s n_k + n_k\partial_s V + \eta_{kls} n_l)\}\,, \\
\phi =& \sqrt{1-\zeta^2}\,,
\end{aligned}
\tag{6.4}
$$

with $\vec{b}[\vec{v}]$ given again by (6.2). In eqs. (6.1)–(6.4) $\partial_x = \partial_1$ is the partial derivative with respect to the position x, $\partial_2 \equiv 0$, $\Omega_T \equiv \Omega \times [0, T]$, and $\Omega \equiv (0, 1)$ (remember that we are working with scaled dimensionless variables). Remember that the spinorial diffusive model without pseudomagnetic field QSDE1 (6.1), (6.2) can be regarded as a particular case of the spinorial diffusive model with pseudomagnetic field QSDE2 (6.3), (6.4), and can obviously be obtained by putting $\zeta = 0$, $\vec{\omega} = 0$ in (6.3), (6.4).

We have discretized eqs. (6.1), (6.3) in space with the Crank-Nicolson finite-difference scheme (see e.g. [43] for details), obtaining a set of ODE which have been solved by means of the Matlab routine ode23s. More precisely, we have discretized the first and second derivative operators by means of centered finite differences: for arbitrary smooth functions $u = u(x)$, $v = v(x)$,

$$
\begin{aligned}
(\partial_x u)|_{x=x_i} \approx& \frac{u_{i+1} - u_{i-1}}{2\triangle x} \qquad 1 \le i \le N-1\,, \\
(\partial_x(u\,\partial_x v))|_{x=x_i} \approx& \frac{1}{2\triangle x^2}[u_{i+1}(v_{i+1} - v_i) + u_i(v_{i+1} - 2v_i + v_{i-1}) \\
& - u_{i-1}(v_i - v_{i-1})] \qquad 1 \le i \le N-1\,,
\end{aligned}
\tag{6.5}
$$

where the points $\{x_i\,,\, i = 0 \ldots N\}$ are the nodes of the uniformely spaced discretization grid, $\triangle x = x_{i+1} - x_i$ and $u_i = u(x_i)$ for $1 \le i \le N-1$. We point out that, if u, v are smooth enough, the approximations in (6.5) are accurate up to $O(\triangle x^2)$, as $\triangle x \to 0$.

We simulated a ballistic diode to which a certain bias is applied: we chose initial and boundary conditions corresponding to a state of global equilibrium with zero applied voltage and zero spin, and we observed the evolution of the system towards a new equilibrium due to the applied potential.

6.2 Numerical results for the models QSDE1, QSDE2.

In this section we present some numerical results related to the models QSDE1 (6.3), (6.4) and QSDE2 (6.3), (6.4). We choose the boundary conditions:

$$
n_0 = C, \quad \vec{n} = 0, \quad V = U \quad \text{on } \partial\Omega = \{0, 1\},\ t > 0, \tag{6.6}
$$

where $U(x) = V_A x$ and $V_A = 80$ is the scaled applied potential, and the initial conditions

$$
n_0(x, 0) = \exp(-V_{\text{eq}}(x)), \quad \vec{n}(x, 0) = 0, \tag{6.7}
$$

where V_{eq} is the equilibrium potential, defined by

$$
-\lambda_D^2 \partial_{xx}^2 V_{\text{eq}} = \exp(-V_{\text{eq}}) - C(x) \quad \text{in } \Omega, \quad V_{\text{eq}}(0) = V_{\text{eq}}(1) = 0.
$$

We choose $\lambda_D^2 = 10^{-3}$. The doping profile corresponds to that of a ballistic diode:

$$C(x) = C_{\min} \quad \text{for } \bar{x} < x < 1 - \bar{x}, \quad C(x) = 1 \quad \text{otherwise},$$

where $C_{\min} = 0.025$ and $\bar{x} = 0.2$. The pseudo-spin polarization and the direction of the local magnetization in the model QSDE2 (6.3), (6.4) are chosen as follows:

$$\zeta = 0.5, \quad \vec{\omega} = (0, 0, 1)^\top.$$

Table 6.1 shows the values of the units which allows for the computation of the physical values from the scaled ones.

space unit	10^{-7} m
time unit	0.5×10^{-13} s
voltage unit	1.25×10^{-2} V
charge density unit	10^{17} m^{-2}
current density unit	2×10^{23} m^{-1} s^{-1}

Table 6.1: Units used for the numerical simulations.

Models QSDE1 (6.1), (6.2) and QSDE2 (6.3), (6.4), with the corresponding initial and boundary conditions (6.6)-(6.7) are discretized with the Crank-Nicolson finite-difference scheme and the space step $\triangle x = 10^{-2}$ (see eq. (6.5)). The resulting nonlinear discrete ODE system is solved by using the Matlab routine ode23s.[1]

Since the initial spin vector is assumed to vanish, the charge density n_0, computed from the model QSDE1, corresponds exactly to the charge density of the standard drift-diffusion model, and the spin vector vanishes at all times. The situation is different in the model QSDE2 since the equations are fully coupled. For the model QSDE2, Figure 6.1 shows the charge density n_0 and the components n_j of the spin vector versus position at various times. The solution at $t = 1$ corresponds to the steady state. We observe a charge built-up of n_0 in the low-doped region of the diode (i.e. where $C = C_{min}$). The spin vector components vary only slightly in this region but their gradients are significant in the high-doped regions close to the contacts. Clearly, the components n_j do not need to be positive and, in fact, they even do not have a definite sign.

The presence of the pseudomagnetic field affects slightly the charge density evolution. Figure 6.2 shows a comparison between the charge density profiles for the models QSDE1, QSDE2 at (scaled) time $t = 0.05$, when the relative difference between the two profiles is maximized.

The models QSDE1 and QSDE2 are well defined only if $|\vec{n}|/n_0 < 1$. We plot this ratio in Figure 6.3 at various times for the model QSDE2. In all the presented cases, the quotient stays below one. This indicates that $b_k[\vec{n}/n_0]$ is well defined also in this model.

We have shown in Theorem 5 that the spin vector of the model QSDE1 converges to zero if the electric potential satisfies certain conditions. In Figure

[1] The routine ode23s solves a system of stiff ODE with a low order method.

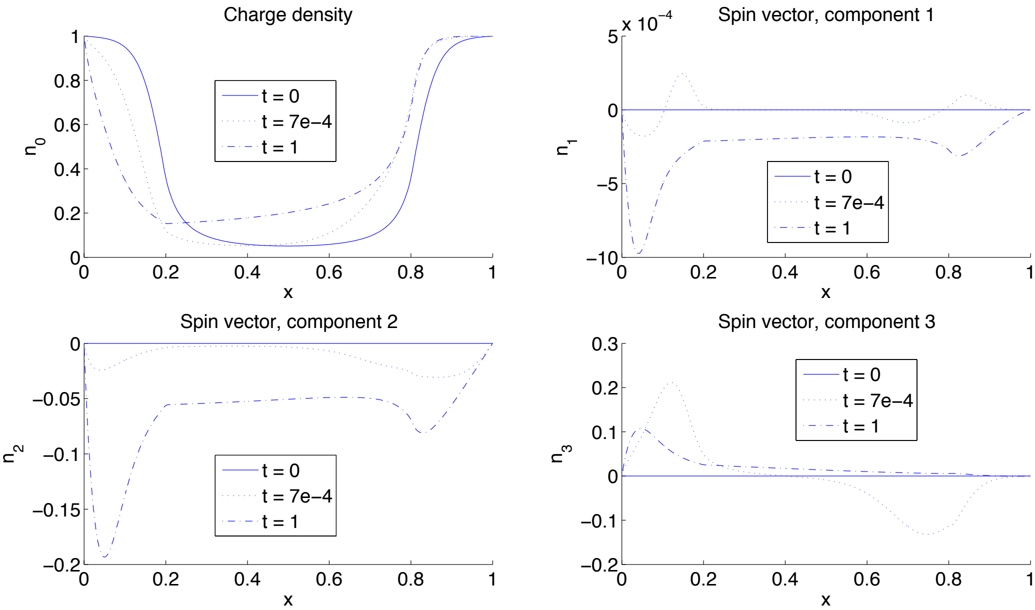

Figure 6.1: Model QSDE2: Charge density and components of the spin vector versus position at times $t = 0$, $t = 7 \cdot 10^{-4}$, and $t = 1$.

6.4, the relative difference $\|n_0(t) - n_0(\infty)\|_2/\|n_0(\infty)\|_2$ versus time is depicted (semilogarithmic plot), where $n_0(\infty)$ denotes the steady-state particle density of model QSDE1 or QSDE2, respectively. The norm $\|\cdot\|_2$ is the discretized L^2 norm, which means, the Euclidean norm on $\mathbb{R}^N$ where N is the number of points in the space grid. The stationary solution is approximated by $n_0(t^*)$ with $t^* = 1$, because we have observed numerically that at $t = t^* = 1$ the solution almost perfectly steady. Whereas the decay of the solution to the model QSDE1 is numerically of exponential type (in agreement with the theoretical results), the decay for the model QSDE2 seems to be exponential only for small times.

In the final Figure 6.5, we present the current-voltage characteristics for the models QSDE1 and QSDE2, i.e. the relation between J_0 at $x = 1$ and the applied bias V_A. The characteristics of model QSDE1 correspond to the current-voltage curve of the standard drift-diffusion model coupled with the Poisson equation. We observe that the additional terms in the definition of J_0 lead to an increase of the particle current density.

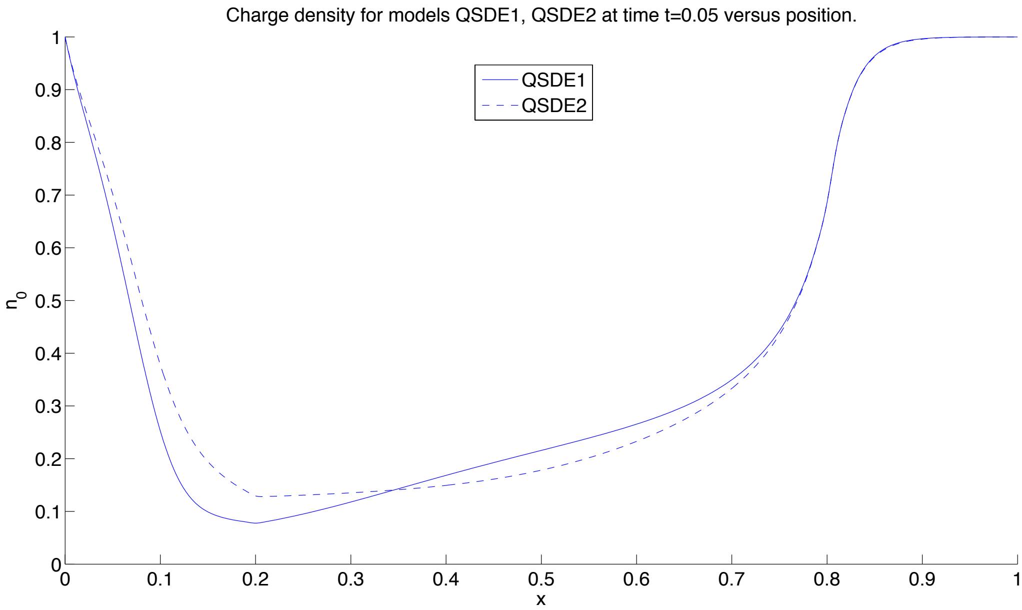

Figure 6.2: Charge density for models QSDE1 and QSDE2 versus position at time $t = 0.05$.

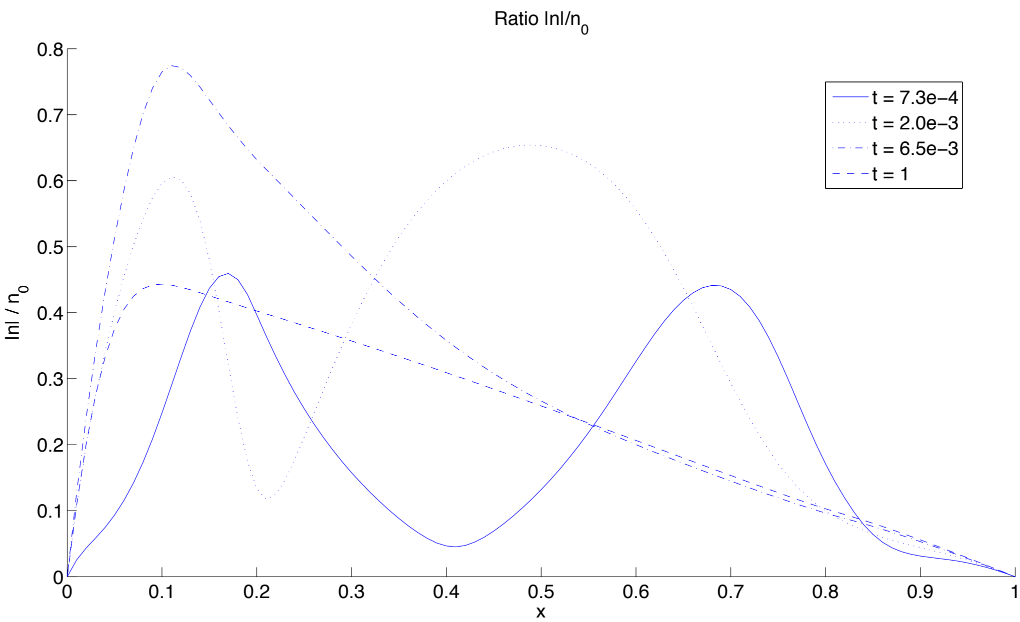

Figure 6.3: Model QSDE2: Ratio $|\vec{n}|/n_0$ versus position at various times.

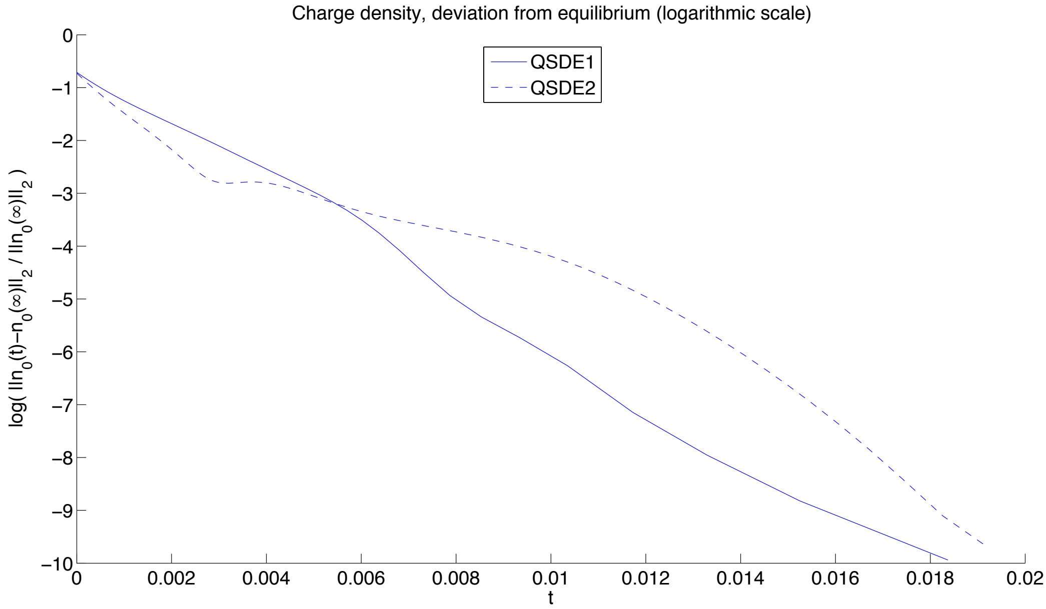

Figure 6.4: Relative difference $\|n_0(t) - n_0(\infty)\|/\|n_0(t)\|$ versus time (semilogarithmic plot) for the models QSDE1 (solid line) and QSDE2 (dashed line).

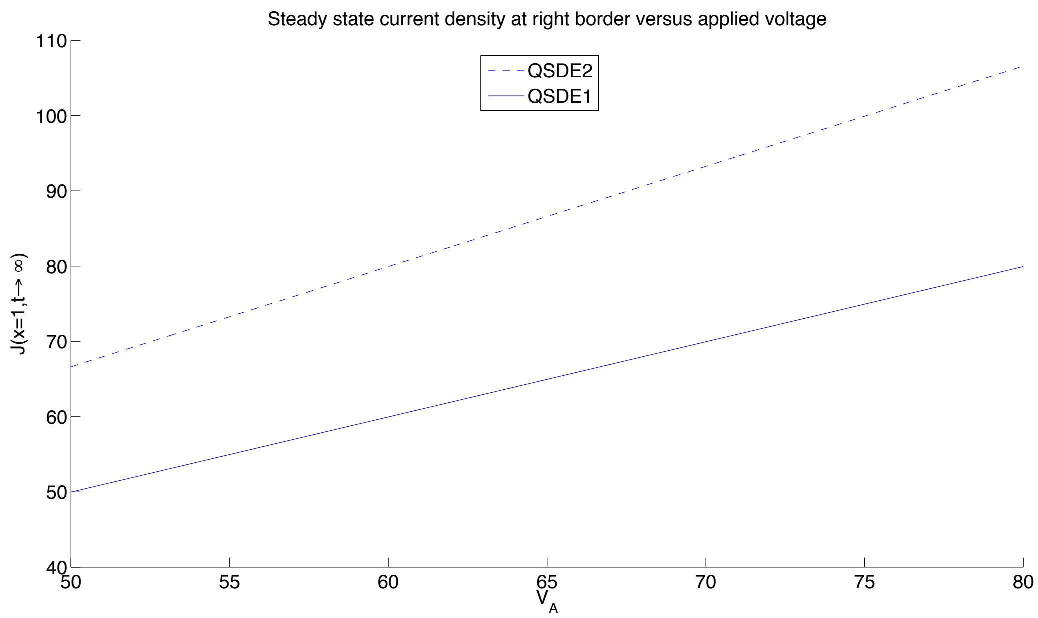

Figure 6.5: Static current-voltage characteristics for the models QSDE1 and QSDE2.

Chapter 7

Conclusions

The subject of our PhD thesis was the description of quantum transport of electrons in graphene by means of fluid models.

After a short introduction, where we presented the carbon-based semiconductor material known as graphene and its main electronic properties, we presented a kinetic model, that is, the collisional Wigner equation (1.33), as the starting point of the derivation of fluid models; several scalings have been applied to the Wigner equations in order to derive models of different kind (diffusive or hydrodynamic).

We defined the quantum equilibrium distribution by means of the quantum minimum entropy principle, i.e. as a minimizer of a suitable quantum entropy functional under the constraints of given fluid-dynamic moments; we computed then a semiclassical expansion of the quantum exponential in the spinorial case, which has been exploited in the subsequent part of this thesis in order to derive explicit fluid models.

We derived two classes of models: two-band models, which are based upon a choice of moments reflecting the splitting of the energy spectrum in two bands (conduction and valence), i.e. involving the band distribution functions $w_\pm$, and spinorial models, which means, evolution equations for fluid moments involving separately all the Pauli components of the Wigner matrix. The first fluid model we presented is the first-order hydrodynamic model (3.44), involving the moments $n_\pm$ (band densities) and $\vec{J}_\pm$ (band currents). Then we derived two diffusive two-band models for the band densities $n_\pm$: a first-order model (3.89) and a second-order model (3.123). Two spinorial hydrodynamic models for the moments n_0 (charge density), $\vec{n}$ (spin vector), $\vec{J}$ (current) have been presented next: a first-order model (4.35) and a second-order model (4.59). Finally two first-order spinorial diffusive models have been derived, namely the QSDE1 model (4.91)–(4.92) and the QSDE2 model (4.107), involving the fluid moments n_0, $\vec{n}$; in particular, to derive the QSDE2 model (4.107) we theorized the existence of a "pseudo-magnetic field" able to interact with the electron pseudospin and providing a strong coupling between the model equations.

During the derivation of each fluid model, semiclassical expansions of the equilibrium distribution for the system have been exploited in order to overcome the intrinsic computational difficulties, which are due to the nonlinearity and nonlocality of the quantum exponential (appearing in the expression of the quantum thermal equilibrium distribution) and to the presence of the pseudospin degree of freedom.

We performed an analysis of the diffusive spinorial model (4.91)–(4.92): we proved, by applying a fixed point argument, the existence of weak solutions and uniqueness of the solution under a regularity condition on the moments; we found an entropy for the model and proved an entropy inequality; we studied the long-time behaviour of the solutions showing, by exploiting an energy method, the decay of the spin vector in several L^p norms.

We obtained some numerical simulations for both the spinorial diffusive models, (4.91)–(4.92) and (4.107), in one space dimension, through a finite difference scheme: we simulated a graphene-based device (namely, a ballistic diode) to which a certain bias is applied, showing the temporal behaviour of the moments and pointing out some noteworthy features of the analyzed fluid models.

It is interesting to compare the models, which have been presented in this thesis, with other existing fluid models for quantum transport of electrons in graphene. However, very few mathematical models of this kind have been considered in literature until today, since both quantum fluid-dynamics and graphene are very recent fields of reseach.

In [48] a hydrodynamic model for electron-hole plasma in graphene is derived employing a statistical closure of a set of two scalar collisional Boltzmann equations (one for each energy band):

$$\begin{aligned}
\partial_t f_e + v_F \frac{\vec{p}}{|\vec{p}|} \cdot \vec{\nabla}_x f_e + e\vec{\nabla}_x \varphi \cdot \vec{\nabla}_p f_e =& St\{f_e, f_e\} + St\{f_e, f_h\} + St_i\{f_e\}\,,\\
\partial_t f_h + v_F \frac{\vec{p}}{|\vec{p}|} \cdot \vec{\nabla}_x f_h - e\vec{\nabla}_x \varphi \cdot \vec{\nabla}_p f_h =& St\{f_h, f_h\} + St\{f_h, f_e\} + St_i\{f_h\}\,;
\end{aligned}$$

here f_e, f_h are the electrons and holes distribution functions, $v_F \approx 10^6$ m/s is the Fermi velocity, e is the absolute value of the electron charge, φ is the electric potential (which is self-consistently given by the Poisson equation), $St_i\{f_e\}$ and $St_i\{f_h\}$ are the collision integrals of electrons and holes, respectively, with impurities and phonons, and $St\{f_e, f_e\}$, $St\{f_e, f_h\}$, $St\{f_h, f_h\}$ are the intercarrier collision integrals.

The fluid model is a system of Euler equations involving the moments Σ_e, Σ_h (electron and hole sheet densities, respectively), $\vec{V}_e$, $\vec{V}_h$ (electron and hole average velocities):

$$\begin{aligned}
\partial_t \Sigma_s + \operatorname{div}(\Sigma_s \vec{V}_s) =& 0 \qquad (s = e, h)\,,\\
\frac{3}{2v_F}\partial_t(\langle p_e\rangle \vec{V}_e) + \frac{v_F}{2}\vec{\nabla}\langle p_e\rangle - e\Sigma_e\vec{\nabla}\varphi =& -\beta_e\vec{V}_e - \beta_{eh}(\vec{V}_e - \vec{V}_h)\,,\\
\frac{3}{2v_F}\partial_t(\langle p_h\rangle \vec{V}_h) + \frac{v_F}{2}\vec{\nabla}\langle p_h\rangle + e\Sigma_h\vec{\nabla}\varphi =& -\beta_h\vec{V}_h - \beta_{eh}(\vec{V}_h - \vec{V}_e)\,,
\end{aligned} \tag{7.1}$$

where $\langle p_e\rangle$, $\langle p_h\rangle$ are the average momentum modulus for electrons and holes, respectively, and they depend only on Σ_e, Σ_h. The average velocities $\vec{V}_e$, $\vec{V}_h$

are assumed to be small: as a consequence, the friction terms are neglected in comparison to the electron-electron and hole-hole collision terms.

The distribution function of each band at thermal equilibrium is chosen to be a Fermi-Dirac distribution:

$$f_s(p) = \left[1 + \exp\left(\frac{v_F|\vec{p}| - \vec{p}\cdot\vec{V}_s - \mu_s}{T}\right)\right]^{-1} \qquad (s = e, h)\,, \tag{7.2}$$

with suitable chemical potentials μ_e, μ_h and average drift velocities $\vec{V}_e$, $\vec{V}_h$. The dynamics of the two energy bands is thus assumed to be decoupled at thermal equilibrium: the coupling between the fluid equations is given by the collision terms. Moreover a first-order Taylor expansion with respect to $\vec{V}_e$, $\vec{V}_h$ of the equilibrium distribution is performed, leading to a linearization of this latter with respect to the average drift velocities:

$$f_s(p) = f_s(p;\vec{V}_s = 0) + \vec{\nabla}_{\vec{V}_s} f_s(p;\vec{V}_s = 0)\cdot\vec{V}_s \qquad (s = e, h)\,. \tag{7.3}$$

The fluid model (7.1) involves band densities and band currents, is of hydrodynamic type and contains no viscous corrections; concerning this general features, it is similar to the first order two-band hydrodynamic model (3.44). However, the differences between the Euler equations (7.1) and the models previously derived in this thesis are many. First of all, model (7.1) is purely semiclassic, which means, no quantum correction is considered in the fluid equations or in the equilibrium distribution: the kinetic equation from which the fluid model is derived is a collisional Boltzmann equation, and the contributions of each band to the equilibrium distribution are reciprocally decoupled, as it happens at leading semiclassical order. In this thesis, instead, the quantum counterpart of the Boltzmann equation, that is, the Wigner equation, has always been the starting point in the derivation of the fluid models, and quantum corrections of at least first order to the equilibrium distribution have always been taken into account, even if simplifying assumptions (like the low scaled Fermi speed hypothesis (1.37) and the strongly mixed state assumption (3.90), (4.36)) have been considered in order to overcome the not trivial difficulties, which naturally arise in the computation of the semiclassical expansion of the quantum exponential in the spinorial case. Moreover, in the derivation of Eq. (7.1), the Fermi-Dirac statistics (see eq. (7.2)) is adopted in order to describe the system, coherently with the fact that the energy spectrum of the Hamiltonian describing massless electrons in graphene (given by Eq. (1.15)) is unbounded from below. On the contrary, all models that have been presented in this thesis are based, for the sake of simplicity, upon the Maxwell-Boltzmann statistics: as a consequence, an additional term has been added to the system Hamiltonian (see Eq. (1.16)) in order to cut off the infinite negative energy branch without destroying the double-cone structure of the energy spectrum near the Dirac points. Concerning the approximations employed in the derivation of the models, we remark that a first order Taylor expansion of the equilibrium distribution with respect to the drift velocities (see eq. (7.3)) have been exploited to derive model (7.1), leading to relevant simplifications in the computations; this technique can be compared with the strongly mixed state hypothesis (see Eqs. (3.90), (4.36)), which has allowed the derivation of second order fluid models that would have been very hard to obtain otherwise.

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