Etude mathématique et numérique de modèles de transport : application à la spintronique

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Summary

This thesis is decomposed into three parts. The main part is devoted to the study of spin polarized currents in semiconductor materials. An hierarchy of microscopic and macroscopic models are derived and analyzed. These models takes into account the spin relaxation and precession mechanisms acting on the spin dynamics in semiconductors. We have essentially two mechanisms : the spin-orbit coupling and the spin-flip interactions. We begin by presenting a semiclassical analysis (via the Wigner transformation) of the Schrödinger equation with spin-orbit hamiltonian. At kinetic level, the spinor Vlasov (or Boltzmann) equation is an equation of distribution function with 2×2 hermitian positive matrix value. Starting then from the spinor form of the Boltzmann equation with different spin-flip and non spin-flip collision operators and using diffusion asymptotic techniques, different continuum models are derived. We derive drift-diffusion, SHE and Energy-Transport models of two-components or spin-vector types with spin rotation and relaxation effects. Two numerical applications are then presented : the simulation of transistor with spin rotational effect and the study of spin accumulation effect in inhomogenous semiconductor interfaces.

In the second part, the diffusion limit of the linear Boltzmann equation with a strong magnetic field is performed. The Larmor radius is supposed to be much smaller than the mean free path. The limiting equation is shown to be a diffusion equation in the parallel direction while in the orthogonal direction, the guiding center motion is obtained. The diffusion constant in the parallel direction is obtained through the study of a new collision operator obtained by averages of the original one. Moreover, a correction to the guiding center motion is derived.

In the third part of this thesis, we are interested in the description of the confinement potential in two-dimensional electron gases. The stationary one dimensional Schrödinger–Poisson system on a bounded interval is considered in the limit of a small Debye length (or small temperature). Electrons are supposed to be in a mixed state with the Boltzmann statistics. Using various reformulations of the system as convex minimization problems, we show that only the first energy level is asymptotically occupied. The electrostatic potential is shown to converge towards a boundary

layer potential with a profile computed by means of a half space Schrödinger–Poisson system.

Key words. *Semiclassical analysis, Wigner transformation, spin-orbit hamiltonian, spinor Boltzmann equation, micro-macro limit, diffusion limit, moment method, entropy minimization, drift-diffusion, SHE, Energy-Transport, two-component models, Spin-FET, finite elements, Gummel iterations, guiding-center approximation, high magnetic field, convex minimization, min-max theorem, concentration-compactness principle, boundary layer.*

Table of contents

Introduction

Ce travail de thèse comporte trois parties. La partie principale porte sur l'étude mathématique et l'analyse numérique des phénomènes de transport en spintronique. Deux autres travaux ont été menés en parallèle. Le premier concerne l'étude de l'asymptotique de diffusion et l'approximation centre-guide de systèmes de particules en présence de champs magnétiques forts. Dans un autre travail, nous nous intéressons à la description du profil de potentiel de confinement dans des gaz d'électrons bidimensionnels en étudiant une asymptotique forte densité du système Schrödinger-Poisson unidimensionnel stationnaire. Nous résumons maintenant chacune des trois parties.

Nous nous intéressons dans la première partie de cette thèse au transport des courants polarisés en spin dans des matériaux à base de semi-conducteur. Le mécanisme essentiel pouvant agir sur l'orientation du spin électronique dans les semi-conducteurs est ce que l'on appelle le couplage spin-orbite. Lorsque la structure étudiée présente une absence de symétrie, le couplage spin-orbite se traduit par l'apparition d'un champ effectif faisant précesser (ou tourner) le vecteur spin pendant les vols libres des électrons. Dans les structures semi-conductrices, on a essentiellement le couplage spin-orbite de Rashba et celui de Dresselhauss. Le terme de Rashba apparaît dans des couches d'accumulations à l'interface entre deux hétérostructures et est due à la forte asymétrie du puits quantique dans lequel se confine le gaz d'électrons bidimensionnel. Le couplage de Dresselhauus quant à lui résulte de l'asymétrie présente dans certains structures cristallines.

Nous dérivons et analysons une hiérarchie de modèles allant du niveau microscopique au niveau macroscopique en tenant compte des différents mécanismes de rotation et de relaxation du spin électronique dans les semi-conducteurs. Au niveau microscopique, l'hamiltonien spin-orbite lié à l'absence de symétrie se représente par la forme suivante

$$H_{SO} = \alpha\hbar\vec{\Omega}(t,x,k)\cdot\vec{\sigma},$$

où $\vec{\sigma}$ est le vecteur des matrices de Pauli (0.0.5), x, k sont respectivement la position et le vecteur d'onde d'une particule ($k \equiv i\hbar\nabla_x$), α est l'ordre du couplage et $\vec{\Omega}$ représente le champ effectif. Dans un premier lieu, nous effectuons une ana-

lyse semi-classique, via la transformation de Wigner, de l'équation de Schrödinger avec un hamiltonien spin-orbite. Suivant l'ordre du couplage spin-orbite par rapport à la constante de Planck adimensionnée, nous dérivons des modèles cinétiques à deux composantes ou spinorielle (avec une fonction de distribution à valeur matricielle). Partant ensuite de la spinor forme de l'équation de Boltzmann (avec différents opérateurs de collisions avec et sans renversement du vecteur spin) et par des techniques d'asymptotiques de diffusion, nous dérivons et analysons plusieurs modèles macroscopiques. Ils sont de type dérive-diffusion, SHE, Energie-Transport, à deux composantes ou spinoriels conservant des effets de rotation et de relaxation du vecteur spin. Nous validons ensuite ces modèles par des cas tests numériques. Deux applications numériques sont présentées : la simulation d'un transistor à effet de rotation de spin et l'étude de l'effet d'accumulation de spin à l'interface entre deux couches semi-conductrices différemment dopées. Cette partie de thèse donne lieu à deux articles en préparation [46, 47].

Mots clés : *Analyse semi-classique, transformation de Wigner, hamiltonien spin-orbite, équation de Boltzmann spinorielle, passage cinétique fluide, limite de diffusion, méthode des moments, minimisation d'entropie, dérive-diffusion, SHE, Energie-Transport, modèles à deux composantes, Spin-FET, éléments finis, itérations Gummel.*

Dans un autre travail, nous considérons une équation cinétique de type Boltzmann linéaire dans des domaines où un champ magnétique fort est appliqué. La présence de ce dernier introduit de fortes oscillations et donc des difficultés pour les simulations numériques. Nous étudions la limite de diffusion en supposant que le champ magnétique est unidirectionnel et tend vers l'infini. Le modèle obtenu est un modèle macroscopique (moins coûteux numériquement que le modèle cinétique). Il est constitué d'une équation diffusive dans la direction parallèle au champ magnétique et d'une dérive représentant l'effet centre-guide en présence d'un champ électrique dans la direction perpendiculaire. Le terme de diffusion contient des moyennes de giration de l'opérateur de collisions utilisé. Nous prouvons la convergence en utilisant des techniques d'entropie pour traiter le comportement diffusif, et en conjuguant par les rotations locales induites par le champ magnétique pour tenir compte des oscillations. Ce travail fait l'objet d'une publication [13].

Mots clés : *limite de diffusion, approximation centre-guide, champ magnétique fort.*

Dans la troisième partie de cette thèse, nous étudions la limite faible longueur de Debye (ou faible température) du système de Schrödinger-Poisson unidimensionnel stationnaire sur un intervalle borné. Les électrons sont supposés dans un mélange d'états avec une statistique de Boltzmann (ou de Fermi-Dirac). En utilisant différentes reformulations du système comme des problèmes de minimisation

convexe, nous montrons qu'asymptotiquement seul le premier niveau d'énergie est occupé. Le potentiel électrostatique converge vers une couche limite avec un profil calculé à l'aide d'un système de Schrödinger-Poisson sur le demi axe réel. Cette partie est publiée dans SIAM-Multiscale Modeling and Simulations [48].

Mots clés : minimisation convexe, théorème min-max, principe de concentration-compacité, couche limite.

Dans la suite de cette introduction nous détaillons et présentons les principaux résultats obtenus dans chacune des trois parties de cette thèse.

I. Modèles de transport en spintronique

I.1 Introduction à la spintronique

Les électrons ne sont pas seulement caractérisés par leur charge électrique mais aussi par leur moment cinétique intrinsèque ou spin. Jusqu'aux années 90', l'électronique ignorais quasiment le spin de l'électron. La spintronique, ou l' électronique de spin, est un nouveau domaine de recherche tentant d'allier l'électronique classique et les propriétés quantiques du spin. Il vise à manipuler le spin des porteurs de charge, et de l'utiliser comme un degré de liberté supplémentaire ou comme un nouveau vecteur de l'information.

La magnétorésistance géante (Giant Magneto-Resistance ou GMR) découverte par Albert Fert et al [55], et la magnétorésistance tunnel, sont les premières manifestations de la spintronique.

Dans des structures électroniques composées de couches magnétiques séparées par une couche paramagnétique, la GMR se traduit par un changement de résistance important observé dans de tels structures lorsque, sous l'effet d'un champ magnétique extérieur (ou sous l'effet de l'accumulation des spins à l'interface M/PM), les aimantations macroscopiques des couches magnétiques successives basculent d'un état antiparallèle à un état parallèle aligné.

Un effet similaire à la magnétorésistance géante, appelé magnétorésistance tunnel, a été observé dans des jonctions tunnel métal/isolant/métal, dans lesquels les deux électrodes métalliques sont magnétiques. Cet effet magnétorésistif a été utilisé, dans les années quatre-vingt dix, pour développer des mémoires magnétiques à accès aléatoire ou MRAM (Magnetic Random Access Memories). Dans ces mémoires, l'information n'est plus stockée sous la forme d'une charge, comme c'est le cas des mémoires semi-conductrices de type DRAM ou Flash, mais sous la forme d'une direction d'aimantation dans la jonction tunnel magnétique.

Pour utiliser le spin comme un porteur de l'information, il faut que cette dernière

ne soit pas perdue durant son transport. En d'autres termes, il faut disposer de porteurs dont l'orientation du spin est parfaitement définie. Cette notion conduit naturellement aux courants polarisés en spin : essentiellement liée dans les semi-conducteurs aux différences relatives des densités de spin-up et spin-down. Notons que dans les métaux ferromagnétiques, la notion de courants polarisés en spin est surtout liée à la différence de mobilité des spin-up et spin-down. Bien que les premières recherches dans ce domaine ont été menées pour des structures composées de multi-couches magnétiques, les chercheurs portent actuellement une attention particulière à l'étude des courants polarisés en spin dans les semi-conducteurs. La raison est la découverte du long temps de vie du spin et la présence des mécanismes pouvant agir sur la dynamique du spin électronique dans les semi-conducteurs.

I.1.1 Mécanismes agissant sur le spin dans les semi-conducteurs

Ces mécanismes sont dus au couplage spin-orbite qui est un effet relativiste lié au mouvement de l'électron autour de son noyau. Ils peuvent être classés en deux catégories.

- **Mécanisme d'Elliot-Yafet.** L'interaction spin-orbite mélange les états de spin-up et down. Les intéractions instantanées entre les particules et le cristal (ou l'environnement) peuvent alors être accompagnées d'un retournement de l'orientation du vecteur spin, selon le mécanisme dit d'Elliot-Yafet [103, 56]. Bien que les intéractions avec renversement du spin soient des événements rares dans les semi-conducteurs [24], elles peuvent être suffisantes dans les zones à faible mobilité (ou forte densité) pour faire disparaître la cohérence en spin (ou faire relaxer le vecteur spin). C'est le mécanisme de relaxation d'Elliot-Yafet.
- **Mécanisme de relaxation de D'yakonov-Perel.** Lorsque le système présente une asymétrie d'inversion, le couplage spin-orbite va se traduire par l'apparition d'un champ magnétique (qu'on appelle champ effectif) faisant précesser le vecteur spin pendant les vols libres des porteurs de charge. Le couplage spin-orbite se décompose en deux termes :
  - *Couplage spin-orbite de Rashba [27].* Ce couplage apparaît dans les couches d'accumulations à l'interface entre deux hétéro-structures et dû à la forte asymétrie du puits quantique dans lequel se confine le gaz d'électrons bidimensionnel (2DEG). Le vecteur de précession de spin associé au couplage de Rashba pour un 2DEG formé dans un plan (xy) est donné par [82, 27] :

$$\vec{\Omega}_R = \frac{2a_{46}E_z}{\hbar}(-k_y e_x + k_x e_y) \tag{0.0.1}$$

    avec a_{46} est une constante dépendant du matériel, $\hbar$ est la constante de Planck, E_z est le champ électrique de confinement dans la direction z per-

pendiculaire au plan (xy), $k = (k_x, k_y)$ est le vecteur d'onde de particule dans le plan (xy) et e_x, e_y dénotent les vecteurs unitaires suivant les axes des x et des y.

– *Couplage de Dresselhauss [43].* C'est un couplage spin-orbite qui résulte de l'asymétrie présente dans certaines structures cristallines. Le vecteur de précession de Dresselhauss s'écrit sous la forme

$$\vec{\Omega}_D = \frac{2a_{42}}{\hbar}(k_x e_x - k_y e_y), \tag{0.0.2}$$

où a_{42} est un paramètre dépendant de la structure.

FIG. 1 – Dynamique du vecteur spin sous l'action du vecteur de précession de Rashba dans un 2DEG et dans un fil quantique 1DEG.

Le mécanisme de D'yakonov-Perel lié à l'existence d'un champ magnétique effectif représente le mécanisme essentiel de relaxation du spin électronique dans les hétéro-structures semi-conductrices [45, 103]. Le module du champ effectif lié au terme de Rashba (0.0.1), soit la vitesse de rotation de spin, dépend de E_z. Elle peut donc être contrôlée à l'aide du champ électrique de confinement par un potentiel extérieur appliqué au système (potentiel de grille). Néanmoins, ce contrôle n'est efficace que si l'on se place dans de bonnes conditions. En effet, dans un gaz d'électrons $2D$, la direction du champ $\vec{\Omega}_R$ (0.0.1) dépend du vecteur d'onde k. Ce vecteur se redistribue de façon aléatoire dans le plan à l'issu de chaque intéraction subie par la particule (voir Figure 1). Dans un régime fortement collisionnel, les particules subissent beaucoup de chocs. La dynamique du champ de Rashba ressemble dans ce cas à une marche au hasard et la cohérence de spin est donc relaxée via le mécanisme de relaxation de D'yakonov-Perel.

Pour éviter ce problème, une solution consiste à confiner les électrons dans la direction y en plus du confinement dans la direction z. Le transport dans le gaz se fait alors dans une seule direction de l'espace. On définit un fil quantique

ou $1DEG$. Dans ce cas, le champ effectif de Rashba est donné par

$$\vec{\Omega}_R^{1D} = \alpha k_x e_y,$$

pour un certain paramètre α. Sa direction ne dépend pas de k et donc $\vec{\Omega}_R^{1D}$ ne change pas de direction avec les intéractions instantanées des particules. L'effet de Rashba est dans ce cas efficace pour contrôler la dynamique du vecteur spin dans le fil quantique. Si le vecteur spin des électrons injectés dans le fil est parallèle à ce dernier, la rotation de spin s'effectue dans un même plan perpendiculaire à $\vec{\Omega}_R^{1D}$. La période de rotation varie avec la tension de grille appliquée. Ce mécanisme est vérifié numériquement, voir Chapitre 3 de cette thèse.

Le vecteur de Dresselhauss, quant à lui, n'est pas contrôlable par une voie externe et il induit aussi un mécanisme de relaxation de spin de type D'yakonov Perel [45]. D'autres mécanismes de relaxation de spin existent dans la littérature, voir [103].

I.1.2 Transistor à effet de rotation de spin

Après le MRAM, la recherche actuelle se dirige vers la fabrication des composantes intégrant des matériaux magnétiques et semi-conducteurs dans une même hétéro-structure dite "hybride". La possibilité de contrôler la vitesse de rotation du vecteur spin dans les hétéro-structures via le couplage spin-orbite de Rashba a conduit deux chercheurs américains Datta et Das à proposer en 1990 [30] un transistor à effet de rotation de spin ou spin-FET (spin Field Effect Transistor). Il s'agit d'un transistor à haute mobilité électronique HEMT (High Electron Mobility Transistor) dans lequel les zones fortement dopées de source et de drain sont remplacées par des contacts ferromagnétiques. La source agit comme un polariseur en spin. Dans le semi-conducteur, les spins vont précesser autour d'un certain champ effectif. Leur vitesse angulaire peut être modulée par la tension de la grille. Le contact de drain, quant à lui, agit comme un analyseur : si le spin est orienté parallèlement à l'aimantation du drain, le courant dans ce dernier est important. Dans le cas contraire, le courant est faible. A part les contraintes de dimensionnement, plusieurs obstacles s'opposent à la réalisation du spin-FET, notamment les problèmes d'injection et de collection de spin aux interfaces FM/SC, SC/FM.

I.2 Description des modèles utilisés

Dans cette première partie de la thèse, nous nous intéressons à la dérivation des modèles de transport tenant compte de différents mécanismes agissant sur le spin

électronique dans les semi-conducteurs décrits ci-dessus. Nous dérivons et analysons une hiérarchie de modèles allant du niveau microscopique (avec l'équation de Schrödinger) au niveau macroscopique en passant par des modèles cinétiques (Chapitre 1, 2). Nous présentons ensuite quelques applications numériques (Chapitre 3). Dans cette section nous présentons les modèles utilisés pour décrire le transport des courants polarisés en spin dans les semi-conducteurs. Plus particulièrement, nous décrivons comment sont introduit dans les équations, pour différentes échelles de modélisation, les mécanismes de relaxation dûs aux couplages spin-orbite et aux intéractions avec renversement de spin.

I.2.1 Modèle quantique

En mécanique quantique, une particule de spin 1/2 (électron) plongée dans un potentiel V peut être décrite par une fonction d'onde $\Psi(t,x) = (\psi^{\uparrow}(t,x), \psi^{\downarrow}(t,x))$ à valeur vectoriel dans $\mathbb{C}^2$. Les composantes $\psi^{\uparrow}(t,x)$ et $\psi^{\downarrow}(t,x)$ représentent les fonctions d'ondes des particules avec spin-up et spin-down respectivement. La fonction Ψ vérifie l'équation de Schrödinger suivante :

$$i\hbar\partial_t\Psi = (H_0 + H_{SO})(\Psi) \tag{0.0.3}$$

où H_0 est l'hamiltonien standard de l'énergie cinétique plus l'énergie potentiel

$$H_0 = (\frac{-\hbar^2}{2m}\Delta_x + V)I_2,$$

m est la masse effective d'un electron et I_2 est la matrice identité de $\mathbb{C}^2$. L'hamiltonien spin-orbite, noté par H_{SO}, s'écrit sous la forme générale suivante :

$$H_{SO} = \alpha\hbar\vec{\Omega}(t,x,k)\cdot\vec{\sigma} \tag{0.0.4}$$

où $\vec{\sigma}$ est le vecteur $\vec{\sigma} = (\sigma_1, \sigma_2, \sigma_3)$ des trois célèbres matrices de Pauli,

$$\sigma_1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \sigma_2 = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \quad \sigma_3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \tag{0.0.5}$$

et α est l'ordre du couplage. Ici, k est le vecteur d'onde, $k \equiv -i\hbar\nabla_x$. En effet, selon [76, 49] l'hamitonien de l'intéraction spin-orbite, dérivé de l'équation de Dirac à quatre composantes [29], est donné par

$$H_{SO} = \frac{i\hbar^2}{4m^2c^2}(\nabla_x V \times \nabla_x)\cdot\vec{\sigma}. \tag{0.0.6}$$

L'hamiltonien de Rashba s'écrit ([27]),

$$H_R = \alpha i\hbar(\vec{\sigma}_1\partial_y - \vec{\sigma}_2\partial_x)$$

pour un gas d'électrons formé dans le plan (xy) et l'hamiltonien de Dresselhauss est donné par [43]

$$H_D = \alpha i\hbar(\vec{\sigma}_1\partial_x - \vec{\sigma}_2\partial_y).$$

Rappelons qu'en physique quantique $|\Psi(t,x)|^2 = |\psi^\uparrow|^2 + |\psi^\downarrow|^2$ représente la probabilité de présence d'une particule en x à l'instant t et que l'on a $\int_{\mathbb{R}^3} \|\Psi(t,x)\|^2 dx = 1$. Les quantités macroscopiques telles que la matrice densité et courant sont définies à partir de Ψ comme suit

$$N(t,x) = \Psi(t,x)\otimes\overline{\Psi}(t,x), \quad J(t,x) = \frac{\hbar}{2i}[\nabla_x\Psi(t,x)\otimes\overline{\Psi}(t,x) - \Psi(t,x)\otimes\nabla_x\overline{\Psi}(t,x)],$$

où $\otimes$ désigne le produit tensoriel de deux vecteurs.

I.2.2 Modèles cinétiques et macroscopiques

En microélectronique classique, le transport des charges est décrit au niveau cinétique par une grandeur statistique : la fonction de distribution scalaire $f(t,x,v)$. Cette fonction représente une densité dans l'espace des phases décrit par la position x et la vitesse v à l'instant t. Autrement dit, $f(t,x,v)dxdv$ correspond au nombre de particules se trouvant à l'instant t dans un volume $dxdv$ autour du point (x,v). L'évolution de cette fonction est décrite par l'équation de Vlasov ou Boltzmann dans un cadre collisionnel [22, 28, 65, 100].

En spintronique, un ensemble de particules de spin 1/2 est décrit au niveau cinétique par une fonction de distribution à valeurs dans l'ensemble des matrices carrées hermitiennes d'ordre 2 ($\mathcal{H}_2(\mathbb{C})$). L'équation de Vlasov spinorielle avec intéractions spin-orbite s'écrit

$$\partial_t F + v\cdot\nabla_x F + \mathcal{F}\cdot\nabla_v F = \frac{\alpha i}{2}[\vec{\Omega}\cdot\vec{\sigma}, F], \tag{0.0.7}$$

où $\mathcal{F}(t,x) = -\nabla_x V(t,x)$ est la force extérieure exercée sur les particules , et supposée conservative donc dérivant d'un certain potentiel V. Dans cette description cinétique, le couplage spin-orbite est donné par le terme de droite de l'équation (0.0.7), où α est l'ordre du couplage, $\vec{\Omega}(t,x,v)$ est le champ effectif associé et $[A,B] = AB - BA$ désigne le commutateur des deux matrices. La fonction de distribution admet dans ce cas quatre degrés de liberté : un pour la distribution des charges et trois pour la distribution des spins. En effet, la matrice identité I_2 et les trois matrices de Pauli (0.0.5) constituent une base de $\mathcal{H}_2(\mathbb{C})$. Décomposons F dans cette base de la manière suivante

$$F(t,x,v) = \frac{1}{2}f_c(t,x,v)I_2 + \vec{f_s}(t,x,v)\cdot\vec{\sigma} \tag{0.0.8}$$

et injectons la dans (0.0.7). Nous obtenons

$$\begin{cases} \partial_t f_c + v\cdot\nabla_x f_c - \nabla_x V\cdot\nabla_v f_c = 0 \\ \partial_t \vec{f_s} + v\cdot\nabla_x \vec{f_s} - \nabla_x V\cdot\nabla_v \vec{f_s} + \alpha\vec{\Omega}\times\vec{f_s} = 0. \end{cases}$$

On obtient une équation scalaire sur $f_c = tr(F)$, où $tr(F)$ est la trace de F et f_c représente la fonction de distribution des charges que l'on utilise en microélectronique. La fonction $\vec{f_s}$ est une fonction vectorielle à valeurs dans $\mathbb{R}^3$. Elle représente la fonction de distribution des spins. Avec la décomposition (0.0.8), le commutateur représentant l'effet spin-orbite dans l'équation (0.0.7) devient un produit vectoriel entre $\vec{\Omega}$ et $\vec{f_s}$. Ce dernier introduit un effet de rotation du vecteur distribution des spins $\vec{f_s}$ autour du champ effectif $\vec{\Omega}$. De plus, les valeurs propres de $F(t,x,v)$ pour tout $(t,x,v) \in \mathbb{R}^+ \times \mathbb{R}^6$ sont données par

$$f^{\uparrow}(t,x,v) = \frac{1}{2} f_c(t,x,v) + |\vec{f_s}|(t,x,v),$$
$$f^{\downarrow}(t,x,v) = \frac{1}{2} f_c(t,x,v) - |\vec{f_s}|(t,x,v),$$

où $|\vec{f_s}|$ est le module de $\vec{f_s}$. Elles représentent les fonctions de distributions des particules avec "spin-up" et "spin-down" respectivement. Ceci montre que $f_c = f^{\uparrow} + f^{\downarrow}$ est la fonction de distribution de l'ensemble total des particules sans tenir compte de leur spin (ou distribution des charges) et $|\vec{f_s}| = \frac{1}{2}(f^{\uparrow} - f^{\downarrow})$ est ce qu'on appelle la fonction de distribution de polarisation en spin. Cette décomposition appliquée à toute quantité spinorielle (ou matricielle à valeur dans $\mathcal{H}_2(\mathbb{C})$) sera appelée décomposition en partie charge et partie spin.

Si l'on veut prendre en compte, en plus des intéractions spin-orbite, les collisions entre les particules (ou avec le crystal), avec et sans retournement de spin, l'équation de Vlasov est alors remplacée par la "spinor" forme de l'équation de Boltzmann (ou l'équation de Boltzmann spinorielle)

$$\partial_t F + v \cdot \nabla_x F - \nabla_x V \cdot \nabla_v F = \frac{Q(F)}{\tau} + \frac{\alpha i}{2}[\vec{\Omega} \cdot \vec{\sigma}, F] + Q_{sf}(F)$$

où Q est l'opérateur de collisions sans renversement de spin et τ est le temps moyen entre deux collisions successives. Les intéractions avec renversement de spin (ou spin-flip interactions) sont données par l'opérateur Q_{sf} admettant la forme réduite suivante

$$Q_{sf} = \frac{tr(F) I_2 - F}{\tau_{sf}}, \tag{0.0.9}$$

où τ_{sf} est le temps de relaxation du vecteur spin. Cette expression nous dit que si les intéractions avec retournement de spin sont nombreuses ou si τ_{sf} est petit et tend vers zéro, alors la fonction de distribution F tend vers une distribution scalaire. Autrement dit, Q_{sf} fait relaxer la distribution des spins donnée par la décomposition (0.0.8) vers zéro (mécanisme de relaxation d'Elliot-Yafet). Différents opérateurs de collisions sans renversement de spin seront considérés dans la suite comme les collisions électrons-phonons, élastiques, inélastiques, etc...

En microélectronique, les modèles macroscopiques ou fluides s'intéressent à l'évolution des quantités moyennées en vitesse de la fonction de distribution tels que la densité $n(t,x) = \int_{\mathbb{R}^3} f(t,x,v)dv$, le courant $j(t,x) = \int_{\mathbb{R}^3} vf(t,x,v)dv$, et l'énergie $\mathcal{W}(t,x) = \int_{\mathbb{R}^3} \frac{|v|^2}{2} f(t,x,v)dv$. Ces modèles moins précis que les modèles cinétiques (d'un point de vue physique) possèdent une avantage d'être en général moins coûteux du point de vue numérique. Différents modèles existent dans la littérature et sont obtenus à partir des modèles cinétiques par différents processus. Les modèles hydrodynamiques comme les équations d'Euler et de Navier-Stokes sont obtenus avec une limite hydrodynamique reposant sur la méthode de moments [3, 22, 66, 71, 70, 99]. Une hiérarchie d'autres modèles fluides existent tels que le modèle SHE (Spherical Harmonic Expansion) [32, 23], ET (Energie-Transport) [10, 12, 42, 36] et le modèle de dérive-diffusion [20, 95]. Ces différents modèles sont obtenus à partir de l'équation de Boltzmann suivant le mécanisme collisionnel dominant [8] et via la limite de diffusion. Cette limite consiste à perturber la fonction de distribution autour d'un équilibre thermodynamique local (la Maxwellienne) par un petit paramètre représentant le rapport entre le libre parcourt moyen et la longueur macroscopique caractéristique. Nous citons d'autres travaux concernant l'obtention rigoureuse des modèles macroscopiques à partir des équations cinétiques [2, 4, 40, 41, 67, 72, 73].

Modèles macroscopiques en spintronique. Les modèles macroscopiques (et cinétiques) utilisés pour décrire le transport des courants polarisés en spin sont de deux types. On a d'une part les modèles à deux composantes et d'autre part les modèles spinoriels ou matriciels. Dans la description à deux composantes, les électrons sont supposés avoir deux types de spin : électron avec spin-up et électron avec spin-down. Chaque type de particules est décrit par une équation cinétique ou macroscopique et les deux équations sont couplées par des termes d'échanges dûs aux intéractions avec renversement de spin. Par exemple, le modèle de dérive diffusion à deux composantes s'écrit [89, 101, 102]

$$\begin{cases} \partial_t n_{\uparrow(\downarrow)} + div_x j_{\uparrow(\downarrow)} = \dfrac{n_{\downarrow(\uparrow)} - n_{\uparrow(\downarrow)}}{\tau_{sf}}, \\ j_{\uparrow(\downarrow)} = -D_{\uparrow(\downarrow)}(\nabla_x n_{\uparrow(\downarrow)} + \nabla_x V n_{\uparrow(\downarrow)}), \end{cases}$$

où $n_{\uparrow(\downarrow)}$ est la densité des particules avec spin-up (spin-down), $j_{\uparrow(\downarrow)}$ est le courant et $D_{\uparrow(\downarrow)}$ est la constante de diffusion correspondant au type de particules. Le terme de droite de cette équation est un terme de relaxation caractérisé par τ_{sf}, temps de renversement de spin phénoménologique (spin-flip time) ou temps de relaxation, qui peut prendre en compte à la fois la relaxation via le mécanisme d'Elliot-Yafet et la relaxation via le mécanisme de D'yakonov-Perel. Les modèles à deux composantes ont été initialement utilisés pour décrire le transport de spin dans les métaux ferromagnétiques. Ils sont ensuite utilisés dans les semi-conducteurs pour étudier par

exemple la propagation d'un courant polarisé en spin à travers l'interface entre deux régions semi-conductrices de différents dopages [89] (voir aussi Chapitre 3). Dans ce type de modèles, l'effet du mécanisme de D'yakonov-Perel est pris en compte de manière très simplifiée dans le temps phénoménologique τ_{sf}. L'approche spinorielle ou matricielle, qui permet d'incorporer dans le modèle le mécanisme de D'yakonov-Perel de manière microscopique, est une description plus générale du transport polarisé en spin dans les semi-conducteurs. Dans cette description, la variable de spin est une quantité vectorielle à valeurs dans $\mathbb{R}^3$ et les différents mécanismes de relaxation et de rotation décrits auparavant peuvent être pris en compte comme on vient de l'expliquer sur l'équation de Boltzmann.

I.3 Résumé des résultats

Chapitre 1. Le chapitre 1 est consacré à l'analyse semi-classique de l'équation de Schrödinger avec hamiltonien spin-orbite. Dans la première partie de ce chapitre, nous étudions la limite semi-classique d'une équation de Schrödinger de la forme

$$i\varepsilon\partial_t\Psi^\varepsilon = -\frac{\varepsilon^2}{2}\Delta_x\Psi^\varepsilon + V^\varepsilon\Psi^\varepsilon + \alpha\Omega_\varepsilon^W(t,x,i\varepsilon\nabla_x)\cdot\vec{\sigma}\Psi^\varepsilon, \tag{0.0.10}$$

avec

$$\Psi^\varepsilon(t=0) = \Psi_I^\varepsilon, \tag{0.0.11}$$

et ε est la constante de Planck adimensionnée. L'hamiltonien spin-orbite est représenté par l'opérateur de Weyl $\Omega_\varepsilon^W(t,x,i\varepsilon\nabla_x)\cdot\vec{\sigma}$ associé au symbol $\vec{\Omega}_\varepsilon(t,x,\xi)\cdot\vec{\sigma}$ donné par

$$\Omega_\varepsilon^W(t,x,i\varepsilon\nabla_x)\cdot\vec{\sigma}(\Psi) = \frac{1}{(2\pi)^3}\int_{\mathbb{R}^3_\xi}\int_{\mathbb{R}^3_y}\vec{\Omega}_\varepsilon\left(t,\frac{x+y}{2},\varepsilon\xi\right)\cdot\vec{\sigma}(\Psi(y))e^{i(x-y)\cdot\xi}d\xi dy.$$

La limite semi-classique ($\varepsilon\to 0$) conduit à de modèles cinétiques. Cette limite est étudiée en appliquant des résultats de convergence importants dans la théorie de la limite semi-classique via la transformée de Wigner [64, 80]. De nombreux résultats mathématiques concernant l'étude de l'équation de Schrödinger ainsi que sa limite semi-classique peuvent être trouvés dans la littérature [7, 11, 25, 26, 64, 80, 84, 85, 86]. En comparant l'ordre du couplage spin-orbite α avec ε, deux cas sont étudiés. Si α est du même ordre que ε, alors la limite semi-classique conduit à la "spinor" forme de l'équation de Vlasov. Plus précisément, la transformation de Wigner associée à Ψ^ε et définie par

$$W^\varepsilon(\Psi^\varepsilon,\Psi^\varepsilon)(t,x,\xi) = (2\pi)^{-3}\int_{\mathbb{R}^3}e^{i\eta\cdot\xi}\Psi^\varepsilon(t,x-\varepsilon\frac{\eta}{2})\otimes\overline{\Psi^\varepsilon}(t,x+\varepsilon\frac{\eta}{2})d\eta$$

converge dans un certain sens (voir Chapitre 1) vers W^0. Si $\alpha=\mathcal{O}(\varepsilon)$, W^0 vérifie

$$\partial_t W^0 + \xi\cdot\nabla_x W^0 - \nabla_x V\cdot\nabla_\xi W^0 = i[W^0,\vec{\Omega}\cdot\vec{\sigma}],$$

$$W^0(0,x,\xi) = W_I,$$

où V, $\vec{\Omega}$ et W_I sont respectivement les limites de V^ε, $\vec{\Omega}_\varepsilon$ et $W^\varepsilon(\Psi_I^\varepsilon, \Psi_I^\varepsilon)$ quand $\varepsilon \to 0$. Par ailleurs, si α est supposé constant par rapport à ε ($\alpha = \mathcal{O}(1)$), on obtient à la limite un modèle cinétique à deux composantes avec un "splitting" entre les niveaux d'énergie up et down d'ordre $|\vec{\Omega}|$. La limite est vérifiée dans ce cas en dehors de l'ensemble E des (t,x,ξ) dans $\mathbb{R}^+ \times \mathbb{R}^6_{x,\xi}$ où $\vec{\Omega}$ s'annule

$$E = \left\{ (t,x,\xi) \in \mathbb{R}^+ \times \mathbb{R}^6 / \ \vec{\Omega}(t,x,\xi) = 0 \right\}.$$

En d'autres termes, nous avons $W^0(t,x,\xi) = \dfrac{1}{2} w_c(t,x,\xi) I_2 + w_s(t,x,\xi) \dfrac{\vec{\Omega}}{|\vec{\Omega}|} \cdot \vec{\sigma}$ pour tout $(t,x,\xi) \in \mathbb{R}^+ \times \mathbb{R}^6 \setminus \overline{E}$ où $\overline{E}$ est l'adhérence de E. En plus, les valeurs propres de W^0, $w_\uparrow = \dfrac{w_c}{2} + w_s$ et $w_\downarrow = \dfrac{w_c}{2} - w_s$, satisfont

$$\begin{cases} \partial_t w_\uparrow + \nabla_\xi \lambda_\uparrow \cdot \nabla_x w_\uparrow - \nabla_x \lambda_\uparrow \cdot \nabla_\xi w_\uparrow = 0 \quad \text{sur } (\mathbb{R}^+ \times \mathbb{R}^6_{x,\xi}) \setminus \overline{E} \\ \\ \partial_t w_\downarrow + \nabla_\xi \lambda_\downarrow \cdot \nabla_x w_\downarrow - \nabla_x \lambda_\downarrow \cdot \nabla_\xi w_\downarrow = 0 \quad \text{sur } (\mathbb{R}^+ \times \mathbb{R}^6_{x,\xi}) \setminus \overline{E}. \end{cases}$$

Les énergies totales up et down, $\lambda_\uparrow$ and $\lambda_\downarrow$, sont respectivement données par

$$\lambda_\uparrow(t,x,\xi) = \frac{|\xi|^2}{2} + V + |\vec{\Omega}|, \quad \lambda_\downarrow(t,x,\xi) = \frac{|\xi|^2}{2} + V - |\vec{\Omega}|.$$

Lorsque les courbes caractéristiques atteignent E, les deux modes d'énergies $\lambda_\uparrow$ et $\lambda_\downarrow$ se croisent et un problème de transfert d'énergie entre eux peut apparaître. Plusieurs travaux mathématiques existent pour décrire l'évolution semi-classique d'un système au delà d'un croisement de modes et pour quantifier le transfert d'énergie en termes de mesures de Wigner à double échelle et formule de Landau-Zener. Nous renvoyons le lecteur aux travaux de Patrick Gérard et Clotilde Fermanian-Kammerer sur ce sujet [50, 51, 52, 53, 54].

La deuxième partie du premier chapitre est consacrée à la dérivation d'un modèle de sous-bande couplé cinétique/quantique. Ce type de modèle décrit le transport des particules dans des systèmes partiellement confinés tels que les gaz d'électrons bidimensionnels. Dans ces systèmes de particules, les différentes directions de l'espace ne jouent pas le même rôle. Le gaz d'électrons est confiné dans une (ou plusieurs directions) et le transport s'effectue dans les autres directions. Dans la direction du confinement l'échelle spatiale est généralement petite et une description quantique est nécessaire ; dans la direction du transport les électrons se comportent d'une façon classique et un modèle cinétique ou fluide peut être utilisé. Cette approche de couplage directionnel a été récemment développée au sein de l'équipe MIP de l'institut de mathématiques de Toulouse. Dans [15], un modèle de sous-bande quantique/cinétique est dérivé d'un modèle entièrement quantique par le biais d'une

limite semi-classique partielle. L'analyse du modèle obtenu a été ensuite effectuée dans [14]. La thèse de N. Vauchelet dirigée par N. Ben Abdallah et F. Méhats [98] a été consacrée à la dérivation et l'étude mathématique et numérique d'un modèle couplé quantique/fluide à savoir Dérive-Diffusion-Schrödinger-Poisson (voir aussi [17, 19, 90]). D'autres modèles adiabatiques quantique/fluide sont dérivés comme les modèles Schrödinger/SHE et Schrödinger/ET [18]. Notons enfin qu'une autre stratégie de couplage quantique/classique à savoir le couplage spatial existe [6, 9, 34]. Cette approche consiste à découper le domaine d'étude en plusieurs zones. Chaque zone est décrite par un modèle quantique ou classique et le couplage se fait par des conditions d'interfaces.

Ici, le confinement a lieu dans une seule direction de l'espace notée z et le transport s'effectue dans la direction orthogonale $\mathbf{x}$. Nous étudions la limite semi-classique partielle de l'équation de Schrödinger avec terme spin-orbite en suivant [15]. Le point de départ est l'équation de Schrödinger adimensionnée suivante

$$\begin{cases} i\varepsilon\partial_t\Psi^\varepsilon = -\dfrac{\varepsilon^2}{2}\Delta_{\mathbf{x}}\Psi^\varepsilon - \dfrac{1}{2}\partial_z^2\Psi^\varepsilon + V^\varepsilon\Psi^\varepsilon + \varepsilon\Omega_\varepsilon^W(t,\mathbf{x},z,i\nabla_\varepsilon)\cdot\vec{\sigma}(\Psi^\varepsilon), \\ \Psi^\varepsilon(0,\mathbf{x},z) = \Psi_I^\varepsilon(\mathbf{x},z), \end{cases} \tag{0.0.12}$$

avec $(\mathbf{x},z)\in\mathbb{R}^2\times[0,1]$, $\Psi^\varepsilon = \Psi^\varepsilon(t,\mathbf{x},z)$ et $\nabla_\varepsilon = (\varepsilon\nabla_{\mathbf{x}},\partial_z)$. Les sous bandes sont définies par les éléments propres de l'opérateur de Schrödinger $-\frac{1}{2}\partial_z^2 + V^\varepsilon$ dans la direction z

$$\begin{cases} -\frac{1}{2}\partial_z^2\chi_p^\varepsilon + V^\varepsilon\chi_p^\varepsilon = \epsilon_p^\varepsilon\chi_p^\varepsilon \\ \chi_p^\varepsilon(t,\mathbf{x},.)\in H_0^1(0,1), \quad \displaystyle\int_0^1 \chi_p^\varepsilon\chi_q^\varepsilon = \delta_{pq}. \end{cases} \tag{0.0.13}$$

La limite $\varepsilon\to 0$, conduit à un modèle de sous bande quantique/cinétique. Plus précisément, la matrice densité donnée par $N^\varepsilon = \Psi^\varepsilon(t,\mathbf{x},z)\otimes\overline{\Psi^\varepsilon}(t,\mathbf{x},z)$ converge dans un certain sens vers N avec

$$N(t,\mathbf{x},z) = \sum_{p\geq 1}\left(\int_{\mathbb{R}^2} F_p(t,\mathbf{x},\xi_{\mathbf{x}})d\xi_{\mathbf{x}}\right)|\chi_p(t,\mathbf{x},z)|^2$$

où χ_p sont les fonctions propres pour $\varepsilon = 0$ et $\xi_{\mathbf{x}}$ est la variable dual associée à $\mathbf{x}$. La fonction de distribution de la $p$ième sous bande satisfait

$$\begin{cases} \partial_t F_p + \xi_{\mathbf{x}}\cdot\nabla_{\mathbf{x}}F_p - \nabla_{\mathbf{x}}\epsilon_p\cdot\nabla_{\xi_{\mathbf{x}}}F_p = i[F_p,\vec{\Omega}_p\cdot\vec{\sigma}], \\ + \text{ conditions initiales} \end{cases}$$

où le champ effectif du $p$ième sous bande, $\vec{\Omega}_p$, est donné par

$$\vec{\Omega}_p(t,\mathbf{x},\xi_{\mathbf{x}}) = \int_0^1 \vec{\Omega}(t,\mathbf{x},z,\xi_{\mathbf{x}})|\chi_p(t,\mathbf{x},z)|^2 dz. \tag{0.0.14}$$

En appliquant ces résultats à l'hamiltonien spin-orbite (0.0.6), l'équation cinétique de la $p$ième sous bande s'écrit alors

$$\partial_t F_p + \xi_{\mathbf{x}} \cdot \nabla_{\mathbf{x}} F_p - \nabla_{\mathbf{x}} \epsilon_p \cdot \nabla_{\xi_{\mathbf{x}}} F_p = i\alpha_p(t,\mathbf{x})[\sigma_2 v_1 - \sigma_1 v_2, F_p]$$

avec

$$\alpha_p(t,\mathbf{x}) = \int_0^1 \partial_z V(t,\mathbf{x},z)|\chi_p(t,\mathbf{x},z)|^2 dz.$$

L'effet spin-orbite obtenu n'est autre que l'effet de Rashba utilisé dans la littérature pour modéliser le couplage spin-orbite dans les 2DEG [103, 27]. De plus, nous obtenons une relation explicite reliant l'ordre du couplage α_p et le potentiel de confinement.

Chapitre 2. Dans ce chapitre, nous dérivons rigoureusement une hiérarchie de modèles macroscopiques vectoriels ou à deux composantes. Nous partons de l'équation de Boltzmann adimensionnée dans un scaling de diffusion

$$\frac{\partial F^\varepsilon}{\partial t} + \frac{1}{\varepsilon}(v.\nabla_x F^\varepsilon - \nabla_x V.\nabla_v F^\varepsilon) = \frac{1}{\varepsilon^2} Q(F^\varepsilon) + \frac{\alpha}{\varepsilon}\left[\frac{i}{2}\vec{\Omega}(x,v).\vec{\sigma}, F^\varepsilon\right] + Q_{sf}(F^\varepsilon), \quad (0.0.15)$$

où ε est le libre parcourt moyen adimensionné. Nous rappelons que Q_{sf} est l'opérateur de collisions avec renversement de spin donné par (0.0.9). Différents opérateurs de collisions Q sans retournement de spin sont considérés. Suivant le mécanisme collisionnel dominant, nous dérivons de modèles macroscopiques de type dérive diffusion avec statistique de Boltzmann ou de Fermi-Dirac, SHE, ET, à deux composantes ou vectoriels gardant des effets de rotations et de relaxation du spin électronique. Nous commençons par considérer l'approximation BGK linéaire de l'opérateur de collisions électron-phonon avec une statistique de Boltzmann donnée par

$$Q(F) = \int_{\mathbb{R}^3} \alpha(v,v')[\mathcal{M}(v)F(v') - \mathcal{M}(v')F(v)]dv, \quad (0.0.16)$$

où α est la section efficace supposée bornée par des bornes supérieures et inférieures strictement positives. La fonction $\mathcal{M}$ est la maxwellienne

$$\mathcal{M}(v) = \frac{1}{(2\pi)^{\frac{3}{2}}} e^{-\frac{1}{2}|v|^2}, \quad \forall v \in \mathbb{R}^3. \quad (0.0.17)$$

Cet opérateur fait relaxer F vers la maxwellienne quand le libre parcourt moyen tend vers zero. Puisque les collisions avec renversement de spin sont rares dans les semiconducteurs [24], nous supposons que Q_{sf} est une perturbation d'ordre ε de Q. Ceci justifie que Q_{sf} est considéré d'ordre un dans le scaling de diffusion (0.0.15). Nous étudions la limite de diffusion $\varepsilon \to 0$ pour différents ordres du couplage spin-orbite α par rapport à ε. Le chapitre 2 est organisé de la manière suivante.

Nous nous intéressons tout d'abord à l'étude des propriétés fondamentales de l'équation de Boltzmann avec terme spin-orbite (0.0.15). Nous montrons l'existence et l'unicité de solutions faibles vérifiant le principe de maximum. Autrement dit nous montrons que si initialement $F^\varepsilon(t=0,x,v) := F_{in}(x,v)$ est une fonction à valeurs dans l'ensemble des matrices carrées hermitiennes et positives que l'on note par $\mathcal{H}_2^+(\mathbb{C})$, alors $F^\varepsilon(t,x,v) \in \mathcal{H}_2^+(\mathbb{C})$, $\forall t > 0$ et $\forall (x,v) \in \mathbb{R}^6$. Nous établissons en plus des estimations à priori nécessaires pour passer à la limite.

La deuxième partie est consacrée à la dérivation des modèles cinétiques et macroscopiques à deux composantes. Nous nous plaçons dans un régime où le couplage spin-orbite est fort de sorte que la période de rotation du vecteur spin T autour de $\vec{\Omega}$ est petite devant le temps caractéristique $\bar{t}$. La limite $\eta := \dfrac{T}{\bar{t}} \to 0$ est appelée "limite de decohérence". Cette limite fait relaxer la partie spin de la fonction de distribution parallèlement au champ effectif considéré $\vec{\Omega}(t,x,v)$. Dans le cas où la direction de $\vec{\Omega}$ ne dépend pas de v, nous obtenons un modèle cinétique à deux composantes en projetant le vecteur distribution de spin suivant la direction de $\vec{\Omega}(t,x,.)$. Partant ensuite de ce dernier modèle cinétique et appliquant une limite de diffusion (ou fluide), nous pouvons dériver des modèles macroscopiques à deux composantes. Par ailleurs, si $\vec{\Omega}$ change de direction avec la vitesse v, une limite de décohérence appliquée à la spinor forme de l'équation de Boltzmann suivie d'une limite de diffusion fait relaxer la distribution de spin vers 0 et on obtient à la limite un modèle macroscopique scalaire sur la densité des charges. Notons que cette relaxation de spin est bien connue en spintronique des semi-conducteurs et n'est autre que le mécanisme de relaxation de D'yakonov-Perel [45, 103] présenté au début de ce chapitre introductoire. Ces résultats sont ensuite vérifiés rigoureusement en passant à la limite $\varepsilon \to 0$ dans l'équation (0.0.15) en présence d'un couplage spin-orbite ultra-fort : supposant $\alpha = \mathcal{O}(\dfrac{1}{\varepsilon})$. Nous montrons aussi que la limite de diffusion dans ce cas aboutit à un modèle diffusif à 2 composantes si $\dfrac{\vec{\Omega}}{|\vec{\Omega}|}$ ne dépend pas de v et à un modèle scalaire sinon.

Section 2.5 concerne la dérivation d'un modèle vectoriel de type dérive-diffusion avec des effets de rotation et de relaxation du vecteur spin. Remarquons tout d'abord que si les intéractions spin-orbite sont faibles telles que $\alpha = \mathcal{O}(\varepsilon)$ alors, formellement $F^\varepsilon \to F_0$ lorsque ε tend vers 0 avec $Q(F_0) = 0$. Ceci implique que $F_0 = N(t,x)\mathcal{M}(v)$ (voir Chapitre 2). En plus, en intégrant l'équation (0.0.15) par rapport à v et passant à la limite, la matrice densité N vérifie

$$\partial_t N + div_x(\mathbb{D}(\nabla_x N + \nabla_x V N)) = \frac{i}{2}[\vec{H}_e \cdot \vec{\sigma}, N] + Q_{sf}(N)$$

où $\mathbb{D}$ est une matrice symétrique définie positive. Le champ effectif résultant de cette

limite est donné par

$$\vec{H}_e(x) = \int_{\mathbb{R}^3} \vec{\Omega}(x,v)\mathcal{M}(v)dv.$$

En pratique, $\vec{\Omega}$ est impaire par rapport à v (voir vecteur de Rashba et de Dresselhauss par exemple). Ceci implique, puisque $\mathcal{M}$ est paire par rapport à v, que $\vec{H}_e = 0$ et on perd l'effet spin-orbite à la limite dans ce cas. Ainsi, pour garder de traces de l'effet spin-orbite au niveau macroscopique, on étudie la limite de diffusion en supposant que le terme spin-orbite est d'ordre $\frac{1}{\varepsilon}$ ($\alpha = \mathcal{O}(1)$) si $\vec{\Omega}$ est impaire par rapport à v. Nous dérivons un modèle vectoriel de type dérive-diffusion conservant des effets de rotation et de relaxation du vecteur spin et l'un de ces principaux résultats à savoir le principe de maximum est vérifié.

En suivant la même stratégie qu'on vient de présenter, d'autres modèles macroscopiques à deux composantes ou matriciels peuvent être dérivés. Nous présentons à la fin du 2ème chapitre un modèle de type SHE dans le cas où les collisions prises en comptes sont les collisions élastiques. Nous discutons ensuite la construction des opérateurs de collisions non linéaires conservant certains moments tels que la masse et l'énergie par le principe de minimisation d'entropie. Nous utilisons ensuite ces opérateurs pour dérivés des modèles de type Energie-Transport et Dérive-Diffusion avec une statistique de Fermi-Dirac par le bias de la méthode des moments.

Chapitre 3. Dans ce chapitre, deux applications numériques sont présentées. La première concerne la simulation d'un transistor à effet de rotation de spin. En suivant le travail de [19, 90], un modèle de sous-bande de dérive diffusion Schrödinger-Poisson avec effets de relaxation et de rotation du vecteur spin dus au couplage de Rashba est dérivé et utilisé pour la simulation. Le dispositif considéré est un MOSFET à double grille (voir [98] pour plus de détails). Nous considérons un cas simple en supposant que le transport s'effectue dans une seule direction de l'espace. Le vecteur de precession de Rashba ne change pas de direction dans ce cas. Nous ne considérons pas des contacts ohmic ferromagnétiques. Nous injectons un courant polarisé en spin dans le plan du dispositif avec une densité de spin parallèle à la direction du transport. Nous montrons numériquement l'efficacité de l'effet de Rashba pour contrôler l'orientation du vecteur spin dans le canal. La direction de spin à l'arrivé au drain est entièrement déterminée par le potentiel de grille V_{gs} et le courant de drain oscille en fonction de V_{gs} dans ce cas.

Le deuxième exemple étudié est l'effet de l'accumulation de spin à l'interface entre deux régions semi-conductrices. C'est un effet bien connu en spintronique des semi-conducteurs [89, 88]. Deux modèles sont utilisés. Cet effet sera représenté tout d'abord en utilisant un modèle de dérive-diffusion à deux composantes couplé avec l'équation de Poisson. Nous utilisons ensuite un modèle vectoriel de dérive diffusion

couplé toujours avec l'équation de Poisson afin d'étudier l'effet de precession de Rashba sur la densité d'accumulation.

II. Diffusion et champs magnétiques forts (Chapter 4)

II.1 Introduction et position du problème

Le confinement magnétique est une approche importante utilisée dans beaucoup de dispositifs de production d'énergie par fusion nucléaire (tokamaks, plasmas ionosphériques, etc...). De puissants champs magnétiques sont utilisés dans de tels dispositifs. Le confinement est basé sur la propriété des particules de décrire une trajectoire en hélice autour d'une ligne de champ magnétique. En effet, le mouvement d'une particule de masse m et de charge q plongée dans un champ électrique $\vec{E}$ et un champ magnétique constante $\vec{B} = Be_z$, où e_z est un vecteur unitaire, est décrit par l'équation de mouvement suivante :

$$m\frac{dv}{dt} = q(\vec{E} + B(v \times e_z)), \tag{0.0.18}$$

où v est le vecteur vitesse. La solution générale de l'équation homogène associée (pour $\vec{E} = 0$) est donnée par

$$\overline{v}(t) = \mathcal{R}(w_c t)v_0 \quad \text{avec} \quad \mathcal{R}(\tau) = \begin{pmatrix} \cos\tau & -\sin\tau & 0 \\ \sin\tau & \cos\tau & 0 \\ 0 & 0 & 1 \end{pmatrix} \tag{0.0.19}$$

où $w_c = \dfrac{qB}{m}$ est la fréquence du cyclotron et $v_0 \in \mathbb{R}^3$. Une quantité importante prise en considération dans la suite est la gyropériode T_c. Il s'agit du temps qu'elle met une particule de masse m et de charge q soumise à un champ magnétique constant B pour faire une rotation d'angle 2π. On a

$$T_c = \frac{2\pi}{w_c} = \frac{2\pi m}{qB}. \tag{0.0.20}$$

En intégrant l'équation (0.0.19), le rayon vecteur $\overline{x}(t)$, $\dot{\overline{x}}(t) = \overline{v}(t)$, vérifie

$$\begin{cases} \overline{x}^{\perp}(t) = & \overline{x}^{\perp}(0) + \dfrac{1}{w_c}(e_z \times v_0^{\perp}) - \dfrac{|v_0^{\perp}|}{w_c}\mathcal{R}(w_c t + \dfrac{\pi}{2})\dfrac{v_0^{\perp}}{|v_0^{\perp}|} \\ \overline{x}^{\parallel}(t) = & \overline{x}^{\parallel}(0) + v_0^{\parallel}t, \end{cases}$$

où $\overline{x}^{\perp}$ et $\overline{x}^{\parallel}$ sont respectivement la partie perpendiculaire et la partie parallèle de $\overline{x}$ par rapport au champ magnétique (ou e_z). C'est l'équation paramétrée d'une hélice de centre de rotation $\overline{x}_c(t) = \left(\overline{x}^{\perp}(0) + \dfrac{1}{w_c}(e_z \times v_0^{\perp}), \overline{x}^{\parallel}(0) + v_0^{\parallel}t\right)$ qu'on appelle centre-guide et de rayon de rotation

$$r_L = \frac{|v_0^{\perp}|}{w_c} = \frac{m|v_0^{\perp}|}{qB}, \tag{0.0.21}$$

appelé rayon de Larmor et qui est inversement proportionnel au module du champ magnétique B. Ceci implique que, lorsque B augmente et tend vers l'infini, le rayon de Larmor tend vers zéro et les particules sont piégées le long de la ligne du champ magnétique. En présence d'un champ électrique, la solution de (0.0.18) est donnée par la solution générale de l'équation homogène $\overline{v}$ plus une solution particulière v_{part} de (0.0.18). On a $v_{part}^{\parallel} = \dfrac{q\vec{E}^{\parallel}}{m}t$ et on cherche une solution particulière stationnaire dans la direction perpendiculaire. Ceci implique que $\vec{B} \times v_{part}^{\perp} = \vec{E}$ et donc

$$v_{part}^{\perp} = \frac{\vec{E} \times \vec{B}}{B^2}. \tag{0.0.22}$$

On en déduit que le rayon vecteur en présence d'un champ électrique est donné par

$$\begin{cases} x^{\perp}(t) = & x^{\perp}(0) + \frac{1}{w_c}(e_z \times v_0^{\perp}) + \dfrac{\vec{E} \times \vec{B}}{B^2}t - r_L \mathcal{R}(w_c t + \dfrac{\pi}{2})\dfrac{\vec{v}_0^{\perp}}{v_0^{\perp}} \\ x^{\parallel}(t) = & x^{\parallel}(0) + (v_0^{\parallel} + \dfrac{q\vec{E}^{\parallel}}{m})t. \end{cases}$$

Par conséquent, un champ électrique perpendiculaire à $\vec{B}$ n'accélère pas les particules mais crée une dérive uniforme du centre-guide dans la direction $\vec{E} \times \vec{B}$ avec une vitesse (appelée vitesse de dérive du centre-guide) inversement proportionnelle à B^2, et donnée exactement par (0.0.22).

La présence d'un champ magnétique fort dans les équations cinétiques (Vlasov, Boltzmann) introduit de fortes oscillations et donc des difficultés pour la simulation numérique. La question de trouver des modèles approximatifs moins coûteux numériquement que les modèles cinétiques est très importante dans ce sujet. Différents modèles approximatifs existent dans la littérature tels que les modèles centre-guide et gyrocinétiques. Ces modèles consistent à moyenner le mouvement sur la gyropériode tout en supposant que B tend vers l'infini. Nous référons à une liste de travaux physiques sur ce type de modèles [77, 81, 87, 44]. De point de vue mathématique, E. Sonnendrücker et E. Frénod ont étudié la limite champ magnétique fort du système Vlasov et Vlasov-Poisson par des techniques d'homogénéisation [59, 60]. Dans [59], il a été montré que l'approximation centre-guide de l'équation de Vlasov $3D$ conduit à une équation cinétique unidimensionnelle dans la direction du champ magnétique. La dérive du centre-guide est obtenue ensuite dans [60] en étudiant la limite centre-guide de l'équation de Vlasov $2D$ (dans la direction perpendiculaire au champ) dans un échelle de temps suffisamment long. L'investigation de l'équation de Vlasov et du système Vlasov-Poisson en présence d'un champ magnétique fort est intensivement étudiée pour différents régimes asymptotiques [57, 58, 61, 62, 68, 69, 96, 97].

Dans toutes les références précédentes, le transport est supposé balistique (sans collisions). Nous sommes intéressés ici par des régimes où les collisions sont importantes et nous étudions l'asymptotique de diffusion de l'équation de Boltzmann en

présence d'un champ magnétique fort. L'équation de Boltzmann dans le scaling de diffusion s'écrit [95, 67]

$$\varepsilon\partial_t f_\varepsilon + (\mathbf{v}\cdot\nabla_{\mathbf{r}} f_\varepsilon + \mathbf{E}\cdot\nabla_{\mathbf{v}} f_\varepsilon) + \alpha(\mathbf{v}\times e_z)\cdot\nabla_{\mathbf{v}} f_\varepsilon = \frac{Q(f_\varepsilon)}{\varepsilon}$$

où $\mathbf{r} = (x, y, z)$ est le vecteur position, $\mathbf{v} = (v_x, v_y, v_z)$ est la variable vitesse, et $\varepsilon = \frac{\tau}{\bar{t}} \ll 1$ est le libre parcourt moyen adimensionné avec $\bar{t}$ et le temps caractéristique. Le champ magnétique est supposé constant et parallèle à l'axe des z de vecteur unitaire e_z. Nous notons par $\mathbf{r}_\perp = (x, y)$ et $\mathbf{v}_\perp = (v_x, v_y)$ les variables orthogonales. Le paramètre α^{-1} représente la gyropériode adimensionnée où

$$\alpha = \bar{t} w_c = \frac{2\pi\bar{t}}{T_c}.$$

Nous considérons dans ce travail pour simplifier la forme BGK linéaire de l'opérateur des collisions electron-phonon donné par (0.0.16)-(0.0.17). Le modèle fluide obtenu lorsque ε tend vers zéro est alors de type dérive-diffusion. Si la gyropériode est plus grande que le temps de relaxation τ ou si α est constante devant ε ($\alpha = \mathcal{O}(1)$) alors l'effet du champ magnétique disparaît à la limite. D'autre part, si T_c est du même ordre que le temps de relaxation ou bien si $\alpha = \mathcal{O}(\varepsilon^{-1})$, l'équation de Boltzmann devient

$$\partial_t f_\varepsilon^{\mathcal{B}} + \frac{1}{\varepsilon}(\mathbf{v}\cdot\nabla_{\mathbf{r}} f_\varepsilon^{\mathcal{B}} + \mathbf{E}\cdot\nabla_{\mathbf{v}} f_\varepsilon^{\mathcal{B}}) + \frac{\mathcal{B}}{\varepsilon^2}(\mathbf{v}\times e_z)\cdot\nabla_{\mathbf{v}} f_\varepsilon^{\mathcal{B}} = \frac{Q(f_\varepsilon^{\mathcal{B}})}{\varepsilon^2} \tag{0.0.23}$$

où $\mathcal{B}$ est une constante strictement positive telle que $\alpha = \dfrac{\mathcal{B}}{\varepsilon}$. Ce scaling de diffusion est utilisé généralement pour les plasmas et les gas binaires. La matrice de diffusion dans le modèle limite admet une composante antisymétrique dans ce cas générée par le champ magnétique. Ce résultat est prouvé par P. Degond et al [31, 35, 39] pour des collisions avec des murs. D'autres résultats formels concernant les gaz binaires se trouvent aussi dans [33, 37, 38, 83].

Dans ce travail, nous considérons une situation où la gyropériode T_c est plus petite que le temps de relaxation. Ce qui revient à supposer que $\mathcal{B}$ est grand et tend vers l'infini. Nous allons voir que le scaling de diffusion standard (0.0.23) n'est pas convenable pour décrire, quand $\varepsilon \to 0$ et $\mathcal{B} \to +\infty$, la dynamique du centre-guide dans la direction perpendiculaire au champ magnétique. Il décrit seulement le transport diffusif dans la direction parallèle. Un autre scaling est proposé pour lequel la limite de diffusion avec $\mathcal{B} \to +\infty$ conduit à un modèle de dérive-diffusion dans la direction parallèle au champ magnétique et dans la direction perpendiculaire, le transport est dominé par la dérive du centre-guide. Afin de mieux comprendre ce qui se passe à la limite, nous considérons l'approximation du temps de relaxation de l'opérateur de collisions

$$Q(f) = n(t,x)\mathcal{M}(v) - f, \quad n(t,x) = \int_{\mathbb{R}^3} f(t,x,v)dv. \tag{0.0.24}$$

En prenant un développement de Hilbert de $f_\varepsilon^{\mathcal{B}}$ de la forme

$$f_\varepsilon^{\mathcal{B}} = f_0^{\mathcal{B}} + \varepsilon f_1^{\mathcal{B}} + \mathcal{O}(\varepsilon^2)$$

et en injectant dans (0.0.23), on trouve

$$\begin{cases} Q(f_0^{\mathcal{B}}) - \mathcal{B}(\mathbf{v}\times e_z)\cdot\nabla_{\mathbf{v}} f_0^{\mathcal{B}} = 0 \\ Q(f_1^{\mathcal{B}}) - \mathcal{B}(\mathbf{v}\times e_z)\cdot\nabla_{\mathbf{v}} f_1^{\mathcal{B}} = \mathbf{v}\cdot\nabla_{\mathbf{r}} f_0^{\mathcal{B}} + \mathbf{E}\cdot\nabla_{\mathbf{v}} f_0^{\mathcal{B}}. \end{cases}$$

La première équation implique que $f_0^{\mathcal{B}} = n_{\mathcal{B}}(t,\mathbf{r})\mathcal{M}(\mathbf{v})$ et la deuxième équation devient

$$-f_1^{\mathcal{B}} - \mathcal{B}(\mathbf{v}\times e_z)\cdot\nabla_{\mathbf{v}} f_1^{\mathcal{B}} = (\nabla_{\mathbf{r}} n_{\mathcal{B}} - \mathbf{E}\, n_{\mathcal{B}})\mathbf{v}\mathcal{M}. \tag{0.0.25}$$

En intégrant (0.0.23) par rapport à $\mathbf{v}$ et en passant à la limite, nous obtenons l'équation de continuité

$$\partial_t n_{\mathcal{B}} + div_{\mathbf{r}} j_{\mathcal{B}} = 0$$

où $j_{\mathcal{B}} = \int_{\mathbb{R}^3} \mathbf{v} f_1^{\mathcal{B}} d\mathbf{v}$ est le courant. D'autre part, avec (0.0.25) $j_{\mathcal{B}}$ se calcule explicitement et nous avons $j_{\mathcal{B}} = -\mathbb{D}_{\mathcal{B}}(\nabla_{\mathbf{r}} n_{\mathcal{B}} - \mathbf{E}\, n_{\mathcal{B}})$ où

$$\mathbb{D}_{\mathcal{B}} = \begin{pmatrix} \frac{1}{1+\mathcal{B}^2} & \frac{\mathcal{B}}{1+\mathcal{B}^2} & 0 \\ -\frac{\mathcal{B}}{1+\mathcal{B}^2} & \frac{1}{1+\mathcal{B}^2} & 0 \\ 0 & 0 & 1 \end{pmatrix}.$$

La matrice de diffusion $\mathbb{D}_{\mathcal{B}}$ n'est pas symétrique. En plus, $\mathbb{D}_{\mathcal{B}} = \mathbb{D}_{\mathcal{B}}^S + \mathbb{D}_{\mathcal{B}}^{AS}$ avec $\mathbb{D}_{\mathcal{B}}^S = \begin{pmatrix} \frac{1}{1+\mathcal{B}^2} & 0 & 0 \\ 0 & \frac{1}{1+\mathcal{B}^2} & 0 \\ 0 & 0 & 1 \end{pmatrix}$ est une matrice symétrique définie positive avec différents coefficients de diffusion suivant la direction parallèle et la direction perpendiculaire. La partie antisymétrique est donnée par : $\mathbb{D}_{\mathcal{B}}^{AS} = \dfrac{\mathcal{B}}{1+\mathcal{B}^2}\begin{pmatrix} 0 & 1 & 0 \\ -1 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}$. L'équation limite s'écrit alors

$$\partial_t n_B - div_{\mathbf{r}}\left(\mathbb{D}_{\mathcal{B}}^S(\nabla_{\mathbf{r}} n_{\mathcal{B}} - \mathbf{E}\, n_{\mathcal{B}})\right) + \frac{\mathcal{B}}{1+\mathcal{B}^2}(\mathbf{E}\times e_z).\nabla_{\mathbf{r}} n_{\mathcal{B}} = 0.$$

La partie antisymétique de la matrice de diffusion donnant l'effet centre guide est d'ordre $\dfrac{1}{\mathcal{B}}$. Ainsi quand $\mathcal{B}$ tend vers l'infini, nous obtenons une équation de dérive-diffusion $1D$ dans la direction z avec ce scaling.

Puisque le champ magnétique confine les particules dans la direction perpendiculaire $\mathbf{r}_\perp = (x,y)$, et afin de capter la dynamique du centre-guide dans cette direction, nous proposons de faire le changement de variable : $\mathbf{r}_\perp \to (\sqrt{\mathcal{B}})\mathbf{r}_\perp$. Ce rééchelonnement implique les changements suivants

$$\nabla_{\mathbf{r}} \to \begin{pmatrix} \sqrt{\mathcal{B}}\nabla_{\mathbf{r}_\perp} \\ \partial_z \end{pmatrix},\ \mathbf{E} \to \begin{pmatrix} \sqrt{\mathcal{B}}\mathbf{E}_\perp \\ E_z \end{pmatrix}.$$

Pour simplifier la présentation, nous posons $\mathcal{B} = \dfrac{1}{\eta^2}$ où η est un petit paramètre destiné à tendre vers zéro. Dans ce travail, la fonction de distribution dépend de deux petits paramètres ε et η. Elle vérifie l'équation de Boltzmann adimensionnée suivante

$$\begin{cases} \dfrac{\partial f^{\varepsilon\eta}}{\partial t} + \dfrac{\mathcal{T}_z f^{\varepsilon\eta}}{\varepsilon} + \dfrac{\mathcal{T}_\perp f^{\varepsilon\eta}}{\varepsilon\eta} + \dfrac{(\mathbf{v}\times\mathbf{e}_z)}{\varepsilon^2\eta^2}\cdot\nabla_{\mathbf{v}} f^{\varepsilon\eta} = \dfrac{Q(f^{\varepsilon\eta})}{\varepsilon^2} \\ f^{\varepsilon\eta}(t=0) = f_0(\mathbf{r},\mathbf{v}). \end{cases} \tag{0.0.26}$$

Ici, $\mathcal{T}_\perp$ and $\mathcal{T}_z$ sont respectivement les parties perpendiculaire et parallèle de l'opérateur de transport

$$\mathcal{T}_\perp = \mathbf{v}_\perp\cdot\nabla_{\mathbf{r}_\perp} + \mathbf{E}_\perp\cdot\nabla_{\mathbf{v}_\perp}, \quad \mathcal{T}_z = v_z\partial_z + E_z\partial_{v_z}.$$

II.2 Résultats obtenus

Nous étudions le cas où ε tend vers zéro pour η donné et ensuite η tend vers zéro et le cas où ε et η tendent vers zéro simultanément. Le premier résultat concerne la limite de diffusion $\varepsilon \to 0$ pour η fixé. Nous montrons que $(f^{\varepsilon\eta})_\varepsilon$ converge dans un certain sens (voir Chapitre 4) vers $\rho_\eta(t,\mathbf{r})\mathcal{M}(\mathbf{v})$ et la densité ρ_η vérifie

$$\partial_t\rho_\eta - \mathrm{div}(\mathbb{D}^\eta(\nabla\rho_\eta - \rho_\eta\mathbf{E})) = 0. \tag{0.0.27}$$

La matrice de diffusion $\mathbb{D}^\eta$ est donnée par la formule

$$\mathbb{D}^\eta = \int \begin{pmatrix} \frac{1}{\eta}\mathbf{v}_\perp \\ v_z \end{pmatrix} \otimes \begin{pmatrix} \eta\mathbf{X}^\eta_\perp \\ X^\eta_z \end{pmatrix} d\mathbf{v},$$

$\mathbf{X}^\eta = \begin{pmatrix} \mathbf{X}^\eta_\perp \\ X^\eta_z \end{pmatrix}$ étant l'unique solution de

$$-Q(\mathbf{X}^\eta) + \frac{\mathbf{v}\times e_z}{\eta^2}\cdot\nabla_{\mathbf{v}}(\mathbf{X}^\eta) = \begin{pmatrix} \dfrac{1}{\eta^2}\mathbf{v}_\perp \\ v_z \end{pmatrix}\mathcal{M}(\mathbf{v}) \quad \text{and} \quad \int_{\mathbb{R}^3}\mathbf{X}^\eta(\mathbf{v})d\mathbf{v} = 0. \tag{0.0.28}$$

Dans l'approximation du temps de relaxation $\sigma(\mathbf{v},\mathbf{v}') = \frac{1}{\tau}$, la matrice $\mathbb{D}^\eta$ se calcule explicitement

$$\mathbb{D}^\eta = \tau\begin{pmatrix} \frac{\eta^2}{\tau^2+\eta^4} & \frac{\tau}{\tau^2+\eta^4} & 0 \\ -\frac{\tau}{\tau^2+\eta^4} & \frac{\eta^2}{\tau^2+\eta^4} & 0 \\ 0 & 0 & 1 \end{pmatrix}.$$

À la limite $\eta \to 0$, le bloc supérieure de cette matrice se réduit à $\mathcal{I} = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}$ et sa partie symétrique est d'ordre η^2. Nous obtenons ces résultats dans le cas où

la section σ est non constante. Nous développons rigoureusement $\mathbf{X}^\eta$ par rapport à η jusqu'à l'ordre η^4. Ceci nous donne un développement des parties symétrique et antisymétrique de $\mathbb{D}^\eta$ en fonction de η. Nous montrons que la diffusion est d'ordre 1 dans la direction parallèle et d'ordre η^2 dans la direction perpendiculaire. La partie antisymétrique $\mathbb{D}^\eta_{as}$ agit dans la direction perpendiculaire. Elle est donnée par la matrice $\mathcal{I}$ à l'ordre principale ce qui conduit à la dérive du centre-guide. En plus, le développement de $\mathbb{D}^\eta_{as}$ donne une correction d'ordre η à la dynamique du centre-guide. Nous renvoyons le lecteur au Chapitre 4 pour plus de détails.

Le deuxième résultat concerne la limite simultanée $\varepsilon, \eta \to 0$. Nous montrons que $f^{\varepsilon\eta} \to \rho(t,\mathbf{r})\mathcal{M}(\mathbf{v})$ avec

$$\begin{cases} \partial_t \rho + \partial_z \mathrm{J}_z + \nabla_{\mathbf{r}} \cdot (\rho \mathbf{E} \times \mathbf{e}_z) = 0 \\ \rho(0,\mathbf{r}) = \displaystyle\int_{\mathbb{R}^3} f_0(\mathbf{r},\mathbf{v})\, d\mathbf{v} \end{cases} \tag{0.0.29}$$

Le courant parallèle est donné par

$$\mathrm{J}_z = -D_z(\partial_z \rho - E_z \rho)$$

où D_z est la constante de diffusion

$$D_z = \int_{\mathbb{R}^3} \mathrm{X}_z^{(0)} v_z d\mathbf{v},$$

et $\mathrm{X}_z^{(0)}$ est le terme d'ordre zéro de X_z^η. C'est une fonction isotrope (invariante par rotation autour de e_z) vérifiant

$$-\overline{\overline{Q}}(\mathrm{X}_z^{(0)}) = v_z \mathcal{M}, \quad \int_{\mathbb{R}^3} \mathrm{X}_z^{(0)}(\mathbf{v}) d\mathbf{v} = 0$$

avec

$$\overline{\overline{Q}}(f)(\mathbf{v}) = \int_{\mathbb{R}^3} \overline{\overline{\sigma}}(\mathbf{v},\mathbf{v}')[\mathcal{M}(\mathbf{v}) f(\mathbf{v}') - \mathcal{M}(\mathbf{v}') f(\mathbf{v})] d\mathbf{v}'$$

et

$$\overline{\overline{\sigma}}\,(\mathbf{v},\mathbf{v}') = \frac{1}{4\pi^2} \int_0^{2\pi} \int_0^{2\pi} \sigma\left(\mathcal{R}(\tau)\mathbf{v}, \mathcal{R}(\tau')\mathbf{v}'\right)\, d\tau d\tau'.$$

L'équation limite (0.0.29) est composée d'un courant de dérive-diffusion dans la direction parallèle et d'une dérive due au mouvement du centre-guide dans la direction perpendiculaire. Le coefficient de diffusion parallèle D_z est obtenu via l'analyse d'un opérateur de collisions avec une section efficace moyennée sur les cercles de gyration autour du champ magnétique.

III. Confinement (Chapitre 5)

III.1 Motivation et description du problème

Afin de mieux contrôler le transport électronique, de nombreux dispositifs électroniques sont basés sur la réduction de la dimensionalité en confinant les électrons dans une ou plusieurs directions de l'espace. Parmi eux, nous avons les gas d'électrons bidimensionnels (2DEG) [1, 74] dont les électrons sont confinés dans une seule direction.

Le système Schrödinger-Poisson est l'un des modèles les plus appropriés pour décrire le transport quantique balistique (sans collisions) des particules chargés dans les semi-conducteurs ainsi qu'en chimie quantique. Dans [94, 93, 92], la simulation du transport électronique dans les gaz d'électrons bidimensionnels balistiques a été réalisée grâce à la dérivation d'un modèle approché permettant de tenir compte de manière moyennée de l'effet du potentiel de confinement sur le transport quantique. Le modèle proposé admet un avantage considérable d'être moins coûteux numériquement et de rester en accord complet avec le model $3D$ de point de vue physique. L'analyse rigoureuse de cette approximation a ensuite été effectuée dans [16, 91] dans le cas où le profil du potentiel de confinement V_c et l'échelle spatiale de ses variations ε sont supposés donnés. Dans [16], l'approximation est justifiée en effectuant une étude asymptotique lorsque ε tend vers zéro de la solution du système de Schrödinger-Poisson tridimensionnel suivant

$$i\partial_t \psi^\varepsilon = -\frac{1}{2}\Delta_{x,z}\psi^\varepsilon + V^\varepsilon \psi^\varepsilon + V_c^\varepsilon \psi^\varepsilon,$$

$$V^\varepsilon = \frac{1}{4\pi\sqrt{|x|^2+z^2}} * (|\psi^\varepsilon|^2),$$

où $x \in \mathbb{R}^2$ et $z \in \mathbb{R}$ est la direction de confinement. Le potentiel V^ε est le potentiel auto-consistant et V_c^ε est le potentiel de confinement imposé au système et donné par

$$V_c^\varepsilon = \frac{1}{\varepsilon^2} V_c(\frac{z}{\varepsilon}), \tag{0.0.30}$$

où V_c est une fonction donnée. Le cas stationnaire dans un domaine borné est traité dans [91].

Le but de ce travail est en quelque sorte de justifier le scaling (0.0.30) par l'analyse d'un système de Schrödinger-Poisson unidimensionnel (dans la direction de confinement z). De ce fait, nous ignorons le transport des particules dans la direction orthogonale à l'axe des z en supposant par exemple que le système est invariant dans cette direction. Le paramètre ε n'est pas donné mais calculé en fonction de la longueur de Debye adimensionnée. Le système est supposé fermé et occupe l'intervalle $[0, 1]$. Les

électrons se répartissent dans ce cas sur des niveaux d'énergies discrets qui sont les valeurs propres de l'opérateur de Schrödinger $-\frac{d^2}{dz^2}+V$. La densité totale de particules est la superposition des densités de tous les niveaux d'énergies avec un facteur d'occupation donné par la statistique de Boltzmann. Le potentiel electrostatique de confinement est noté par V_ε. Le point de départ est le système Schrödinger-Poisson unidimensionnel stationnaire vérifié par V_ε suivant

$$\begin{cases} -\dfrac{d^2\varphi_p}{dz^2}+V\varphi_p=\mathcal{E}_p\varphi_p \qquad z\in[0,1], \\ \varphi_p\in H^1(0,1),\ \varphi_p(0)=0,\ \varphi_p(1)=0,\ \displaystyle\int_0^1\varphi_p\varphi_q=\delta_{pq} \\ -\varepsilon^3\dfrac{d^2V}{dz^2}=\dfrac{1}{\mathcal{Z}}\displaystyle\sum_{p=1}^{+\infty}e^{-\mathcal{E}_p}|\varphi_p|^2, \quad \mathcal{Z}=\displaystyle\sum_{p=1}^{+\infty}e^{-\mathcal{E}_p} \\ V(0)=0, \quad \dfrac{dV}{dz}(1)=0. \end{cases} \tag{0.0.31}$$

Le scaling menant à ce système sera détaillé. Le paramètre ε est donné en fonction de la longueur de Debye adimensionnée, λ_D, par

$$\varepsilon^3=(\frac{\lambda_D}{L})^2, \quad \lambda_D=\sqrt{\frac{k_BT\varepsilon_0\varepsilon_r}{e^2N}} \tag{0.0.32}$$

avec L est la longueur caractéristique dans la direction z, e est la charge élémentaire, et $N=\dfrac{N_s}{L}$ est la densité volumique moyenne avec N_s le nombre total de particules (ou la densité surfacique). Le paramètre ε est supposé petit et tend vers zéro. Ceci correspond à la limite faible longueur de Debye ou faible température ou forte densité (vu la relation (0.0.32)). A la limite ($\varepsilon\to 0$), les fonctions d'ondes se concentrent au point $z=0$. Afin d'analyser cette couche limite, un zoom est effectué au voisinage de $z=0$ via le changement de variables suivant

$$\varphi_p(z)=\frac{1}{\sqrt{\varepsilon}}\psi_p(\frac{z}{\varepsilon}), \quad \mathcal{E}_p=\frac{1}{\varepsilon^2}E_p, \quad V(z)=\frac{1}{\varepsilon^2}U(\frac{z}{\varepsilon}), \quad \xi=\frac{z}{\varepsilon}. \tag{0.0.33}$$

L'équation de Poisson dans (0.0.31) devient $-\dfrac{d^2U}{d\xi^2}=\dfrac{1}{\tilde{\mathcal{Z}}}\displaystyle\sum_{p=1}^{+\infty}e^{\frac{-E_p}{\varepsilon^2}}|\psi_p|^2$ avec $\tilde{\mathcal{Z}}=\displaystyle\sum_{p=1}^{+\infty}e^{\frac{-E_p}{\varepsilon^2}}$. Les valeurs propres $(E_p)_p$ sont simples, distinctes et forment une suite croissante par rapport à p pour tout $\varepsilon>0$. Nous montrerons de plus l'existence d'un gap strictement positif séparant le premier niveau d'énergie E_1 et les autres $E_p(p\geq 2)$ uniformément par rapport à ε. Ceci implique que les facteurs d'occupations $e^{\frac{-E_p}{\varepsilon^2}}$ pour $p\geq 2$ sont tous négligeables devant le premier ($p=1$) quand ε devient petit. Il est donc naturel de prétendre que le modèle (0.0.31) est asymptotiquement proche

de

$$\begin{cases} -\dfrac{d^2\tilde{\varphi}_1}{dz^2} + \tilde{V}\tilde{\varphi}_1 = \tilde{\mathcal{E}}_1\tilde{\varphi}_1 \qquad z \in [0,1], \\ \tilde{\mathcal{E}}_1 = \inf\limits_{\varphi\in H_0^1(0,1),\|\varphi\|_{L^2}=1} \left\{ \displaystyle\int_0^1 |\varphi'|^2 + \int_0^1 \tilde{V}\varphi^2 \right\}, \\ -\varepsilon^3 \dfrac{d^2\tilde{V}}{dz^2} = |\tilde{\varphi}_1|^2, \\ \tilde{V}(0) = 0, \quad \dfrac{d\tilde{V}}{dz}(1) = 0 \end{cases} \tag{0.0.34}$$

dans lequel seul le premier niveau d'énergie est pris en compte. Ceci est en accord avec les simulations numériques [94]. Dans ce travail, nous montrons rigoureusement que ces deux modèles sont asymptotiquement proches et nous estimons leur différence en fonction de ε. Nous montrons qu'elle décroît exponentiellement. De plus, nous prouvons qu'à la limite $\varepsilon \to 0$, le potentiel $\tilde{V}_\varepsilon$ solution de (0.0.34) converge vers un potentiel de couche limite de la forme $\dfrac{1}{\varepsilon^2}U_0(\dfrac{\cdot}{\varepsilon})$ avec un profil U_0 vérifiant un système de Schrödinger-Poisson unidimensionnel sur le demi axe réel :

$$\begin{cases} -\dfrac{d^2\psi_1}{d\xi^2} + U\psi_1 = E_1\psi_1 \qquad \xi \in [0,+\infty[, \\ E_1 = \inf\limits_{\psi\in H_0^1(\mathbb{R}^+),\|\psi\|_{L^2}=1} \left\{ \displaystyle\int_0^{+\infty} |\psi'|^2 + \int_0^{+\infty} U\psi^2 \right\}, \\ -\dfrac{d^2U}{d\xi^2} = |\psi_1|^2, \\ U(0) = 0, \quad \dfrac{dU}{d\xi} \in L^2(\mathbb{R}^+). \end{cases} \tag{0.0.35}$$

III.2 Résultats obtenus

Les modèles (0.0.31) et (0.0.34) sont bien posés et admettent des solutions uniques. L'étude du problème Schrödinger-Poisson sur un domaine borné est effectuée par F. Nier [84, 85, 86] en le reformulant en un problème de minimisation convexe. Le système limite (0.0.35) quand à lui est posé sur $[0,\infty[$. Le premier résultat du Chapitre 5 concerne l'étude de ce modèle (Théorème 5.1.1). Nous sommes amenés à étudier aussi un problème de minimisation posé sur un domaine non borné. Cette étude est réalisée grace au principe de concentration-compacité introduit par P. L. Lions [79]. Le deuxième résultat concerne la comparaison de différents systèmes présentés ci-dessus. Nous obtenons le théorème suivant.

Theorem 0.0.1. *Soit V_ε, $\tilde{V}_\varepsilon$ et U_0 les potentiels satisfaisant* (0.0.31), (0.0.34) *et* (0.0.35) *respectivement. Les estimations suivantes sont vérifiées*

$$\|V_\varepsilon - \tilde{V}_\varepsilon\|_{H^1(0,1)} = \mathcal{O}(e^{-\frac{c}{\varepsilon^2}}),$$

$$\|\tilde{V}_\varepsilon - \frac{1}{\varepsilon^2} U_0(\frac{\cdot}{\varepsilon})\|_{H^1(0,1)} = \mathcal{O}(e^{-\frac{c}{\varepsilon}}),$$

où c est une constante générique strictement positive et indépendante de ε.

III.3 Commentaires

Le choix de condition au bord de type Newmann pour le potentiel au point $z = 1$ est justifié dans certaines situations physiques [5]. Les conditions de Dirichlet sont plus habituelles dans ce type de modèle. Dans ce cas, l'analyse peut être effectuée mais comporte des complexités techniques liées au fait qu'une autre couche limite apparaît au point $z = 1$ et que les valeurs propres admettent asymptotiquement une multiplicité double. Pour simplifier, nous avons donc imposé des conditions de type Newmann en $z = 1$.

Il est plus naturel d'utiliser une statistique de Fermi-Dirac dans la limite forte densité. Cette étude peut être généralisée au cas Fermi-Dirac avec quelques complications techniques (voir dernière section du Chapitre 5 pour plus de détails).

Enfin, le problème multidimensionnel est beaucoup plus compliqué. La localisation de la couche limite dans ce cas peut dépendre de la géométrie de bord du domaine considéré. Ce type de problème est présent dans l'étude de l'équation de Schrödinger avec champ magnétique [21, 75].

References

[1] T. Ando, A. B. Fowler, and F. Stern, *Electronic properties of two-dimensional electron systems*, Rev. Mod. Phys., 54, 2 (1982), p. 437.

[2] C. Bardos, F. Golse, and C. D. Levermore, *Fluid dynamic limits of kinetic equations. II. Convergence proofs for the Boltzmann equation*, Comm. Pure Appl. Math., 46 (1993), pp. 667–753.

[3] C. Bardos, F. Golse, and D. Levermore, *Fluid dynamic limits of kinetic equations. I. Formal derivations*, J. Statist. Phys., 63 (1991), pp. 323–344.

[4] ——, *The acoustic limit for the Boltzmann equation*, Arch. Rational. Mech. Ana., 153 (2000), pp. 177–204.

[5] G. Bastard, *Wave mechanics applied to semiconductor heterostructures*, Les éditions de physiques, 1996.

[6] N. Ben Abdallah, *A hybrid kinetic-quantum model for stationary electron transport*, J. Stat. Phys., 90 (1998), pp. 627–662.

[7] ——, *On a multidimensional Schrödinger-Poisson scattering model for semiconductors*, J. Math. Phys., 41 (2000), pp. 4241–4261.

[8] N. Ben Abdallah and P. Degond, *On a hierarchy of macroscopic models for semiconductors*, J. Math. Phys., 37 (1996), pp. 3306–3333.

[9] N. Ben Abdallah, P. Degond, and I. Gamba, *Coupling one dimensional time dependent classical and quantum transport models*, J. Math. Phys., 43 (2002), pp. 1–24.

[10] N. Ben Abdallah, P. Degond, and S. Génieys, *An Energy-Transport model derived from the Boltzmann equation of semiconductors*, J. Stat. Phys., 84 (1996), pp. 205–231.

[11] N. Ben Abdallah, P. Degond, and P. A. Markowich, *On a One-Dimensional Schrödinger-Poisson Scattering Model*, ZAMP, 48 (1997), pp. 35–55.

[12] N. Ben Abdallah, S. Desvillettes, and S. Génieys, *On the convergence of the Boltzmann for the semiconductors toward the energy transport model*, J. Stat. Phys., 98 (2000), pp. 835–870.

[13] N. Ben Abdallah and R. El Hajj, *Diffusion and guiding center approximation for particle transport in strong magnetic fields*, Kinetic and Related Models, Vol. 1, No. 3 (2008), pp. 124–146.

[14] N. Ben Abdallah and F. Méhats, *On a Vlasov Schrödinger Poisson model*, Comm. Partial Differential Equations, 29 (2004), pp. 173–206.

[15] N. Ben Abdallah and F. Méhats, *Semiclassical analysis of the Schrödinger equation with a partially confining potential*, J. Math. Pures Appl. (9), 84 (2005), pp. 580–614.

[16] N. Ben Abdallah, F. Méhats, and O. Pinaud, *Adiabatic approximation of the Schrödinger-Poisson system with a partial confinement*, SIAM J. Math. Anal., 36 (2004/2005), pp. 986–1013.

[17] N. Ben Abdallah and F. Méhats, *On a Vlasov-Schrödinger-Poisson Model* , Comm. Partial Differential Equations, 29 (2004), pp. 173–206.

[18] N. Ben Abdallah, F. Méhats, and C. Negulescu, *Adiabatic quantum-fluid transport models*, Comm. Math. Sci., 4 (2006), pp. 621–650.

[19] N. Ben Abdallah, F. Méhats, P. Pietra, and N. Vauchelet, *A drift-diffusion subband model for the simulation of the double-gate mosfet*, IEEE-NANO 2005, Conference on Nanotechnology, Nagoya.

[20] N. Ben Abdallah, F. Méhats, and N. Vauchelet, *Analysis of a Drift-Diffusion-Schrödinger-Poisson model*, C.R. Acad. Sci. Paris, Ser. I 335, pp. 1007–1012.

[21] V. Bonnaillie, *On the fundamental state energy for a Schrödinger operator with magnetic field in domains with corners*, Asymptotic Analysis, 41 (2005), pp. 215–258.

[22] F. Bouchut, F. Golse, and M. Pulvirenti, *Kinetic equations and asymptotic theory*, B. perthame, L. Desvillettes Eds, Series in Appl. Math., bf 4, Gauthier-Villars (2000).

[23] J. P. Bourgade, *On spherical harmonics expansion type models for electron-phonon collisions*, Math. Methods Appl. Sci., 23 (2003), pp. 247–271.

[24] A. Bournel, *Magnéto-électronique dans des dispositifs à semiconducteurs*, Ann. Phys. Fr, 25 (2000), pp. 1–167.

[25] F. Brezzi and P. A. Markowich, *A mathematical analysis of quantum transport in three dimensional systems*, Anna. di Matematica Pura Applicata, 160 (1991), pp. 171–191.

[26] ——, *The three-dimensional Wigner-Poisson problem : existence, uniqueness and approximation*, Math. Methods Appl. Sci., 14 (1991), pp. 35–61.

[27] Y. A. Bychkov and E. I. Rashba, *Oscillatory effects and the magnetic susceptibility of carriers in inversion layers*, Journal of Physics C : Solid State Physics, 17 (1984), pp. 6039–6045.

[28] C. Cercignani, *The Boltzmann equation and its applications*, Springer-Verlag, Berlin, 1988.

[29] E. U. Condon and G. H. Shortley, *The theory of atomic spectra*, Cambridge University Press, Cambridge, 1953.

[30] S. Datta and B. Das, *Electronic analog of the electro-optic modulator*, Applied Physics Letters, 56 (1990), pp. 665–667.

[31] P. Degond, *A model of near-wall conductivity and its application to plasma thrusters*, SIAM J. Appl. Math., 58 (1998), pp. 1138–1162 (electronic).

[32] ——, *An infinite system of diffusion equations arising in transport theory : the coupled Spherical Harmonic Expansion model*, Math. Models Methods Appl. Sci., 11 (2001), pp. 903–932.

[33] P. Degond, *Asymptotic continuum models for plasmas and disparate mass gaseous binary mixtures*, Material Substructures in Complex Bodies, Elsevier, (2007).

[34] P. Degond and A. El Ayyadi, *A coupled Schrödinger drift-diffusion model for quantum semiconductor device simulations*, J. Comp. Phys., 181 (2002), pp. 222–259.

[35] P. Degond, V. Latocha, S. Mancini, and A. Mellet, *Diffusion dynamics of an electron gas confined between two plates*, Methods Appl. Anal., 9 (2002), pp. 127–150.

[36] P. Degond, C. D. Levermore, and C. Schmeiser, *A note on the energy-transport limit of the semiconductor Boltzmann equation*, IMA Vol. Math. Appl., 135 (2004), pp. 137–153.

[37] P. Degond and B. Lucquin-Desreux, *The asymptotics of collision operators for two species of particles of disparate masses*, Math. Models Methods Appl. Sci., 6 (1996), pp. 405–436.

[38] P. Degond and B. Lucquin-Desreux, *Transport coefficients of plasmas and disparate mass binary gases*, Transport Theory Statist. Phys., 25 (1996), pp. 595–633.

[39] P. Degond and S. Mancini, *Diffusion driven by collisions with the boundary*, Asymptot. Anal., 27 (2001), pp. 47–73.

[40] P. Degond, F. Méhats, and C. Ringhofer, *Quantum hydrodynamic models derived from the entropy principle*, Contemp. Math. 371, Amer. Math. Soc., Providence RI (2005).

[41] ——, *Quantum energy-transport and drift-diffusion models*, J. Stat. Phys., 118 (2005), pp. 625–667.

[42] P. Degond and C. Schmeiser, *Macroscopic models for semiconductor heterostructures*, J. Math. Phys., 39 (1998), pp. 4634–4663.

[43] G. Dresselhaus, *Spin-Orbit Coupling Effects in Zinc Blende Structures*, Phys. Rev., 100 (1955), pp. 580–586.

[44] D. H. E. Dubin, J. A. Krommes, C. Oberman, and W. W. Lee, *Nonlinear gyrokinetic equations*, Physics of Fluids, 26 (1983), pp. 3524–3535.

[45] M. I. D'yakonov and V. Y. Kachorovskii, *spin relaxation of two-dimensional electrons in noncentrosymmetric semiconductors*, Sov. Phys. Semicond., 20 (1986), pp. 110–112.

[46] R. El Hajj, *On an hierarchy of kinetic and macroscopic models for semiconductor Spintronics*, in preparation.

[47] R. El Hajj, *On spin transport models and application to numerical simulation of transistors with spin rotational effect*, in preparation.

[48] R. El Hajj and N. Ben Abdallah, *High density limit of the stationary one dimensional Schrödinger–Poisson system*, Multiscale Modeling and Simulation, 7 (2008), pp. 124–146.

[49] R. J. Elliott, *Theory of the Effect of Spin-Orbit Coupling on Magnetic Resonance in Some Semiconductors*, Phys. Rev., 96 (1954), pp. 266–279.

[50] C. Fermanian-Kammerer and P. Gérard, *Mesures semi-classiques et croisement de modes*, Séminaire Équations aux dérivées partielles (Polytechnique) (1999-2000), Art. No. 17, 13 p.

[51] ——, *Une formule de Landau-Zener pour un croisement non dégénéré et involutif de codimension 3*, C. R. Math. Acad. Sci. Paris, 335 (2002), pp. 915–920.

[52] ——, *A Landau-Zener formula for non-degenerated involutive codimension 3 crossings*, Ann. Henri Poincaré, 4 (2003), pp. 513–552.

[53] C. Fermanian-Kammerer and P. Gerard, *A Landau-Zener formula for two-scaled Wigner measures*, in Dispersive transport equations and multiscale models (Minneapolis, MN, 2000), vol. 136 of IMA Vol. Math. Appl., Springer, New York, 2004, pp. 167–177.

[54] C. Fermanian-Kammerer and P. Gérard, *Two-scale Wigner measures and the Landau-Zener formulas*, in Multiscale methods in quantum mechanics, Trends Math., Birkhäuser Boston, Boston, MA, 2004, pp. 59–68.

[55] A. Fert, A. Friederich, and al, *Giant Magnetoresistance of (001)Fe/(001)Cr Magnetic Superlattices*, Phys. Rev. Lett., 61 (1988), p. 2472.

[56] G. Fishman and G. Lampel, *Spin relaxation of photoelectrons in p-type gallium arsenide*, Phys. Rev. B, 16 (1977), pp. 820–831.

[57] E. Frenod and K. Hamdache, *Homogenisation of transport kinetic equations with oscillating potentials*, Proc. Roy. Soc. Edinburgh Sect. A, 126 (1996), pp. 1247–1275.

[58] E. Frénod, P.-A. Raviart, and E. Sonnendrücker, *Two-scale expansion of a singularly perturbed convection equation*, J. Math. Pures Appl. (9), 80 (2001), pp. 815–843.

[59] E. Frénod and E. Sonnendrücker, *Homogenization of the Vlasov equation and of the Vlasov-Poisson system with a strong external magnetic field*, Asymptot. Anal., 18 (1998), pp. 193–213.

[60] E. Frénod and E. Sonnendrücker, *Long time behavior of the two-dimensional Vlasov equation with a strong external magnetic field*, Math. Models Methods Appl. Sci., 10 (2000), pp. 539–553.

[61] E. Frénod and E. Sonnendrücker, *The finite Larmor radius approximation*, SIAM J. Math. Anal., 32 (2001), pp. 1227–1247 (electronic).

[62] E. Frénod and F. Watbled, *The Vlasov equation with strong magnetic field and oscillating electric field as a model for isotop resonant separation*, Electron. J. Differential Equations, (2002, No. 06), p. 20 (electronic).

[63] P. Gérard, *Mesures semi-classiques et ondes de Bloch*, Séminaire sur les Équations aux Dérivées Partielles, École Polytech., (1991), pp. Exp. No. XVI, 19.

[64] P. Gérard, P. A. Markowich, N. J. Mauser, and F. Poupaud, *Homogenization limits and Wigner transforms*, Comm. Pure Appl. Math., 50 (1997), pp. 323–379.

[65] R. T. Glassey, *The Cauchy problem in kinetic theory*, Society for Industrial and Applied Mathematics (SIAM), Philadelphia, PA, 1996.

[66] F. Golse and D. Levermore, *Stokes-Fourier and acoustic limits for the Boltzmann equations : Convergence proofs*, Comm. Pure Appl. Math., 55 (2002), pp. 336–393.

[67] F. Golse and F. Poupaud, *Limite fluide des équations de Boltzmann des semi-conducteurs pour une statistique de Fermi-Dirac*, Asymptotic Anal., 6 (1992), pp. 135–160.

[68] F. Golse and L. Saint-Raymond, *The Vlasov-Poisson system with strong magnetic field*, J. Math. Pures Appl. (9), 78 (1999), pp. 791–817.

[69] F. Golse and L. Saint-Raymond, *The Vlasov-Poisson system with strong magnetic field in quasineutral regime*, Math. Models Methods Appl. Sci., 13 (2003), pp. 661–714.

[70] F. Golse and L. Saint-Raymond, *Hydrodynamics limit for the Boltzmann equation*, Lecture Porto Ercole, (2004).

[71] ——, *The Navier-Stokes limit of the Boltzmann equation for bounded collision kernels*, Invent Math., 155 (2004), pp. 81–161.

[72] T. Goudon, P. E. Jabin, and A. Vasseur, *Hydrodynamic limit for the Vlasov-Navier-Stokes equations, I. Light particles regime*, Indiana Univ. Math. J., 53 (2004), pp. 1495–1515.

[73] ——, *Hydrodynamic limit for the Vlasov-Navier-Stokes equations, II. Fine particles regime*, Indiana Univ. Math. J., 53 (2004), pp. 1517–1536.

[74] J. Harris, C. T. Foxon, K. Barnham, D. Lacklison, J. Hewett, and C. White, *Two-dimensional electron gas strutures with mobilities in excess of* $3.10^6 cm^2 V^1 S^1$, J. Appl. Phys., 61 (1986), p. 1219.

[75] B. Helffer and A. Mohamed, *Semiclassical analysis for the ground state energy of a Schrödinger operator with magnetic wells*, J. Funct. Anal., 138 (1996), pp. 40–81.

[76] L. D. Landau and E. M. Lifshitz, *Quantum Mechanics*, Pergamon Press, Oxford, 1991.

[77] W. W. Lee, *Gyrokinetic approach in particle simulation*, Physics of Fluids, 26 (1983), pp. 556–562.

[78] C. D. Levermore, *Moment closure hierarchies for kinetic theories*, J. Stat. Phys., 83 (1996), pp. 1021–1065.

[79] P. Lions, *The concentration-compactness principle in the Calculus of Variations. The locally compact case, part 1*, Ann. Inst. Henri Poincaré, analyse non linéaire, 1 (1984), pp. 109–145.

[80] P.-L. Lions and T. Paul, *Sur les mesures de Wigner*, Rev. Mat. Iberoamericana, 9 (1993), pp. 553–618.

[81] R. G. Littlejohn, *Hamiltonian formulation of guiding center motion*, Phys. Fluids, 24 (1981), pp. 1730–1749.

[82] G. Lommer, F. Malcher, and U. Rössler, *spin splitting in semiconductor heterostructures for $B \to 0$*, Phys. Rev. Lett., 60 (1988), pp. 728–731.

[83] B. Lucquin-Desreux, *Diffusion of electrons by multicharged ions*, Math. Models Methods Appl. Sci., 10 (2000), pp. 409–440.

[84] F. Nier, *A stationary Schrödinger-Poisson System Arising from the modelling of electronic devices*, Forum Math., 2 (1990), pp. 489–510.

[85] ——, *A variational formulation of Schrödinger-Poisson Systems in Dimension $d \leq 3$*, Comm. Partial Differential Equations, 18 (1993), pp. 1125–1147.

[86] ——, *Schrödinger-Poisson Systems in Dimension $d \leq 3$:The Whole-space case*, Proc. Roy. Soc. Edinburgh Sect. A, 123 (1993), pp. 1179–1201.

[87] T. G. Northrop, *The guiding center approximation to charged particle motion*, Annals of Physics, 15 (1961), pp. 79–101.

[88] Y. V. Pershin, *Accumulation of electron spin polarization at semiconductor interfaces*, Phys. Rev. B, 68 (2003), p. 233309.

[89] Y. V. Pershin and V. Privman, *Focusing of spin polarization in semiconductors by inhomogeneous doping*, Phys. Rev. Lett., 90 (2003), p. 256602.

[90] P. Pietra and N. Vauchelet, *Modeling and simulation of the diffusive transport in a nanoscale double-gate mosfet*, submitted.

[91] O. Pinaud, *Adiabatic approximation of the Schrödinger-Poisson system with a partial confinement : the stationnary case*, J. Math. Phys., 45 (2004), p. 2029.

[92] E. Polizzi, *Modélisation et simulation numériques du transport quantique balistique dans les nanostructures semi-conductrices*, PhD. Thesis, INSA, Toulouse, France, (2001).

[93] E. Polizzi and N. Ben Abdallah, *Self-consistent three dimensional model for quantum ballistic transport in open systems*, Phys. Rev B., 66 (2002), pp. 245301–245309.

[94] ——, *subband decomposition approach for the simulation of quantum electron transport in nanostructures*, J. Comp. Phys., 202 (2005), pp. 150–180.

[95] F. Poupaud, *Diffusion approximation of the linear semiconductor Boltzmann equation : analysis of boundary layers*, Asymptotic Anal., 4 (1991), pp. 293–317.

[96] L. Saint-Raymond, *The gyrokinetic approximation for the Vlasov-Poisson system*, Math. Models Methods Appl. Sci., 10 (2000), pp. 1305–1332.

[97] L. Saint-Raymond, *Control of large velocities in the two-dimensional gyrokinetic approximation*, J. Math. Pures Appl. (9), 81 (2002), pp. 379–399.

[98] N. Vauchelet, *Modélisation mathématique du transport diffusif de charges partiellement quantiques*, Thesis, Université Paul Sabatier-Toulouse III, (2006).

[99] C. Villani, *Limite hydrodynamiques de l'équation de Boltzmann*, Séminaire Bourbaki, 53ème année (2000–2001), p. n0 893.

[100] ——, *A review of mathematical topics in collisional kinetic theory*, in Handbook of mathematical fluid dynamics 1, North-Holland Amsterdam, 2002.

[101] Z. G. Yu and M. E. Flatté, *Electric-field dependent spin diffusion and spin injection into semiconductors*, Phys. Rev. B, 66 (2002), p. 201202.

[102] Z. G. Yu and M. E. Flatté, *Spin diffusion and injection in semiconductor structures : electric field effects*, Phys. Rev. B, 66 (2002), p. 235302.

[103] I. Zutic, J. Fabian, and S. D. Sarma, *Spintronics : Fundamentals and applications*, Reviews of Modern Physics, 76 (2004), p. 323.

Part I

Transport models for semiconductor spintronics

Chapter 1

Semiclassical analysis of the Schrödinger equation with spin-orbit hamiltonian

Abstract

The aim of this first chapter is the derivation of kinetic type models for semiconductor spintronics. In the first part, a semi-classical analysis of the Schrödinger equation with general spin-orbit hamiltonian is performed. Two situations are discussed. First, if the spin-orbit hamiltonian (H_{SO}) is considered as a perturbative term with order ε (the scaled planck constant) of the total energy hamiltonian (H_0), then the semi-classical limit ($\varepsilon \to 0$) leads to the so called "spinor" kinetic equation. However if $H_{SO} = \mathcal{O}(H_0)$, a two component kinetic model is obtained at the limit. The second part of this chapter is dedicated to the study of the semi classical limit of a partially confined electron gas in one direction of the space (z). A partial semi-classical limit is applied following the work of N. Ben Abdallah and F. Méhats [1]. The limit model in this case couples an infinity quasi-static Schrödinger equations describing the energy levels in the confinement direction and an infinity Vlasov equations in the transport directions with Rashba spin-orbit coupling. Moreover, an explicit expression relying the order of the Rashba effect and the confinement potential is derived.

1.1 Introduction

The study of spin related phenomenae in semi-conductor devices attracts a huge attention by the physical community. The main reason is the possibility to control the spin vector direction due to the existence of mechanisms acting on the spin dynamics. The must important mechanism existing is the spin-orbit coupling. This kind of spin-dependent interactions results generally from a lack of symmetry in the structure. It manifests itself by the appearance of an effective magnetic field which makes precess the spin vector during the free paths of the particles. There are two main types of spin-orbit interactions in semiconductor heterostructures. The Dresselhaus spin-orbit interactions [5] results from asymmetry present in certain crystal lattices like zing blende structures. The Rashba spin-orbit interactions arises due to the asymmetry of quantum wells formed at the interface of semiconductor heterostructures [3]. The spin-orbit hamiltonian takes the following general form [24]

$$H_{SO} = \alpha\hbar\vec{\Omega}(t,x,k)\cdot\vec{\sigma} \tag{1.1.1}$$

where $\vec{\sigma}$ is the vector of the Pauli spin matrices given by (A.2.1), (t,x,k) are respectively the time, the position and the wave vector of the electron ($k \equiv i\hbar\nabla_x$), α is the strength of the spin-orbit coupling and $\vec{\Omega}$ represents the effective field or the precession vector. Let us give some examples. In the Elliot-Yafet mechanism of relaxation [24], the spin-orbit hamiltonian is given by

$$H_{SO} = i\frac{\hbar^2}{4m^2c^2}(\nabla_x V\times\nabla_x)\cdot\vec{\sigma}. \tag{1.1.2}$$

The Rashba spin-orbit hamiltonian writes as [3]

$$H_R = \alpha i\hbar\left(\sigma_1\partial_{x_2} - \sigma_2\partial_{x_1}\right),$$

and the Dresselhauss spin-orbit interactions can be represented by the following hamiltonian [5]

$$H_D = \alpha i\hbar\left(\sigma_1\partial_{x_1} - \sigma_2\partial_{x_2}\right).$$

In this chapter, different kinetic models describing the spin transport in semiconductor spintronic devices will be rigorously derived. A semi-classical analysis of the Schrödinger equation with spin-orbit hamiltonian using the theory of Wigner transform is performed. It leads, according to the order of the spin-orbit coupling with respect to the scaled Planck constant, either to a spinor kinetic equation with 2×2 hermitian matrix value distribution function or to a two-component kinetic model. This is the subject of the next section. The third section is concerned with the derivation of subband kinetic/quantum model for partially confined systems.

1.2 Schrödinger equation with general spin-orbit Hamiltonian

This part is dedicated to the study of the semi classical limit of the Schrödinger equation with spin-orbit hamiltonian. The starting equation will be the following scaled linear Schrödinger equation :

$$i\varepsilon\partial_t\Psi^\varepsilon = -\frac{\varepsilon^2}{2}\Delta_x\Psi^\varepsilon + V^\varepsilon\Psi^\varepsilon + \alpha\Omega_\varepsilon^W(t,x,i\varepsilon\nabla_x)\cdot\vec{\sigma}\Psi^\varepsilon \tag{1.2.1}$$

subject to the following initial condition

$$\Psi^\varepsilon(t=0) = \Psi_I^\varepsilon. \tag{1.2.2}$$

Here, $\Omega_\varepsilon^W(t,x,i\varepsilon\nabla_x)\cdot\vec{\sigma}$ is the Weyl operator associated to the complex 2×2 matrix valued symbol $\vec{\Omega}_\varepsilon(t,x,\xi)\cdot\vec{\sigma}$ on $\mathbb{R}^3_x\times\mathbb{R}^3_\xi$ defined by

$$\Omega_\varepsilon^W(t,x,i\varepsilon\nabla_x)\cdot\vec{\sigma}(\Psi) = \frac{1}{(2\pi)^3}\int_{\mathbb{R}^3_\xi}\int_{\mathbb{R}^3_y}\vec{\Omega}_\varepsilon\left(t,\frac{x+y}{2},\varepsilon\xi\right)\cdot\vec{\sigma}(\Psi(y))e^{i(x-y)\cdot\xi}d\xi dy. \tag{1.2.3}$$

This operator represents the spin-orbit hamiltonian with $\vec{\Omega}_\varepsilon$ is the effective field and α is the spin-orbit coupling order. We recall that the wave function $\Psi^\varepsilon(t,x) = (\psi_\uparrow^\varepsilon(t,x),\psi_\downarrow^\varepsilon(t,x))$ is a function of the time $t\in\mathbb{R}^+$ and the position $x\in\mathbb{R}^3$ with $\mathbb{C}^2$ vector value. The potential V^ε is given and regular (satisfying Assumption 1.2.4). The parameter ε is a scaled Planck constant intended to go to zero. To perform rigourously this semi classical limit, we will apply some interesting convergence results using Wigner transform techniques. A review of these techniques can be found in [13]. The Wigner transform is a powerful tool introduced initially by Wigner in [23]. Many important convergence results for semi classical limit have been then obtained using this transform. We cite for instance the works of Gérard [12], Lions and Paul [15] and Markowich and Mauser [16].

The order of the spin-orbit coupling with respect to ε will obviously play an important role in this semi classical limit. We treat here two cases : $\alpha = \mathcal{O}(\varepsilon)$ and $\alpha = \mathcal{O}(1)$. In the first case ($\alpha = \mathcal{O}(\varepsilon)$), the spin-orbit coupling is considered as a perturbation part of the total energy symbol $P^\varepsilon(t,x,\xi) = \left(\frac{|\xi|^2}{2} + V^\varepsilon(t,x)\right) I_2$ and the semi classical limit leads to the spinor kinetic equation. This result is cited in Theorem 1.2.1. However, when $\alpha = \mathcal{O}(1)$, a splitting between the two energy levels of the spin-up and spin-down species will occur with energy gap of order $|\vec{\Omega}|$ where $\vec{\Omega}$ denotes the limit of $\vec{\Omega}_\varepsilon$ when ε goes to zero. The semi-classical limit leads to a two-component kinetic model in this case. This is the subject of the second theorem of this section, Theorem 1.2.2.

Theorem 1.2.1 (**case** $\alpha = \mathcal{O}(\varepsilon)$)**.** *Under Assumptions 1.2.4, 1.2.5, 1.2.6 and 1.2.10, we have the following results.*

1. *The Wigner transform $W^\varepsilon(\Psi_I^\varepsilon, \Psi_I^\varepsilon)$, defined by (1.2.12), converges in $\mathcal{S}'(\mathbb{R}^3_x \times \mathbb{R}^3_\xi, \mathcal{M}_2(\mathbb{C}))$ to $W_I \in \mathcal{M}_b(\mathbb{R}^3_x \times \mathbb{R}^3_\xi, \mathcal{M}_2(\mathbb{C}))$.*
2. *The Wigner transform $W^\varepsilon(\Psi^\varepsilon, \Psi^\varepsilon)$ of the solution of (1.2.1)-(1.2.2) converges in*
   $L^\infty(\mathbb{R}^+, \mathcal{S}'(\mathbb{R}^3_x \times \mathbb{R}^3_\xi, \mathcal{M}_2(\mathbb{C})))$ weak $\star$ topology to $W^0 \in C^0(\mathbb{R}^+, \mathcal{M}_b(\mathbb{R}^6, \mathcal{H}_2^+(\mathbb{C})))$. Moreover, if $\alpha = \mathcal{O}(\varepsilon)$ then, W^0 satisfies the spinor Boltzmann equation :
   $$\partial_t W^0 + \xi \cdot \nabla_x W^0 - \nabla_x V \cdot \nabla_\xi W^0 = i[W^0, \vec{\Omega} \cdot \vec{\sigma}] \tag{1.2.4}$$
   $$W^0(0, x, \xi) = W_I \tag{1.2.5}$$
   where V and $\vec{\Omega}$ denote respectively the limits of V^ε and $\vec{\Omega}_\varepsilon$ as $\varepsilon \to 0$.
3. *For every $T > 0$, the macroscopic quantities $N^\varepsilon, J^\varepsilon$ given by Definition 1.2.7 converge in $L^\infty((0,T); \mathcal{M}_b(\mathbb{R}^3_x, \mathcal{M}_2(\mathbb{C})))$ weak $\star$ topology to :*
   $$N(t,x) = \int_{\mathbb{R}^3} W^0(t,x,\xi) d\xi,$$
   and
   $$J(t,x) = \int_{\mathbb{R}^3} v W^0(t,x,\xi) d\xi.$$

In this theorem as in the sequel, if E is a Banach space, $\mathcal{S}'(\mathbb{R}^3, E)$ denotes the E-valued tempered distributions and $\mathcal{M}_b(\mathbb{R}^3, E)$ is the space of E-valued bounded measures. Moreover, $\mathcal{M}_2(\mathbb{C})$ denotes the space of 2×2 complex matrices and $\mathcal{H}_2^+(\mathbb{C})$ is the space of hermitian positive definite matrices. The second Theorem is concerned with the case $\alpha = \mathcal{O}(1)$.

Theorem 1.2.2 (**case** $\alpha = \mathcal{O}(1)$)**.** *Under the same assumptions as for Theorem 1.2.1 and if $\alpha = \mathcal{O}(1)$ with respect to ε, then the spin part of the Wigner measure associated to $(\Psi^\varepsilon)_\varepsilon$, W^0, given by the above theorem is parallel to $\vec{\Omega}$ outside the set*

$$E = \left\{ (t,x,\xi) \in \mathbb{R}^+ \times \mathbb{R}^6 / \ \vec{\Omega}(t,x,\xi) = 0 \right\}. \tag{1.2.6}$$

In other words, we have $W^0(t,x,\xi) = \frac{1}{2} w_c(t,x,\xi) I_2 + w_s(t,x,\xi) \frac{\vec{\Omega}}{|\vec{\Omega}|} \cdot \vec{\sigma}$ for all $(t,x,\xi) \in \mathbb{R}^+ \times \mathbb{R}^6 \setminus \overline{E}$ with $\overline{E}$ is the closure of E. In addition, the eigenvalues of W^0 given by $w_\uparrow = \frac{w_c}{2} + w_s$ and $w_\downarrow = \frac{w_c}{2} - w_s$ satisfy the following two-kinetic model

$$\begin{cases} \partial_t w_\uparrow + \nabla_\xi \lambda_\uparrow \cdot \nabla_x w_\uparrow - \nabla_x \lambda_\uparrow \cdot \nabla_\xi w_\uparrow = 0 \quad \text{on } (\mathbb{R}^+ \times \mathbb{R}^6_{x,\xi}) \setminus \overline{E} \\ \\ \partial_t w_\downarrow + \nabla_\xi \lambda_\downarrow \cdot \nabla_x w_\downarrow - \nabla_x \lambda_\downarrow \cdot \nabla_\xi w_\downarrow = 0 \quad \text{on } (\mathbb{R}^+ \times \mathbb{R}^6_{x,\xi}) \setminus \overline{E}. \end{cases} \tag{1.2.7}$$

The up and down total energies, $\lambda_\uparrow$ and $\lambda_\downarrow$, are respectively given by

$$\lambda_\uparrow(t,x,\xi)=\frac{|\xi|^2}{2}+V+|\vec{\Omega}|,\quad \lambda_\downarrow(t,x,\xi)=\frac{|\xi|^2}{2}+V-|\vec{\Omega}|. \tag{1.2.8}$$

Remark 1.2.3. *Outside $E=\{(t,x,\xi)\in\mathbb{R}^+\times\mathbb{R}^6/\ \vec{\Omega}(t,x,\xi)=0\}$, the eigenvalues $\lambda_\uparrow$ and $\lambda_\downarrow$ are distincts and of constant multiplicity 1. The distribution functions $w_\uparrow$ and $w_\downarrow$ propagate along the hamiltonian curves (or the characteristics curves) associated with $\lambda_\uparrow$ and $\lambda_\downarrow$ outside E. However, when the classical trajectories reach E, a crossing of the two energy levels occurs and some energy transfer between the two modes is expected to happen above the crossing. Many works have been devoted to describe the semi-classical evolution through crossings and to quantify the energy transfer in terms of two-scale Wigner measures and Landau-Zener formula. We refer the reader to the works of Patrick Gérard and Clotilde Fermanian-Kammerer [6, 7, 8, 9, 10] and references therein.*

1.2.1 Analysis of the Schrödinger equation with spin-orbit term

This subsection is concerned with the analysis of (1.2.1)-(1.2.2). Some assumptions on the potential V^ε, the initial data Ψ_I^ε and the effective field of the spin-orbit coupling $\vec{\Omega}_\varepsilon$ are needed.

Assumption 1.2.4. *We assume that $(\varepsilon,t,x)\mapsto V^\varepsilon(t,x)$ is a real nonnegative function belonging to $C^0([0,1]_\varepsilon,C^1\cap W^{1,\infty}(\mathbb{R}^+\times\mathbb{R}^3))$.*

Assumption 1.2.5. *We assume that the initial data $(\Psi_I^\varepsilon)_\varepsilon$ belongs to $H^1(\mathbb{R}^3,\mathbb{C}^2)$ and satisfies the following energy estimate*

$$\mathcal{E}^\varepsilon(\Psi_I^\varepsilon):=\int_{\mathbb{R}^3}(|\Psi_I^\varepsilon|^2+\varepsilon^2\|\nabla_x\otimes\Psi_I^\varepsilon\|_2^2)dx\le C,$$

for some constant $C>0$ independent on ε.

In this text, $|.|$ and $\|.\|_2$ denote respectively the Euclidian vector and matrix norms.

Assumption 1.2.6. *We suppose that $\vec{\Omega}_\varepsilon(t,x,\xi)$ belongs to $C^0([0,1]_\varepsilon,C^1(\mathbb{R}^+\times\mathbb{R}^6_{x,\xi}))^3$. In addition, there exists $m>0$ such that for all $\alpha,\beta\in\mathbb{N}^*$ with $\alpha+\beta\le 1$, there exists $C_{\alpha,\beta}(t)$ a positive continuous function independent of ε such that $\forall l,k\in\{1,2,3\}$*

$$\left|\frac{\partial^{\alpha+\beta}}{\partial x_k^\alpha\partial\xi_l^\beta}\vec{\Omega}_\varepsilon\right|\le C_{\alpha,\beta}(t)(1+|\xi|)^{m-\beta}. \tag{1.2.9}$$

Definition 1.2.7. *Let $\Psi^\varepsilon \in C^0(\mathbb{R}^+, H^1(\mathbb{R}^3_x, \mathbb{C}^2))$ be the solution of (1.2.1). The associated particle and current densities are defined by*

$$N^\varepsilon(t,x) = \Psi^\varepsilon(t,x) \otimes \overline{\Psi^\varepsilon}(t,x) \tag{1.2.10}$$

and

$$J^\varepsilon(t,x) = \frac{\varepsilon}{2i}[\nabla_x \Psi^\varepsilon(t,x) \otimes \overline{\Psi^\varepsilon}(t,x) - \Psi^\varepsilon(t,x) \otimes \overline{\nabla_x \Psi^\varepsilon(t,x)}]. \tag{1.2.11}$$

Definition 1.2.8. *Let $\phi_1, \phi_2 \in \mathcal{S}'(\mathbb{R}^3_x, \mathbb{C}^2)$ (the space of tempered distributions), the Wigner matrix associated to ϕ_1 and ϕ_2 is the $\mathcal{M}_2(\mathbb{C})$-valued distribution on $\mathbb{R}^3_x \times \mathbb{R}^3_\xi$ defined by*

$$W^\varepsilon(\phi_1,\phi_2)(x,\xi) = (2\pi)^{-3} \int_{\mathbb{R}^3} e^{i\eta\cdot\xi} \phi_1(x - \varepsilon\frac{\eta}{2}) \otimes \overline{\phi}_2(x + \varepsilon\frac{\eta}{2}) d\eta. \tag{1.2.12}$$

We refer the reader to [13, 15] for a detailed study of this transformation and its application to the semi classical analysis. The first proposition ensures the existence of solution of (1.2.1)- (1.2.2) and gives energy estimate.

Proposition 1.2.9. *Under Assumptions 1.2.4, 1.2.5 and for any $\varepsilon \in [0,1]$,* (1.2.1)-(1.2.2) *admits a unique weak solution*

$$\Psi^\varepsilon \in C^0(\mathbb{R}^+, H^1(\mathbb{R}^3, \mathbb{C}^2)) \cap C^1(\mathbb{R}^+, H^{-1}(\mathbb{R}^3, \mathbb{C}^2)) \tag{1.2.13}$$

and the sequence $(\Psi^\varepsilon)_\varepsilon$ is bounded in $C^0(\mathbb{R}^+, L^2(\mathbb{R}^3, \mathbb{C}^2))$.

Proof. Since the Pauli matrices are hermitian, it is simple to verify that the hamiltonian $H_\varepsilon = (-\frac{\varepsilon^2}{2}\Delta_x + V)I_2 + \alpha\Omega^W(t,x,i\varepsilon\nabla)\cdot\vec{\sigma}$ (with I_2 is the 2×2 identity matrix) is a self adjoint operator on its domain $H^2(\mathbb{R}^3,\mathbb{C}^2)$ in $L^2(\mathbb{R}^3,\mathbb{C}^2)$. Then, applying the Stone's Theorem (see [22, 20]), equation (1.2.1) admits a unique weak solution satisfying (1.2.13). Moreover, taking the scalar product of (1.2.1) with Ψ^ε in $\mathbb{C}^2$, integrating with respect to x and taking the imaginary part, one gets $\partial_t(\int_{\mathbb{R}^3} |\Psi^\varepsilon|^2 dx) = 0$ which gives the mass conservation

$$\int_{\mathbb{R}^3} |\Psi^\varepsilon|^2 dx = \int_{\mathbb{R}^3} |\Psi^\varepsilon_I|^2 dx. \tag{1.2.14}$$

■

Assumption 1.2.10. *The energy estimate is propagated with the weak solutions $(\Psi^\varepsilon)_\varepsilon$ of* (1.2.1)-(1.2.2). *This means that there exists a continuous function $C(t)$ independent of ε such that*

$$\forall t \geq 0, \quad \mathcal{E}^\varepsilon(\Psi^\varepsilon) = \int_{\mathbb{R}^3} (|\Psi^\varepsilon|^2 + \varepsilon^2 \|\nabla_x \otimes \Psi^\varepsilon\|_2^2) dx \leq C(t). \tag{1.2.15}$$

Notice that Assumption 1.2.10 is verified in practice when taking Rashba, Dresselhauss, or Elliot-Yafet spin-orbit hamiltonian. Indeed, taking for instance

$$i\varepsilon\partial_t\Psi^\varepsilon = -\frac{\varepsilon^2}{2}\Delta_x\Psi^\varepsilon + V^\varepsilon\Psi^\varepsilon + i\varepsilon^2(\vec{\sigma}\times\nabla_x V^\varepsilon).\nabla_x\Psi^\varepsilon$$

multiplying by $\overline{\partial_t\Psi^\varepsilon}$, integrating with respect to x and taking the real part, one finds

$$\frac{\varepsilon^2}{4}\partial_t\int_{\mathbb{R}^3}\|\nabla_x\otimes\Psi^\varepsilon\|_2^2dx+\frac{1}{2}\int_{\mathbb{R}^3}V^\varepsilon\partial_t(|\Psi^\varepsilon|^2)dx=\varepsilon^2\Im\left(\int_{\mathbb{R}^3}(\vec{\sigma}\times\nabla_x V^\varepsilon).\nabla_x\Psi^\varepsilon.\overline{\partial_t\Psi^\varepsilon}dx\right) \tag{1.2.16}$$

where $\Im(z)$ denotes the imaginary part of $z\in\mathbb{C}$. In addition, by an integration by part

$$\begin{aligned}
&\Im\left(\int_0^t\int_{\mathbb{R}^3}(\vec{\sigma}\times\nabla_x V^\varepsilon)\cdot\nabla_x\Psi^\varepsilon\cdot\overline{\partial_s\Psi^\varepsilon}dsdx\right) \qquad (1.2.17)\\
&=\frac{1}{2i}\int_0^t\int_{\mathbb{R}^3}\left[(\vec{\sigma}\times\nabla_x V^\varepsilon)\cdot\nabla_x\Psi^\varepsilon\cdot\overline{\partial_s\Psi^\varepsilon}-\overline{(\vec{\sigma}\times\nabla_x V^\varepsilon)\cdot\nabla_x\Psi^\varepsilon}\cdot\partial_s\Psi^\varepsilon\right]dsdx\\
&=\frac{1}{2i}\int_0^t\int_{\mathbb{R}^3}\left[\partial_s(\overline{(\vec{\sigma}\times\nabla_x V^\varepsilon)\cdot\nabla_x\Psi^\varepsilon})\cdot\Psi^\varepsilon-\Psi^\varepsilon\cdot\overline{(\vec{\sigma}\times\nabla_x V^\varepsilon)\cdot\nabla_x\partial_s\Psi^\varepsilon}\right]dsdx\\
&\quad-\frac{1}{2i}\int_{\mathbb{R}^3}\overline{(\vec{\sigma}\times\nabla_x V^\varepsilon)\cdot\nabla_x\Psi^\varepsilon(t,x)}\cdot\Psi^\varepsilon(t,x)dx+\frac{1}{2i}\int_{\mathbb{R}^3}\overline{(\vec{\sigma}\times\nabla_x V^\varepsilon(0,x))\cdot\nabla_x\Psi_I^\varepsilon}\cdot\Psi_I^\varepsilon dx\\
&=\frac{1}{2i}\int_0^t\int_{\mathbb{R}^3}\overline{(\vec{\sigma}\times\nabla_x\partial_s V^\varepsilon)\cdot\nabla_x\Psi^\varepsilon}\cdot\Psi^\varepsilon dsdx-\frac{1}{2i}\int_{\mathbb{R}^3}\overline{(\vec{\sigma}\times\nabla_x V^\varepsilon)\cdot\nabla_x\Psi^\varepsilon(t,x)}\cdot\Psi^\varepsilon(t,x)dx\\
&\qquad+\frac{1}{2i}\int_{\mathbb{R}^3}\overline{(\vec{\sigma}\times\nabla_x V^\varepsilon(0,x))\cdot\nabla_x\Psi_I^\varepsilon}\cdot\Psi_I^\varepsilon dx.
\end{aligned}$$

Moreover, it is simple to show that for any regular function U we have

$$\left|\frac{i}{2}\int_{\mathbb{R}^3}\overline{(\vec{\sigma}\times\nabla_x U)\cdot\nabla_x\Psi^\varepsilon}\cdot\Psi^\varepsilon dx\right|\leq\sup_{\mathbb{R}^3}(|\nabla_x U|)\left(\int_{\mathbb{R}^3}\|\nabla_x\otimes\Psi^\varepsilon\|_2^2dx\right)^{\frac{1}{2}}\left(\int_{\mathbb{R}^3}|\Psi^\varepsilon|^2\right)^{\frac{1}{2}}.$$

Applying this inequality to all the terms of the right hand side of (1.2.17), one finds thanks to Assumptions 1.2.4 and 1.2.5 and Young's formula

$$\begin{aligned}
&\varepsilon^2\Im\left(\int_0^t\int_{\mathbb{R}^3}(\vec{\sigma}\times\nabla_x V^\varepsilon)\cdot\nabla_x\Psi^\varepsilon\cdot\overline{\partial_s\Psi^\varepsilon}dsdx\right)\leq\\
&\qquad C_1(t)+\frac{\varepsilon^2}{8}(\int_{\mathbb{R}^3}\|\nabla_x\otimes\Psi^\varepsilon\|_2^2dx+\int_0^t\int_{\mathbb{R}^3}\|\nabla_x\otimes\Psi^\varepsilon\|_2^2dsdx), \qquad (1.2.18)
\end{aligned}$$

with a continuous function $C_1(t)$ independent of ε. Finally, integrating (1.2.16) with respect to t and with (1.2.18), we obtain

$$\varepsilon^2\int_{\mathbb{R}^3}\|\nabla_x\otimes\Psi^\varepsilon\|_2^2dx\leq C_2(t)+\varepsilon^2\int_0^t\int_{\mathbb{R}^3}\|\nabla_x\otimes\Psi^\varepsilon\|_2^2dsdx.$$

Applying the Gronwall's Lemma and with the mass conservation (1.2.14), one deduces (1.2.15).

1.2.2 Semiclassical limit

In this subsection, a brief proof of the two above theorems will be presented. We use a main theorem in the semi-classical analysis due to Gérard, Markovich and al in [13] to passing to the limit. More precisely we will use Theorem 6.1 of [13].

Proof of Theorem 1.2.1 and Theorem 1.2.2. The first point of Theorem 1.2.1 results from the boundedness of Ψ_I^ε in $L^2(\mathbb{R}^3, \mathbb{C}^2)$ (see [13]). Let $P_\varepsilon(t,x,\xi) = \left(\frac{|\xi|^2}{2} + V^\varepsilon\right) I_2$, then equation (1.2.1) rewrites as

$$\varepsilon\partial_t\Psi^\varepsilon + i\left(P_\varepsilon^W(t,x,i\varepsilon\nabla_x) + \alpha\Omega_\varepsilon^W(t,x,i\varepsilon\nabla_x)\cdot\vec{\sigma}\right)(\Psi^\varepsilon) = 0. \tag{1.2.19}$$

We begin by the first case : $\alpha = \mathcal{O}(\varepsilon)$ and we take $\alpha = \varepsilon$ for simplicity. By taking a Hilbert expansions of V^ε and $\vec{\Omega}_\varepsilon$ with respect to ε

$$V^\varepsilon = V + \varepsilon V^1 + o(\varepsilon), \quad \vec{\Omega}_\varepsilon = \vec{\Omega} + \varepsilon\vec{\Omega}_1 + o(\varepsilon),$$

we have

$$P_\varepsilon + \varepsilon\vec{\Omega}_\varepsilon\cdot\vec{\sigma} = P_0(t,x,\xi) + \varepsilon(V_1 I_2 + \vec{\Omega}\cdot\vec{\sigma}) + o(\varepsilon),$$

with $P_0(t,x,\xi) = \left(\frac{|\xi|^2}{2} + V(t,x)\right) I_2$. Let $\lambda(t,x,\xi) = \frac{|\xi|^2}{2} + V(t,x)$ be the unique eigenvalue of $P_0(t,x,\xi)$ of multiplicity 2, and applying Theorem 6.1 of [13] then, $W^\varepsilon(\Psi^\varepsilon,\Psi^\varepsilon)$ converges weak $\star$ in $L^\infty(\mathbb{R}^+, \mathcal{S}'(\mathbb{R}^3_x\times\mathbb{R}^3_v, \mathcal{M}_2(\mathbb{C})))$ to
$W^0 \in C^0(\mathbb{R}^+, \mathcal{M}_b(\mathbb{R}^6, \mathcal{H}_2^+(\mathbb{C})))$. In addition, W^0 satisfies

$$\partial_t W^0 + \{\lambda, W^0\} = [W^0, F_\lambda] \quad \text{on } (\mathbb{R}^+\times\mathbb{R}^6_{x,\xi})\setminus E, \tag{1.2.20}$$

with $F_\lambda = [\Pi_\lambda, \{\lambda,\Pi_\lambda\}] + i\Pi_\lambda(V_1 I_2 + \vec{\Omega}\cdot\vec{\sigma})\Pi_\lambda$, Π_λ is the orthogonal projection on the eigenspace associated to λ, and $\{\ \}$ denotes the Poisson bracket :

$$\{\lambda, W^0\} = \nabla_\xi\lambda\cdot\nabla_x W^0 - \nabla_x\lambda\cdot\nabla_\xi W^0.$$

The set E represents a closed subset of $\mathbb{R}^+\times\mathbb{R}^3_x\times\mathbb{R}^3_\xi$ such that, for every $(t,x,\xi)\notin E$, the eigenvalues of P_0 can be ordered as follows, see [13],

$$\lambda_1(t,x,\xi) < \ldots < \lambda_d(t,x,\xi)$$

where, for $1\le q\le d$, the multiplicity of $\lambda_q(t,x,\xi)$ does not depend on (t,x,ξ). Here, we have one eigenvalue $\lambda(t,x,\xi)$ ($d=1$) of multiplicity two for every $(t,x,\xi)\in\mathbb{R}^+\times\mathbb{R}^6$. We choose then $E=\emptyset$. Moreover, we have $\Pi_\lambda = I_2$ then, $F_\lambda = i(V_1 I_2 + \vec{\Omega}\cdot\vec{\sigma})$ and equation (1.2.20) yields (1.2.4). For the convergence of the macroscopic quantities, we refer the reader also to [13].

We assume now that $\alpha = \mathcal{O}(1)$ and we take $\alpha = 1$, then the principal order (with respect to ε) of the symbol of the pseudo-differential operator in equation (1.2.19) multiplied by $-i$ is given by $P_0(t,x,\xi)+\vec{\Omega}(t,x,\xi)\cdot\vec{\sigma}$. It admits two simple eigenvalues $\lambda_\uparrow$ and $\lambda_\downarrow$ given by

$$\lambda_\uparrow = \frac{|\xi|^2}{2} + V(t,x) + |\vec{\Omega}(x,\xi)|, \quad \lambda_\downarrow = \frac{|\xi|^2}{2} + V(t,x) - |\vec{\Omega}(x,\xi)|.$$

Denoting by $\Pi_\uparrow$ and $\Pi_\downarrow$ the orthogonal projections on the eigenspaces associated to $\lambda_\uparrow$ and $\lambda_\downarrow$ respectively, one can easily verify that

$$\Pi_\uparrow = \frac{1}{2}\left(I_2 + \frac{\vec{\Omega}\cdot\vec{\sigma}}{|\vec{\Omega}|}\right), \text{ and } \Pi_\downarrow = \frac{1}{2}\left(I_2 - \frac{\vec{\Omega}\cdot\vec{\sigma}}{|\vec{\Omega}|}\right) \quad \text{on } (\mathbb{R}^+\times\mathbb{R}^6)\setminus E$$

where E is given by (1.2.6). From Theorem 6.1 of [13], the weak limit of $W^\varepsilon(\Psi^\varepsilon,\Psi^\varepsilon)$, W^0, is given by $W^0 = W^0_\uparrow + W^0_\downarrow$. The up and down functions $W^0_\uparrow$ and $W^0_\downarrow$ are a two continuously t-dependent positive matrix valued measures on $\mathbb{R}^6_{x,\xi}$ satisfying

$$\partial_t W^0_{\uparrow(\downarrow)} + \{\lambda_{\uparrow(\downarrow)}, W^0_{\uparrow(\downarrow)}\} = [W^0_{\uparrow(\downarrow)}, F_{\uparrow(\downarrow)}] \quad \text{on } (\mathbb{R}^+\times\mathbb{R}^6_{x,\xi})\setminus\overline{E}, \tag{1.2.21}$$

with $F_{\uparrow(\downarrow)} = [\Pi_{\uparrow(\downarrow)}, \{\lambda_{\uparrow(\downarrow)}, \Pi_{\uparrow(\downarrow)}\}] + i\Pi_{\uparrow(\downarrow)}(V_1 I_2 + \vec{\Omega}_1\cdot\vec{\sigma})\Pi_{\uparrow(\downarrow)}$. Moreover, we have $W^0_{\uparrow(\downarrow)} = \Pi_{\uparrow(\downarrow)} W^0 \Pi_{\uparrow(\downarrow)}$ and if we pose $W^0 = \dfrac{w_c}{2} I_2 + \vec{w}_s\cdot\vec{\sigma}$, then a straightforward calculation gives

$$W^0_\uparrow = \left(\frac{w_c}{2} + \frac{\vec{w}_s\cdot\vec{\Omega}}{|\vec{\Omega}|}\right)\Pi_\uparrow \text{ and } W^0_\downarrow = \left(\frac{w_c}{2} - \frac{\vec{w}_s\cdot\vec{\Omega}}{|\vec{\Omega}|}\right)\Pi_\downarrow \quad \text{on } (\mathbb{R}^+\times\mathbb{R}^6_{x,\xi})\setminus\overline{E}. \tag{1.2.22}$$

We deduce that

$$\begin{aligned} W^0 &= \frac{1}{2}\left(\frac{w_c}{2} + \frac{\vec{w}_s\cdot\vec{\Omega}}{|\vec{\Omega}|}\right)\left(I_2 + \frac{\vec{\Omega}\cdot\vec{\sigma}}{|\vec{\Omega}|}\right) + \frac{1}{2}\left(\frac{w_c}{2} - \frac{\vec{w}_s\cdot\vec{\Omega}}{|\vec{\Omega}|}\right)\left(I_2 - \frac{\vec{\Omega}\cdot\vec{\sigma}}{|\vec{\Omega}|}\right) \\ &= \frac{w_c}{2} I_2 + \frac{\vec{w}_s\cdot\vec{\Omega}}{|\vec{\Omega}|^2}\vec{\Omega}\cdot\vec{\sigma} \quad \text{on } (\mathbb{R}^+\times\mathbb{R}^6_{x,\xi})\setminus\overline{E}. \end{aligned}$$

This implies that the spin part of W^0, $\vec{w}_s$ is parallel to $\vec{\Omega}$. Let $w_s(t,x,\xi) = \dfrac{\vec{w}_s\cdot\vec{\Omega}}{|\vec{\Omega}|}$ and let $w_\uparrow = \dfrac{w_c}{2} + w_s$ and $w_\downarrow = \dfrac{w_c}{2} - w_s$ be the eigenvalues of W^0, we have, from (1.2.22), $W^0_\uparrow = w_\uparrow\Pi_\uparrow$ and $W^0_\downarrow = w_\downarrow\Pi_\downarrow$. Equation (1.2.21) yields (1.2.7). Indeed, we have

$$\partial_t W^0_{\uparrow(\downarrow)} + \{\lambda_{\uparrow(\downarrow)}, W^0_{\uparrow(\downarrow)}\} = (\partial_t w_{\uparrow(\downarrow)} + \{\lambda_{\uparrow(\downarrow)}, w_{\uparrow(\downarrow)}\})\Pi_{\uparrow(\downarrow)} + w_{\uparrow(\downarrow)}\{\lambda_{\uparrow(\downarrow)}, \Pi_{\uparrow(\downarrow)}\}.$$

In addition, using the identity $[\vec{a}\cdot\vec{\sigma},\vec{b}\cdot\vec{\sigma}] = 2i(\vec{a}\times\vec{b})\cdot\vec{\sigma}$ for any two vectors $\vec{a}$ and $\vec{b}$, one has

$$\begin{aligned}
[W_\uparrow^0, F_\uparrow] &= [w_\uparrow\Pi_\uparrow, [\Pi_\uparrow, \{\lambda_\uparrow, \Pi_\uparrow\}]] + [w_\uparrow\Pi_\uparrow, i\Pi_\uparrow(V_1 I_2 + \vec{\Omega}_1\cdot\vec{\sigma})\Pi_\uparrow] \\
&= \frac{w_\uparrow}{4}\left[\Pi_\uparrow, \left[\frac{\vec{\Omega}\cdot\vec{\sigma}}{|\vec{\Omega}|}, \left\{\lambda_\uparrow, \frac{\vec{\Omega}}{|\vec{\Omega}|}\right\}\cdot\vec{\sigma}\right]\right] + 0 \\
&= \frac{iw_\uparrow}{2}\left[\Pi_\uparrow, \left(\frac{\vec{\Omega}}{|\vec{\Omega}|}\times\left\{\lambda_\uparrow, \frac{\vec{\Omega}}{|\vec{\Omega}|}\right\}\right)\cdot\vec{\sigma}\right] \\
&= \frac{-w_\uparrow}{2}\frac{\vec{\Omega}}{|\vec{\Omega}|}\times\left(\frac{\vec{\Omega}}{|\vec{\Omega}|}\times\left\{\lambda_\uparrow, \frac{\vec{\Omega}}{|\vec{\Omega}|}\right\}\right)\cdot\vec{\sigma} \\
&= \frac{-w_\uparrow}{2}\left(\left\{\lambda_\uparrow, \frac{\vec{\Omega}}{|\vec{\Omega}|}\right\}.\frac{\vec{\Omega}}{|\vec{\Omega}|}\right)\frac{\vec{\Omega}\cdot\vec{\sigma}}{|\vec{\Omega}|} + \frac{w_\uparrow}{2}\frac{\vec{\Omega}.\vec{\Omega}}{|\vec{\Omega}|^2}\left\{\lambda_\uparrow, \frac{\vec{\Omega}}{|\vec{\Omega}|}\right\}\cdot\vec{\sigma} \\
&= \frac{w_\uparrow}{2}\left\{\lambda_\uparrow, \frac{\vec{\Omega}}{|\vec{\Omega}|}\right\}\cdot\vec{\sigma} = w_\uparrow\{\lambda_\uparrow, \Pi_\uparrow\}.
\end{aligned}$$

Similarly, $[W_\downarrow^0, F_\downarrow] = w_\downarrow\{\lambda_\downarrow, \Pi_\downarrow\}$ and we conclude that

$$(\partial_t w_{\uparrow(\downarrow)} + \{\lambda_{\uparrow(\downarrow)}, w_{\uparrow(\downarrow)}\})\Pi_{\uparrow(\downarrow)} + w_{\uparrow(\downarrow)}\{\lambda_{\uparrow(\downarrow)}, \Pi_{\uparrow(\downarrow)}\} = w_{\uparrow(\downarrow)}\{\lambda_{\uparrow(\downarrow)}, \Pi_{\uparrow(\downarrow)}\}$$

which gives system (1.2.7).

1.3 Semi-classical limit of the Schrödinger equation with Spin-Orbit term and partially confining potential

1.3.1 Introduction and main result

The starting equation in this section is the following scaled Schrödinger equation

$$\begin{cases} i\varepsilon\partial_t\Psi^\varepsilon = -\dfrac{\varepsilon^2}{2}\Delta_{\mathbf{x}}\Psi^\varepsilon - \dfrac{1}{2}\partial_z^2\Psi^\varepsilon + V^\varepsilon\Psi^\varepsilon + \varepsilon\Omega_\varepsilon^W(t,\mathbf{x},z,i\nabla_\varepsilon)\cdot\vec{\sigma}(\Psi^\varepsilon) \\ \Psi^\varepsilon(0,\mathbf{x},z) = \Psi_I^\varepsilon(\mathbf{x},z) \end{cases} \tag{1.3.1}$$

where $(\mathbf{x},z)\in\mathbb{R}^2\times[0,1]$, $\Psi^\varepsilon = \Psi^\varepsilon(t,\mathbf{x},z)$ and $\nabla_\varepsilon = (\varepsilon\nabla_{\mathbf{x}}, \partial_z)$. Let us denote the spatial domain by

$$\mathcal{D} = \mathbb{R}^2\times(0,1).$$

The position variables in the longitudinal directions are denoted by $\mathbf{x}\in\mathbb{R}^2$ and z is used for the transversal direction (or confinement one). For any $\xi\in\mathbb{R}^3$, we

will write $\xi = (\xi_{\mathbf{x}}, \xi_z)$ where $\xi_{\mathbf{x}} \in \mathbb{R}^2$ and $\xi_z \in \mathbb{R}$ are respectively the longitudinal and transversal parts of ξ. The Weyl operator $\Omega_\varepsilon^W(t, \mathbf{x}, z, i\nabla_\varepsilon) \cdot \vec{\sigma}$ represents in this section the following operator

$$\Omega_\varepsilon^W(t, \mathbf{x}, z, i\nabla_\varepsilon)\cdot\vec{\sigma}(\psi) = \frac{1}{(2\pi)^2}\int_{\mathbb{R}^2_{\xi_{\mathbf{x}}}}\int_{\mathbb{R}^2_{\mathbf{y}}} \vec{\Omega}_\varepsilon\left(t, \frac{\mathbf{x}+\mathbf{y}}{2}, z, \varepsilon\xi_{\mathbf{x}}, i\partial_z\right)\cdot\vec{\sigma}(\psi(\mathbf{y}, z))e^{i(\mathbf{x}-\mathbf{y})\cdot\xi_{\mathbf{x}}}d\xi_{\mathbf{x}}d\mathbf{y}.$$

Here, for every $(t, \mathbf{x}, z, \xi_{\mathbf{x}}) \in \mathbb{R}^+ \times \mathcal{D} \times \mathbb{R}^2_{\xi_{\mathbf{x}}}$, $\vec{\Omega}(t, \mathbf{x}, z, \xi_{\mathbf{x}}, i\partial_z)$ is a vector valued differential operator which is the image of $i\partial_z$ by some regular vector valued function $\vec{\Omega}(t, \mathbf{x}, z, \xi_{\mathbf{x}}, .)$. The confinement in the z direction is modeled through the following boundary conditions

$$\Psi^\varepsilon(t, \mathbf{x}, z = 0) = \Psi^\varepsilon(t, \mathbf{x}, z = 1) = 0. \tag{1.3.2}$$

Thanks to this assumption, the transverse Hamiltonian $(-\frac{1}{2}\partial_z^2 + V^\varepsilon)I_2$ has a discrete spectrum and a complete set of eigenfunctions. Let $\chi_p^\varepsilon(t, \mathbf{x}, .)$ and $\epsilon_p^\varepsilon(t, \mathbf{x})$ be the eigenfunctions and eigenvalues of $-\frac{1}{2}\partial_z^2 + V^\varepsilon$ with homogenous boundary conditions, they satisfy

$$\begin{cases} -\frac{1}{2}\partial_z^2\chi_p^\varepsilon + V^\varepsilon\chi_p^\varepsilon = \epsilon_p^\varepsilon\chi_p^\varepsilon \\ \chi_p^\varepsilon(t, \mathbf{x}, .) \in H_0^1(0, 1), \quad \displaystyle\int_0^1 \chi_p^\varepsilon\chi_q^\varepsilon = \delta_{pq}. \end{cases} \tag{1.3.3}$$

For any $(t, \mathbf{x}) \in \mathbb{R}^+ \times \mathbb{R}^2$, $\left(\chi_p^\varepsilon(t, \mathbf{x}, .)\right)_{p\geq 1}$ is an orthonormal basis of $L^2(0, 1)$, $(\epsilon_p^\varepsilon)_{p\geq 1}$ are simple as eigenvalues of $-\frac{1}{2}\partial_z^2 + V^\varepsilon$. The eigenvalues of the transverse Hamiltonian $(-\frac{1}{2}\partial_z^2 + V^\varepsilon)I_2$ are then ϵ_p^ε and are of multiplicity two. Let us denote by $\mathcal{H}_p^\varepsilon(t, \mathbf{x})$ the p-th eigenspace which is given by

$$\mathcal{H}_p^\varepsilon(t, \mathbf{x}) = span\left\{\begin{pmatrix} \chi_p^\varepsilon \\ 0 \end{pmatrix}, \begin{pmatrix} 0 \\ \chi_p^\varepsilon \end{pmatrix}\right\} \subset (L^2(0, 1))^2$$

and by $\Pi_p^\varepsilon(t, \mathbf{x})$ the orthogonal projector on $\mathcal{H}_p^\varepsilon(t, \mathbf{x})$. For $\varepsilon = 0$, we shall use the notation Π_p and ϵ_p instead of Π_p^0 and ϵ_p^0. As in the previous section we take the following assumptions

Assumption 1.3.1. *For any $T > 0$, $(\varepsilon, t, \mathbf{x}, z) \mapsto V^\varepsilon(t, \mathbf{x}, z)$ is a real nonnegative function belonging to $C^0([0, 1]_\varepsilon, C^1 \cap W^{1,\infty}([0, T] \times \mathbb{R}^2, L^\infty(0, 1)))$.*

Assumption 1.3.2. *The initial data Ψ_I^ε belongs to $H_0^1(\mathcal{D}, \mathbb{C}^2)$ and there exists $C > 0$ independent of ε such that*

$$\int\int_{\mathcal{D}} (|\Psi_I^\varepsilon|^2 + \varepsilon^2\|\nabla_{\mathbf{x}} \otimes \Psi_I^\varepsilon\|_2^2 + |\partial_z\Psi_I^\varepsilon|^2)d\mathbf{x}dz \leq C.$$

Assumption 1.3.3. *The effective field* $\vec{\Omega}_\varepsilon(t,\mathbf{x},z,\xi_\mathbf{x},\xi_z)$ *belongs to* $C^0([0,1]_\varepsilon, C^1(\mathbb{R}^+\times \mathcal{D}\times\mathbb{R}^3_\xi))^3$ *such that* (1.2.9) *holds. In addition, we assume that* $\vec{\Omega}_\varepsilon$ *satisfies the following expansion*

$$\vec{\Omega}_\varepsilon = \vec{\Omega}(t,\mathbf{x},z,\xi_\mathbf{x}) + \varepsilon\vec{\Omega}_1(t,\mathbf{x},z,\xi_\mathbf{x},\xi_z) + o(\varepsilon) \tag{1.3.4}$$

with $\vec{\Omega}\in C^1(\mathbb{R}^+\times\mathcal{D}\times\mathbb{R}^2_{\xi_\mathbf{x}})$ *and* $\vec{\Omega}_1\in C^1(\mathbb{R}^+\times\mathcal{D}\times\mathbb{R}^3_{\xi_\mathbf{x},\xi_z})$.

Definition 1.3.4. *Let*

$$\mathcal{H} = L^2((0,1),\mathbb{C}^2).$$

This is an Hilbert space equipped with the L^2 *norm. The unknown* Ψ^ε *of* (1.3.1) *is an* $\mathcal{H}$*-valued function on* $\mathbb{R}^+\times\mathbb{R}^2$. *In the sequel,* $\mathcal{H}\overline{\otimes}\mathcal{H}$ *will denote the space of bilinear forms on* $\mathcal{H}\times\mathcal{H}$. *It can be identified to* $L^2((0,1)^2,\mathcal{M}_2(\mathbb{C}))$ *: the set of linear combination of simple tensors of the form* $(\Phi_1\otimes\overline{\Phi}_2)(z,z')$ *for any* $\Phi_1,\Phi_2\in\mathcal{H}$ *and where*

$$\begin{aligned}(\Phi_1\otimes\overline{\Phi}_2)(\Psi_1,\Psi_2) &= \int_0^1\int_0^1 \Phi_1(z)\otimes\overline{\Phi}_2(z') : \overline{\Psi_1(z)\otimes\overline{\Psi}_2(z')}dzdz' \\ &= \left(\int_0^1 \Phi_1(z)\cdot\overline{\Psi}_1(z)dz\right)\left(\overline{\int_0^1 \Phi_2(z')\cdot\overline{\Psi}_2(z')dz'}\right)\end{aligned}$$

$\forall\Psi_1,\Psi_2\in\mathcal{H}$.

Definition 1.3.5. *Let* Φ_1,Φ_2 *be two* $\mathcal{H}$*-valued distribution belonging to* $\mathcal{S}'(\mathbb{R}^2_\mathbf{x},\mathcal{H})$. *For any* $\varepsilon>0$, *the partial Wigner transform is given by*

$$W^\varepsilon(\Phi_1,\Phi_2)(\mathbf{x},\xi_\mathbf{x},z',z) = (2\pi)^{-2}\int_{\mathbb{R}^2} e^{i\eta\cdot\xi_\mathbf{x}}\Phi_1(\mathbf{x}-\varepsilon\frac{\eta}{2},z)\otimes\overline{\Phi}_2(\mathbf{x}+\varepsilon\frac{\eta}{2},z')d\eta. \tag{1.3.5}$$

This defines a continuous sesquilinear mapping from $\mathcal{S}'(\mathbb{R}^2_\mathbf{x},\mathcal{H})\times\mathcal{S}'(\mathbb{R}^2_\mathbf{x},\mathcal{H})$ *to* $\mathcal{S}'(\mathbb{R}^2_\mathbf{x}\times\mathbb{R}^2_{\xi_\mathbf{x}},\mathcal{H}\overline{\otimes}\mathcal{H})$.

Under Assumptions 1.3.1, 1.3.2, equation (1.3.1) admits a unique weak solution $\Psi^\varepsilon\in C^0(\mathbb{R}^+,H^1_0(\mathcal{D},\mathbb{C}^2))\cap C^1(\mathbb{R}^+,H^{-1}(\mathcal{D},\mathbb{C}^2))$ satisfying the mass conservation (see the previous section). We assume moreover that the energy estimate is propagated

$$\forall t>0,\quad \int\int_\mathcal{D}(|\Psi^\varepsilon|^2+\varepsilon^2\|\nabla_\mathbf{x}\otimes\Psi^\varepsilon\|_2^2+|\partial_z\Psi^\varepsilon_I|^2)d\mathbf{x}dz\le C(t) \tag{1.3.6}$$

where $C(t)$ is a continuous function of t independent of ε.

Definition 1.3.6. *Let* Ψ^ε *be the solution of* (1.3.1). *The associated macroscopic quantities are now given by*

$$N^\varepsilon(t,\mathbf{x},z,z') = \Psi^\varepsilon(t,\mathbf{x},z)\otimes\overline{\Psi^\varepsilon}(t,\mathbf{x},z') \tag{1.3.7}$$

and

$$J^\varepsilon(t,\mathbf{x},z,z') = \frac{\varepsilon}{2i}[\nabla_\mathbf{x}\Psi^\varepsilon(t,\mathbf{x},z)\otimes\overline{\Psi^\varepsilon}(t,\mathbf{x},z') - \Psi^\varepsilon(t,\mathbf{x},z)\otimes\nabla_\mathbf{x}\overline{\Psi^\varepsilon}(t,\mathbf{x},z')]. \tag{1.3.8}$$

We are now read to give the main result of this section. This is the subject of the next Theorem.

Theorem 1.3.7. *Assume that Assumptions 1.3.1, 1.3.2 and 1.3.3 hold. Then, up to extraction of subsequences, we have the following results at the limit $\varepsilon \mapsto 0$.*

1. *For any $p \in \mathbb{N}^*$, $W^\varepsilon(\Pi_p^\varepsilon(0,\mathbf{x})\Psi_I^\varepsilon, \Pi_p^\varepsilon(0,\mathbf{x})\Psi_I^\varepsilon)$ converges in $\mathcal{S}'(\mathbb{R}^4_{\mathbf{x},\xi_\mathbf{x}}, \mathcal{H}\overline{\otimes}\mathcal{H})$ to*

$$F_{p,I}(\mathbf{x},\xi_\mathbf{x})\chi_p(0,\mathbf{x},z)\chi_p(0,\mathbf{x},z') \in \mathcal{M}_b(\mathbb{R}^4_{\mathbf{x},\xi_\mathbf{x}}, \mathcal{H}\overline{\otimes}\mathcal{H}).$$

   Moreover, $F_{p,I}(\mathbf{x},\xi_\mathbf{x}) \in \mathcal{H}_2^+(\mathbb{C})$ for all $(\mathbf{x},\xi_\mathbf{x}) \in \mathbb{R}^4$.

2. *The Wigner transform $W^\varepsilon(\Psi^\varepsilon,\Psi^\varepsilon)$ of the solution of (1.3.1) converges in $L^\infty(\mathbb{R}^+, \mathcal{S}'(\mathbb{R}^4_{\mathbf{x},\xi_\mathbf{x}}, \mathcal{H}\overline{\otimes}\mathcal{H}))$ weak $\star$ to*

$$W^0 = \sum_p F_p(t,\mathbf{x},\xi_\mathbf{x})\chi_p(t,\mathbf{x},z)\chi_p(t,\mathbf{x},z') \in C^0(\mathbb{R}^+, \mathcal{M}_b(\mathbb{R}^4_{\mathbf{x},\xi_\mathbf{x}}, \mathcal{H}\overline{\otimes}\mathcal{H})) \tag{1.3.9}$$

   with $F_p(t,\mathbf{x},\xi_\mathbf{x}) \in \mathcal{H}_2^+(\mathbb{C})$. It solves

$$\begin{cases} \partial_t F_p + \xi_\mathbf{x}\cdot\nabla_\mathbf{x} F_p - \nabla_\mathbf{x}\epsilon_p\cdot\nabla_{\xi_\mathbf{x}} F_p = i[F_p, \vec{\Omega}_p\cdot\vec{\sigma}], \\ F_p(0,\mathbf{x},\xi_\mathbf{x}) = F_{p,I}(\mathbf{x},\xi_\mathbf{x}), \end{cases} \tag{1.3.10}$$

   where the effective field on the p-th subband, $\vec{\Omega}_p$, is given by

$$\vec{\Omega}_p(t,\mathbf{x},\xi_\mathbf{x}) = \int_0^1 \vec{\Omega}(t,\mathbf{x},z,\xi_\mathbf{x})|\chi_p(t,\mathbf{x},z)|^2 dz. \tag{1.3.11}$$

3. *For every $T>0$, the particle and current densities N^ε and J^ε given by (1.3.7)-(1.3.8) converge in $L^\infty((0,T), \mathcal{M}_b(\mathbb{R}^2_\mathbf{x}, \mathcal{H}\overline{\otimes}\mathcal{H}))$ weak $\star$ to*

$$\begin{aligned} N(t,\mathbf{x},z,z') &= \sum_{p\geq 1}\left(\int_{\mathbb{R}^2} F_p(t,\mathbf{x},\xi_\mathbf{x})d\xi_\mathbf{x}\right)\chi_p(t,\mathbf{x},z)\chi_p(t,\mathbf{x},z') \\ J(t,\mathbf{x},z,z') &= \sum_{p\geq 1}\left(\int_{\mathbb{R}^2} v F_p(t,\mathbf{x},\xi_\mathbf{x})d\xi_\mathbf{x}\right)\chi_p(t,\mathbf{x},z)\chi_p(t,\mathbf{x},z'). \end{aligned}$$

1.3.2 Application : subband model with Rashba spin-orbit effect

If we consider the general spin-orbit hamiltonian given by (1.1.2), the Schrödinger equation with physical dimensional variables writes

$$i\hbar\partial_t\Psi^\varepsilon = -\frac{\hbar^2}{2m}\Delta_{\mathbf{x},z}\Psi^\varepsilon + V^\varepsilon\Psi^\varepsilon + i\frac{\hbar^2}{4m^2c^2}(\vec{\sigma}\times\nabla_{\mathbf{x},z}V^\varepsilon)\cdot\nabla_{\mathbf{x},z}\Psi^\varepsilon \tag{1.3.12}$$

with $\hbar$ is the Planck constant, m is the effective mass of an electron and c denotes the speed of light. Let respectively, L and l be the longitudinal and transversal length

scales. Here, we are interested in situations where the length scale in the confinement direction z, l, is much smaller than the length scale in the non confinement one. In other words, let ε be the ratio between the two length scales l and L, we assume that

$$\varepsilon := \frac{l}{L} << 1.$$

This leads, up to rescaling of equation (1.3.12), to

$$i\varepsilon\partial_t\Psi^\varepsilon = -\frac{\varepsilon^2}{2}\Delta_{\mathbf{x}}\Psi^\varepsilon - \frac{1}{2}\partial_z^2\Psi^\varepsilon + V^\varepsilon\Psi^\varepsilon + i\beta(\vec{\sigma}\times\nabla_\varepsilon V^\varepsilon)\cdot\nabla_\varepsilon\Psi^\varepsilon \tag{1.3.13}$$

where $\nabla_\varepsilon = (\varepsilon\nabla_{\mathbf{x}}, \nabla_z)$ and $\beta = \dfrac{\hbar^2}{4m^2c^2l^2}$. If $\overline{V}$ and $\bar{t}$ denote the potential and time scales, to obtain (1.3.13) we have taken the following hypotheses

$$\overline{V} = \frac{\overline{h}^2}{ml^2} \quad \text{and} \quad \frac{\overline{V}\bar{t}}{\hbar} = \frac{1}{\varepsilon}.$$

The constant β is a dimensionless quantity. We shall assume that β is small and is of order ε and we take $\beta = \varepsilon$ for simplicity. A straightforward computation gives

$$\begin{aligned}(\vec{\sigma}\times\nabla_\varepsilon V^\varepsilon)\cdot\nabla_\varepsilon\psi^\varepsilon &= \partial_z V^\varepsilon(\sigma_2(\varepsilon\partial_x) - \sigma_1(\varepsilon\partial_y))\Psi^\varepsilon \\ &\quad +\varepsilon\sigma_3(\partial_x V^\varepsilon(\varepsilon\partial_y) - \partial_y V^\varepsilon(\varepsilon\partial_x))\Psi^\varepsilon \\ &\quad +\varepsilon(\sigma_1\partial_y V^\varepsilon - \sigma_2\partial_x V^\varepsilon)\partial_z\Psi^\varepsilon\end{aligned}$$

where (x, y) are the components of $\mathbf{x}\in\mathbb{R}^2$. This implies that $i(\vec{\sigma}\times\nabla_\varepsilon V^\varepsilon)\cdot\nabla_\varepsilon = \Omega_\varepsilon^W(t, \mathbf{x}, z, i\nabla_\varepsilon)\cdot\vec{\sigma}$ with $\vec{\Omega}_\varepsilon = \vec{\Omega} + \varepsilon\vec{\Omega}_1 + o(\varepsilon)$ such that

$$\vec{\Omega}(t, \mathbf{x}, z, \xi) = \partial_z V(-\xi_{\mathbf{x}}^2, \xi_{\mathbf{x}}^1, 0), \quad \vec{\Omega}_1(t, \mathbf{x}, z, \xi) = (\partial_y V\xi_z, -\partial_x V\xi_z, \partial_x V\xi_{\mathbf{x}}^2 - \partial_y V\xi_{\mathbf{x}}^1)$$

and where V is the limit of V^ε when ε goes to zero and $\xi = (\xi_{\mathbf{x}}^1, \xi_{\mathbf{x}}^2, \xi_z)$. Applying Theorem 1.3.7, one finds the following Boltzmann equation in the p-th subband

$$\partial_t F_p + \xi_{\mathbf{x}}\cdot\nabla_{\mathbf{x}}F_p - \nabla_{\mathbf{x}}\epsilon_p\cdot\nabla_{\xi_{\mathbf{x}}}F_p = i\alpha_p(t, \mathbf{x})[\sigma_2\xi_{\mathbf{x}}^1 - \sigma_1\xi_{\mathbf{x}}^2, F_p]$$

where

$$\alpha_p(t, \mathbf{x}) = \int_0^1 \partial_z V(t, \mathbf{x}, z)|\chi_p(t, \mathbf{x}, z)|^2 dz. \tag{1.3.14}$$

Remark 1.3.8. *The spin-orbit effect obtained in this limit is nothing but the Rashba effect used generally in the literature [3, 24] to describe the spin-orbit interactions in bidimensional gases. Moreover, an explicit relation between the confinement potential and the strength of the Rashba spin-orbit coupling is obtained, relation* (1.3.14).

1.3.3 Proof of Theorem 1.3.7

Theorem 1.3.7 can be proved by following the work of N. Ben Abdallah and F. Mehats [1]. We present here the ideas of the proof and we refer to [1] for details. For the general properties of the Wigner transform (1.3.5) we refer the reader to [1, 13, 15]. Let us summarize some of these properties.
We introduce the following space of $\mathcal{H}\overline{\otimes}\mathcal{H}$-valued test functions :

$$\mathcal{A} = \{\phi \in C_c^0(\mathbb{R}^2_{\mathbf{x}} \times \mathbb{R}^2_{\xi_{\mathbf{x}}}, \mathcal{H}\overline{\otimes}\mathcal{H}) \quad / \quad (\mathcal{F}_{\xi_{\mathbf{x}}}\phi)(\mathbf{x},\eta) \in L^1(\mathbb{R}^2_\eta, C_c^0(\mathbb{R}^2_{\mathbf{x}}, \mathcal{H}\overline{\otimes}\mathcal{H}))\} \tag{1.3.15}$$

with $\mathcal{F}_{\xi_{\mathbf{x}}}\phi$ be the Fourier transform with respect to $\xi_{\mathbf{x}}$. This space equipped with

$$\|\mathcal{F}_{\xi_{\mathbf{x}}}\phi\|_{L^1(\mathbb{R}^2_\eta,(C_c^0(\mathbb{R}^2_{\mathbf{x}},\mathcal{H}\overline{\otimes}\mathcal{H}))}$$

is a separable Banach space.

Proposition 1.3.9. *Let (Ψ^ε) be a bounded family of $L^2(\mathbb{R}^2_{\mathbf{x}}, \mathcal{H})$ functions. Then, the sequence $W^\varepsilon(\Psi^\varepsilon, \Psi^\varepsilon)$ is uniformly bounded in $\mathcal{A}'$. Namely, we have*

$$\|W^\varepsilon(\Psi^\varepsilon, \Psi^\varepsilon)\|_{\mathcal{A}'} \leq \|\Psi^\varepsilon\|_{L^2(\mathbb{R}^2_{\mathbf{x}},\mathcal{H})}. \tag{1.3.16}$$

There exists a bounded measure with 2×2 hermitian and non negative matrix value, W^0, such that, up to extraction of subsequence, $W^\varepsilon(\Psi^\varepsilon, \Psi^\varepsilon)$ converges to W^0 in $\mathcal{A}'$ weak $\star$; W^0 is called the Wigner measure associated to this subsequence of (Ψ^ε). Moreover, assume that (Ψ^ε) is $\varepsilon-$ oscillatory :

$$\varepsilon^2 \int_{\mathbb{R}^2} \|\nabla_{\mathbf{x}} \otimes \Psi^\varepsilon\|_2^2 d\mathbf{x} \leq C \tag{1.3.17}$$

with $C > 0$ independent of ε and the following compactness property holds :

$$\lim_{n\to+\infty} \limsup_{\varepsilon\to 0} \|(Id - \mathbb{P}_n^\varepsilon)\Psi^\varepsilon\|_{L^2(\mathbb{R}^2,\mathcal{H})} = 0. \tag{1.3.18}$$

We denote by Id the identity function on $\mathcal{H}$ and $(\mathbb{P}_n^\varepsilon)_{n\in\mathbb{N}}$ is a sequence of functions in $C^0([0,1]_\varepsilon \times \mathbb{R}^2, Com(\mathcal{H}))$ such that $\lim_{n\to\infty} \mathbb{P}_n^0 = Id$ in the $\mathcal{L}(\mathcal{H})$ weak $\star$ topology, locally uniformly with respect to x. Then,

$$N^\varepsilon \rightharpoonup \int_{\mathbb{R}^3} W^0(.,\xi_{\mathbf{x}}) d\xi_{\mathbf{x}} \quad in \quad \mathcal{M}_b(\mathbb{R}^3, \mathcal{H}\overline{\otimes}\mathcal{H}) \text{ weak } \star, \tag{1.3.19}$$

$$J^\varepsilon \rightharpoonup \int_{\mathbb{R}^3} \xi_{\mathbf{x}} W^0(.,\xi_{\mathbf{x}}) d\xi_{\mathbf{x}} \quad in \quad \mathcal{M}_b(\mathbb{R}^3, \mathcal{H}\overline{\otimes}\mathcal{H}) \text{ weak } \star, \tag{1.3.20}$$

where the quantities N^ε and J^ε are given by Definition 1.3.6.

Lemma 1.3.10. *Let $T > 0$ be fixed and let $(\phi_1^\varepsilon(t,\mathbf{x}))$ and $(\phi_2^\varepsilon(t,\mathbf{x}))$ be two families bounded in $L^\infty((0,T),L^2(\mathbb{R}^2_{\mathbf{x}},\mathcal{H}))$. Consider an $\mathcal{L}(\mathcal{H})$-valued function $(\varepsilon,t,\mathbf{x},\xi_{\mathbf{x}})\mapsto P_\varepsilon(t,\mathbf{x},\xi_{\mathbf{x}})$ belonging to $C^0([0,1],C^1(\mathbb{R}^+\times\mathbb{R}^4_{\mathbf{x},\xi_{\mathbf{x}}},\mathcal{L}(\mathcal{H})))$ and satisfying, for some $M\geq 0$,*

$$\forall\alpha\in\mathbb{N}^3\times\mathbb{N}^3/|\alpha|\leq 1:\|\partial^\alpha_{\mathbf{x},\xi_{\mathbf{x}}}P_\varepsilon(\mathbf{x},\xi_{\mathbf{x}})\|_{\mathcal{L}(\mathcal{H})}\leq C_\alpha(1+|\xi_{\mathbf{x}}|)^M$$

with $C_\alpha>0$ independent of ε. Then, we have

$$W^\varepsilon(P^W_\varepsilon(t,\mathbf{x},i\varepsilon\nabla_{\mathbf{x}})\phi_1^\varepsilon,\phi_2^\varepsilon)=P_\varepsilon W^\varepsilon(\phi_1^\varepsilon,\phi_2^\varepsilon)+\frac{\varepsilon}{2i}\{P_\varepsilon,W^\varepsilon(\phi_1^\varepsilon,\phi_2^\varepsilon)\}+\varepsilon r_1^\varepsilon \tag{1.3.21}$$

$$W^\varepsilon(\phi_1^\varepsilon,P^W_\varepsilon(t,\mathbf{x},i\varepsilon\nabla_{\mathbf{x}})\phi_2^\varepsilon)=W^\varepsilon(\phi_1^\varepsilon,\phi_2^\varepsilon)P^*_\varepsilon+\frac{\varepsilon}{2i}\{W^\varepsilon(\phi_1^\varepsilon,\phi_2^\varepsilon),P^*_\varepsilon\}+\varepsilon r_2^\varepsilon \tag{1.3.22}$$

where $r_1^\varepsilon\rightharpoonup 0$ and $r_2^\varepsilon\rightharpoonup 0$ in $\mathcal{S}'(\mathbb{R}^4,\mathcal{H}\overline{\otimes}\mathcal{H})$ weak $\star$ uniformly with respect to $t\in(0,T)$. Here, $\{p,q\}$ denotes the Poisson bracket of two functions $p(\mathbf{x},\xi)$ and $q(\mathbf{x},\xi)$, given by

$$\{p,q\}(\mathbf{x},\xi)=\nabla_\xi p(\mathbf{x},\xi).\nabla_{\mathbf{x}}q(\mathbf{x},\xi)-\nabla_{\mathbf{x}}p(\mathbf{x},\xi).\nabla_\xi q(\mathbf{x},\xi). \tag{1.3.23}$$

Before going on, one needs the following lemma which summarizes the regularities of the eigenelements of the transversal Schrödinger operator.

Lemma 1.3.11. *Let $(\epsilon_p^\varepsilon,\chi_p^\varepsilon)_\varepsilon$ satisfying* (1.3.3)*. Then, under Assumption 1.3.1, ϵ_p^ε, χ_p^ε have the same regularity as V^ε. Namely, the function $(\varepsilon,t,\mathbf{x})\mapsto\epsilon_p^\varepsilon(t,\mathbf{x})$ belongs to $C^0([0,1]_\varepsilon,C^1\cap W^{1,\infty}([0,T]\times\mathbb{R}^2))$ and $(\varepsilon,t,\mathbf{x},z)\mapsto\chi_p^\varepsilon(t,\mathbf{x},z)\in C^0([0,1]_\varepsilon,C^1\cap W^{1,\infty}([0,T]\times\mathbb{R}^2_{\mathbf{x}},H^2(0,1)))$ for any $T>0$. Moreover, let Π_p^ε be the orthogonal projector on the p-th eigenspace and let $\partial_t\Pi_p^\varepsilon$ and $\nabla_{\mathbf{x}}\Pi_p^\varepsilon$ be their derivatives defined by the following commutators :*

$$\partial_t\Pi_p^\varepsilon=[\partial_t,\Pi_p^\varepsilon],\quad \nabla_{\mathbf{x}}\Pi_p^\varepsilon=[\nabla_{\mathbf{x}},\Pi_p^\varepsilon].$$

For any $p\geq 1$ and $T>0$, Π_p^ε is a self-adjoint operator on $\mathcal{L}(\mathcal{H})$ and the function $(\varepsilon,t,\mathbf{x})\mapsto\Pi_p^\varepsilon$ as well as their derivatives with respect to t and $\mathbf{x}$ are continuously bounded functions of $(\varepsilon,t,\mathbf{x})\in[0,1]\times[0,T]\times\mathbb{R}^2$ valued in $\mathcal{L}(\mathcal{H})$.

Proof. This is a standard result using the perturbation theory of linear operators (see for instance [14, 22]). ■

We proceed now to the proof of the first point of Theorem 1.3.7. Under Assumption 1.3.2 and by (1.3.16), we have, up to extraction of subsequence,

$$W^\varepsilon(\Psi_I^\varepsilon,\Psi_I^\varepsilon)\rightharpoonup W_I^0\quad\text{as }\varepsilon\to 0$$

in $A'_{\mathcal{H}}$ weak $\star$, where W_I^0 is a bounded measure with 2×2 hermitian, nonnegative matrix value. Moreover, in view of Lemma 1.3.11, $\Pi_p^\varepsilon(0,\mathbf{x})\varphi$ converges strongly to $\Pi_p(0,\mathbf{x})\varphi$ as $\varepsilon\to 0$ in $\mathcal{A}$ for every $\varphi\in\mathcal{A}$. Therefore,

$$\Pi_p^\varepsilon(0,\mathbf{x})W^\varepsilon(\Psi_I^\varepsilon,\Psi_I^\varepsilon)\Pi_p^\varepsilon(0,\mathbf{x})\rightharpoonup \Pi_p(0,\mathbf{x})W_I^0\Pi_p(0,\mathbf{x})\quad\text{in }\mathcal{A}'\text{ weak }\star$$

and thanks to Lemma 1.3.10 and the self adjointness of Π_p^ε, one obtains

$$W^\varepsilon(\Pi_p^\varepsilon(0,\mathbf{x})\Psi_I^\varepsilon,\Pi_p^\varepsilon(0,\mathbf{x})\Psi_I^\varepsilon)\rightharpoonup \Pi_p(0,\mathbf{x})W_I^0\Pi_p(0,\mathbf{x})\quad\text{in }\mathcal{A}'\text{ weak }\star.$$

Moreover, we have $W_I^0\in\mathcal{M}_b(\mathbb{R}^4,\mathcal{H}\overline{\otimes}\mathcal{H})$ with $W_I^0(\mathbf{x},\xi_\mathbf{x},z,z')\in\mathcal{H}_2^+(\mathbb{C})$ for all $(\mathbf{x},\xi_\mathbf{x},z,z')\in\mathbb{R}^4\times[0,1]^2$. Let $F_{p,I}=\int_0^1\int_0^1 W_I^0(\mathbf{x},\xi_\mathbf{x},z,z')\chi_p(0,\mathbf{x},z)\chi_p(0,\mathbf{x},z')dzdz'$, then $F_{p,I}(\mathbf{x},\xi_\mathbf{x})\in\mathcal{H}_2^+(\mathbb{C})$ and

$$\Pi_p(0,\mathbf{x})W_I^0\Pi_p(0,\mathbf{x})=F_{p,I}(\mathbf{x},\xi_\mathbf{x})\chi_p(0,\mathbf{x},z)\chi_p(0,\mathbf{x},z').$$

For the second point of the theorem, let

$$W_{p,q}^\varepsilon=W^\varepsilon(\Pi_p^\varepsilon\Psi^\varepsilon,\Pi_q^\varepsilon\Psi^\varepsilon).$$

An analogous analysis using (1.3.6) and (1.3.16) shows that

$$W_{p,q}^\varepsilon\rightharpoonup W_{p,q}^0:=\Pi_pW^0\Pi_q,\quad\text{as }\varepsilon\to 0$$

in $L^\infty((0,T),\mathcal{A}')$ weak $\star$ for every $T>0$, where W^0 denotes the weak $\star$ limit of $W^\varepsilon(\Psi^\varepsilon,\Psi^\varepsilon)$ in $L^\infty((0,T),\mathcal{A}')$. It is a bounded measure belonging to $L^\infty((0,T),\mathcal{M}_b(\mathbb{R}^4,\mathcal{H}\otimes\mathcal{H}))$ with $\mathcal{H}_2^+(\mathbb{C})$ matrix value. It remains now to compute $W_{p,q}^0$ for every $p,q\in\mathbb{N}$.

Lemma 1.3.12. *let $\Psi_p^\varepsilon=\Pi_p^\varepsilon\Psi^\varepsilon$. Then,*

$$\Psi_p^\varepsilon\in C^0(\mathbb{R}^+,H^1(\mathbb{R}^2,\mathcal{H}))\cap C^0(\mathbb{R}^+,L^2(\mathbb{R}^2,H^2((0,1),\mathbb{C}^2))\cap C^1(\mathbb{R}^+,L^2(\mathbb{R}^2,\mathcal{H}))$$

and satisfies

$$i\varepsilon\partial_t\Psi_p^\varepsilon=-\frac{\varepsilon^2}{2}\Delta_\mathbf{x}\Psi_p^\varepsilon+\epsilon_p^\varepsilon\Psi_p^\varepsilon+R_p^\varepsilon+\varepsilon\Pi_p^\varepsilon\Omega_\varepsilon^W(t,\mathbf{x},z,i\nabla_\varepsilon).\vec{\sigma}(\Psi^\varepsilon)\tag{1.3.24}$$

with

$$R_p^\varepsilon=i\varepsilon(\partial_t\Pi_p^\varepsilon)\Psi^\varepsilon+\frac{\varepsilon^2}{2}\nabla_\mathbf{x}\Pi_p^\varepsilon\cdot\nabla_\mathbf{x}\Psi^\varepsilon+\frac{\varepsilon^2}{2}\mathrm{div}_\mathbf{x}((\nabla_\mathbf{x}\Pi_p^\varepsilon)\Psi^\varepsilon).$$

In addition, for any $T>0$

$$\lim_{N\to+\infty}\sup_{\varepsilon\in(0,1]}\sup_{t\in[0,T]}\left\|\sum_{p\geq N}\Psi_p^\varepsilon(t,.)\right\|_{L^2(\mathbb{R}^2,\mathcal{H})}=0.\tag{1.3.25}$$

We refer also to [1] for the proof of this lemma. We deduce that, for every $p, q \in \mathbb{N}$, $W^\varepsilon_{p,q}$ satisfies

$$\begin{aligned}
\partial_t W^\varepsilon_{p,q} &= W^\varepsilon(\partial_t \Psi^\varepsilon_p, \Psi^\varepsilon_q) + W^\varepsilon(\Psi^\varepsilon_p, \partial_t \Psi^\varepsilon_q) \\
&= \frac{i\varepsilon}{2}\left(W^\varepsilon(\Delta_{\mathbf{x}}\Psi^\varepsilon_p, \Psi^\varepsilon_q) - W^\varepsilon(\Psi^\varepsilon_p, \Delta_{\mathbf{x}}\Psi^\varepsilon_q)\right) - \frac{i}{\varepsilon}\left(W^\varepsilon(\epsilon^\varepsilon_p \Psi^\varepsilon_p, \Psi^\varepsilon_q) - W^\varepsilon(\Psi^\varepsilon_p, \epsilon^\varepsilon_q \Psi^\varepsilon_q)\right) \\
&+ W^\varepsilon((\partial_t \Pi^\varepsilon_p)\Psi^\varepsilon, \Psi^\varepsilon_q) + W^\varepsilon(\Psi^\varepsilon_p, (\partial_t \Pi^\varepsilon_q)\Psi^\varepsilon) - \frac{i\varepsilon}{2}\left(W^\varepsilon([\Delta_{\mathbf{x}}, \Pi^\varepsilon_p]\Psi^\varepsilon, \Psi^\varepsilon_q) - W^\varepsilon(\Psi^\varepsilon_q, [\Delta_{\mathbf{x}}, \Pi^\varepsilon_q]\Psi^\varepsilon)\right) \\
&- iW^\varepsilon(\Pi^\varepsilon_p \Omega^W_\varepsilon(t, \mathbf{x}, z, i\nabla_\varepsilon).\vec{\sigma}(\Psi^\varepsilon), \Psi^\varepsilon_q) + iW^\varepsilon(\Psi^\varepsilon_p, \Pi^\varepsilon_q \Omega^W_\varepsilon(t, \mathbf{x}, z, i\nabla_\varepsilon).\vec{\sigma}(\Psi^\varepsilon)). \qquad (1.3.26)
\end{aligned}$$

Multiplying this equation by ε and getting formally ε goes to zero, one gets

$$(\epsilon_p - \epsilon_q) W^0_{p,q} = 0.$$

Since $\epsilon_p \neq \epsilon_q$ if $p \neq q$, one deduces that $W^0_{p,q} = 0$, or $\Pi_p W^0 \Pi_q = 0$ for $p \neq q$. This result can be checked rigorously in the distribution sense. That is to wit,

$$W^\varepsilon_{p,q} \rightharpoonup 0 \quad \text{if } p \neq q \quad \text{in } \mathcal{D}'(\mathbb{R}^+_t \times \mathbb{R}^4_{\mathbf{x},\xi_{\mathbf{x}}}, \mathcal{H}\overline{\otimes}\mathcal{H}).$$

See [1] for details. Remark that we have, by construction of $\mathcal{H}\overline{\otimes}\mathcal{H}$,

$$W^0 = \sum_{p,q} \Pi_p W^0 \Pi_q$$

and thus

$$W^0 = \sum_{p \in \mathbb{N}^*} \Pi_p W^0 \Pi_p := \sum_{p \in \mathbb{N}^*} \Pi_p W^0 \Pi_p.$$

Let us now calculate the equation verified by $W^0_{p,p}$. For abuse of notations, we shall use W^0_p instead of $W^0_{p,p}$. For this we will perform the limit of (1.3.26) for $p = q$ and for a given $T > 0$. Applying Lemma 1.3.10 and with the boundedness of ϵ^ε_p, Π^ε_p and all its derivatives with respect to t and $\mathbf{x}$, one can pass to the limit on all the terms of the right hand side of (1.3.26) in $L^\infty((0,T), \mathcal{A}')$ weak $\star$, to find

$$\Pi_p\left(\partial_t W^0_p + \xi_{\mathbf{x}} \cdot \nabla_{\mathbf{x}} W^0_p - \nabla_{\mathbf{x}} \epsilon_p \cdot \nabla_{\xi_{\mathbf{x}}} W^0_p\right)\Pi_p = i\Pi_p[W^0_p, \vec{\Omega}(t, \mathbf{x}, z, \xi_{\mathbf{x}})]\Pi_p. \quad (1.3.27)$$

See [1] for more details on the obtention of the left hand side of this equation. Let us just explain the ideas for the obtention of the right hand side. View Assumption 1.3.3, the properties of Π^ε_p (Lemma 1.3.11) and Lemma 1.3.10, one can write

$$W^\varepsilon(\Pi^\varepsilon_p \Omega^W_\varepsilon(t, \mathbf{x}, z, i\nabla_\varepsilon) \cdot \vec{\sigma}(\Psi^\varepsilon), \Psi^\varepsilon_p) = \Pi^\varepsilon_p \Omega^W_\varepsilon(t, \mathbf{x}, z, \xi_{\mathbf{x}}) \cdot \vec{\sigma} W^\varepsilon(\Psi^\varepsilon, \Psi^\varepsilon)\Pi^\varepsilon_p + r^\varepsilon$$

where the both sides are bounded in $L^\infty((0,T), \mathcal{A}')$ and r^ε tends to 0 uniformly on $[0,T]$ in $\mathcal{A}'$ weak $\star$. Passing to the limit, we have

$$W^\varepsilon(\Pi^\varepsilon_p \Omega^W_\varepsilon(t, \mathbf{x}, z, i\nabla_\varepsilon) \cdot \vec{\sigma}(\Psi^\varepsilon), \Psi^\varepsilon_p) \rightharpoonup \Pi_p \vec{\Omega}(t, \mathbf{x}, z, \xi_{\mathbf{x}}) \cdot \vec{\sigma} W^0 \Pi_p = \Pi_p \vec{\Omega}(t, \mathbf{x}, z, \xi_{\mathbf{x}}) \cdot \vec{\sigma} W^0_p \Pi_p$$

since $W^0 = \sum_{q\in\mathbb{N}^*} W^0_q = \sum_{q\in\mathbb{N}^*} \Pi_q W^0 \Pi_q$. Using the same arguments, we have also

$$W^\varepsilon(\Psi^\varepsilon_p, \Pi^\varepsilon_p \Omega^W_\varepsilon(t,\mathbf{x},z,i\nabla_\varepsilon)\cdot\vec{\sigma}(\Psi^\varepsilon)) \rightharpoonup \Pi_p W^0_p \vec{\Omega}(t,\mathbf{x},z,\xi_\mathbf{x})\cdot\vec{\sigma}\Pi_p.$$

We deduce then, by passing to the limit in (1.3.26) for $p = q$, that W^0_p satisfies (1.3.27) in the sense of distributions $\mathcal{S}'((0,T)\times\mathbb{R}^4, \mathcal{H}\overline{\otimes}\mathcal{H})$ and that $\partial_t W^\varepsilon_p$ is bounded in $L^\infty((0,T), \mathcal{S}'(\mathbb{R}^4, \mathcal{H}\overline{\otimes}\mathcal{H}))$. Thus, W^ε_p is equicontinuous in t with values in $\mathcal{S}'$ and converges locally uniformly with respect to t. One deduces that $W^0_p \in C^0(\mathbb{R}^+, \mathcal{M}_b(\mathbb{R}^4, \mathcal{H}\overline{\otimes}\mathcal{H}))$ and for the continuity of W^0 stated in (1.3.9), it suffices to remark that (1.3.25) and (1.3.16) imply the uniform convergence of the series

$$\sum_{p\in\mathbb{N}^*} W^\varepsilon_p \in C^0([0,T], \mathcal{A}').$$

Finally, since $W^0_p = \Pi_p W^0_p \Pi_p$ then,

$$W^0_p(t,\mathbf{x},\xi_\mathbf{x},z,z') = F_p(t,\mathbf{x},\xi_\mathbf{x})\chi_p(t,\mathbf{x},z)\chi_p(t,\mathbf{x},z')$$

with F_p is an $\mathcal{H}^+_2(\mathbb{C})$ matrix valued function and (1.3.27) yields the first equation of (1.3.10).

The third item of Theorem 1.3.7 is a direct consequence of Proposition 1.3.9, of (1.3.9) and the uniform convergence of the series. The ε-oscillatory property is assured by the energy estimate (1.3.6) and the compactness property (1.3.18) holds true by setting

$$\mathbb{P}^\varepsilon_n = \sum_{p\le n} \Pi^\varepsilon_p$$

and thanks to (1.3.25) and Lemma 1.3.11.

References

[1] N. Ben Abdallah and F. Méhats, *Semiclassical analysis of the Schrödinger equation with a partially confining potential*, J. Math. Pures Appl. (9), 84 (2005), pp. 580–614.

[2] J. A. Bittencourt, *Fundamentals of plasma physics*, Pergamon Press, Oxford, 1986.

[3] Y. A. Bychkov and E. I. Rashba, *Oscillatory effects and the magnetic susceptibility of carriers in inversion layers*, Journal of Physics C : Solid State Physics, 17 (1984), pp. 6039–6045.

[4] S. Datta and B. Das, *Electronic analog of the electro-optic modulator*, Applied Physics Letters, 56 (1990), pp. 665–667.

[5] G. Dresselhaus, *Spin-orbit coupling effects in zinc blende structures*, Phys. Rev., 100 (1955), pp. 580–586.

[6] C. Fermanian-Kammerer and P. Gérard, *Mesures semi-classiques et croisement de modes*, Séminaire Équations aux dérivées partielles (Polytechnique) (1999-2000), Art. No. 17, 13 p.

[7] ——, *Une formule de Landau-Zener pour un croisement non dégénéré et involutif de codimension 3*, C. R. Math. Acad. Sci. Paris, 335 (2002), pp. 915–920.

[8] ——, *A Landau-Zener formula for non-degenerated involutive codimension 3 crossings*, Ann. Henri Poincaré, 4 (2003), pp. 513–552.

[9] C. Fermanian-Kammerer and P. Gerard, *A Landau-Zener formula for two-scaled Wigner measures*, in Dispersive transport equations and multiscale models (Minneapolis, MN, 2000), vol. 136 of IMA Vol. Math. Appl., Springer, New York, 2004, pp. 167–177.

[10] C. Fermanian-Kammerer and P. Gérard, *Two-scale Wigner measures and the Landau-Zener formulas*, in Multiscale methods in quantum mechanics, Trends Math., Birkhäuser Boston, Boston, MA, 2004, pp. 59–68.

[11] A. Fert, A. Friederich, and al, *Giant magnetoresistance of (001)fe/(001)cr magnetic superlattices*, Phys. Rev. Lett., 61 (1988), pp. 2472–2475.

[12] P. Gérard, *Mesures semi-classiques et ondes de Bloch*, (1991), pp. Exp. No. XVI, 19.

[13] P. Gérard, P. A. Markowich, N. J. Mauser, and F. Poupaud, *Homogenization limits and Wigner transforms*, Comm. Pure Appl. Math., 50 (1997), pp. 323–379.

[14] T. Kato, *Perturbation theory for linear operators*, Springer-Verlag, Berlin, Heidelberg, 1966.

[15] P.-L. Lions and T. Paul, *Sur les mesures de Wigner*, Rev. Mat. Iberoamericana, 9 (1993), pp. 553–618.

[16] P. A. Markowich and N. J. Mauser, *The classical limit of a self-consistent quantum-Vlasov equation in* $3D$, Math. Models Methods Appl. Sci., 3 (1993), pp. 109–124.

[17] P. A. Markowich, N. J. Mauser, and F. Poupaud, *A Wigner-function approach to (semi)classical limits : electrons in a periodic potential*, J. Math. Phys., 35 (1994), pp. 1066–1094.

[18] P. A. Markowich, C. A. Ringhofer, and C. Schmeiser, *Semiconductor equations*, Springer-Verlag, Vienna, 1990.

[19] M. S. Mock, *Analysis of mathematical models of semiconductor devices*, vol. 3 of Advances in Numerical Computation Series, Boole Press, Dún Laoghaire, 1983.

[20] A. Pazy, *Semigroups of linear operators and applications to partial differential equations*, vol. 44 of Applied Mathematical Sciences, Springer-Verlag, New York, 1983.

[21] Y. P. Raizer, *Gas Discharge Physics*, Springer, Berlin, 1997.

[22] M. Reed and B. Simon, *Methods of modern mathematical physics.*, Academic Press, New York, second ed., 1975. Functional analysis.

[23] E. Wigner, *On the quantum correction for thermodynamic equilibrium*, Phys. Rev., 40 (1932), pp. 749–759.

[24] I. Zutic, J. Fabian, and S. D. Sarma, *Spintronics : Fundamentals and applications*, Reviews of Modern Physics, 76 (2004), p. 323.

Chapter 2

On an hierarchy of kinetic and macroscopic models for spintronics

Abstract

In this chapter an hierarchy of kinetic and macroscopic models for semiconductor spintronics is presented and analyzed. We begin by presenting and studying the so called "spinor" Boltzmann equation. Starting with a rescaled version of the Boltzmann equation with different spin-flip and non spin-flip collision operators, different continuum models are derived. By comparing the strength of the spin-orbit scattering with the scaled mean free paths, we explain how some models existing in the literature (like the two-component models) can be obtained from the spinor Boltzmann equation. A new spin-vector drift diffusion model keeping spin relaxation and spin precession effects due to the spin-orbit coupling in semiconductor structures is derived and some of its mathematical properties are checked. Other spin-vector diffusif models like Spherical Harmonic Expansion (SHE) , Energy-Transport and Drift-Diffusion with Fermi-Dirac statistics models are derived by means of the moment method and entropy minimization principle.

2.1 Introduction

The electrons are not only characterized by their electric charge but also by their intrinsic kinetic moment or the so called "spin". The spintronics is a new booming domain of research which tries to control the spin and to use it as an additional degree of freedom or a new vector of information. Although the first researches in this domain were led essentially for structures based on magnetic multilayers [22], the spin dependent properties of the electron transport in semiconductors have recently attracted several attentions. There are typically two class of mechanisms [23] which make relax the spin vector in semiconductors. In one side, we have according to the Elliot-Yafet mechanism [49, 23] the instantaneous interactions of the particles with the crystal accompanied with reversal of the spin direction. They will be called the spin-flip interactions. These events are rare in semiconductors : typically less than one interaction up one thousand return the spin orientation [7]. The second category of mechanisms are relative to the effect on spin-orbit coupling of the asymmetry inversion that can exist in the system. They can be characterized by an effective magnetic field which makes precess the spin vector during the free path of the particles. The ability to control this effective magnetic field could allow spin control and manipulation in semiconductor heterostructures.

Many theoretical models are used by the physical community for spin-polarized transport [35, 36, 38, 41, 42, 44, 46, 47, 49]. In microelectronics the drift-diffusion system is one of the most used model for modelling the transport of charged particles in semiconductors [32, 33], Plasma [5], Gas Discharges [39], etc. The drift-diffusion model, which describes the macroscopic behavior of the particles, is a very well suited model for numerical simulations. Two types of drift-diffusion approximations are essentially used in spintronics : the so called two-component drift-diffusion model and the spin polarization vector or density matrix based approximation. In the two-component description, the electrons are considered to be of two types, namely, having spin up or down. Each type of electrons is described by the usual drift-diffusion equation with additional terms related to sources and relaxation of the electron spin polarization, see [46, 47, 36]. The two-component model has been used initially for spin transport in ferromagnetic metals, it was used also in studies of propagation of spin-polarized electrons through a semiconductor region with variable level of doping [36]. In this kind of model, the mechanism of spin relaxation (such the spin-orbit interaction for instance) is not specified. The spin-vector (or density matrix) approach is a more general description in which the spin variable (the density or the distribution function for example) is a vector quantity and the mechanisms acting on the spin dynamics can be taken into account.

The aim of this chapter is to derive and analyse macroscopic models for semi-

conductor spintronics from the general spinor Boltzmann equation. The starting equation is the following scaled Boltzmann equation

$$\frac{\partial F^\varepsilon}{\partial t}+\frac{1}{\varepsilon}(v\cdot\nabla_x F^\varepsilon-\nabla_x V\cdot\nabla_v F^\varepsilon)=\frac{1}{\varepsilon^2}Q(F^\varepsilon)+\frac{\alpha}{\varepsilon}\left[\frac{i}{2}\vec{\Omega}(x,v)\cdot\vec{\sigma},F^\varepsilon\right]+Q_{sf}(F^\varepsilon), \quad (2.1.1)$$

under the initial condition

$$F^\varepsilon(0,x,v)=F_{in}(x,v), \quad (2.1.2)$$

where $\varepsilon>0$ is a small positive parameter. It represents the scaled mean free paths. The parameter α is the scaled strength of the spin-orbit scattering. The operator Q is the collision operator and Q_{sf} represents the spin-flip interactions (or interactions accompanied with reversal of spin's direction). We use the following relaxation time approximation of Q_{sf}

$$Q_{sf}(F)=\frac{tr(F)I_2-2F}{\tau_{sf}}, \quad (2.1.3)$$

with $\tau_{sf}>0$ is the spin relaxation time. This operator makes relax, when τ_{sf} goes to zero, the matrix distribution function to a scalar one. Since the spin-flip interactions are not frequent in semiconductor structures as we mentioned above, τ_{sf} is not small and we assume that Q_{sf} is a perturbation part of the collision operator. This is natural then to consider Q_{sf} of order one in the diffusion scaling (2.1.1). The diffusion limit $\varepsilon\to 0$ leads to macroscopic diffusion models (Drift-Diffusion, SHE, etc...) according to the dominant scattering mechanisms. We refer to [1, 2, 12, 14, 19, 27, 37, 25, 43] for the rigorous derivation of macroscopic models from kinetic equations. Different kind of scattering operators are considered in this work. We consider first the collision operator for a Boltzmann statistics in the linear BGK approximation given by :

$$Q(F)=\int_{\mathbb{R}^3}\alpha(v,v')[\mathcal{M}(v)F(v')-\mathcal{M}(v')F(v)]dv'. \quad (2.1.4)$$

The function $\mathcal{M}$ is the normalized Maxwellian

$$\mathcal{M}(v)=\frac{1}{(2\pi)^{\frac{3}{2}}}e^{-\frac{1}{2}|v|^2}, \quad \forall v\in\mathbb{R}^3. \quad (2.1.5)$$

The chapter is organized a follows. In the next section, we fix some notations used along this chapter. The study of the Boltzmann equation is carried out in Section 2.3. Existence and uniqueness of weak solutions of (2.1.1) is presented. It is a standard result of Boltzmann type equations. In the spinor Boltzmann description, the distribution function shall be a matrix valued function from $\mathbb{R}^+\times\mathbb{R}^6$ into the space of 2×2 hermitian and positive matrices ($\mathcal{H}_2^+(\mathbb{C})$). We prove that equation

(2.1.1) preserves the positivity and the self adjointness of the distribution function during the time. In other terms, the following maximum principle holds :

if $F_{in}(x,v) \in \mathcal{H}_2^+(\mathbb{C}), \forall (x,v) \in \mathbb{R}^6$ then, $F^\varepsilon(t,x,v) \in \mathcal{H}_2^+(\mathbb{C}), \forall t > 0$ and $(x,v) \in \mathbb{R}^6$.

This means that if F^ε satisfies (2.1.1), then $(F^\varepsilon)^*$ is also a solution of (2.1.1). Moreover, if $F_{in} \in \mathcal{H}_2^+(\mathbb{C})$ and if we decompose F^ε into spin-dependent and spin-independent parts as

$$F^\varepsilon(t,x,v) = \frac{1}{2} f_c^\varepsilon(t,x,v) I_2 + \vec{f_s^\varepsilon}(t,x,v) \cdot \vec{\sigma}$$

where f_c^ε is the charge distribution and $\vec{f_s^\varepsilon}$ is the spin distribution then, we have $\frac{1}{2} f_c^\varepsilon(t,x,v) \geq |\vec{f_s}|(t,x,v)$ for every $(t,x,v) \in \mathbb{R} \times \mathbb{R}^6$.

In the following sections we study the diffusion limit $\varepsilon \to 0$ for different order of α with respect to ε. Section 2.4 is dedicated to the derivation of two-component models from the spinor Boltzmann equation. We begin by discussing what we call the decoherence limit. This limit corresponds to keeping ε constant and to taking α goes to $+\infty$. It corresponds to taking a large spin-orbit coupling so that the ratio between the period of rotations (T) induced by the spin-orbit effect and the used time scale ($\bar{t}$) is small and goes to zero. This limit makes relax the spin part of the distribution function to the direction parallel to $\vec{\Omega}$. If the direction of $\vec{\Omega}$ does not depend on v, a two-component kinetic model is obtained which yields two-component macroscopic model at the diffusion limit. In the next subsection, we study the diffusion limit of (2.1.1) with $\boldsymbol{\alpha = \mathcal{O}(\frac{1}{\varepsilon})}$. This situation occurs in structures where the spin-orbit coupling is high such that the rotational period T is of the same order of the mean free path time τ and where $\frac{T}{\bar{t}} = \varepsilon$. Similarly, if the direction of $\vec{\Omega}$ does not depend on v, the spin vector direction tends towards $\vec{\Omega}$ and one gets at the limit a two component drift-diffusion model. However, if the direction of $\vec{\Omega}$ depends on v, the spin information is lost at the limit. In other words, the spin vector relaxes towards zero and we obtain the standard scalar drift-diffusion model for the charge density (or the total density) used in microelectronics. This spin relaxation corresponds to the D'yakonov-Perel mechanism. It happens since the effective field changes frequently direction due to the numerous interactions that a particle undergo on its trajectory in the diffusion regime under investigation.

In Section 2.5, we are interested by the derivation of general spin-vector drift-diffusion model with spin rotation and relaxation effects. Suppose first that α is of the same order as ε ($\boldsymbol{\alpha = \mathcal{O}(\varepsilon)}$) and take $\alpha = \varepsilon$ for simplicity. This means that the order of the spin-orbit coupling is small in such a way that the rotation angle of the spin vector around the effective field $\vec{\Omega}$ is small during the free paths of the

particles. In this case, F^ε converges to $N(t,x)\mathcal{M}(v)$ (in the weak sense see Section 2.5) such that N is a positive hermitian matrix satisfying the following equation

$$\partial_t N + \mathrm{div}_x(\mathbb{D}(\nabla_x N + \nabla_x V N)) = \frac{i}{2}[\vec{H}_e \cdot \vec{\sigma}, N] + \frac{tr(N)I_2 - N}{\tau_{sf}},$$

where $\mathbb{D}$ is a positive definite matrix and the effective field is an $\mathcal{M}$-weighted averaging of $\vec{\Omega}$ with respect to v :

$$\vec{H}_e(x) = \int_{\mathbb{R}^3} \vec{\Omega}(x,v)\mathcal{M}(v)dv.$$

Remark that if $\vec{\Omega}$ is an odd vector with respect to v then $\vec{H}_e = 0$ and no rotation effect appears at the limit. This is generally the case of the spin-orbit effective fields in semiconductor heterostructures (Rashba or Dresselhauss vectors). To keep trace of the spin-orbit interactions at the diffusion limit when $\vec{\Omega}$ is an odd vector, one has to take a time scale such that $\boldsymbol{\alpha = \mathcal{O}(1)}$ with respect to ε. Applying this idea, a general spin-vector drift-diffusion model will be rigourously derived (Theorem 2.5.2) and one of its main property to wit the conservation of the positivity and the self-adjointness of the density matrix during the time (maximum principle) will be checked (see Theorem 2.5.3).

Following the same strategy, other two-component or spin-vector fluid models can be derived. Section 2.6 is dedicated to the derivation of spin-vector SHE (Spherical Harmonic Expansion) model when taking dominant elastic collisions. Finally, in Section 2.7 we discuss the derivation of Energy-Transport and Drift-Diffusion with Fermi-Dirac statistics models using the moment method and entropy minimization principle. We note that the method used is inspired from the works of P. Degond and C. Ringhofer [17, 18] for derivation of quantum hydrodynamic models. Other works on derivation and numerical study of quantum fluid models exist [15, 16, 13, 24].

2.2 Assumptions and notations

Let us begin by introducing some assumptions and notations.

Assumption 2.2.1. *The cross-section, $\alpha(.,.)$, of the collision operator* (2.1.4) *belongs to $W^{1,\infty}(\mathbb{R}^6)$ and is assumed to be symmetric and bounded from above and below :*

$$\exists \alpha_1, \alpha_2 > 0, \quad 0 < \alpha_1 \leq \alpha(v,v') \leq \alpha_2, \quad \forall v, v' \in \mathbb{R}^3.$$

Assumption 2.2.2. *For any fixed $T > 0$, the potential $(t,x) \mapsto V(t,x)$ is a non negative real function belonging to $C^1([0,T], W^{1,\infty}(\mathbb{R}^3))$.*

We will use $\mathcal{M}_2(\mathbb{C})$ to denote the space of 2×2 complex matrices ; $\mathcal{H}_2(\mathbb{C})$ denotes the subspace of hermitian matrices and $\mathcal{H}_2^+(\mathbb{C})$ the subspace of hermitian positive matrices. We will denote by $\|.\|_2$ and $\langle .,.\rangle_2$ the Frobenuis norm and the associated Frobenuis inner product

$$\langle A,B\rangle_2 = \Re(A:\overline{B}) = \Re(\sum_{i,j=1}^{2} A_{ij}\overline{B}_{ij}), \quad \|A\|_2^2 = \langle A,A\rangle_2 = \sum_{i,j=1}^{2} |A_{ij}|^2$$

where for $z\in\mathbb{C}$, $\Re(z)$ is the real part of z and for any two complex matrices $A,B\in\mathcal{M}_2(\mathbb{C})$

$$A:B=\sum_{i,j} A_{ij}B_{ij}.$$

Definition 2.2.3. *We define the space $\mathbb{L}^2_{\mathcal{M}}$ by*

$$\mathbb{L}^2_{\mathcal{M}} = \{F=F(x,v)\in\mathcal{H}_2(\mathbb{C}) \text{ such that } \int_{\mathbb{R}^6}\frac{\|F(x,v)\|_2^2}{\mathcal{M}}dxdv<+\infty\}. \qquad (2.2.1)$$

This is an Hilbert space equipped with the following scalar product

$$\langle F,G\rangle_{\mathcal{M}} = \int_{\mathbb{R}^6}\frac{\langle F,G\rangle_2}{\mathcal{M}}dxdv,$$

and $\|.\|_{\mathcal{M}}$ will denote the norm associated to $\langle .,.\rangle_{\mathcal{M}}$. The same space with scalar valued functions will be denoted by $L^2_{\mathcal{M}}$ instead of $\mathbb{L}^2_{\mathcal{M}}$.

2.3 Study of spinor Boltzmann type models

The aim of this section is to study the properties of the spinor Boltzmann equation with the spin-orbit term. Existence and uniqueness of weak solution of (2.1.1) will be shown and some a priori estimates on the solution independent of the parameters α and ε will be given (Theorem 2.3.2). The contents of this first part review some well known results on linear Boltzmann type equations. We begin by defining the notion of weak solution of (2.1.1).

Definition 2.3.1 (weak solution)**.** *For a fixed time $T>0$, a function $F^\varepsilon\in L^2([0,T];\mathbb{L}^2_{\mathcal{M}})$ is called weak solution of* (2.1.1) *if it satisfies :*

$$\begin{aligned}-\int_0^T\int_{\mathbb{R}^6}\langle F^\varepsilon,\partial_t\psi\rangle_2 dtdxdv - \frac{1}{\varepsilon}\int_0^T\int_{\mathbb{R}^6}\langle F^\varepsilon, v\cdot\nabla_x\psi-\nabla_x V\cdot\nabla_v\psi\rangle_2 dtdxdv = \\ \frac{1}{\varepsilon^2}\int_0^T\int_{\mathbb{R}^6}\langle Q(F^\varepsilon),\psi\rangle_2 dtdxdv + \frac{\alpha}{\varepsilon}\int_0^T\int_{\mathbb{R}^6}\langle\frac{i}{2}[\vec{\Omega}(x,v)\cdot\vec{\sigma},F^\varepsilon],\psi\rangle_2 dtdxdv \\ +\int_0^T\int_{\mathbb{R}^6}\langle Q_{sf}(F^\varepsilon),\psi\rangle_2 dtdxdv + \int_{\mathbb{R}^6}\langle F_{in},\psi(0)\rangle_2 dxdv, \quad (2.3.1)\end{aligned}$$

for all $\psi \in C_c^1([0,T)\times\mathbb{R}^6;\mathcal{H}_2(\mathbb{C}))$.

Theorem 2.3.2. *For all fixed* $\varepsilon>0$, $\alpha>0$, $T\geq 0$, $F_{in}\in\mathbb{L}^2_{\mathcal{M}}$ *and under Assumptions 2.2.1, 2.2.2, the model* (2.1.1)-(2.1.2) *admits a unique weak solution* $F^\varepsilon\in C^0([0,T];\mathbb{L}^2_{\mathcal{M}})$ *satisfying*

$$\|F^\varepsilon(t)\|_{\mathbb{L}^2_{\mathcal{M}}}\leq C,\quad \|N^\varepsilon\|_{L^2_{t,x}([0,T]\times\mathbb{R}^3)}\leq C\quad \forall t>0, \tag{2.3.2}$$

$$\|F^\varepsilon-\mathcal{P}(F^\varepsilon)\|^2_{L^2_t(\mathbb{L}^2_M)}\leq C\varepsilon^2, \tag{2.3.3}$$

where $C>0$ *is a general constant independent of* α *and* ε. *Here,* $\mathcal{P}$ *is the orthogonal projection on* $Ker(Q)$ *which satisfies :* $\mathcal{P}(F^\varepsilon)=N^\varepsilon\mathcal{M}$ *with* $N^\varepsilon:=\int_{\mathbb{R}^3}F^\varepsilon dv$. *In addition the following maximum principle holds : if* $F_{in}(x,v)\in\mathcal{H}_2^+(\mathbb{C}),\forall(x,v)\in\mathbb{R}^6$ *then* $F(t,x,v)\in\mathcal{H}_2^+(\mathbb{C})\ \forall t\in[0,T],\ (x,v)\in\mathbb{R}^6$.

The next proposition summarizes some fundamental properties of the collision operator (2.1.4). Since it acts only on the speed variable v, t and x are considered as a parameters and are omitted in the next proposition for the sake of simplicity.

Proposition 2.3.3 (**Properties of the collision operator** (2.1.4))**.** *Under Assumption 2.2.1, the collision operator given by* (2.1.4) *satisfies the following properties.*

(i) For all $F\in\mathbb{L}^2_{\mathcal{M}}$, *we have the mass conservation :*

$$\int_{\mathbb{R}^3}Q(F)(v)dv=0.$$

(ii) The mapping $Q:\mathbb{L}^2_{\mathcal{M}}\to\mathbb{L}^2_{\mathcal{M}}$ *is a linear, continuous, selfadjoint and nonpositive operator.*

(iii) The kernel of Q *is*

$$Ker(Q)=\{F\in\mathbb{L}^2_{\mathcal{M}},\ \text{such that } \exists N\in\mathcal{H}_2(\mathbb{C}),F(v)=N\mathcal{M}(v)\}.$$

(iv) Let $\mathcal{P}$ *be the orthogonal projection on* $KerQ$, *then we have the following coercivity inequality*

$$-\langle Q(F),F\rangle_{\mathcal{M}}\geq\alpha_1\|F-\mathcal{P}(F)\|^2_{\mathcal{M}}. \tag{2.3.4}$$

(v) The range of Q, $\mathcal{R}(Q)$, *is a closed subset of* $\mathbb{L}^2_{\mathcal{M}}$ *such that*

$$\mathcal{R}(Q)=Ker(Q)^\perp=\left\{F\in\mathbb{L}^2_{\mathcal{M}},\ \text{such that }\int_{\mathbb{R}^3}F(v)dv=\begin{pmatrix}0&0\\0&0\end{pmatrix}\right\}.$$

Proof. The first point (i) is a direct consequence of Assumption 2.2.1. The linearity of Q is obvious. Let $F, G \in \mathbb{L}^2_{\mathcal{M}}$, we have

$$\langle Q(F), G\rangle_{\mathcal{M}} = \Re\left(\int_{\mathbb{R}^3} \alpha(v,v')\mathcal{M}(v')\mathcal{M}(v)\left[\frac{F(v')}{\mathcal{M}(v')} - \frac{F(v)}{\mathcal{M}(v)}\right] : \overline{\frac{G(v)}{\mathcal{M}(v)}} dvdv'\right). \tag{2.3.5}$$

Using the symmetry of the cross-section α, one can write

$$\langle Q(F), G\rangle_{\mathcal{M}} = -\frac{1}{2}\Re\left(\int_{\mathbb{R}^3} \alpha(v,v')\mathcal{M}(v')\mathcal{M}(v)\left[\frac{F(v')}{\mathcal{M}(v')} - \frac{F(v)}{\mathcal{M}(v)}\right] : \overline{\left[\frac{G(v')}{\mathcal{M}(v')} - \frac{G(v)}{\mathcal{M}(v)}\right]} dvdv'\right). \tag{2.3.6}$$

This implies that Q is selfadjoint and negative operator on $\mathbb{L}^2_{\mathcal{M}}$. By Assumption 2.2.1 and the fact that $\int_{\mathbb{R}^3} \|F(v)\|_2 dv \leq \|F\|_{\mathcal{M}}$, (2.3.5) gives

$$|\langle Q(F), G\rangle_{\mathcal{M}}| \leq C\|F\|_{\mathcal{M}}\|G\|_{\mathcal{M}},$$

which yields the continuity of Q. The third point is obvious using the equality (2.3.6). Namely, the following equivalences hold :

$$(F \in KerQ) \Leftrightarrow (\langle Q(F), F\rangle_{\mathcal{M}} = 0) \Leftrightarrow (\exists N \in \mathcal{H}_2(\mathbb{C}),\ F(v) = NM(v)).$$

The orthogonal of $KerQ$ is then given by the set :

$$(KerQ)^{\perp} = \left\{ F \in \mathbb{L}^2_{\mathcal{M}},\ \text{such that}\ \int_{\mathbb{R}^3} F(v)dv = \begin{pmatrix} 0 & 0 \\ 0 & 0 \end{pmatrix} \right\}. \tag{2.3.7}$$

Let now $F \in \mathbb{L}^2_{\mathcal{M}}$ and let $G = F - \mathcal{P}F$ where $\mathcal{P}F$ is the orthogonal projection of F on $KerQ$. Then, using the self-adjointness of Q, we have

$$\langle Q(F), F\rangle_{\mathcal{M}} = \langle Q(G), G\rangle_{\mathcal{M}}.$$

Since $G \in (KerQ)^{\perp}$ and with Assumption 2.2.1 we get

$$\begin{aligned} -\langle Q(F), F\rangle_{\mathcal{M}} &= \frac{1}{2}\int \alpha(v,v')\mathcal{M}'\mathcal{M}\|\frac{G'}{\mathcal{M}'} - \frac{G}{\mathcal{M}}\|_2^2 dvdv' \\ &\geq \alpha_1 \int_{\mathbb{R}^3} \frac{\|G\|_2^2}{\mathcal{M}} dv = \alpha_1 \|F - \mathcal{P}F\|^2_{\mathcal{M}}. \end{aligned}$$

For the last point, since Q is selfadjoint we have $\overline{\mathcal{R}(Q)} = (KerQ)^{\perp}$. It remains to show that $\mathcal{R}(Q)$ is closed. Indeed, let $(H_p)_{p\geq 1} \in \mathcal{R}(Q)$ be a sequence converging to $H \in \mathbb{L}^2_{\mathcal{M}}$ with respect to $\|.\|_{\mathcal{M}}$. Writing $H_p = Q(F_p) = Q(G_p)$, where $G_p = F_p - \mathcal{P}F_p$, we have

$$\alpha_1\|G_p - G_q\|^2_{\mathcal{M}} \leq \langle Q(G_p) - Q(G_q), G_p - G_q\rangle_{\mathcal{M}} \leq \|H_p - H_q\|_{\mathcal{M}}\|G_p - G_q\|_{\mathcal{M}}.$$

Therefore, $(G_p)_p$ is a cauchy sequence in $\mathbb{L}^2_{\mathcal{M}}$. There exists $G \in \mathbb{L}^2_{\mathcal{M}}$ such that $(G_p)_p$ converges to G. By the continuity of Q and the uniqueness of the limit, we deduce that $H = Q(G)$.

■

Proof of Theorem 2.3.2. This is a standard result of the Boltzmann type equations using a fixed point theorem and the characteristics method. Let us recall the main ideas of the proof. For notational simplicity, we omit the presence of α and ε (supposing $\alpha = \varepsilon = 1$). We decompose the collision operator as, $Q = Q^+ + Q^-$ when $Q^+(F) = \left(\int_{\mathbb{R}^3} \alpha(v,v')F(v')dv'\right)\mathcal{M}(v)$ and $Q^-(F) = -\nu(v)F$ with $\nu(v) = \int_{\mathbb{R}^3} \alpha(v,v')\mathcal{M}(v')dv'$.

Lemma 2.3.4. *Let $\mathcal{L} = \partial_t + v\cdot\nabla_x - \nabla_x V\cdot\nabla_v$, then for any $F_{in} \in \mathbb{L}^2_{\mathcal{M}}$ and $S \in C^0([0,T];\mathbb{L}^2_{\mathcal{M}})$, the problem*

$$\begin{cases} \mathcal{L}(F) - Q^-(F) - \dfrac{i}{2}[\vec{\Omega}\cdot\vec{\sigma}, F] - Q_{sf}(F) = S \\ F(t=0) = F_{in} \end{cases} \tag{2.3.8}$$

admits a unique weak solution satisfying the following estimate

$$\|F(t)\|_{\mathbb{L}^2_{\mathcal{M}_V}} \leq \|F_{in}\|_{\mathbb{L}^2_{\mathcal{M}_V}} + \int_0^t \|S(s)\|_{\mathbb{L}^2_{\mathcal{M}_V}} ds \tag{2.3.9}$$

with $\mathcal{M}_V = \dfrac{1}{(2\pi)^{\frac{3}{2}}} e^{-\frac{1}{2}|v|^2+V}$. In addition, the maximum principle holds which means that if F_{in}, S are two hermitian positive matrices functions then the solution of (2.3.8), F, is also in $\mathcal{H}_2^+(\mathbb{C})$, $\forall (t,x,v) \in [0,T]\times\mathbb{R}^6$.

Proof. Using the decomposition of any matrix $A \in \mathcal{H}_2(\mathbb{C})$ into spin-dependent and spin-independent parts as $A = A_c I_2 + \vec{A}_s\cdot\vec{\sigma}$, $H_2(\mathbb{C})$ is equivalent to $\mathbb{R}^4$ (we use the identification $A \equiv (A_c, \vec{A}_s)$ for any $A \in \mathcal{H}_2(\mathbb{C})$). Any function $F \in \mathbb{L}^2_{\mathcal{M}}$ is seen as a function in $(L^2_{\mathcal{M}})^4$. Let $F_{in} \equiv (F_c^{in}, \vec{F}_s^{in})$ and $S \equiv (S_c, \vec{S}_s)$, then problem (2.3.8) is equivalent to finding $F \equiv (F_c, \vec{f}_s)$ in $C^0([0,T],(L^2_{\mathcal{M}})^4)$ such that

$$\begin{cases} \mathcal{L}(F) + \mathcal{C}(v)(F) + \mathcal{A}(x,v)(F) = S \\ F(t=0) = F_{in}. \end{cases} \tag{2.3.10}$$

The function $\mathcal{C}(v)$ is the matrix associated to the $-(Q^- + Q_{sf})$ operator given by

$$\mathcal{C}(v) = \begin{pmatrix} \nu(v) & 0 \\ 0 & (\nu(v) + \frac{1}{\tau_{sf}})I_3 \end{pmatrix},$$

I_3 denotes the identity matrix of order three. For all $(x,v) \in \mathbb{R}^6$, $\mathcal{A}(x,v)$ is an antisymmetric 4×4 matrix associated to the spin-orbit anti-joint operator $(\frac{i}{2}[\vec{\Omega}\cdot\vec{\sigma}, .])$.

It has the following form : $\mathcal{A}(x,v) = \begin{pmatrix} 0 & 0 \\ 0 & \mathcal{I}(x,v) \end{pmatrix}$ with 3×3 antisymmetric matrix function $\mathcal{I}(x,v)$. Assuming first that F_{in} and S are regulars, then, thanks to the characteristics method, the solution of (2.3.10) is given by the following integral formula

$$\begin{aligned} F(t,z) = \exp\left(-\int_0^t [\mathcal{C}(\mathcal{Z}(s;z,t)) + \mathcal{A}(\mathcal{Z}(s;z,t))]ds\right)\cdot F_{in} \\ + \int_0^t \exp\left(-\int_s^t [\mathcal{C}(\mathcal{Z}(\tau;z,t)) + \mathcal{A}(\mathcal{Z}(\tau;z,t))]d\tau\right)\cdot S(\mathcal{Z}(s;z,t))ds, \end{aligned} \tag{2.3.11}$$

where $z=(x,v)$ is the variable in the phase space. For any $z=(x,v)\in\mathbb{R}^6$, $t\in[0,T]$, the characteristics $\mathcal{Z}(s;z,t) := (\mathcal{X}(s;z,t),\mathcal{V}(s;z,t))$ satisfy the following differential system

$$\begin{cases} \dfrac{d\mathcal{X}}{ds} = \mathcal{V}(s), \\ \dfrac{d\mathcal{V}}{ds} = E(\mathcal{X}(s)), \qquad E=-\nabla_x V, \\ (\mathcal{X}(t;z,t),\mathcal{V}(t;z,t)) = (x,v). \end{cases}$$

In this case, F given by (2.3.11) is also the weak solution of (2.3.10). By scalar multiplying (2.3.8) by $\frac{F}{\mathcal{M}_V}$ and integrating with respect to t,x, and v (i.e. rigourously choosing it as a test function in the weak formulation), one can find estimate (2.3.9) since Q^- and Q_{sf} are two negative operators on $\mathcal{H}_2(\mathbb{C})$ and $\langle \frac{i}{2}[\vec{\Omega}\cdot\vec{\sigma},F],F\rangle_2 = 0$. Furthermore, using the integral formula (2.3.11), one can verify straightforwardly the maximum principle. If F_{in} and S belong to $\mathbb{L}^2_{\mathcal{M}}$ and $C^0([0,T],\mathbb{L}^2_{\mathcal{M}})$ respectively, these results remain correct and can be obtained by regularization technics. The proof of Lemma 2.3.4 is achieved.

■

To continue the proof of Theorem 2.3.2, we define

$$\begin{aligned} \chi : \mathbb{L}^2_{\mathcal{M}}\times C^0([0,T],\mathbb{L}^2_{\mathcal{M}}) &\longrightarrow C^0([0,T],\mathbb{L}^2_{\mathcal{M}}) \\ (F_{in},S) &\longrightarrow \chi(F_{in},S)=F, \end{aligned}$$

where $\chi(F_{in},S):=F$ is the unique weak solution of (2.3.8) with initial condition F_{in} and source term S. The mapping χ is linear, continuous (in view of estimate (2.3.9)) and satisfies the maximum principle. Moreover, a function F satisfies (2.1.1)-(2.1.2) if and only if $F=\chi(F_{in},Q^+(F))$ which is equivalent to say that F is a fixed point of $\Theta : F\in C^0([0,T],\mathbb{L}^2_{\mathcal{M}}) \mapsto \chi(F_{in},Q^+(F)) \in C^0([0,T],\mathbb{L}^2_{\mathcal{M}})$. To show that Θ admits a unique fixed point, let us define, for every $\delta\geqslant 0$, the norm $\|.\|_\delta$ on $C^0([0,T],\mathbb{L}^2_{\mathcal{M}})$ by

$\|F\|_\delta = \sup_{t\in[0,T]} \left(e^{-\delta t}\|F\|_{\mathbb{L}^2_{\mathcal{M}}}\right)$. All these norms are equivalent to the usual one $\|.\|_0$ (for $\delta = 0$), and one can choose δ small enough so that Θ forms a contracted mapping on $(C^0([0,T],\mathbb{L}^2_{\mathcal{M}}),\|.\|_\delta)$. As a conclusion, problem (2.1.1)-(2.1.2) admits a unique weak solution satisfying the maximum principle (since $Q^+(F)$ conserves the positivity of F and by Lemma 2.3.4) and we have

$$\|F(t)\|_{\mathbb{L}^2_{\mathcal{M}_V}} \leq \|F_{in}\|_{\mathbb{L}^2_{\mathcal{M}_V}} + \int_0^T \int_{\mathbb{R}^6} \langle Q(F), \frac{F}{\mathcal{M}_V}\rangle_2 dsdxdv \qquad \forall t \in [0,T].$$

Furthermore, taking into account the parameters α and ε, the weak solution, F^ε, of (2.1.1)-(2.1.2) satisfies

$$\|F(t)\|_{\mathbb{L}^2_{\mathcal{M}_V}} \leq \|F_{in}\|_{\mathbb{L}^2_{\mathcal{M}_V}} + \frac{1}{\varepsilon^2}\int_0^T \int_{\mathbb{R}^6} \langle Q(F), \frac{F}{\mathcal{M}_V}\rangle_2 dsdxdv \qquad \forall t \in [0,T].$$

Finally, since $\int_{\mathbb{R}^3} \langle Q(F), \frac{F}{\mathcal{M}_V}\rangle_2 dv \leq 0$, one deduces estimates (2.3.2) and the balance deviation inequality (2.3.3) follows from the coercivity inequality (2.3.4).

2.4 Two-component models

This section is concerned with the derivation of two-component kinetic and macroscopic models from the general spinor kinetic equation.

2.4.1 Decoherence limit

We explain in this subsection how the spin-orbit interactions act on the distribution function when the order of this coupling becomes large. We assume that the period of rotation T of the spin vector distribution part around the effective field $\vec{\Omega}$ is small in front of the time scale $\bar{t}$ of the problem. The decoherence limit is the limit $\eta = \dfrac{T}{\bar{t}} \to 0$. This makes relax the spin part of the distribution function F_η of (2.4.1) towards the effective field line. This is the subject of the next proposition.

Proposition 2.4.1. *Assume that $\vec{\Omega}$ satisfies Assumption 2.4.3, $F_{in} \in \mathbb{L}^2_{\mathcal{M}}$ and that Assumptions 2.2.1, 2.2.2 hold. Let $T > 0$ and $F_\eta \in L^2([0,T],\mathbb{L}^2_{\mathcal{M}})$ be the weak solution of*

$$\partial_t F_\eta + v\cdot\nabla_x F_\eta - \nabla_x V\cdot\nabla_v F_\eta = Q(F_\eta) + \frac{i}{2\eta}[\vec{\Omega}\cdot\sigma, F_\eta] + Q_{sf}(F_\eta) \qquad (2.4.1)$$

with $F_\eta(0,x,v) = F_{in}(x,v)$. Then, when η goes to 0, F_η tends to F_0 such that $F_0(t,x,v) = \dfrac{f_c(t,x,v)}{2} I_2 + f_s(t,x,v)\vec{\omega}(x,v)\cdot\vec{\sigma}$ with f_c and f_s belong to $L^2([0,T],L^2_{\mathcal{M}})$. In addition, the charge and spin distribution functions, f_c and f_s, satisfy weakly

$$\partial_t f_c + v \cdot \nabla_x f_c - \nabla_x V \cdot \nabla_v f_c = Q(f_c) \tag{2.4.2}$$

$$\partial_t f_s + v \cdot \nabla_x f_s - \nabla_x V \cdot \nabla_v f_s = Q\left(f_s \vec{\omega}\right) \cdot \vec{\omega} - 2\frac{f_s}{\tau_{sf}} \tag{2.4.3}$$

and $F_0(0,x,v) = F_{in}(x,v)$ *where for any* $(x,v) \in \mathbb{R}^6$, $\vec{\omega}(x,v)$ *is the unit vector of the effective field line.*

Proof. Equation 2.4.1 admits a unique weak solution $F_\eta \in L^2([0,T];\mathbb{L}^2_{\mathcal{M}})$ such that $(F_\eta)_\eta$ is bounded with respect to η (see Section 2.3 for details). There exists $F_0 \in L^2([0,T];\mathbb{L}^2_{\mathcal{M}})$ such that $F_\eta \rightharpoonup F_0$ weakly in $L^2([0,T];\mathbb{L}^2_{\mathcal{M}})$. This implies that $i[\vec{\Omega} \cdot \vec{\sigma}, F_\eta]$ is also bounded in $L^2([0,T];\mathbb{L}^2_{\mathcal{M}})$ with respect to η and $i[\vec{\Omega}\cdot\vec{\sigma}, F_\eta] \rightharpoonup i[\vec{\Omega}\cdot\vec{\sigma}, F_0]$. Multiplying the weak formulation of (2.4.1) by η and taking η tends to zero, we get $i[\vec{\Omega} \cdot \vec{\sigma}, F_0] = 0$. This implies that the spin part of F_0 is parallel to $\vec{\Omega}$ i.e. there exist f_c and f_s in $L^2([0,T];\mathbb{L}^2_{\mathcal{M}})$ such that $F_0 = \dfrac{f_c}{2} I_2 + f_s \vec{\omega} \cdot \vec{\sigma}$. Decomposing (2.4.1) into charge and spin parts by setting $F_\eta = \dfrac{f_c^\eta}{2} + f_s^\eta \cdot \vec{\sigma}$, one has

$$\partial_t f_c^\eta + v \cdot \nabla_x f_c^\eta - \nabla_x V \cdot \nabla_v f_c^\eta = Q(f_c^\eta)$$

$$\partial_t f_s^\eta + v \cdot \nabla_x f_s^\eta - \nabla_x V \cdot \nabla_v f_s^\eta = Q(f_s^\eta) - \frac{1}{\eta}\vec{\Omega} \times f_s^\eta - 2\frac{f_s^\eta}{\tau_{sf}}. \tag{2.4.4}$$

The weak limit of the first equation is (2.4.2). Taking the scalar multiplication of (2.4.4) with $\vec{\omega}$ and passing to the limit weakly in $L^2_{\mathcal{M}}([0,T] \times \mathbb{R}^6)$ one finds (2.4.3). ■

Remark 2.4.2. *If we suppose that the direction of* $\vec{\Omega}$, $\vec{\omega}$, *does not depend on* v *then, we obtain at the decoherence limit a two-component kinetic model describing the evolution of spin-up and spin-down distribution functions* $f^\uparrow$ *and* $f^\downarrow$. *These functions are nothing but the eigenvalues of* F_0 *choosing such that :* $f^\uparrow = f_c + f_s$ *and* $f^\downarrow = f_c - f_s$. *If* f_c, f_s *satisfy* (2.4.2)-(2.4.3), *then* $f^\uparrow$ *and* $f^\downarrow$ *satisfy the following two-component kinetic model*

$$\begin{cases} \partial_t f^\uparrow + v \cdot \nabla_x f^\uparrow - \nabla_x V \cdot \nabla_v f^\uparrow = Q(f^\uparrow) + \dfrac{f^\downarrow - f^\uparrow}{\tau_{sf}}, \\ \partial_t f^\downarrow + v \cdot \nabla_x f^\downarrow - \nabla_x V \cdot \nabla_v f^\downarrow = Q(f^\downarrow) + \dfrac{f^\uparrow - f^\downarrow}{\tau_{sf}}, \end{cases} \tag{2.4.5}$$

subject to the initial conditions : $f^\uparrow(0) = \dfrac{f^c_{in}}{2} + \vec{f}^s_{in} \cdot \vec{\omega}$ *and* $f^\downarrow(0) = \dfrac{f^c_{in}}{2} - \vec{f}^s_{in} \cdot \vec{\omega}$, *where* f^c_{in} *and* $\vec{f}^s_{in}$ *are the charge and spin parts of* F_{in} $\left(F_{in} = \dfrac{f^c_{in}}{2} I_2 + \vec{f}^s_{in}.\vec{\sigma}\right)$. *The model* (2.4.5), *leads then to a two-component macroscopic model in this case (the case when the effective field direction is independent on* v*).*

In the next subsection, we will pass from a spinor Boltzmann equation to a 2-component macroscopic (drift-diffusion) model. We will see also that this asymptotic is possible if the effective field line does not depend on v and it corresponds to taking a diffusion limit of the spinor Boltzmann equation with high spin-orbit coupling (case $\alpha = \mathcal{O}(\frac{1}{\varepsilon})$).

2.4.2 Diffusion limit with strong spin-orbit coupling : two-component Drift-Diffusion model

This part is intended to the study of the diffusion limit ($\varepsilon \to 0$) of (2.1.1) when $\alpha = \mathcal{O}(\frac{1}{\varepsilon})$ with respect to ε. As mentioned in the introduction, the macroscopic model, one obtains in this case, changes wether the direction of $\vec{\Omega}$ depends on v or not. We will see that if the effective field Ω does not change direction with v this scaling gives at the limit a two-component Drift-Diffusion model. For simplicity, we suppose that $\alpha = \dfrac{1}{\varepsilon}$ and the starting equation is then

$$\frac{\partial F^\varepsilon}{\partial t} + \frac{1}{\varepsilon}(v \cdot \nabla_x F^\varepsilon - \nabla_x V \cdot \nabla_v F^\varepsilon) = \frac{1}{\varepsilon^2}\left\{ Q(F^\varepsilon) + \frac{i}{2}[\vec{\Omega}\cdot\vec{\sigma}, F^\varepsilon] \right\} + Q_{sf}(F^\varepsilon), \quad (2.4.6)$$

with initial condition (2.1.2). The operators Q and Q_{sf} are given by (2.1.4) and (2.1.3) respectively. We will use the following form of $\vec{\Omega}$.

Assumption 2.4.3. *We assume that $\vec{\Omega}$ belongs to $C^2(\mathbb{R}^6, \mathbb{R}^3)$ and is given by*

$$\vec{\Omega}(x,v) = \lambda(x,v)\vec{\omega}(x,v), \quad \textit{such that} \quad |\vec{\omega}(x,v)| = 1, \forall (x,v) \in \mathbb{R}^6$$

where λ and $\vec{\omega}$ are two regular respectively scalar and vectorial functions. In addition, we suppose that the following polynomially controls at infinity with respect to v hold

$$C_1(1+|v|)^m \leq |\lambda(x,v)| \leq C_2(1+|v|)^m \quad (2.4.7)$$

$$\sum_{\eta \in \{x_i, v_i\}} |\partial_\eta \vec{\Omega}| + \sum_{\eta,\eta' \in \{x_i,v_i\}} |\partial^2_{\eta\eta'}\vec{\omega}(x,v)| \leq C(1+|v|)^m \quad (2.4.8)$$

for $C_1 > 0$, $C_2 > 0$, $C > 0$ and $m \in \mathbb{N}$.

Definition 2.4.4. *We denote by Q_{SO} the following unbounded operator on $\mathbb{L}^2_{\mathcal{M}}$*

$$Q_{SO} = Q + \frac{i}{2}[\vec{\Omega}\cdot\vec{\sigma}, .] \quad (2.4.9)$$

defined on the following domain

$$\begin{aligned} D(Q_{SO}) &= \left\{ F \in \mathbb{L}^2_{\mathcal{M}} \,/\quad i[\vec{\Omega}\cdot\vec{\sigma}, F] \in \mathbb{L}^2_{\mathcal{M}} \right\} \quad (2.4.10) \\ &= \left\{ F = \frac{tr(F)}{2} I_2 + \vec{f_s}\cdot\sigma \in \mathbb{L}^2_{\mathcal{M}} \,/\quad \vec{\Omega}\cdot\vec{f_s} \in \mathbb{L}^2_{\mathcal{M}} \right\}. \end{aligned}$$

Recalling that $\mathbb{L}^2_{\mathcal{M}}$ denotes the space given by Definition 2.2.3.

In view of the properties of the collision operator listed in Proposition 2.3.3, we present in the following proposition some important properties of Q_{SO}.

Proposition 2.4.5. *Under Assumptions 2.2.1, 2.4.3, the unbounded operator* $(Q_{SO}, D(Q_{SO}))$ *given by* (2.4.9)-(2.4.10) *satisfies the following properties.*

1. *It is a maximal monotone operator on* $\mathbb{L}^2_{\mathcal{M}}$.
2. *Let* $Ker(Q_{SO})$ *be the nul space of* Q_{SO}*, then we have the following characterization :*

$$ker(Q_{SO}) = \Big\{ F = N(x)\mathcal{M}(v)/\ N = \frac{N_c}{2} I_2 + \vec{N}_s \cdot \vec{\sigma} \in L^2(\mathbb{R}^3, \mathcal{H}_2(\mathbb{C})) \\ and\ \vec{N}_s = \begin{cases} 0 & if\ \vec{\omega}\ depends\ on\ v \\ n_s(x)\vec{\omega} & if\ \vec{\omega} = \vec{\omega}(x)\ independent\ on\ v. \end{cases} \Big\} \tag{2.4.11}$$

3. *The range of* Q_{SO} *is given by*

$$Im(Q_{SO}) = \Big\{ G = \frac{g_c}{2} I_2 + \vec{g}_s \cdot \vec{\sigma} \in \mathbb{L}^2_{\mathcal{M}}\ /\ \int_{\mathbb{R}^3} g_c dv = 0 \\ and\ \Big(\int_{\mathbb{R}^3} \vec{g}_s dv \Big) \cdot \vec{\omega} = 0\ if\ \vec{\omega}\ does\ not\ depend\ on\ v \Big\} \tag{2.4.12}$$

Proof. 1. The adjoint of Q_{SO} is given by

$$Q^*_{SO} = Q - \frac{i}{2}[\vec{\Omega} \cdot \vec{\sigma}, .] \tag{2.4.13}$$

defined on $D(Q^*_{SO}) = D(Q_{SO})$. Indeed, by definition

$$D(Q^*_{SO}) = \left\{ F \in \mathbb{L}^2_{\mathcal{M}}/\ G \mapsto \langle F, Q_{SO}(G) \rangle_{\mathcal{M}} \text{ is a bounded operator on } D(Q_{SO}) \right\}.$$

For every $F \in D(Q^*_{SO})$, $G \in D(Q_{SO})$, we have by the self-adjointness of Q

$$\langle F, Q_{SO}(G) \rangle_{\mathcal{M}} = \langle Q(F) - \frac{i}{2}[\vec{\Omega} \cdot \vec{\sigma}, F], G \rangle_{\mathcal{M}}. \tag{2.4.14}$$

This implies

$$\langle \frac{i}{2}[\vec{\Omega} \cdot \vec{\sigma}, F], G \rangle_{\mathcal{M}} = \langle Q(F), G \rangle_{\mathcal{M}} - \langle F, Q_{SO}(G) \rangle_{\mathcal{M}}$$

for every $G \in D(Q_{SO})$. We deduce that for $F \in D(Q^*_{SO})$, $\frac{i}{2}[\vec{\Omega} \cdot \vec{\sigma}, F]$ is a linear and continuous operator on $D(Q_{SO})$ which is dense in $\mathbb{L}^2_{\mathcal{M}}$. It can be then prolonged to a linear continuous operator on $\mathbb{L}^2_{\mathcal{M}}$ which implies that (since $\mathbb{L}^2_{\mathcal{M}}$ is an Hilbert space) $\frac{i}{2}[\vec{\Omega} \cdot \vec{\sigma}, F] \in \mathbb{L}^2_{\mathcal{M}}$ and thus $F \in D(Q_{SO})$ if $F \in D(Q^*_{SO})$. The reciprocal inclusion $(D(Q_{SO}) \subset D(Q^*_{SO}))$ is obvious and from (2.4.14), one deduces that Q^*_{SO} is given

by (2.4.13) on $D(Q_{SO})$. In other side, $\langle i[\vec{\Omega}\cdot\vec{\sigma}, F], F\rangle_{\mathcal{M}} = 0$ for every $F \in \mathbb{L}^2_{\mathcal{M}}$. Then, since Q is a non positive operator, we have

$$\langle Q_{SO}(F), F\rangle_{\mathcal{M}} = \langle Q^*_{SO}(F), F\rangle_{\mathcal{M}} = \langle Q(F), F\rangle_{\mathcal{M}} \leq 0$$

and the operators Q_{SO} and Q^*_{SO} are monotones. Moreover, $D(Q_{SO})$ is dense in $\mathbb{L}^2_{\mathcal{M}}$ and the graph of Q_{SO}, $\mathcal{G}(Q_{SO})$, is closed. Indeed, let $(F_n, Q_{SO}(F_n))_{n\in\mathbb{N}}$ such that $F_n \in D(Q_{SO})$ be a sequence in $\mathcal{G}(Q_{SO})$ converging to (F, G) in $(\mathbb{L}^2_{\mathcal{M}})^2$. We have to prove that $F \in D(Q_{SO})$ and $G = Q_{SO}(F)$. For every $H \in D(Q_{SO})$, one has

$$\langle F_n, Q^*_{SO}(H)\rangle_{\mathcal{M}} = \langle Q_{SO}(F_n), H\rangle_{\mathcal{M}}.$$

By passing to the limit, $n \to +\infty$, one gets

$$\langle F, Q^*_{SO}(H)\rangle_{\mathcal{M}} = \langle G, H\rangle_{\mathcal{M}}$$

for every $H \in D(Q_{SO})$ and since $\overline{D(Q_{SO})} = \mathbb{L}^2_{\mathcal{M}}$, we deduce that $F \in D(Q_{SO})$ and $Q_{SO}(F) = G$. As a consequence, Q_{SO} is a densely defined closed operator such that Q_{SO} and Q^*_{SO} are monotones. It is then a maximal monotone operator on $\mathbb{L}^2_{\mathcal{M}}$.

2. Let $F \in Ker(Q_{SO})$, we have

$$Q(F) + \frac{i}{2}[\vec{\Omega}\cdot\vec{\sigma}, F] = 0. \tag{2.4.15}$$

Taking the scalar product with F in $\mathbb{L}^2_{\mathcal{M}}$, one gets $\langle Q(F), F\rangle_{\mathcal{M}} = 0$. This implies that $Q(F) = 0$ and $F = N(x)\mathcal{M}(v)$ such that $N \in L^2(\mathbb{R}^3, \mathcal{H}_2(\mathbb{C}))$ (see Proposition 2.3.3). Writing $N = \dfrac{N_c}{2} I_2 + \vec{N}_s \cdot \vec{\sigma}$ and inserting it in (2.4.15), we obtain

$$\vec{\Omega} \times \vec{N}_s = 0. \tag{2.4.16}$$

One can deduce simply that $\vec{N}_s = 0$ if $\vec{\Omega}$ changes direction with v and if not, the vector $\vec{N}_s$ is parallel to $\vec{\Omega}$.

3. Since Q_{SO} is a closed and densely defined operator on $\mathbb{L}^2_{\mathcal{M}}$, we have

$$\overline{Im(Q_{SO})} = (KerQ^*_{SO})^{\perp}.$$

Moreover, we have $Ker(Q^*_{SO}) = Ker(Q_{SO})$ and it is simple to verify that the orthogonal of $Ker(Q_{SO})$ is nothing else but the set given (2.4.12). This implies that $Im(Q_{SO}) \subset Ker(Q_{SO})$. In other side, let $G = \dfrac{g_c}{2} I_2 + \vec{g}_s \cdot \vec{\sigma} \in ker(Q_{SO})^{\perp}$ which means that $\displaystyle\int_{\mathbb{R}^3} g_c dv = 0$ and $\left(\displaystyle\int_{\mathbb{R}^3} \vec{g}_s dv\right) \cdot \vec{\omega} = 0$ if $\vec{\omega} = \vec{\omega}(x)$ does not depend on v. Viewing the properties of the collision operator Q (Proposition 2.3.3), there is a

unique function $f_c \in L^2_{\mathcal{M}}(\mathbb{R}^6)$ such that $\int_{\mathbb{R}^3} f_c(x,v)dv = 0$ and $Q(f_c) = g_c$. It remains to verify the existence of a unique $\vec{f_s} \in (L^2_{\mathcal{M}}(\mathbb{R}^6))^3$ such that $(\int_{\mathbb{R}^3} \vec{f_s}dv)\cdot\vec{\omega} = 0$ if $\vec{\omega}$ does not depend on v and

$$Q(\vec{f_s}) - \lambda(\vec{\omega} \times \vec{f_s}) = \vec{g}_s.$$

Since Q_{SO} is a maximal monotone operator, then $\forall\delta > 0$, $\delta Id - Q_{SO}$ is surjective, where Id denotes the identity operator on $\mathbb{L}^2_{\mathcal{M}}$. There exists a vector function $\vec{f_s^\delta}$ such that $\vec{f_s^\delta}\cdot\vec{\sigma} \in D(Q_{SO})$ for any $\delta > 0$ and $(\delta Id - Q_{SO})(\vec{f_s^\delta}\cdot\vec{\sigma}) = \vec{g}_s\cdot\vec{\sigma}$. Then,

$$\delta\vec{f_s^\delta} - Q(\vec{f_s^\delta}) + \lambda\vec{\omega}\times\vec{f_s^\delta} = \vec{g}_s,$$

for all $\delta > 0$. We have to prove now that the sequence $(\vec{f_s^\delta})_\delta$ is bounded in $(L^2_{\mathcal{M}}(\mathbb{R}^6))^3$. We argue by contradiction and assume the existence of a subsequence denoted also by $(\vec{f_s^\delta})_\delta$ such that $\|\vec{f_s^\delta}\| \xrightarrow[\delta\to 0]{} +\infty$ with $\|.\|$ is the norm in $(L^2_{\mathcal{M}}(\mathbb{R}^6))^3$. Denoting by $\vec{\mathbf{f}_s^\delta} = \dfrac{f_s^\delta}{\|f_s^\delta\|}$, we have

$$\delta\vec{\mathbf{f}_s^\delta} - Q(\vec{\mathbf{f}_s^\delta}) + \lambda\vec{\omega}\times\vec{\mathbf{f}_s^\delta} = \frac{\vec{g}_s}{\|\vec{f_s^\delta}\|}, \tag{2.4.17}$$

and $\|\vec{\mathbf{f}_s^\delta}\| = 1$. Then, by passing to the limit weakly in $(L^2_{\mathcal{M}})^3$, we have $\vec{\mathbf{f}_s^\delta} \rightharpoonup \vec{\mathbf{f}_s}$ in $(L^2_{\mathcal{M}})^3$ such that

$$-Q(\vec{\mathbf{f}_s}) + \lambda\vec{\omega}\times\vec{\mathbf{f}_s} = 0$$

which implies that $\vec{\mathbf{f}_s} = 0$ if $\vec{\omega}$ depends on v and $\vec{\mathbf{f}_s} = n_s(t,x)\vec{\omega}(t,x)\mathcal{M}$ if not. Moreover, if $\vec{\omega}$ is independent on v, $\vec{g}_s$ satisfies $(\int_{\mathbb{R}^3}\vec{g}_s dv)\cdot\vec{\omega} = 0$. Then, integrating (2.4.17) with respect to v and multiplying by $\vec{\omega}$, the same condition is also satisfied by $(\vec{\mathbf{f}_s^\delta})$: $\int_{\mathbb{R}^3}\vec{\mathbf{f}_s^\delta}dv\cdot\vec{\omega} = 0$ for every $\delta > 0$. Getting $\delta \to 0$, one deduces that $n_s = (\int_{\mathbb{R}^3}\vec{\mathbf{f}_s}dv)\cdot\vec{\omega} = 0$. Hence, $\vec{\mathbf{f}_s^\delta} \rightharpoonup \vec{\mathbf{f}_s} = 0$. In other side, let us show that $\vec{\mathbf{f}_s^\delta} \to \vec{\mathbf{f}_s}$ strongly in $(L^2_{\mathcal{M}})^3$. This implies that $\|\vec{\mathbf{f}_s}\| = 1$, since $\|\vec{\mathbf{f}_s^\delta}\| = 1\ \forall\delta > 0$ which is in contradiction with $\vec{\mathbf{f}_s} = 0$. Indeed, rewriting equation (2.4.17) as follows

$$(\delta + \nu(v))\vec{\mathbf{f}_s^\delta} + \lambda\vec{\omega}\times\vec{\mathbf{f}_s^\delta} = \vec{\mathbf{g}_s^\delta} + Q^+(\vec{\mathbf{f}_s^\delta}), \tag{2.4.18}$$

with $\nu(v) = \int_{\mathbb{R}^3}\alpha(v,v')\mathcal{M}(v')dv'$, $Q^+(\vec{\mathbf{f}_s^\delta}) = \int_{\mathbb{R}^3}\alpha(v,v')\vec{\mathbf{f}_s^\delta}(v')dv'\mathcal{M}(v)$ and $\vec{\mathbf{g}_s^\delta} = \dfrac{\vec{g}_s}{\|\vec{f_s^\delta}\|}$. The solution of (2.4.18) can be computed explicitly. Indeed, without loss of generality, assume that $\vec{\omega} = (w_1, w_2, w_3)$ is such that $w_3 \neq 0$, $\|\vec{\omega}\| = 1$, and complete it to an orthonormal basis of $\mathbb{R}^3$: $(\varepsilon_1, \varepsilon_2, \vec{\omega})$. The change-of-basis matrix, P, from

the standard euclidian basis to the new one is an orthogonal matrix (${}^tP \cdot P = I_3$) given by

$$P = \frac{1}{(w_1^2 + w_3^2)^{\frac{1}{2}}} \begin{pmatrix} w_3 & -w_1 w_2 & w_1(w_1^2 + w_3^2)^{\frac{1}{2}} \\ 0 & w_1^2 + w_3^2 & w_2(w_1^2 + w_3^2)^{\frac{1}{2}} \\ -w_1 & -w_2 w_3 & w_3(w_1^2 + w_3^2)^{\frac{1}{2}} \end{pmatrix}. \tag{2.4.19}$$

Let $\vec{\mathbf{F}}_s^{\delta} = {}^tP\vec{\mathbf{f}}_s^{\delta}$ be the new coordinates of $\vec{\mathbf{f}}_s^{\delta}$ in the new basis $(\varepsilon_i)_i$. Then, it satisfies the following equation

$$N_\delta(\vec{\mathbf{F}}_s^{\delta}) = {}^tP(\vec{h}_s^{\delta}), \tag{2.4.20}$$

where $\vec{h}_s^{\delta} = \vec{\mathbf{g}}_s^{\delta} + Q^+(\vec{\mathbf{f}}_s^{\delta})$ is the second member of (2.4.18) and

$$N_\delta = (\delta + \nu(v)) \begin{pmatrix} 1 & -\tilde{\lambda} & 0 \\ \tilde{\lambda} & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}, \quad \tilde{\lambda}(x,v) = \frac{\lambda(x,v)}{\delta + \nu(v)}. \tag{2.4.21}$$

It is simple to verify that $\vec{h}_s^{\delta}$ converges strongly in $(L^2_{\mathcal{M}})^3$ to $Q^+(\vec{\mathbf{f}}_s)$. Moreover, N_δ is invertible and

$$N_\delta^{-1} = \frac{1}{\delta + \nu(v)} \begin{pmatrix} \frac{1}{1+\tilde{\lambda}^2} & \frac{\tilde{\lambda}}{1+\tilde{\lambda}^2} & 0 \\ \frac{-\tilde{\lambda}}{1+\tilde{\lambda}^2} & \frac{1}{1+\tilde{\lambda}^2} & 0 \\ 0 & 0 & 1 \end{pmatrix}.$$

It is a bounded matrix with respect to δ uniformly with respect to $(x,v) : \|N_\delta^{-1}\|_2 \leq \dfrac{2}{\delta + \alpha_1}$ if the cross section $\alpha(v,v')$ satisfies Assumption 2.2.1. As a conclusion, we have

$$\vec{\mathbf{f}}_s^{\delta} = P \cdot N_\delta^{-1} \cdot {}^tP(\vec{h}_s^{\delta})$$

with $(\vec{h}_s^{\delta})_\delta$ is a strongly convergent sequence in $(L^2_{\mathcal{M}})^3$ and N_δ^{-1} is a uniformly bounded matrix with respect to δ. Then, $(\vec{\mathbf{f}}_s^{\delta})_\delta$ converges strongly in $(L^2_{\mathcal{M}})^3$. The proof of the proposition is completed.

■

The following lemma follows from the last proposition.

Lemma 2.4.6. *There exists a unique $\vec{\chi}_s \in (\mathbb{L}^2_{\mathcal{M}})^3$ satisfying*

$$Q(\vec{\chi}_s) + \lambda(\vec{\omega} \times \vec{\chi}_s) = v \cdot \nabla_x \vec{\omega}\mathcal{M} \tag{2.4.22}$$

under the following condition

$$\left(\int_{\mathbb{R}^3} \vec{\chi}_s(x,v) dv \right) \cdot \vec{\omega} = 0, \quad \forall x \in \mathbb{R}^3. \tag{2.4.23}$$

Theorem 2.4.7. *Let $T > 0$, $F_{in} \in \mathbb{L}^2_{\mathcal{M}}$ and assume that Assumptions 2.2.1, 2.2.2, 2.4.3 hold and that the direction of the effective field $\vec{\omega}$ is independent on v. Then, the sequence of weak solutions, $(F^\varepsilon)_{\varepsilon>0}$, of (2.4.6)-(2.1.2) converges weakly in $L^2([0,T];\mathbb{L}^2_{\mathcal{M}})$, when ε goes to zero, to $N(t,x)\mathcal{M}(v)$ with $N \in L^2([0,T]\times\mathbb{R}^3, \mathcal{H}_2^+(\mathbb{C}))$ and such that*

$$N(t,x) = \frac{n_c(t,x)}{2} I_2 + n_s(t,x)\vec{\omega}(x)\cdot\vec{\sigma} \tag{2.4.24}$$

(the spin part of N is parallel to $\vec{\omega}$). In addition, the spin-up and spin-down densities, $n^\uparrow = n_c + n_s$ and $n^\downarrow = n_c - n_s$ satisfy the following two-component drift-diffusion model

$$\begin{cases} \partial_t n^\uparrow - \mathrm{div}_x(\mathbb{D}_1(\nabla_x n^\uparrow + \nabla_x V n^\uparrow)) = \dfrac{n^\downarrow - n^\uparrow}{\tau(x)} \\ \\ \partial_t n^\downarrow - \mathrm{div}_x(\mathbb{D}_1(\nabla_x n^\downarrow + \nabla_x V n^\downarrow)) = \dfrac{n^\uparrow - n^\downarrow}{\tau(x)} \end{cases} \tag{2.4.25}$$

where $\mathbb{D}_1$ is a symmetric positive definite matrix given by (2.5.10). We obtain at the limit a modified spin relaxation time given by

$$\tau(x) = \frac{2\tau_{sf}}{2 + \tau_{sf}\chi(x)}$$

where $\chi(x)$ is a positive function

$$\chi(x) = -\int_{\mathbb{R}^3} \frac{Q(\vec{\chi}_s)\cdot\vec{\chi}_s}{\mathcal{M}} dv \geq 0 \tag{2.4.26}$$

with $\vec{\chi}_s$ satisfies (2.4.22).

Proof. With estimate (2.3.2), there exist $F \in L^2([0,T],\mathbb{L}^2_{\mathcal{M}})$ and $N \in L^2([0,T]\times\mathbb{R}^3;\mathcal{H}_2^+(\mathbb{C}))$ such that $F^\varepsilon \rightharpoonup F$ and $N^\varepsilon \rightharpoonup N$ in the corresponding spaces and $N = \displaystyle\int_{\mathbb{R}^3} F dv$ (since $N^\varepsilon = \int_{\mathbb{R}^3} F^\varepsilon dv$, $\forall\varepsilon > 0$). Multiplying (2.4.6) by ε^2 and passing to the weak limit $\varepsilon \to 0$, one gets in the distribution sence

$$Q(F) + \frac{i}{2}[\vec{\omega}\cdot\vec{\sigma}, F] = 0.$$

Since $\vec{\omega}$ is independent on v and with (2.4.11), $F = N(t,x)\mathcal{M}(v)$ such that the density matrix N can be written as (2.4.24). Let $N^\varepsilon = \dfrac{n_c^\varepsilon}{2} I_2 + \vec{n}_s^\varepsilon\cdot\vec{\sigma}$ and $F^\varepsilon = \dfrac{f_c^\varepsilon}{2} I_2 + \vec{f}_s^\varepsilon\cdot\vec{\sigma}$ with $n_c^\varepsilon = \displaystyle\int_{\mathbb{R}^3} f_c^\varepsilon dv$ and $\vec{n}_s^\varepsilon = \displaystyle\int_{\mathbb{R}^3} \vec{f}_s^\varepsilon dv$. Then, $n_c^\varepsilon \rightharpoonup n_c$ in $L^2([0,T]\times\mathbb{R}^3)$ and $\vec{n}_s^\varepsilon \rightharpoonup n_s\vec{\omega}$ in $(L^2([0,T]\times\mathbb{R}^3))^3$ (or $\vec{n}_s^\varepsilon\cdot\vec{\omega} \rightharpoonup n_s$) where n_c and n_s are the charge and spin parts of N (2.4.24). Integrating equation (2.4.6) with respect to v, one obtains the following continuity equations

$$\begin{cases} \partial_t n_c^\varepsilon + \mathrm{div}_x j_c^\varepsilon = 0 \\ \partial_t \vec{n}_s^\varepsilon + \nabla_x \cdot J_s^\varepsilon = \dfrac{-1}{\varepsilon^2}\displaystyle\int_{\mathbb{R}^3} (\vec{\Omega}\times\vec{f}_s^\varepsilon) dv - \frac{2\vec{n}_s^\varepsilon}{\tau_{sf}} \end{cases} \tag{2.4.27}$$

where the charge and spin currents, j_c^ε ans J_s^ε, are given by

$$j_c^\varepsilon = \frac{1}{\varepsilon}\int_{\mathbb{R}^3} v f_c^\varepsilon dv \quad J_s^\varepsilon = \frac{1}{\varepsilon}\int_{\mathbb{R}^3} (v \otimes \vec{f}_s^\varepsilon) dv.$$

These continuity equations can be obtained weakly by taking test functions constants with respect to v in the weak formulation (2.3.1) (this choice of test functions is possible, see the next section). Moreover, using estimate (2.3.3), there is R^ε in $L^2([0,T];\mathbb{L}^2_{\mathcal{M}})$ bounded with respect to ε such that $F^\varepsilon = N^\varepsilon \mathcal{M} + \varepsilon R^\varepsilon$. In terms of spin and charge parts, we have

$$\begin{cases} \vec{f}_s^\varepsilon = \vec{n}_s^\varepsilon \mathcal{M} + \varepsilon \vec{r}_s^\varepsilon, \quad f_c^\varepsilon = n_c^\varepsilon \mathcal{M} + \varepsilon r_c^\varepsilon \\ \|\vec{r}_s^\varepsilon\|_{L^2_t((L^2_{\mathcal{M}})^3)} \leq C, \quad \|r_c^\varepsilon\|_{L^2_t(L^2_{\mathcal{M}})} \leq C \end{cases} \tag{2.4.28}$$

where $C > 0$ is a general constant independent of ε. Thus, $j_c^\varepsilon = \displaystyle\int_{\mathbb{R}^3} v r_c^\varepsilon dv$ and $(j_c^\varepsilon)_\varepsilon$ is bounded with respect to ε in $L^2([0,T]\times\mathbb{R}^3)$. It converges weakly to a function j_c in $L^2([0,T]\times\mathbb{R}^3)$ and by passing to the limit on the first equation of (2.4.27), we have

$$\partial_t n_c + \mathrm{div}_x j_c = 0. \tag{2.4.29}$$

Moreover, multiplying the second equation of (2.4.27) by $\vec{\omega}$, we get

$$\partial_t(\vec{n}_s^\varepsilon \cdot \vec{\omega}) + \mathrm{div}_x(J_s^\varepsilon(\vec{\omega})) = J_s^\varepsilon : (\nabla_x \otimes \vec{\omega}) - \frac{2\vec{n}_s^\varepsilon}{\tau_{sf}} \tag{2.4.30}$$

where $J_s^\varepsilon(\vec{\omega}) = \dfrac{1}{\varepsilon}\displaystyle\int_{\mathbb{R}^3} (v \otimes \vec{f}_s^\varepsilon)(\vec{\omega}) dv = \frac{1}{\varepsilon}\int_{\mathbb{R}^3} v(\vec{f}_s^\varepsilon \cdot \vec{\omega}) dv = \int_{\mathbb{R}^3} v(\vec{r}_s^\varepsilon \cdot \vec{\omega}) dv$ bounded with respect to ε. Let us denote by j_s the weak limit of $J_s^\varepsilon(\vec{\omega})$ in $L^2([0,T]\times\mathbb{R}^3)$. Besides, let $S^\varepsilon := J_s^\varepsilon : (\nabla_x \otimes \vec{\omega})$. Then, $S^\varepsilon = \dfrac{1}{\varepsilon}\displaystyle\int_{\mathbb{R}^3} (v \cdot \nabla_x \vec{\omega}) \cdot \vec{f}_s^\varepsilon dv$ which is also bounded with respect to ε in $L^2([0,T]\times\mathbb{R}^3)$ and converges weakly to a certain function $S \in L^2([0,T]\times\mathbb{R}^3)$. By passing to the weak limit $\varepsilon \to 0$, (2.4.30) yields the following continuity equation

$$\partial_t n_s + \mathrm{div}_x(j_s) = S - \frac{2n_s}{\tau_{sf}}. \tag{2.4.31}$$

To close this equation, one has to express j_s and S according to n_s. For this, taking the Frobenius inner product of (2.4.6) with $\dfrac{\theta_1 \vec{\omega} \cdot \vec{\sigma}}{\mathcal{M}}$ where θ_1 is given by (2.5.8) and integrating with respect to v yields

$$\begin{aligned} J_s^\varepsilon(w) = -\varepsilon \int_{\mathbb{R}^3} \partial_t(\vec{f}_s^\varepsilon \cdot \vec{\omega}) \frac{\theta_1}{\mathcal{M}} dv - \int_{\mathbb{R}^3} v \cdot (\nabla_x + \nabla_x V)(\vec{n}_s^\varepsilon \cdot \vec{\omega}) \theta_1 dv - \int_{\mathbb{R}^3} \vec{n}_s^\varepsilon \cdot (v \cdot \nabla_x \vec{\omega}) \theta_1 dv \\ - \varepsilon \int_{\mathbb{R}^3} (v \cdot \nabla_x - \nabla_x V \cdot \nabla_v)(\vec{r}_s^\varepsilon \cdot \vec{\omega}) \frac{\theta_1}{\mathcal{M}} dv - \frac{\varepsilon}{\tau_{sf}} \int_{\mathbb{R}^3} \frac{(\vec{f}_s^\varepsilon \cdot \vec{\omega}) \theta_1}{\mathcal{M}} dv, \end{aligned}$$

up to straightforward computations using the self-adjointness of the collision operator Q and the expansion of $\vec{f}_s^{\varepsilon}$ around the equilibrium (2.4.28). Taking ε goes, to zero one obtains

$$\begin{aligned} J_s^{\varepsilon}(\vec{\omega}) \rightharpoonup j_s &= -\mathbb{D}_1(\nabla_x n_s + \nabla_x V n_s) - \int_{\mathbb{R}^3} (v\cdot\nabla_x\vec{\omega})\cdot\vec{\omega} n_s\theta_1 dv \\ &= -\mathbb{D}_1(\nabla_x n_s + \nabla_x V n_s) \quad (\text{since } \|\vec{\omega}\| = 1) \end{aligned} \tag{2.4.32}$$

with $\mathbb{D}_1 = \displaystyle\int_{\mathbb{R}^3} (\theta_1 \otimes v) dv$. To rigourously find the relation between j_s and n_s, one has to use the weak formulation of (2.4.6) with $\dfrac{\theta_1\vec{\omega}\cdot\vec{\sigma}}{\mathcal{M}}\phi(t,x)$, $\phi \in C_c^1([0,T)\times\mathbb{R}^3)$, as test function and passing then to the limit (see the next section for details). A similar computation gives also

$$j_c = -\mathbb{D}_1(\nabla_x n_c + \nabla_x V n_c). \tag{2.4.33}$$

Finally, we shall express the limit of $S^{\varepsilon} := \dfrac{1}{\varepsilon}\displaystyle\int_{\mathbb{R}^3} (v\cdot\nabla_x\vec{\omega})\cdot\vec{f}_s^{\varepsilon}$, S, in terms of n_s. Taking the inner product of (2.4.6) with $\dfrac{\vec{\chi}_s\cdot\vec{\sigma}}{\mathcal{M}}$, where $\vec{\chi}_s$ satisfies (2.4.22)-(2.4.23), and integrating with respect to v, one obtains

$$\begin{aligned} S^{\varepsilon} = \varepsilon\int_{\mathbb{R}^3} \partial_t\vec{f}_s^{\varepsilon}\cdot\frac{\vec{\chi}_s}{\mathcal{M}}dv + \int_{\mathbb{R}^3}(v\cdot\nabla_x\vec{n}_s^{\varepsilon} + v\cdot\nabla_x V\vec{n}_s^{\varepsilon})\cdot\vec{\chi}_s dv \\ + \varepsilon\int_{\mathbb{R}^3}(v\cdot\nabla_x - \nabla_x V\cdot\nabla_v)\vec{r}_s^{\varepsilon}\cdot\frac{\vec{\chi}_s}{\mathcal{M}}dv + \frac{\varepsilon}{\tau_{sf}}\int_{\mathbb{R}^3}\frac{\vec{f}_s^{\varepsilon}\cdot\chi_s}{\mathcal{M}}dv. \end{aligned}$$

By passing to the limit $\varepsilon\to 0$,

$$S = \int_{\mathbb{R}^3} v\cdot\nabla_x(n_s\vec{\omega})\cdot\vec{\chi}_s dv + \int_{\mathbb{R}^3} v\cdot\nabla_x V n_s(\vec{\omega}\cdot\vec{\chi}_s)dv. \tag{2.4.34}$$

This limit can be rigourously verified by taking $\dfrac{\vec{\chi}_s\cdot\vec{\sigma}}{\mathcal{M}}\phi(t,x)$, with $\phi\in C_c^1([0,T)\times\mathbb{R}^3)$, as test function in (2.3.1). This choice is valid since $\dfrac{\vec{\chi}_s}{\mathcal{M}}$ is polynomially increasing at infinity with respect to v (see Lemma 2.4.8). Moreover, multiplying (2.4.22) by $\vec{\omega}$, we have $Q(\vec{\chi}_s\cdot\vec{\omega}) = 0$ with $\displaystyle\int_{\mathbb{R}^3}\vec{\chi}_s\cdot\vec{\omega}dv = 0$ which implies that $\vec{\chi}_s\cdot\vec{\omega} = 0$. In addition, if we multiply (2.4.22) by $\dfrac{\vec{\chi}_s}{\mathcal{M}}$ and integrate with respect to v, we get

$$\int_{\mathbb{R}^3}(v\cdot\nabla_x\vec{\omega})\cdot\vec{\chi}_s dv = \int_{\mathbb{R}^3}\frac{Q(\vec{\chi}_s)\cdot\vec{\chi}_s}{\mathcal{M}}dv = -\chi(x)\le 0.$$

Consequently, the charge and spin densities n_c and n_s satisfy

$$\begin{cases} \partial_t n_c - \mathrm{div}_x(\mathbb{D}_1(\nabla_x n_c + n_c\nabla_x V)) = 0 \\ \partial_t n_s - \mathrm{div}_x(\mathbb{D}_1(\nabla_x n_s + n_s\nabla_x V)) = -\dfrac{2n_s}{\tau_{sf}} - \chi(x)n_s \end{cases}$$

which yields (2.4.25).

■

Lemma 2.4.8. *Let $\vec{\chi}_s$ be the solution of* (2.4.22)-(2.4.23)*. Then under Assumption 2.2.1 and Assumption 2.4.3, one has*

$$\frac{|\vec{\chi}_s|}{\mathcal{M}} \leq C(1+|v|)^{m+1}, \sum_{\eta\in\{x_i,v_i\}} \frac{\partial_\eta|\vec{\chi}_s|}{\mathcal{M}} \leq C(1+|v|)^{m'},$$

with C is a general positive constant and $m' \in \mathbb{N}$.

Proof. Rewriting equation (2.4.22) as

$$-\nu(v)\vec{\chi}_s + \lambda(\vec{\omega}\times\vec{\chi}_s) = (v\cdot\nabla_x\vec{\omega} - Q^+(\vec{\chi}_s))\mathcal{M}(v) \tag{2.4.35}$$

with $\nu(v) = \displaystyle\int_{\mathbb{R}^3} \alpha(v,v')\mathcal{M}(v')dv'$, $Q^+(\vec{\chi}_s) = \displaystyle\int_{\mathbb{R}^3} \alpha(v,v')\vec{\chi}_s(v')dv'$ and applying the same computations we have made for resolving equation (2.4.18), one finds

$$\frac{\vec{\chi}_s}{\mathcal{M}} = P\cdot N^{-1}\cdot {}^tP(v\cdot\nabla_x\vec{\omega} - Q^+(\vec{\chi}_s)).$$

The matrix P is given by (2.4.19) and

$$N^{-1} = \frac{-1}{\nu}\begin{pmatrix} \frac{1}{1+\tilde{\lambda}^2} & \frac{\tilde{\lambda}}{1+\tilde{\lambda}^2} & 0 \\ \frac{-\tilde{\lambda}}{1+\tilde{\lambda}^2} & \frac{1}{1+\tilde{\lambda}^2} & 0 \\ 0 & 0 & 1 \end{pmatrix}, \qquad \tilde{\lambda}(x,v) = \frac{-\lambda(x,v)}{\nu(v)}.$$

The matrices P and N^{-1} are uniformly bounded with respect to (x,v), $\|P\|_2 = \sqrt{3}$ and $\|N^{-1}\|_2 \leq \dfrac{2}{\alpha_1}$ (with Assumption 2.2.1). Therefore, using Assumption 2.4.3, we deduce that $\dfrac{|\vec{\chi}_s|}{\mathcal{M}} \leq C(1+|v|)^{m+1}$. Similarly, by differentiating (2.4.35) with respect to x or v, one can obtain the second estimates on $\dfrac{\partial_\eta|\vec{\chi}_s|}{\mathcal{M}}$. ∎

2.5 A general spin-vector Drift-Diffusion model

This section is concerned with the diffusion limit when the spin-orbit coupling is of order one with respect to ε ($\alpha = \mathcal{O}(1)$). This scaling is useful to get a spin vector continuum model with rotation effects when the effective field of the spin-orbit coupling is odd with respect to v. Here we take a general effective field $\vec{\Omega}^\varepsilon$ as follows

$$\vec{\Omega}^\varepsilon(x,v) = \frac{1}{\varepsilon}\vec{\Omega}_o(x,v) + \vec{\Omega}_e(x,v), \tag{2.5.1}$$

where $\vec{\Omega}_o$ is odd with respect to v and $\vec{\Omega}_e$ is even with respect to v. For instance, $\vec{\Omega}_o$ can be the effective magnetic field following from the spin-orbit interactions (Rashba [10], Dresselhauss [20]) or the odd part of an applied magnetic field and $\vec{\Omega}_e$

can represent the even part of an applied field. The starting scaled spinor Boltzmann equation is

$$\frac{\partial F^\varepsilon}{\partial t}+\frac{1}{\varepsilon}(v\cdot\nabla_x F^\varepsilon-\nabla_x V\cdot\nabla_v F^\varepsilon)=\frac{1}{\varepsilon^2}Q(F^\varepsilon)+\frac{i}{2}[\vec{\Omega}^\varepsilon(x,v)\cdot\vec{\sigma},F^\varepsilon]+Q_{sf}(F^\varepsilon),\quad(2.5.2)$$

with the initial condition (2.1.2) and the operators Q, Q_{sf} are respectively given by (2.1.4) and (2.1.3). Let us rewrite the weak formulation of (2.5.2). A function $F^\varepsilon\in L^2([0,T];\mathbb{L}^2_{\mathcal{M}})$ is called weak solution of (2.5.2) if it satisfies :

$$\begin{aligned}-\int_0^T\int_{\mathbb{R}^6}\langle F^\varepsilon,\partial_t\psi\rangle_2 dtdxdv-\frac{1}{\varepsilon}\int_0^T\int_{\mathbb{R}^6}\langle F^\varepsilon,v\cdot\nabla_x\psi-\nabla_x V\cdot\nabla_v\psi\rangle_2 dtdxdv=\\ \frac{1}{\varepsilon^2}\int_0^T\int_{\mathbb{R}^6}\langle Q(F^\varepsilon),\psi\rangle_2 dtdxdv+\int_0^T\int_{\mathbb{R}^6}\langle\frac{i}{2}[\vec{\Omega}^\varepsilon(x,v)\cdot\vec{\sigma},F^\varepsilon],\psi\rangle_2 dtdxdv\\ +\int_0^T\int_{\mathbb{R}^6}\langle Q_{sf}(F^\varepsilon),\psi\rangle_2 dtdxdv+\int_{\mathbb{R}^6}\langle F_{in},\psi(0)\rangle_2 dxdv,\quad(2.5.3)\end{aligned}$$

for all $\psi\in C^1_c([0,T)\times\mathbb{R}^6;\mathcal{H}_2(\mathbb{C}))$.

Assumption 2.5.1. *We assume that $\vec{\Omega}_o(x,v)$ and $\vec{\Omega}_e(x,v)$ are respectively two regular odd and even vectors with respect to v. In addition, we suppose that $\vec{\Omega}_o$ is compactly supported with respect to x and there exist a constant $C_0>0$ and $m\in\mathbb{N}$ such that*

$$|\vec{\Omega}_o(v)|+\sum_{\eta\in\{x_i,v_i\}}|\partial_\eta\vec{\Omega}_o(v)|\leq C_0(1+|v|)^m.\quad(2.5.4)$$

The main results of this section is stated in the following two theorems.

Theorem 2.5.2. *Let $T>0$, $F_{in}\in\mathbb{L}^2_{\mathcal{M}}$ and assume that Assumption 2.2.1, Assumption 2.2.2 and Assumption 2.5.1 hold. Let for all $\varepsilon>0$ $F^\varepsilon\in C^0([0,T];\mathbb{L}^2_{\mathcal{M}})$ be the weak solution of (2.5.2)-(2.1.2). Then, the matrix density $N^\varepsilon:=\int_{\mathbb{R}^3}F^\varepsilon(t,x,v)dv$ converges weakly in $L^2([0,T]\times\mathbb{R}^3,\mathcal{H}_2(\mathbb{C}))$ to N which satisfies the following equation*

$$\begin{aligned}\partial_t N-\mathrm{div}_x\{\mathbb{D}_1(\nabla_x N+N\nabla_x V)-i\mathbb{D}_2[\vec{\sigma},N]\}=\\ \frac{i}{2}[\vec{\Omega}\cdot\vec{\sigma},N]+(\mathbb{D}_4-tr(\mathbb{D}_4))(\vec{N}_s)\cdot\vec{\sigma}+Q_{sf}(N)\quad(2.5.5)\end{aligned}$$

with initial condition $N(0,x)=\int_{\mathbb{R}^3}F_{in}(x,v)dv$, and where $\vec{N}_s$ is the spin density part of N. In addition, if we decompose N as : $N=\frac{N_c}{2}I_2+\vec{N}_s\cdot\vec{\sigma}$, then the charge and spin densities satisfy

$$\begin{cases} \partial_t N_c - \mathrm{div}_x(\mathbb{D}_1(\nabla_x N_c + \nabla_x V N_c)) = 0 \\ \\ \partial_t \vec{N}_s - \mathrm{div}_x(\mathbb{D}_1 \cdot (\nabla_x \otimes \vec{N}_s + \nabla_x V \otimes \vec{N}_s) + 2(\mathbb{D}_2^k \times \vec{N}_s)_{k=1,2,3}) = \\ \qquad\qquad -\vec{\Omega} \times \vec{N}_s + (\mathbb{D}_4 - tr\mathbb{D}_4)(\vec{N}_s) - 2\dfrac{\vec{N}_s}{\tau_{sf}}. \end{cases} \tag{2.5.6}$$

Here

$$\vec{\Omega} = \mathrm{div}_x \mathbb{D}_2 - \mathbb{D}_3(\nabla_x V) + H_e, \quad H_e(x) = \int_{\mathbb{R}^3} \vec{\Omega}_e(x,v)\mathcal{M}(v)dv \tag{2.5.7}$$

and the matrices $\mathbb{D}_1$, $\mathbb{D}_2$, $\mathbb{D}_3$ and $\mathbb{D}_4$ are given by (2.5.10). For two matrices A and B, $A \cdot B$ is the product of A and B and $\mathrm{div}_x(A) = \nabla_x \cdot A = (\sum_k \partial_k A_{ki})_i$; $\mathbb{D}_2^k$ is the k^{th} row of $\mathbb{D}_2$. We use $\nabla_x \otimes \vec{N}_s$ to denote the transpose of the Jacobian matrix of $\vec{N}_s$: $\nabla_x \otimes \vec{N}_s = (\partial_{x_i} \vec{N}_s^j)_{ij}$.

Theorem 2.5.3 (**Maximum principle**). *Let $N_{in} \in L^2(\mathbb{R}^3, \mathcal{H}_2^+(\mathbb{C}))$ be given and under the same hypothesis as for the last theorem, there exists a unique weak solution $N(t,x) = \dfrac{N_c(t,x)}{2} I_2 + N_s(t,x).\vec{\sigma} \in C^0([0,T], L^2(\mathbb{R}^3, \mathcal{H}_2(\mathbb{C}))$ for any $T > 0$ of (2.5.6) with $N(0,x) = N_{in}(x)$. In addition, for all $t \geq 0$ and $x \in \mathbb{R}^3$, N(t,x) is an Hermitian and positive matrix ($N(t,x) \in \mathcal{H}_2^+(\mathbb{C})$).*

Remark 2.5.4. *The right hand side of the limit equation (2.5.6) is the sum of a rotational term around a certain field $\vec{\Omega}$ (2.5.7) and a relaxation terms arising from the spin-flip and non spin-flip scattering operators ($\mathbb{D}_4 - tr(\mathbb{D}_4)$ is a negative matrix since $\mathbb{D}_4$ is a symmetric positive definite matrix). The limiting effective field (2.5.7) contains an averaging of the even part $\vec{\Omega}_e$ and keeps traces via the matrices $\mathbb{D}_2$ and $\mathbb{D}_3$ from the odd part $\vec{\Omega}_o$ of the effective field in the kinetic equation.*

Before beginning the proof of these theorems, we have to introduce the four matrices $\mathbb{D}_1$, $\mathbb{D}_2$, $\mathbb{D}_3$ and $\mathbb{D}_4$ appearing in the limit model (2.5.6). These matrices keep traces from the collision operator and the spin-orbit interactions considered. This is the aim of the two following propositions.

Proposition 2.5.5. *There exist a unique $\theta_1 \in (L^2_{\mathcal{M}})^3$ and $\theta_2 \in (L^2_{\mathcal{M}})^3$ such that*

$$-Q(\theta_1 I_2) = v\mathcal{M}(v)I_2, \quad \int_{\mathbb{R}^3} \theta_1(v)dv = 0, \tag{2.5.8}$$

$$-Q(\theta_2 I_2) = \vec{\Omega}_o(v)\mathcal{M}(v)I_2, \quad \int_{\mathbb{R}^3} \theta_2(v)dv = 0, \tag{2.5.9}$$

where I_2 is the 2×2 identity matrix.

Proof. Using the properties of the collision operator introduced in Proposition 2.3.3 and since $\int_{\mathbb{R}^3} v\mathcal{M}(v)I_2 = \begin{pmatrix} 0 & 0 \\ 0 & 0 \end{pmatrix}$, there exists $\vartheta_1 \in (\mathbb{L}^2_{\mathcal{M}})^3$ such that $-Q(\vartheta_1) = vM(v)I_2$. The uniqueness of ϑ_1 is guarantied under the condition $\int_{\mathbb{R}^3} \vartheta_1(v)dv = 0$. It remains to prove that ϑ_1 is a scalar matrix. For this, we decompose ϑ_1 in the orthogonal basis $\{I_2, \sigma_1, \sigma_2, \sigma_3\}$ of the set of 2×2 hermitian matrices and we use the linearity of Q. Since $\vec{\Omega}_o$ is odd with respect to v, one can check similarly the existence of θ_2 satisfying (2.5.9).

■

Proposition 2.5.6. *Let $\mathbb{D}_1$, $\mathbb{D}_2$, $\mathbb{D}_3$ and $\mathbb{D}_4$ be the 3×3 matrices defined respectively by*

$$\begin{aligned} \mathbb{D}_1 &= \int_{\mathbb{R}^3} (\theta_1(v) \otimes v)dv \quad , \mathbb{D}_2 = \int_{\mathbb{R}^3} (v \otimes \theta_2(v))dv, \\ \mathbb{D}_3 &= \int_{\mathbb{R}^3} (\vec{\Omega}_o(v) \otimes \theta_1(v))dv \quad , \mathbb{D}_4 = \int_{\mathbb{R}^3} (\theta_2(v) \otimes \vec{\Omega}_o(v))dv \end{aligned} \tag{2.5.10}$$

where θ_1, θ_2 are given by (2.5.8), (2.5.9). The matrices $\mathbb{D}_1$ and $\mathbb{D}_4$ are symmetric positive definite and ${}^t\mathbb{D}_3 = \mathbb{D}_2$.

Proof. The components of $\mathbb{D}_1$ verify

$$\begin{aligned} \mathbb{D}_1^{ij} &= \int_{\mathbb{R}^3} \theta_1^i(v).v_j dv = \frac{1}{2}\int_{\mathbb{R}^3} \frac{\theta_1^i(v)I_2 : v_j\mathcal{M}(v)I_2}{\mathcal{M}}dv \\ &= -\frac{1}{2}\int_{\mathbb{R}^3} \frac{\theta_1^i(v)I_2 : Q(\theta_1^j I_2)}{\mathcal{M}}dv = -\frac{1}{2}\langle \theta_1^i I_2, Q(\theta_1^j I_2)\rangle_{\mathcal{M}}. \end{aligned}$$

Identically, one can calculate the components of $\mathbb{D}_2, \mathbb{D}_3$ and $\mathbb{D}_4$ to find :

$$\mathbb{D}_2^{ij} = -\frac{1}{2}\langle \theta_2^i I_2, Q(\theta_1^j I_2)\rangle_{\mathcal{M}}, \quad \mathbb{D}_3^{ij} = -\frac{1}{2}\langle \theta_1^i I_2, Q(\theta_2^j I_2)\rangle_{\mathcal{M}}, \quad \mathbb{D}_4^{ij} = -\frac{1}{2}\langle \theta_2^i I_2, Q(\theta_2^j I_2)\rangle_{\mathcal{M}}.$$

The selfadjointness of Q provides that $\mathbb{D}_1$ and $\mathbb{D}_4$ are symmetric and that ${}^t\mathbb{D}_3 = \mathbb{D}_2$. To prove the positivity of $\mathbb{D}_1$ (or $\mathbb{D}_4$), let $X \in \mathbb{R}^3$, and let $f_X^1 = \sum_{i=1}^{3} X_i\theta_1^i I_2$. Then, since $f_X^1 \in (KerQ)^\perp$, from (2.3.4) we have

$$\begin{aligned} \langle \mathbb{D}_1 X, X\rangle &= \sum_{i,j} \mathbb{D}_1^{ij} X_i X_j = -\frac{1}{2}\sum_{i,j} \langle \theta_1^i Id, Q(\theta_1^j Id)\rangle_{\mathcal{M}} X_i X_j \\ &= -\frac{1}{2}\langle \sum_i X_i\theta_1^i Id, Q(\sum_j X_j\theta_1^j Id)\rangle_{\mathcal{M}} = -\frac{1}{2}\langle f_X^1, Q(f_X^1)\rangle_{\mathcal{M}} \geq \frac{\alpha_1}{2}\|f_X^1\|^2_{\mathcal{M}} \geq 0. \end{aligned}$$

Moreover, if $X \in \mathbb{R}^3$ such that $\langle \mathbb{D}_1 X, X\rangle = 0$ then, $f_X^1 = 0$. This implies, by the linearity of Q, that : $\sum_{i=1}^{3} X_i Q(\theta_1^i I_2) = 0$ and then $\sum_{i=1}^{3} X_i v_i \mathcal{M} = 0$. Finally, since $(v_i\mathcal{M})_i$ is a family of linearly independent elements in $L^2_{\mathcal{M}}$, we deduce that $X = 0$. Thus, $\mathbb{D}_1$ (respectively $\mathbb{D}_4$) is a symmetric positive definite matrix.

■

2.5.1 Diffusion limit : formal approach

In this section, we will derive the model (2.5.6) by formally passing to the limit $\varepsilon \to 0$.

Proposition 2.5.7. *If the solution of* (2.5.2)-(2.1.2), F^ε, *has an Hilbert expansion with respect to* ε *in the form :* $F^\varepsilon = F^0 + \varepsilon F^1 + \mathcal{O}(\varepsilon)$, *then* $F^0(t,x,v) = N(t,x)\mathcal{M}(v)$ *and the density matrix* N *satisfies* (2.5.5).

Proof. By inserting the expansion of F^ε in (2.5.2) and comparing the terms corresponding to the same order of ε, we get

$$Q(F^0) = 0, \tag{2.5.11a}$$

$$Q(F^1) = (v \cdot \nabla_x - \nabla_x V \cdot \nabla_v)F^0 - \frac{i}{2}[\vec{\Omega}_o \cdot \vec{\sigma}, F^0]. \tag{2.5.11b}$$

Therefore, $F^0 = N(t,x)\mathcal{M}(v)$ and

$$F^1 = -\theta_1 \cdot (\nabla_x N + N\nabla_x V) + \frac{i}{2}\theta_2 \cdot [\vec{\sigma}, N],$$

where θ_1, θ_2 are given by (2.5.8) and (2.5.9) respectively. Integrating equation (2.5.2) with respect to v yields

$$\partial_t N^\varepsilon + \mathrm{div}_x J^\varepsilon = S^\varepsilon + Q_{sf}(N^\varepsilon), \tag{2.5.12}$$

where $N^\varepsilon = \displaystyle\int_{\mathbb{R}^3} F^\varepsilon dv$, $J^\varepsilon = \frac{1}{\varepsilon}\int_{\mathbb{R}^3} vF^\varepsilon(t,x,v)dv$ and $S^\varepsilon = \frac{i}{2}\displaystyle\int_{\mathbb{R}^3} [\vec{\Omega}^\varepsilon(x,v)\cdot\vec{\sigma}, F^\varepsilon(t,x,v)]dv$. In addition, using the Hilbert expansion of F^ε, one can calculate formally the limit of each term of the last equation. Indeed, we have

$$\begin{aligned} J^\varepsilon &= \frac{1}{\varepsilon}\int_{\mathbb{R}^3} vF^\varepsilon(v)dv = \frac{1}{\varepsilon}(\int_{\mathbb{R}^3} v\mathcal{M}(v)dv)N + \int_{\mathbb{R}^3} vF^1 dv + \mathcal{O}(\varepsilon) \\ &= 0 + \int_{\mathbb{R}^3} vF^1(v)dv + \mathcal{O}(\varepsilon) = -\mathbb{D}_1(\nabla_x N + N\nabla_x V) + \frac{i}{2}\mathbb{D}_2([\vec{\sigma}, N]) + \mathcal{O}(\varepsilon), \end{aligned} \tag{2.5.13}$$

and

$$\begin{aligned} 2S^\varepsilon &= \frac{i}{\varepsilon}\int_{\mathbb{R}^3} [\vec{\Omega}_o\cdot\vec{\sigma}, F^\varepsilon] + i\int_{\mathbb{R}^3} [\vec{\Omega}_e\cdot\vec{\sigma}, F^\varepsilon]dv = i\int_{\mathbb{R}^3} [\vec{\Omega}_o\cdot\vec{\sigma}, F^1]dv + i[H_e\cdot\vec{\sigma}, N] + \mathcal{O}(\varepsilon) \\ &= -i\int_{\mathbb{R}^3} [\vec{\Omega}_o\cdot\vec{\sigma}, \theta_1\cdot(\nabla_x N + N\nabla_x V)]dv - \frac{1}{2}\int_{\mathbb{R}^3} [\vec{\Omega}_o(v)\cdot\vec{\sigma}, \theta_2\cdot[\vec{\sigma}, N]]dv + i[H_e\cdot\vec{\sigma}, N] + \mathcal{O}(\varepsilon). \end{aligned}$$

Then, by a straightforward computation, one finds

$$2S^\varepsilon = -i[\mathbb{D}_3(\nabla_x + \nabla_x V)\cdot\vec{\sigma}, N] - \frac{1}{2}\sum_{i,j=1}^{3} \mathbb{D}_4^{ij}[\vec{e}_i\cdot\vec{\sigma}, [\vec{e}_j\cdot\vec{\sigma}, N]] + i[H_e\cdot\vec{\sigma}, N] + \mathcal{O}(\varepsilon), \tag{2.5.14}$$

where $\{\vec{e}_1, \vec{e}_2, \vec{e}_3\}$ is the euclidian basis of $\mathbb{R}^3$. Let $N = \frac{N_c}{2} I_2 + \vec{N}_s \cdot \vec{\sigma}$, then with Lemma A.2.2 and the double cross product formula, $\vec{a} \times (\vec{b} \times \vec{c}) = (\vec{a} \cdot \vec{c})\vec{b} - (\vec{a} \cdot \vec{b})\vec{c}$, one obtains

$$\begin{aligned}
\sum_{i,j=1}^{3} \mathbb{D}_4^{ij} [\vec{e}_i \cdot \vec{\sigma}, [\vec{e}_j \cdot \vec{\sigma}, N]] &= -4 \sum_{i,j=1}^{3} \mathbb{D}_4^{ij} \vec{e}_i \times (\vec{e}_j \times \vec{N}_s) \cdot \vec{\sigma} \\
&= -4 \sum_{i,j=1}^{3} \mathbb{D}_4^{ij} (\vec{N}_s^i \vec{e}_j - \vec{e}_i \cdot \vec{e}_j \vec{N}_s) \cdot \vec{\sigma}, \qquad (\vec{N}_s^i = \vec{N}_s \cdot \vec{e}_i) \\
&= -4(\mathbb{D}_4(\vec{N}_s) - tr(\mathbb{D}_4)\vec{N}_s) \cdot \vec{\sigma}.
\end{aligned}$$

Replacing (2.5.13) and (2.5.14) in (2.5.12), passing to the limit $\varepsilon \to 0$, and using the fact that ${}^t\mathbb{D}_2 = \mathbb{D}_3$ which implies that

$$\mathrm{div}_x(\mathbb{D}_2[\vec{\sigma}, N]) = [(\mathrm{div}(\mathbb{D}_2) + \mathbb{D}_3(\nabla_x)) \cdot \vec{\sigma}, N],$$

one obtains (2.5.5). ■

2.5.2 Diffusion limit : the rigorous approach

This part is devoted to the proof of Theorem 2.5.2. The first Lemma is a consequence of estimate (2.3.2).

Lemma 2.5.8. *Let $T > 0$ and let $F^\varepsilon \in C^0([0,T]; \mathbb{L}^2_{\mathcal{M}})$ be the weak solution of (2.5.2). There exist $F \in L^2([0,T], \mathbb{L}^2_{\mathcal{M}})$ and $N \in L^2([0,T] \times \mathbb{R}^3, \mathcal{H}_2(\mathbb{C}))$ such that*

$$F^\varepsilon \rightharpoonup F \quad in \quad L^2_t(\mathbb{L}^2_{\mathcal{M}}) - weak \quad and \quad N^\varepsilon \rightharpoonup N \quad in \quad L^2_{t,x}(\mathcal{H}_2(\mathbb{C})) - weak. \tag{2.5.15}$$

In addition, we have $N(t,x) = \displaystyle\int_{\mathbb{R}^3} F(t,x,v)dv$ a.e. $(t,x) \in \mathbb{R}^+ \times \mathbb{R}^3$.

Definition 2.5.9. *For all $\varepsilon \in \mathbb{R}^+$, we define the current J^ε and the source spin-orbit term S^ε by*

$$J^\varepsilon(t,x) = \frac{1}{\varepsilon} \int_{\mathbb{R}^3} v F^\varepsilon(t,x,v)dv, \tag{2.5.16}$$

$$S^\varepsilon(t,x) = \frac{i}{2} \int_{\mathbb{R}^3} [\vec{\Omega}^\varepsilon(x,v) \cdot \vec{\sigma}, F^\varepsilon(t,x,v)]dv. \tag{2.5.17}$$

Lemma 2.5.10. *The current J^ε and the term S^ε given by (2.5.16), (2.5.17) are respectively bounded in $L^2([0,T] \times \mathbb{R}^3, (\mathcal{H}_2(\mathbb{C}))^3)$ and $L^2([0,T] \times \mathbb{R}^3, \mathcal{H}_2(\mathbb{C}))$ with respect to ε.*

Proof. By (2.3.3), there exists $R^\varepsilon \in L^2([0,T], \mathbb{L}^2_{\mathcal{M}})$ such that

$$F^\varepsilon = N^\varepsilon \mathcal{M} + \varepsilon R^\varepsilon \quad \text{and} \quad \|R^\varepsilon\|_{L^2_t(\mathbb{L}^2_{\mathcal{M}})} \leq C. \tag{2.5.18}$$

The current is then equal to : $J^\varepsilon(t,x) = \displaystyle\int_{\mathbb{R}^3} vR^\varepsilon(t,x,v)dv$, and for all $(t,x) \in \mathbb{R}^+ \times \mathbb{R}^3$, we have with the Cauchy-Schwartz inequality

$$\begin{aligned}\int_0^T \int_{\mathbb{R}^3} \|J^\varepsilon(t,x)\|^2_{(\mathcal{H}_2(\mathbb{C}))^3} dtdx &\leq \int_0^T \int_{\mathbb{R}^3} \left(\int_{\mathbb{R}^3} |v| \|R^\varepsilon\|_2 dv \right)^2 dtdx \\ &\leq \|R^\varepsilon\|^2_{L^2_t(\mathbb{L}^2_{\mathcal{M}})} \left(\int_{\mathbb{R}^3} |v|^2 \mathcal{M} dv \right).\end{aligned}$$

Then, with (2.5.18), J^ε is bounded in $L^2_{t,x}((\mathcal{H}_2(\mathbb{C}))^3)$. By proceeding analogously, we obtain the boundedness of S^ε in $L^2_{t,x}(\mathcal{H}_2(\mathbb{C}))$.

■

Proof of Theorem 2.5.2 : As a consequence of Lemma 2.5.10, there exist $J \in L^2([0,T] \times \mathbb{R}^3, (\mathcal{H}_2(\mathbb{C}))^3)$ and $S \in L^2([0,T] \times \mathbb{R}^3, \mathcal{H}_2(\mathbb{C}))$ such that

$$J^\varepsilon \rightharpoonup J \quad \text{in} \quad L^2_{t,x}((\mathcal{H}_2(\mathbb{C}))^3) - weak \quad \text{and} \quad S^\varepsilon \rightharpoonup S \quad \text{in} \quad L^2_{t,x}(\mathcal{H}_2(\mathbb{C})) - weak.$$

If we pass formally to the limit in the equation (2.5.12) we get the continuity equation

$$\partial_t N + \mathrm{div}_x J = S + Q_{sf}(N). \tag{2.5.19}$$

In order to complete the limit equation (2.5.19), we have to find the relation between J, S and N. Indeed, multiplying equation (2.5.2) with $\dfrac{\theta^1 I_2}{\mathcal{M}}$ and integrating with respect to v yields :

$$J^\varepsilon = -\int_{\mathbb{R}^3} (v\cdot\nabla_x F^\varepsilon - \nabla_x V\cdot\nabla_v F^\varepsilon + \varepsilon\partial_t F^\varepsilon)\frac{\theta^1}{\mathcal{M}}dv + \frac{i\varepsilon}{2}\int_{\mathbb{R}^3}[\vec{\Omega}^\varepsilon\cdot\vec{\sigma}, F^\varepsilon]\frac{\theta^1}{\mathcal{M}}dv + \varepsilon\int_{\mathbb{R}^3} Q_{sf}(F^\varepsilon)\frac{\theta^1}{\mathcal{M}}dv.$$

By passing to the limit, $\varepsilon \to 0$, we get

$$\begin{aligned} J &= -\int_{\mathbb{R}^3} v\cdot(\nabla_x N + \nabla_x V N)\theta^1 dv + \frac{i}{2}\int_{\mathbb{R}^3}[\vec{\Omega}_o\cdot\vec{\sigma}, N]\theta^1 dv \\ &= -\mathbb{D}_1(\nabla_x N + \nabla_x V N) + \frac{i}{2}\mathbb{D}_2[\vec{\sigma}, N]. \end{aligned} \tag{2.5.20}$$

To find the relation between S and N, we apply the operation : $\dfrac{i}{2}\displaystyle\int_{\mathbb{R}^3}\frac{[\theta_2\cdot\vec{\sigma},.]}{\mathcal{M}}dv$ on (2.5.2). This yields

$$\begin{aligned} S^\varepsilon - \frac{i}{2}\int_{\mathbb{R}^3}[\vec{\Omega}_e\cdot\vec{\sigma}, F^\varepsilon]dv &= -\frac{i}{2}\int_{\mathbb{R}^3}[\theta_2\cdot\vec{\sigma}, \varepsilon\partial_t F^\varepsilon + v\cdot\nabla_x F^\varepsilon - \nabla_x V\cdot\nabla_v F^\varepsilon]\frac{dv}{\mathcal{M}} \\ &\quad -\frac{\varepsilon}{4}\int_{\mathbb{R}^3}[\theta_2\cdot\vec{\sigma}, [\vec{\Omega}^\varepsilon\cdot\vec{\sigma}, F^\varepsilon]]\frac{dv}{\mathcal{M}} + \frac{i\varepsilon}{2}\int_{\mathbb{R}^3}[\theta_2\cdot\vec{\sigma}, Q_{sf}(F^\varepsilon)]\frac{dv}{\mathcal{M}}. \end{aligned}$$

Taking ε goes to zero and using $\mathbb{D}_3 = {}^t\mathbb{D}_2$, the last equation becomes (see the proof of Proposition 2.5.7 for calculation details)

$$\begin{aligned} S &= -\frac{i}{2}\int_{\mathbb{R}^3}[\theta_2\cdot\vec{\sigma}, v\cdot(\nabla_x N + \nabla_x V N)]dv - \frac{1}{4}\int_{\mathbb{R}^3}[\theta_2\cdot\vec{\sigma},[\vec{\Omega}_o\cdot\vec{\sigma},N]]dv + \frac{i}{2}[H_e\cdot\vec{\sigma},N] \\ &= -\frac{i}{2}[\mathbb{D}_3(\nabla_x+\nabla_x V)\cdot\vec{\sigma},N] + (\mathbb{D}_4 - tr(\mathbb{D}_4))(\vec{N}_s)\cdot\vec{\sigma} + \frac{i}{2}[H_e\cdot\vec{\sigma},N]. \qquad (2.5.21) \end{aligned}$$

For rigorous analysis, we have to use the weak formulation of (2.5.2) with different test functions. Remark first that (2.5.3) is also verified for test functions lie in the following space

$$\begin{aligned} \mathcal{T} = \{&\psi(t,x,v)\in C^1([0,T)\times\mathbb{R}^6,\mathcal{H}_2(\mathbb{C})) \text{ compactly supported with respect to } t \text{ and } x \\ &\text{and } \psi \text{ and all its derivatives are polynomially increasing with respect to } v \\ &\text{i.e}: \exists n\in\mathbb{N}, C\in\mathbb{R}_+/ \quad \|\psi(t,x,v)\|_2 + \sum_{s\in\{t,x_i,v_i\}}\|\partial_s\psi\|_2 \le C(1+|v|)^n\}. \qquad (2.5.22) \end{aligned}$$

In particular, if we take $\psi = \phi(t,x)\in C_c^1([0,T)\times\mathbb{R}^3,\mathcal{H}_2(\mathbb{C}))$ in (2.5.3), we obtain

$$\begin{aligned} -\int_0^T\int_{\mathbb{R}^3}\langle N^\varepsilon,\partial_t\phi\rangle_2 dtdx - \frac{1}{\varepsilon}\int_0^T\int_{\mathbb{R}^6}\langle F^\varepsilon, v.\nabla_x\phi\rangle_2 dtdxdv = \\ \int_0^T\int_{\mathbb{R}^3}\langle\frac{i}{2}\int_{\mathbb{R}^3}[\vec{\Omega}^\varepsilon(v).\vec{\sigma},F^\varepsilon]dv,\phi\rangle_2 dtdx + \int_0^T\int_{\mathbb{R}^3}\langle Q_{sf}(F^\varepsilon),\phi\rangle_2 dtdxdv \\ + \int_{\mathbb{R}^6}\langle F_{in},\phi(0,x)\rangle_2 dxdv. \qquad (2.5.23) \end{aligned}$$

This is nothing else but the weak formulation of the continuity equation (2.5.12) with initial condition

$$N^\varepsilon(0,x) = \int_{\mathbb{R}^3} F_{in}(x,v)dv. \qquad (2.5.24)$$

Passing to the limit $\varepsilon\to 0$ in (2.5.23), one finds the limit continuity equation (2.5.19) in the distribution sense.

It remains now to rigorously rely the current J and the term S with the density N. For this, one needs the following lemma which can be proved as Lemma 2.4.8.

Lemma 2.5.11. *Let θ_1 and θ_2 be given by* (2.5.8), (2.5.9). *Then, under Assumption 2.2.1 and Assumption 2.5.1, we have*

$$\frac{|\theta_1|}{\mathcal{M}} \le C(1+|v|), \quad \sum_{i=1}^3\frac{|\partial_{v_i}\theta_1|}{\mathcal{M}} \le C(1+|v|^2), \qquad (2.5.25)$$

$$\frac{|\theta_2|}{\mathcal{M}}+\sum_{i=1}^{3}\frac{|\partial_{x_i}\theta_2|}{\mathcal{M}}\leq C(1+|v|)^m,\quad \sum_{i=1}^{3}\frac{|\partial_{v_i}\theta_2|}{\mathcal{M}}\leq C(1+|v|)^{m+1},\tag{2.5.26}$$

where C stands for a generic nonnegative constant.

This lemma shows that for all $\phi\in C_c^1([0,T)\times\mathbb{R}^3,\mathcal{H}_2(\mathbb{C}))$ each component of the vectorial function $\psi=\phi(t,x)\dfrac{\theta_1}{\mathcal{M}}$ belongs to $\mathcal{T}$. Using it as a test function in the weak formulation (2.5.3), we get

$$\begin{aligned}\int_0^T\int_{\mathbb{R}^3}\langle J^\varepsilon,\phi(t,x)\rangle_2 dtdx=\varepsilon\int_0^T\int_{\mathbb{R}^6}\langle F^\varepsilon,\partial_t\phi\rangle_2\frac{\theta_1}{\mathcal{M}}dtdxdv+\int_0^T\int_{\mathbb{R}^6}\langle F^\varepsilon,v\cdot\nabla_x\phi-v\cdot\nabla_xV\phi\rangle_2\frac{\theta_1}{\mathcal{M}}\\ -\int_0^T\int_{\mathbb{R}^6}\langle F^\varepsilon,\phi\rangle_2\frac{\nabla_xV\cdot\nabla_v\theta_1}{\mathcal{M}}dtdxdv+\varepsilon\int_0^T\int_{\mathbb{R}^6}\langle\frac{i}{2}[\vec{\Omega}^\varepsilon(x,v)\cdot\vec{\sigma},F^\varepsilon],\phi\rangle_2\frac{\theta_1}{\mathcal{M}}dtdxdv\\ +\varepsilon\int_0^T\int_{\mathbb{R}^6}\langle Q_{sf}(F^\varepsilon),\phi(t,x)\rangle_2\frac{\theta_1}{\mathcal{M}}dtdxdv+\varepsilon\int_{\mathbb{R}^6}\langle F_{in},\phi(0,x)\rangle_2\frac{\theta_1}{\mathcal{M}}dxdv.\end{aligned}\tag{2.5.27}$$

Lemma 2.5.12. *Let $\vec{\Omega}$ be a general vector field ($\vec{\Omega}=\vec{\Omega}_o$ or $\vec{\Omega}_e$), then $[\vec{\Omega}\cdot\vec{\sigma},F^\varepsilon]$ converges weakly to $[\vec{\Omega}\cdot\vec{\sigma},N]\mathcal{M}$ in $L^2([0,T],\mathbb{L}^2_{\mathcal{M}})$.*

Proof. For all $\psi\in L^2([0,T],\mathbb{L}^2_{\mathcal{M}})$, we have

$$\int_0^T\int_{\mathbb{R}^6}\frac{\langle[\vec{\Omega}\cdot\vec{\sigma},F^\varepsilon],\psi\rangle_2}{\mathcal{M}}dtdxdv=-\int_0^T\int_{\mathbb{R}^6}\frac{\langle F^\varepsilon,[\vec{\Omega}\cdot\vec{\sigma},\psi]\rangle_2}{\mathcal{M}}dtdxdv$$

$$\xrightarrow[\varepsilon\to0]{}-\int_0^T\int_{\mathbb{R}^6}\langle N,[\vec{\Omega}\cdot\vec{\sigma},\psi]\rangle_2 dtdxdv=\int_0^T\int_{\mathbb{R}^6}\langle[\vec{\Omega}\cdot\vec{\sigma},N],\psi\rangle_2 dtdxdv.$$

■

Using this lemma and with (2.5.25), it is simply to verify that we can pass to the limit in all the terms of equation (2.5.3). We obtain at the limit

$$\begin{aligned}\int_0^T\int_{\mathbb{R}^3}\langle J,\phi(t,x)\rangle_2 dtdx&=\int_0^T\int_{\mathbb{R}^6}\langle N,(\nabla_x\phi-\nabla_xV\phi)\cdot v\rangle_2\theta_1 dtdxdv\\ &\quad+\int_0^T\int_{\mathbb{R}^6}\langle\frac{i}{2}[\vec{\Omega}_o(x,v)\cdot\vec{\sigma},N],\phi\rangle_2\theta_1 dtdxdv\\ &=\int_0^T\int_{\mathbb{R}^3}\langle N,\mathbb{D}_1(\nabla_x\phi-\nabla_xV\phi)\rangle_2 dtdx+\int_0^T\int_{\mathbb{R}^3}\langle\frac{i}{2}[\mathbb{D}_2\cdot\vec{\sigma},N],\phi\rangle_2 dtdx.\end{aligned}$$

This is the weak formulation of the current (2.5.20). Finally, to find weakly the relation between S and N given by (2.5.21), we choose now $\psi=\dfrac{i[\theta_2\cdot\vec{\sigma},\phi(t,x)]}{2\mathcal{M}}$ for an arbitrary $\phi\in C_c^1([0,T)\times\mathbb{R}^3,\mathcal{H}_2(\mathbb{C}))$ as a test function in (2.5.3). In view of

(2.5.26) and Assumption 2.5.1, this is an admissible test function (i.e belongs to $\mathcal{T}$). One has

$$\int_0^T\int_{\mathbb{R}^3}\langle S^\varepsilon,\phi(t,x)\rangle_2 dtdx-\int_0^T\int_{\mathbb{R}^6}\langle\frac{i}{2}[\vec{\Omega}_e\cdot\vec{\sigma},F^\varepsilon],\phi\rangle_2 dtdxdv=-\varepsilon\int_0^T\int_{\mathbb{R}^6}\langle F^\varepsilon,\frac{i}{2}[\theta_2\cdot\vec{\sigma},\partial_t\phi]\rangle_2\frac{dtdxdv}{\mathcal{M}}$$
$$-\int_0^T\int_{\mathbb{R}^6}\langle F^\varepsilon,\frac{i}{2}[(v\cdot\nabla_x-v\cdot\nabla_x V)\theta_2\cdot\vec{\sigma},\phi]\rangle_2\frac{dtdxdv}{\mathcal{M}}-\int_0^T\int_{\mathbb{R}^6}\langle F^\varepsilon,\frac{i}{2}[\theta_2\cdot\vec{\sigma},v\cdot\nabla_x\phi]\rangle_2\frac{dtdxdv}{\mathcal{M}}$$
$$+\int_0^T\int_{\mathbb{R}^6}\langle F^\varepsilon,\frac{i}{2}[\nabla_x V\cdot\nabla_v(\theta_2\cdot\vec{\sigma}),\phi]\rangle_2\frac{dtdxdv}{\mathcal{M}}-\frac{\varepsilon}{4}\int_0^T\int_{\mathbb{R}^6}\langle i[\vec{\Omega}^\varepsilon(x,v).\vec{\sigma},F^\varepsilon],i[\theta_2\cdot\vec{\sigma},\phi]\rangle_2\frac{dtdxdv}{\mathcal{M}}$$
$$-\frac{\varepsilon}{2}\int_0^T\int_{\mathbb{R}^6}(Q_{sf}\langle F^\varepsilon),i[\theta_2\cdot\vec{\sigma},\phi]\rangle_2\frac{dtdxdv}{\mathcal{M}}-\frac{\varepsilon}{2}\int_{\mathbb{R}^6}\langle F_{in},i[\theta_2\cdot\vec{\sigma},\phi(0,x)]\rangle_2\frac{dxdv}{\mathcal{M}},\quad(2.5.28)$$

where, to obtain the left hand side of this equation, we have used the self adjointness of Q and the following identity.

Lemma 2.5.13. *For each A, B and C in $\mathcal{M}_2(\mathbb{C})$, we have*

$$\langle A,[B,C]\rangle_2=\langle C^*,[A^*,B]\rangle_2.\quad(2.5.29)$$

One verifies easily that we can pass to the limit at all the terms of (2.5.28) to obtain

$$\int_0^T\int_{\mathbb{R}^3}\langle S,\phi(t,x)\rangle_2 dtdx-\int_0^T\int_{\mathbb{R}^3}\langle\frac{i}{2}[H_e\cdot\vec{\sigma},N],\phi\rangle_2 dtdx=$$
$$-\int_0^T\int_{\mathbb{R}^6}\langle N,\frac{i}{2}[(v\cdot\nabla_x-v\cdot\nabla_x V)\theta_2\cdot\vec{\sigma},\phi]\rangle_2 dtdxdv-\int_0^T\int_{\mathbb{R}^6}\langle N,\frac{i}{2}[\theta_2\cdot\vec{\sigma},v\cdot\nabla_x\phi]\rangle_2 dtdxdv$$
$$-\frac{1}{4}\int_0^T\int_{\mathbb{R}^6}\langle[\vec{\Omega}_o(x,v)\cdot\vec{\sigma},N],[\theta_2\cdot\vec{\sigma},\phi]\rangle_2 dtdxdv.$$

This can be rewritten, using identity (2.5.29) and the selfadjointness of all our matrices, as follows

$$\int_0^T\int_{\mathbb{R}^3}\langle S,\phi(t,x)\rangle_2 dtdx=\int_0^T\int_{\mathbb{R}^6}\langle\frac{i}{2}[(v\cdot\nabla_x-v\cdot\nabla_x V)\theta_2\cdot\vec{\sigma},N],\phi\rangle_2 dtdxdv$$
$$+\int_0^T\int_{\mathbb{R}^6}\langle\frac{i}{2}[\theta_2.\vec{\sigma},N],v\cdot\nabla_x\phi\rangle_2 dtdxdv-\frac{1}{4}\int_0^T\int_{\mathbb{R}^3}\langle[\theta_2\cdot\vec{\sigma},[\vec{\Omega}_o\cdot\vec{\sigma},N]],\phi\rangle_2 dtdxdv$$
$$+\int_0^T\int_{\mathbb{R}^3}\langle\frac{i}{2}[H_e\cdot\vec{\sigma},N],\phi\rangle_2.$$

This is the weak formulation of equation (2.5.21). The proof of Theorem 2.5.2 is achieved.

2.5.3 Maximum Principle (Proof of Theorem 2.5.3)

The existence of weak solution of (2.5.5) can be readily verified using semi-groupe technics and the fact that $\mathbb{D}_1$ and $\mathbb{D}_4$ are two symmetric definite positive matrices.

Let us just show that, for all (t,x), $N(t,x) := \frac{N_c(t,x)}{2} I_2 + \vec{N}_s(t,x)\cdot\vec{\sigma}$ is a non negative matrix. It is sufficient to verify that $\frac{N_c}{2} \geq \|\vec{N}_s\|$ since the eigenvalues of N are $\frac{N_c}{2} \pm \|\vec{N}_s\|$. All the following computations can be made rigourously using the weak form of (2.5.6). Taking the scalar product of the second equation of (2.5.6) with $\vec{N}_s$, we get

$$\|\vec{N}_s\|\partial_t(\|\vec{N}_s\|) - \mathrm{div}_x(\mathbb{D}_1\cdot(\nabla_x\otimes\vec{N}_s + \nabla_x V\otimes\vec{N}_s))\cdot\vec{N}_s = 2(\mathbb{D}_3(\nabla_x)\times\vec{N}_s)\cdot\vec{N}_s + (\mathbb{D}_4 - tr\mathbb{D}_4)(\vec{N}_s)\cdot\vec{N}_s - 2\frac{\|\vec{N}_s\|^2}{\tau_{sf}}. \quad (2.5.30)$$

Lemma 2.5.14. *We have*

$$\mathrm{div}_x(\mathbb{D}_1\cdot(\nabla_x\otimes\vec{N}_s + \nabla_x V\otimes\vec{N}_s))\cdot\vec{N}_s = \|\vec{N}_s\|\mathrm{div}_x(\mathbb{D}_1(\nabla_x\|\vec{N}_s\| + \nabla_x V\|\vec{N}_s\|)) - \mathbb{D}_1\cdot(\nabla_x\otimes\vec{N}_s) : (\nabla_x\otimes\vec{N}_s) + \nabla_x\|\vec{N}_s\|\cdot\mathbb{D}_1(\nabla_x\|\vec{N}_s\|).$$

Proof. We have

$$\begin{aligned}
\mathrm{div}_x(\mathbb{D}_1(\nabla_x)\|\vec{N}_s\|^2) &= \mathrm{div}_x(\mathbb{D}_1(\nabla_x)(\vec{N}_s\cdot\vec{N}_s)) = \sum_i \partial_i(\sum_j \mathbb{D}_1^{ij}\partial_j(\vec{N}_s\cdot\vec{N}_s))\\
&= 2\sum_i \partial_i(\sum_j \mathbb{D}_1^{ij}(\partial_j\vec{N}_s\cdot\vec{N}_s)) = 2\sum_{i,j,k}\partial_i(\mathbb{D}_1^{ij}\partial_j\vec{N}_s^k\vec{N}_s^k)\\
&= 2\sum_{i,j,k}\partial_i(\mathbb{D}_1^{ij}\partial_j\vec{N}_s^k)\vec{N}_s^k + 2\sum_{i,j,k}\mathbb{D}_1^{ij}\partial_j\vec{N}_s^k\partial_i\vec{N}_s^k\\
&= 2\sum_{i,k}\partial_i(\mathbb{D}_1\cdot(\nabla_x\otimes\vec{N}_s))_{ik}\vec{N}_s^k + 2\sum_{i,k}(\mathbb{D}_1\cdot(\nabla_x\otimes\vec{N}_s))_{ik}\partial_i\vec{N}_s^k\\
&= 2\mathrm{div}_x(\mathbb{D}_1\cdot(\nabla_x\otimes\vec{N}_s))\cdot\vec{N}_s + 2\mathbb{D}_1\cdot(\nabla_x\otimes\vec{N}_s) : (\nabla_x\otimes\vec{N}_s).
\end{aligned}$$

In other side, we have

$$\begin{aligned}
\mathrm{div}_x(\mathbb{D}_1(\nabla_x\|\vec{N}_s\|^2)) &= 2\mathrm{div}_x(\|\vec{N}_s\|\mathbb{D}_1(\nabla_x\|\vec{N}_s\|))\\
&= 2\nabla_x\|\vec{N}_s\|\cdot\mathbb{D}_1(\nabla_x\|\vec{N}_s\|) + 2\|\vec{N}_s\|\mathrm{div}_x(\mathbb{D}_1(\nabla_x\|\vec{N}_s\|)).
\end{aligned}$$

Identifying these two equations, one obtains

$$\begin{aligned}
\mathrm{div}_x(\mathbb{D}_1\cdot(\nabla_x\otimes\vec{N}_s))\cdot\vec{N}_s &= \|\vec{N}_s\|\mathrm{div}_x(\mathbb{D}_1(\nabla_x\|\vec{N}_s\|)) + \nabla_x\|\vec{N}_s\|\cdot\mathbb{D}_1(\nabla_x\|\vec{N}_s\|)\\
&\quad -\mathbb{D}_1\cdot(\nabla_x\otimes\vec{N}_s) : (\nabla_x\otimes\vec{N}_s).
\end{aligned}$$

A similar calculations give

$$\mathrm{div}_x(\mathbb{D}_1\cdot(\nabla_x V\otimes\vec{N}_s)).\vec{N}_s = \|\vec{N}_s\|\mathrm{div}_x(\mathbb{D}_1(\nabla_x V)\|\vec{N}_s\|).$$

■

Therefore, equation (2.5.30) becomes

$$\|\vec{N}_s\|\left\{\partial_t\|\vec{N}_s\| - \mathrm{div}_x(\mathbb{D}_1(\nabla_x\|\vec{N}_s\| + \nabla_x V\|\vec{N}_s\|))\right\} = -\mathbb{D}_1\cdot(\nabla_x\otimes\vec{N}_s):(\nabla_x\otimes\vec{N}_s)$$
$$+2(\mathbb{D}_3(\nabla_x)\times\vec{N}_s)\cdot\vec{N}_s + (\mathbb{D}_4 - tr\mathbb{D}_4)(\vec{N}_s)\cdot\vec{N}_s + \nabla_x\|\vec{N}_s\|\cdot\mathbb{D}_1(\nabla_x\|\vec{N}_s\|) - 2\frac{\|\vec{N}_s\|^2}{\tau_{sf}}$$
$$\leq -\mathbb{D}_1\cdot(\nabla_x\otimes\vec{N}_s):(\nabla_x\otimes\vec{N}_s) + 2(\mathbb{D}_3(\nabla_x)\times\vec{N}_s)\cdot\vec{N}_s$$
$$+(\mathbb{D}_4 - tr\mathbb{D}_4)(\vec{N}_s)\cdot\vec{N}_s + \nabla_x\|\vec{N}_s\|\cdot\mathbb{D}_1(\nabla_x\|\vec{N}_s\|). \quad (2.5.31)$$

Lemma 2.5.15. *We have,*

$$-\mathbb{D}_1\cdot(\nabla_x\otimes\vec{N}_s):(\nabla_x\otimes\vec{N}_s) + 2(\mathbb{D}_3(\nabla_x)\times\vec{N}_s)\cdot\vec{N}_s$$
$$+(\mathbb{D}_4 - tr\mathbb{D}_4)(\vec{N}_s)\cdot\vec{N}_s + \nabla_x\|\vec{N}_s\|\cdot\mathbb{D}_1(\nabla_x\|\vec{N}_s\|)\leq 0. \quad (2.5.32)$$

Proof. Let $W\in(L^2_{\mathcal{M}}(\mathbb{R}^3))^3$ be the solution of

$$Q(W) = {}^t(\nabla_x\otimes\vec{N}_s)(v\mathcal{M}) + (\vec{\Omega}_o\times\vec{N}_s)\mathcal{M}.$$

We have

$$W = -{}^t(\nabla_x\otimes\vec{N}_s)(\theta_1) - \theta_2\times\vec{N}_s.$$

The operator Q is negative on $L^2_{\mathcal{M}}$. Then, $\displaystyle\int_{\mathbb{R}^3}\frac{Q(W)\otimes W}{\mathcal{M}}dv$ is a negative matrix. Indeed, for all $\xi\in\mathbb{R}^3$, we have

$$\left(\int_{\mathbb{R}^3}\frac{Q(W)\otimes W}{\mathcal{M}}dv\right)(\xi)\cdot\xi = \int_{\mathbb{R}^3}\frac{(Q(W)\cdot\xi)(W\cdot\xi)}{\mathcal{M}}dv = \langle Q(W\cdot\xi), W\cdot\xi\rangle_{\mathcal{M}}\leq 0.$$

This implies that, for all $\xi\in\mathbb{R}^3$,

$$\langle Q(W\cdot\xi), W\cdot\xi\rangle_{\mathcal{M}}\geq tr\left(\int_{\mathbb{R}^3}\frac{Q(W)\otimes W}{\mathcal{M}}dv\right)\|\xi\|^2 = \left(\int_{\mathbb{R}^3}\frac{Q(W)\cdot W}{\mathcal{M}}dv\right)\|\xi\|^2.$$

Particularly, taking $\xi = \vec{N}_s$, one gets the following inequality :

$$\|\vec{N}_s\|^2\int_{\mathbb{R}^3}\frac{Q(W)\cdot W}{\mathcal{M}}dv\leq\int_{\mathbb{R}^3}\frac{(Q(W)\cdot\vec{N}_s)(W\cdot\vec{N}_s)}{\mathcal{M}}dv, \quad (2.5.33)$$

which yields (2.5.32). Indeed, we have

$$\begin{aligned}\frac{Q(W)\cdot W}{\mathcal{M}} &= -{}^t(\nabla_x\otimes\vec{N}_s)(v)\cdot{}^t(\nabla_x\otimes\vec{N}_s)(\theta_1) - {}^t(\nabla_x\otimes\vec{N}_s)(v)\cdot(\theta_2\times\vec{N}_s)\\ &\quad -{}^t(\nabla_x\otimes\vec{N}_s)(\theta_1)\cdot(\vec{\Omega}_o\times\vec{N}_s) - (\vec{\Omega}_o\times\vec{N}_s)\cdot(\theta_2\times\vec{N}_s)\\ &= -(\nabla_x\otimes\vec{N}_s)\cdot{}^t(\nabla_x\otimes\vec{N}_s):(v\otimes\theta_1) - (\nabla_x\otimes\vec{N}_s):(v\otimes(\theta_2\times\vec{N}_s))\\ &\quad -(\nabla_x\otimes\vec{N}_s):(\theta_1\otimes(\vec{\Omega}_o\times\vec{N}_s)) - (\vec{\Omega}_o\times\vec{N}_s)\cdot(\theta_2\times\vec{N}_s),\end{aligned}$$

where we have used the following identity : $A(v)\cdot B(w) = ({}^tA\cdot B) : (v\otimes w)$. Integrating with respect to v, the first term of the right hand side of the last equation is $\mathbb{D}_1(\nabla_x\otimes\vec{N}_s) : (\nabla_x\otimes\vec{N}_s)$. In addition,

$$
\begin{aligned}
&(\nabla_x\otimes\vec{N}_s) : \int_{\mathbb{R}^3} v\otimes(\theta_2\times\vec{N}_s)dv = \sum_{i,j}\partial_i\vec{N}_s^j\int_{\mathbb{R}^3} v_i(\theta_2\times\vec{N}_s)_j dv\\
&= \sum_{i,j}\partial_i\left(\vec{N}_s^j\int_{\mathbb{R}^3} v_i(\theta_2\times\vec{N}_s)_j dv\right) - \sum_{i,j}\vec{N}_s^j\int_{\mathbb{R}^3}\partial_i(v_i\theta_2\times\vec{N}_s)_j dv\\
&= \sum_{j}\partial_i\left(\int_{\mathbb{R}^3} v_i(\theta_2\times\vec{N}_s)\cdot\vec{N}_s dv\right) - \sum_{i,j}\vec{N}_s^j\int_{\mathbb{R}^3}(v_i\partial_i\theta_2\times\vec{N}_s)_j dv - \sum_{i,j}\vec{N}_s^j\int_{\mathbb{R}^3}(v_i\theta_2\times\partial_i\vec{N}_s)_j dv\\
&= 0-0-\sum_j((\sum_i\int_{\mathbb{R}^3} v_i\theta_2\partial_i)\times\vec{N}_s)_j\vec{N}_s^j = -\sum_j({}^t\mathbb{D}_2(\nabla_x)\times\vec{N}_s)_j\vec{N}_s^j = -(\mathbb{D}_3(\nabla_x)\times\vec{N}_s)\cdot\vec{N}_s.
\end{aligned}
$$

Similarly, one can verify that $(\nabla_x\otimes\vec{N}_s) : \int_{\mathbb{R}^3}\theta_1\otimes(\vec{\Omega}_o\times\vec{N}_s)dv = -(\mathbb{D}_3(\nabla_x)\times\vec{N}_s)\cdot\vec{N}_s$. Moreover,

$$
\begin{aligned}
&\int_{\mathbb{R}^3}(\vec{\Omega}_o\times\vec{N}_s)\cdot(\theta_2\times\vec{N}_s)dv = \int_{\mathbb{R}^3}((\theta_2\times\vec{N}_s)\times\vec{\Omega}_o)\cdot\vec{N}_s dv\\
&= \left((\int_{\mathbb{R}^3}\vec{\Omega}_o\cdot\theta_2 dv)\vec{N}_s - \int_{\mathbb{R}^3}(\vec{\Omega}_o\cdot\vec{N}_s)\theta_2\right)\cdot\vec{N}_s = (tr(\mathbb{D}_4)-\mathbb{D}_4)(\vec{N}_s)\cdot\vec{N}_s.
\end{aligned}
$$

Finally, a straightforward computations of the right hand side of (2.5.33) yield : $Q(W)\cdot\vec{N}_s = \|\vec{N}_s\|v\cdot\nabla_x(\|\vec{N}_s\|)\mathcal{M}$ and $W\cdot\vec{N}_s = -\|\vec{N}_s\|\theta_1\cdot\nabla_x(\|\vec{N}_s\|)$. Therefore,

$$
\begin{aligned}
\int_{\mathbb{R}^3}\frac{(Q(W)\cdot\vec{N}_s)(W\cdot\vec{N}_s)}{\mathcal{M}} &= -\|\vec{N}_s\|^2\int_{\mathbb{R}^3} v\cdot\nabla_x(\|\vec{N}_s\|)\ \ \theta_1\cdot\nabla_x(\|\vec{N}_s\|)dv\\
&= -\|\vec{N}_s\|^2\mathbb{D}_1(\nabla_x\|\vec{N}_s\|)\cdot\nabla_x\|\vec{N}_s\|.
\end{aligned}
$$

All these computations together with inequality (2.5.33) give (2.5.32).

■

To complete the proof of Theorem 2.5.3, (2.5.31) and (2.5.32) and the first equation of (2.5.6) imply that $(N_c - 2\|\vec{N}_s\|)$ verifies

$$
\partial_t(N_c-2\|\vec{N}_s\|) - \mathrm{div}_x(\mathbb{D}_1(\nabla_x(N_c-2\|\vec{N}_s\|)+\nabla_x V(N_c-2\|\vec{N}_s\|))) \geq 0.
$$

Moreover, since $\dfrac{N_c(0,x)}{2}I_2 + \vec{N}_s(0,x)\cdot\vec{\sigma} = N_{in}(x) \in \mathcal{H}_2^+(\mathbb{C})$ for all $x\in\mathbb{R}^3$, then $N_c(0,.) - 2\|\vec{N}_s(0,.)\| \geq 0$ and we conclude by the maximum principle satisfying by the scalar drift diffusion equation.

2.6 SHE model

Following the same strategy presented in the previous sections, other macroscopic models of two-component or spin vector types can be derived. In this section we are interested in the derivation of the so called SHE model. The Spherical Harmonic Expansion (SHE) model represents a diffusion approximation of the Boltzmann equation when the elastic collisions are supposed to be the dominant scattering mechanism. We refer to [2, 19] and references therein for details about the rigorous derivation of this model and the link with other macroscopic models (Drift-Diffusion, Energy-Transport, etc). The elastic collision operator takes the following form :

$$Q_{el}(F)(v) = \int_{\mathbb{R}^3} \sigma(v, v')\delta(\mathcal{E}(v') - \mathcal{E}(v))(F(v') - F(v))dv' \tag{2.6.1}$$

where, for $v = (\mathcal{E}(v), \omega(v)) \in \mathbb{R}^3$, $\mathcal{E}(v) = \frac{|v|^2}{2}$ is the energy and $\omega(v)$ is the velocity angle. This operator makes relax the distribution function towards a function depending only on the energy of the particles (see Proposition 2.6.1). In other terms, the SHE model describes a situation following the relaxation of the momentum (ω) and preceding the energy relaxation of the particles. It describes an intermediate situation between the kinetic and the diffusion (drift-diffusion) descriptions. Before listing the properties of the elastic operator, we need to recall the Corea formula. For any $\psi \in C^0(\mathbb{R}^3)$ and $\mathcal{E} \in C^1(\mathbb{R}^3, \mathbb{R})$, the Corea formula says

$$\int_{\mathbb{R}^3} \psi(v)dv = \int_{-\infty}^{+\infty} \left(\int_{S_e} \psi(v)dN_e(v) \right) de \tag{2.6.2}$$

where, for any $e \in \mathbb{R}$, $S_e = \{v \in \mathbb{R}^3, \quad \text{such that } \mathcal{E}(v) = e\}$ and $dN_e(v) = \dfrac{dS_e(v)}{\nabla \mathcal{E}(v)}$ with $dS_e(v)$ denotes the Euclidean surface element on S_e. We will also denote, for every $e \in \mathbb{R}$, $N(e) := \displaystyle\int_{S_e} dN_e(v)$.

The following proposition summarizes the main properties of the elastic operator (2.6.1). We refer to [2] for the proof.

Proposition 2.6.1. *The operator Q_{el} (2.6.1) satisfies the following properties.*

1. *$-Q$ is a self-adjoint non negative operator on $L^2(\mathbb{R}^3, \mathcal{H}_2(\mathbb{C}))$.*
2. *The nul set of Q_{el} is given by*

$$N(Q_{el}) = \left\{ F \in L^2(\mathbb{R}^3, \mathcal{H}_2(\mathbb{C})) \ / \ \ F(v) = G(\mathcal{E}(v)) \text{ for some } G \in L^2_N(\mathbb{R}) \right\} \tag{2.6.3}$$

with $L^2_N(\mathbb{R}) = \{F(\mathcal{E}) \in \mathcal{H}_2(\mathbb{C}) / \ \displaystyle\int_{\mathbb{R}} \|F(\mathcal{E})\|_2^2 N(\mathcal{E})d\mathcal{E} < +\infty\}$.

3. *$-Q_{el}$ is coercive on $N(Q_{el})^{\perp}$ and the following coercivity inequality holds for $C > 0$*

$$\langle -Q_{el}(F), F\rangle_{L^2} \geq C\|F - \mathcal{P}(F)\|_{L^2},$$

where $\mathcal{P}(F)(\mathcal{E}) = \displaystyle\int_{S_\mathcal{E}} F(v)dN_\mathcal{E}(v)$ is the orthogonal projection on $N(Q_{el})$.

4. $Im(Q_{el}) = N(Q_{el})^{\perp} = \left\{ F \in L^2(\mathbb{R}^3, \mathcal{H}^2(\mathbb{C})) \;/\; \displaystyle\int_{S_\mathcal{E}} F(v)dN_\mathcal{E}(v) = 0 \; a.e. \mathcal{E} \in \mathbb{R}^+ \right\}.$

As for the previous section, the starting point will be the following scaled Boltzmann equation

$$\frac{\partial F^\varepsilon}{\partial t} + \frac{1}{\varepsilon}(v\cdot\nabla_x F^\varepsilon - \nabla_x V\cdot\nabla_v F^\varepsilon) = \frac{1}{\varepsilon^2}Q_{el}(F^\varepsilon) + \frac{i}{2}[\vec{\Omega}^\varepsilon(x,v)\cdot\vec{\sigma}, F^\varepsilon] + Q_{sf}(F^\varepsilon), \quad (2.6.4)$$

where $\vec{\Omega}^\varepsilon$ is given by (2.5.1) and Q_{el} by (2.6.1). Using the properties of Q_{el}, one can redefine the matrices $\mathbb{D}_i$ (2.5.10) as follows.

Lemma 2.6.2. *Let $\chi_1, \chi_2 \in (L^2(\mathbb{R}^3))^3$ be the unique solutions of*

$$\begin{cases} -Q_{el}(\chi_1) = v, & \displaystyle\int_{S_\mathcal{E}} \chi_1 dN_\mathcal{E}(v) = 0 \; a.e. \; \mathcal{E} \in \mathbb{R}^+, \\ -Q_{el}(\chi_2) = \vec{\Omega}_o, & \displaystyle\int_{S_\mathcal{E}} \chi_2 dN_\mathcal{E}(v) = 0 \; a.e. \; \mathcal{E} \in \mathbb{R}^+, \end{cases} \quad (2.6.5)$$

and let $\mathbb{D}_1, \mathbb{D}_2, \mathbb{D}_3$ and $\mathbb{D}_4$ be the following matrices

$$\begin{aligned} \mathbb{D}_1(\mathcal{E}) &= \int_{S_\mathcal{E}} (\chi_1 \otimes v)dN_\mathcal{E}(v), & \mathbb{D}_2(x,\mathcal{E}) &= \int_{S_\mathcal{E}} (v \otimes \chi_2)dN_\mathcal{E}(v), \\ \mathbb{D}_3(x,\mathcal{E}) &= \int_{S_\mathcal{E}} (\vec{\Omega}_o \otimes \chi_1)dN_\mathcal{E}(v), & \mathbb{D}_4(x,\mathcal{E}) &= \int_{S_\mathcal{E}} (\chi_2 \otimes \vec{\Omega}_o)dN_\mathcal{E}(v). \end{aligned} \quad (2.6.6)$$

Then, for almost $x \in \mathbb{R}^3$ and $\mathcal{E} \in \mathbb{R}^+$, $\mathbb{D}_1(\mathcal{E})$ and $\mathbb{D}_4(x,\mathcal{E})$ are two symmetric positive definite matrices and ${}^t\mathbb{D}_2 = \mathbb{D}_3$. In addition we have,

$$\mathbb{D}_1(\mathcal{E}) \geq C\int_{S_\mathcal{E}} (v \otimes v)dN_\mathcal{E}(v), \quad \mathbb{D}_4(x,\mathcal{E}) \geq C\int_{S_\mathcal{E}} (\vec{\Omega}_o \otimes \vec{\Omega}_o)dN_\mathcal{E}(v), \quad (2.6.7)$$

with a constant $C > 0$ independent on x and $\mathcal{E}$.

The proof of this lemma is straightforward, one can see [2] for details. Taking an Hilbert expansion of F^ε around $\varepsilon = 0$

$$F^\varepsilon = F^0 + \varepsilon F^1 + \varepsilon^2 F^2 + ...,$$

inserting it in (2.6.4) and identifying equal powers of ε, leads to the equations

$$Q_{el}(F^0) = 0, \quad (2.6.8)$$

$$Q_{el}(F^1) = v.\nabla_x F^0 - \nabla_x V.\nabla_v F^0 - \frac{i}{2}[\vec{\Omega}_o \cdot \vec{\sigma}, F^0], \tag{2.6.9}$$

$$Q_{el}(F^2) = \partial_t F^0 + v.\nabla_x F^1 - \nabla_x V.\nabla_v F^1 - \frac{i}{2}[\vec{\Omega}_o \cdot \vec{\sigma}, F^1] - \frac{i}{2}\left[\vec{\Omega}_e \cdot \vec{\sigma}, F^0\right] - Q_{sf}(F^0). \tag{2.6.10}$$

The first equation implies the existence of an energy dependent function $\mathcal{F}(t, x, \mathcal{E})$ such that

$$F^0(t, x, v) = \mathcal{F}(t, x, \mathcal{E}(v)).$$

The right hand side of the second equation (2.6.9) becomes

$$v.\nabla_x F^0 - \nabla_x V.\nabla_v F^0 - \frac{i}{2}[\vec{\Omega}_o \cdot \vec{\sigma}, F^0] = v \cdot (\nabla_x \mathcal{F} - \nabla_x V \partial_{\mathcal{E}} \mathcal{F}) - \frac{i}{2}[\vec{\Omega}_o \cdot \vec{\sigma}, \mathcal{F}]$$

and with (2.6.5), we have

$$F^1 = -\chi_1 \cdot (\nabla_x \mathcal{F} - \nabla_x V \partial_{\mathcal{E}} \mathcal{F}) + \frac{i}{2}[\chi_2 \cdot \vec{\sigma}, \mathcal{F}]. \tag{2.6.11}$$

Using the properties of the Q_{el} (Proposition 2.6.1), equation (2.6.10) admits a solution if and only if the averaging of its right hand side over $S_{\mathcal{E}}$ is equal to zero for almost every $\mathcal{E} \in \mathbb{R}$. This gives after integration over $S_{\mathcal{E}}$

$$N(\mathcal{E})\partial_t \mathcal{F} + \nabla_x.J - \nabla_x V.\partial_{\mathcal{E}} J = S + \frac{i}{2}\left[\int_{S_{\mathcal{E}}} \vec{\Omega}_e(x, v) dN_{\mathcal{E}}(v) \cdot \vec{\sigma}, \mathcal{F}\right] + Q_{sf}(\mathcal{F}) \tag{2.6.12}$$

with

$$J(t, x, \mathcal{E}) = \int_{S_{\mathcal{E}}} v F_1 dN_{\mathcal{E}}(v) \tag{2.6.13}$$

and

$$S = \frac{i}{2}\int_{S_{\mathcal{E}}} [\vec{\Omega}_o \cdot \vec{\sigma}, F^1] dN_{\mathcal{E}}(v). \tag{2.6.14}$$

To obtain the third term of (2.6.12), we proceed as follows. We write for any $\psi = \psi(\mathcal{E}) \in C_0(\mathbb{R})$, a continuous compactly supported function, using the Corea formula (2.6.2),

$$\begin{aligned}\int_{\mathbb{R}^3} \nabla_v F_1 \psi(\mathcal{E}(v)) dv &= -\int_{\mathbb{R}^3} F_1 \nabla_v \psi(\mathcal{E}(v)) dv = -\int_{\mathbb{R}} \int_{S_{\mathcal{E}}} v F_1 \psi'(\mathcal{E}) dN_{\mathcal{E}} d\mathcal{E} \\ &= -\int_{\mathbb{R}} (\int_{S_{\mathcal{E}}} v F_1 dN_{\mathcal{E}}) \psi'(\mathcal{E}) d\mathcal{E} = -\int_{\mathbb{R}} J \psi'(\mathcal{E}) d\mathcal{E}.\end{aligned}$$

One deduces that $\displaystyle\int_{S_{\mathcal{E}}} \nabla_v F_1 dN_{\mathcal{E}} = \partial_{\mathcal{E}} J$. Moreover, an analogous computations as in the proof of Proposition 2.5.7 lead

$$J = -\mathbb{D}_1(\nabla_x \mathcal{F} - \nabla_x V \partial_{\mathcal{E}} \mathcal{F}) + \frac{i}{2}[\mathbb{D}_2(\vec{\sigma}), \mathcal{F}]$$

and

$$S = -\frac{i}{2}[\mathbb{D}_3(\nabla_x - \nabla_x V \partial_{\mathcal{E}}) \cdot \vec{\sigma}, \mathcal{F}] + (\mathbb{D}_4 - tr(\mathbb{D}_4))(\vec{\mathcal{F}}_s) \cdot \vec{\sigma}$$

with $\vec{\mathcal{F}}_s \cdot \vec{\sigma} = \mathcal{F} - \dfrac{tr(\mathcal{F})}{2} I_2$. Thus, to summarize one can deduce the following theorem.

Theorem 2.6.3. *Let $T > 0$, $F_{in} \in L^2([0,T] \times \mathbb{R}^6)$, then under Assumptions 2.2.1, 2.2.2, 2.5.1, the weak solutions F^ε of (2.6.4)-(2.1.2) converges weakly to F in $L^\infty([0,T], L^2(\mathbb{R}^6, \mathcal{H}_2(\mathbb{C})))$ such that $F(t,x,v) = \mathcal{F}(t,x,\frac{|v|^2}{2})$ for some $\mathcal{F}(t,x,\mathcal{E}) \in L^\infty([0,T], L^2_N(dxd\mathcal{E}))$. In addition $\mathcal{F}$ satisfies the following SHE model with spin precession and relaxation effects :*

$$N(\mathcal{E})\partial_t \mathcal{F} + (\nabla_x - \nabla_x V \partial_\mathcal{E}) \cdot \mathcal{J} = \frac{i}{2}[\vec{\Omega}_{SHE} \cdot \vec{\sigma}, \mathcal{F}] + (\mathbb{D}_4 - tr(\mathbb{D}_4))(\vec{\mathcal{F}}_s \cdot \vec{\sigma}) + Q_{sf}(\mathcal{F}),$$

with

$$\mathcal{J} = -\mathbb{D}_1(\nabla_x \mathcal{F} - \nabla_x V \partial_\mathcal{E} \mathcal{F}) + i[\mathbb{D}_2(\vec{\sigma}), \mathcal{F}]$$

$$\vec{\Omega}_{SHE}(x,\mathcal{E}) = (\nabla_x - \nabla_x V \partial_\mathcal{E}) \cdot \mathbb{D}_2(x,\mathcal{E}) + \int_{S_\mathcal{E}} \vec{\Omega}_e(x,v) dN_\mathcal{E}(v)$$

and where $\vec{\mathcal{F}}_s \cdot \vec{\sigma} = \mathcal{F} - \dfrac{tr(\mathcal{F})}{2} I_2$ is the spin part of $\mathcal{F}$.

2.7 Other fluid models for semiconductor spintronics

Review of macroscopic models and moment method. In microelectronics, the macroscopic or fluid models describe the evolution of macroscopic averaged quantities of the distribution function f. These quantities are usually the particle number density $n(t,x)$, the current density $n(t,x)u(t,x)$ (where u is the mean velocity) and the energy density $\mathcal{W}(t,x)$. They are called the moments of f and are given by

$$\begin{pmatrix} n \\ nu \\ \mathcal{W} \end{pmatrix} = \int_{\mathbb{R}^3} \begin{pmatrix} 1 \\ v \\ \frac{|v|^2}{2} \end{pmatrix} f(t,x,v) dv. \tag{2.7.1}$$

These quantities evolve according to balance equations such as mass, momentum, and energy balance. The macroscopic models (Euler, ET, SHE, Drift-Diffusion) can be obtained from the kinetic equation

$$\partial_t f + v \cdot \nabla_x f - \nabla_x V \cdot \nabla_v f = Q(f) \tag{2.7.2}$$

according to the conservations of the collision operator by using the moment method [1, 31, 6, 26, 28, 29, 45]. As an example, assume that the collision operator admits the following conservation properties

$$\int_{\mathbb{R}^3} Q(f) \begin{pmatrix} 1 \\ v \\ \frac{|v|^2}{2} \end{pmatrix} dv = 0. \tag{2.7.3}$$

The moment method consists in multiplying the Boltzmann equation (2.7.2) by $\begin{pmatrix} 1 \\ v \\ \frac{|v|^2}{2} \end{pmatrix}$ and integrating it with respect to v. This gives with (2.7.1) and (2.7.3)

$$\partial_t \begin{pmatrix} n \\ nu \\ \mathcal{W} \end{pmatrix} + \nabla_x \cdot \int_{\mathbb{R}^3} f(t,x,v) \begin{pmatrix} 1 \\ v \\ \frac{|v|^2}{2} \end{pmatrix} v dv = \begin{pmatrix} 0 \\ -n\nabla_x V \\ -nu \cdot \nabla_x V \end{pmatrix}.$$

It can be written also as

$$\begin{cases} \partial_t n + \nabla_x \cdot (nu) = 0 \\ \partial_t (nu) + \nabla_x \cdot \Pi = -n\nabla_x V \\ \partial_t \mathcal{W} + \nabla_x \cdot \Phi = -nu \cdot \nabla_x V, \end{cases} \tag{2.7.4}$$

where $\Pi(t,x)$ and $\Phi(t,x)$ are respectively the pressure tensor and the energy flux given by

$$\Pi = \int_{\mathbb{R}^3} f(v \otimes v) dv \quad \text{and} \quad \Phi = \int_{\mathbb{R}^3} f \frac{|v|^2}{2} v dv.$$

System (2.7.4) is not closed because Π and ϕ can not be expressed in terms of $n, nu, \mathcal{W}$. To close system (2.7.4), one needs to find a distribution function which allows to compute these quantities in terms of the conserved variables (2.7.1). The Levermore's methodology [31] consists in using the entropy minimization principle. Let $n, T \in \mathbb{R}^+$ and $u \in \mathbb{R}^3$ be fixed, the entropy minimization problem is stated as

$$\min_f \left\{ h(f) / \quad \int_{\mathbb{R}^3} f \begin{pmatrix} 1 \\ v \\ \frac{|v|^2}{2} \end{pmatrix} dv = \begin{pmatrix} n \\ nu \\ \mathcal{W} \end{pmatrix} \right\}, \tag{2.7.5}$$

with $\mathcal{W} = \frac{n|u|^2}{2} + \frac{3}{2} nT$. The entropy h is a convexe function. It describes the statistics of the particles. In the Boltzmann statistics, h is given by

$$h(x) = x(\ln x - 1). \tag{2.7.6}$$

Problem (2.7.5) with (2.7.6) admits a unique solution given by the Maxwellian distribution

$$M_{n,u,T}(v) = \frac{n}{(2\pi T)^{\frac{3}{2}}} \exp\left(-\frac{|v-u|^2}{2T} \right). \tag{2.7.7}$$

The parameters n, u and T are such that n, nu and $\mathcal{W}$ respectively are its density, momentum and energy

$$\int_{\mathbb{R}^3} M_{n,u,T} \begin{pmatrix} 1 \\ v \\ \frac{|v|^2}{2} \end{pmatrix} dv = \begin{pmatrix} n \\ nu \\ \mathcal{W} \end{pmatrix}.$$

Replacing f by $M_{n,u,T}$ in (2.7.4), one obtains the Euler model

$$\begin{cases} \partial_t n + \nabla_x \cdot (nu) = 0, \\ \partial_t (nu) + \nabla_x \cdot (nu \otimes u) + \nabla_x (nT) = -n \nabla_x V, \\ \partial_t \mathcal{W} + \nabla_x \cdot (\mathcal{W} u) + \nabla_x \cdot (nuT) = -nu \cdot \nabla_x V. \end{cases}$$

The Euler model can be obtained from the Boltzmann equation by hydrodynamic limit. It consists in taking the scaled equation

$$\partial_t f^\varepsilon + v \cdot \nabla_x f^\varepsilon - \nabla_x V \cdot \nabla_v f^\varepsilon = \frac{1}{\varepsilon} Q(f^\varepsilon)$$

and getting ε goes to zero. In the hydrodynamic limit, we don't need to know the exact form of the collision operator. It is sufficient to fix some properties satisfied by Q. To obtain for example the Euler model, Q must satisfies the conservation properties (2.7.3) ; the null space (or the local equilibrium) must be given by the maxwellians (2.7.7). In addition, Q must satisfies some entropy decay.

In our case, the distribution is a matrix valued function. To derive maxwellian functions, we propose to study the following entropy problem. Let $\vec{M} = (M_i)_{i=1}^d$ be a vector of 2×2 hermitian matrices, M_i. It represents the vector of the moments of the distribution function. Let $\vec{\mu}(v) = (\mu_i)_{i=1}^d$ be the vector of monomials of v $(1, v, \frac{|v|^2}{2}, \ldots)$. The entropy minimization problem writes as

$$\min_F \{H(F) = tr(h(F))/ \quad \int_{\mathbb{R}^3} \vec{\mu}(v) F dv = \vec{M}\}. \tag{2.7.8}$$

The entropy writes as $H(F) = tr(h(F))$ with h is a convexe function. The expression $h(F)$ refers to the matrix obtained by acting the function h onto F by functional calculus i.e. $h(F)$ has the same eigenbasis as F and has eigenvalues $h(\lambda_s)$ where λ_s are the eigenvalues of F.

The solution of (2.7.8) is easily found and is given by

$$\mathcal{M}_{\vec{\alpha}} = (h')^{-1}(\vec{\alpha} \cdot \vec{\mu}(v))$$

if the derivative of h is invertible. The vector $\vec{\alpha} = (\alpha_i)_{i=1}^d$ is a vector of 2×2 hermitian matrices such that

$$\int_{\mathbb{R}^3} \mathcal{M}_{\vec{\alpha}} \mu_i(v) dv = M_i, \qquad \forall 0 \leq i \leq d. \tag{2.7.9}$$

When h is given by the Boltzmann statistics (2.7.6), the maxwellian becomes

$$\mathcal{M}_{\vec{\alpha}} = \exp(\vec{\alpha} \cdot \vec{\mu}). \tag{2.7.10}$$

2.7.1 Energy-Transport model

The Energy-Transport (ET) model is a diffusion model constituted of a balance equation for the electron density and an energy balance equation [3, 4, 14, 19]. To derive ET Model for semiconductor spintronics, we take the Boltzmann equation in the diffusion scaling (2.5.2). The collision operator Q must now conserve only the mass and the energy. This means

$$\int_{\mathbb{R}^3} Q(f) \begin{pmatrix} 1 \\ \frac{|v|^2}{2} \end{pmatrix} dv = 0. \tag{2.7.11}$$

Following the Levermore's moment method, for any distribution function $F(v)$, we construct the maxwellian $\mathcal{M}_F$ associated to F as the solution of (2.7.8) with h given by (2.7.6), $\vec{\mu}(v) = \begin{pmatrix} 1 \\ \frac{|v|^2}{2} \end{pmatrix}$, and $\vec{M} = \int_{\mathbb{R}^3} F\vec{\mu}(v)dv$. More precisely, $\mathcal{M}_F$ is the solution of

$$\min_G \left\{ H(G) = \langle G, (\log(G) - I_2)\rangle_2 / \quad \int_{\mathbb{R}^3} (G - F) \begin{pmatrix} 1 \\ \frac{|v|^2}{2} \end{pmatrix} dv = 0 \right\}.$$

Then, by (2.7.10)-(2.7.9), $\mathcal{M}_F$ is given by

$$\mathcal{M}_F(v) = \mathcal{M}[A, C] := \exp\left(A + C\frac{|v|^2}{2}\right) \tag{2.7.12}$$

with $A \in \mathcal{H}_2(\mathbb{C})$ and $C \in \mathcal{H}_2(\mathbb{C})$ are such that

$$\int_{\mathbb{R}^3} \mathcal{M}[A, C] \begin{pmatrix} 1 \\ \frac{|v|^2}{2} \end{pmatrix} dv = \int_{\mathbb{R}^3} F \begin{pmatrix} 1 \\ \frac{|v|^2}{2} \end{pmatrix} dv. \tag{2.7.13}$$

Let now the collision operator be given by the following BGK simple form

$$Q(F) = \mathcal{M}[A, C] - F, \tag{2.7.14}$$

where $\mathcal{M}[A, C]$ is defined by (2.7.12) and A and C are relied to F with (2.7.13). Let us, before listing the properties of this operator, gives some properties satisfied by log as function on $\mathcal{H}_2^+(\mathbb{C})$.

Lemma 2.7.1. *1. For all $F \in \mathcal{H}_2^+(\mathbb{C})$, $\log(F)$ is the unique matrix in $\mathcal{H}_2(\mathbb{C})$ satisfying $e^{\log(F)} = F$. Writing $F = f_c I_2 + \vec{f_s} \cdot \vec{\sigma}$, then we have*

$$\log(F) = \frac{1}{2}\log(f_c^2 - |\vec{f_s}|^2)I_2 + \frac{1}{2}\log\left(\frac{f_c - |\vec{f_s}|}{f_c + |\vec{f_s}|}\right)\frac{\vec{f_s}}{|\vec{f_s}|} \cdot \vec{\sigma} \tag{2.7.15}$$

if $\vec{f_s} \neq 0$. Its eigenvalues are then $\log(f_c - |\vec{f_s}|)$ and $\log(f_c + |\vec{f_s}|)$.

2. For all $F, G \in \mathcal{H}_2^+(\mathbb{C})$, the following properties hold.

(a) *If F and G commutate, then* $\log(F \cdot G) = \log(F) + \log(G)$

(b) *If F is invertible then* $\log(F^{-1}) = -\log(F)$

(c) *The function* log *is strictly increasing which means that*

$$\langle (F - G), (\log F - \log G) \rangle_2 \geq 0 \tag{2.7.16}$$

and

$$\langle (F - G), (\log F - \log G) \rangle_2 = 0 \Leftrightarrow F = G. \tag{2.7.17}$$

The collision operator (2.7.14) satisfies the following properties.

(i) By (2.7.13), Q preserves the mass and the energy i.e. (2.7.11) is satisfied.

(ii) Its null space is spanned by the maxwellians. More precisely

$$Q(F) = 0 \Leftrightarrow \exists (A, C) = (A(t,x), C(t,x)) \text{ s.t. } F = \mathcal{M}[A, C] = \exp\left(A + C\frac{|v|^2}{2}\right).$$

(iii) By construction of $\mathcal{M}_F$ and (2.7.16)-(2.7.17), we have the following entropy decay

$$\int_{\mathbb{R}^3} \langle Q(F), \log F \rangle_2 dv \leq 0, \tag{2.7.18}$$

with equality if and only if $F = \mathcal{M}[A, C]$. Indeed, using (2.7.13), we have

$$\int_{\mathbb{R}^3} \langle Q(F), \log(\mathcal{M}[A, C]) \rangle_2 dv = \int_{\mathbb{R}^3} \left\langle \mathcal{M}[A, C] - F, (A + C\frac{|v|^2}{2}) \right\rangle_2 dv = 0.$$

Therefore, with (2.7.16), we have

$$\begin{aligned} \int_{\mathbb{R}^3} \langle Q(F), \log F \rangle_2 dv &= \int_{\mathbb{R}^3} \langle Q(F), \log F - \log(\mathcal{M}[A, C]) \rangle_2 dv \\ &= \int_{\mathbb{R}^3} \langle \mathcal{M}[A, C] - F, \log F - \log(\mathcal{M}[A, C]) \rangle_2 dv \leq 0. \end{aligned}$$

We state now the main result of this subsection which consists on formal derivation of ET model with spin rotation and relaxation effects.

Theorem 2.7.2. *Let F^ε be the solution of* (2.5.2)-(2.1.2) *with Q given by* (2.7.14). *Then, formally, $F^\varepsilon \to F_0$ as $\varepsilon \to 0$, where*

$F_0(t,x,v) = \mathcal{M}[A,C] = \exp\left(A(t,x) + C(t,x)\frac{|v|^2}{2}\right)$ *and* (A,C) *are solutions of*

$$\begin{aligned}
&\partial_t \int_{\mathbb{R}^3} \mathcal{M}[A,C] \begin{pmatrix} 1 \\ \frac{|v|^2}{2} \end{pmatrix} dv \\
&\qquad - \int_{\mathbb{R}^3} \left(\mathcal{T}^2 \mathcal{M}[A,C] - \frac{i}{2}\mathcal{T}\left[\vec{\Omega}_o \cdot \vec{\sigma}, \mathcal{M}[A,C]\right] \right) \begin{pmatrix} 1 \\ \frac{|v|^2}{2} \end{pmatrix} dv \\
&\qquad = -\frac{i}{2} \int_{\mathbb{R}^3} \left[\vec{\Omega}_o \cdot \vec{\sigma}, \mathcal{T}\mathcal{M}[A,C] - \frac{i}{2}[\vec{\Omega}_o \cdot \vec{\sigma}, \mathcal{M}[A,C]] \right] \begin{pmatrix} 1 \\ \frac{|v|^2}{2} \end{pmatrix} dv \\
&+ \frac{i}{2} \int_{\mathbb{R}^3} \left[\vec{\Omega}_e \cdot \vec{\sigma}, \mathcal{M}[A,C] \right] \begin{pmatrix} 1 \\ \frac{|v|^2}{2} \end{pmatrix} dv + \int_{\mathbb{R}^3} Q_{sf}\left(\mathcal{M}[A,C]\right) \begin{pmatrix} 1 \\ \frac{|v|^2}{2} \end{pmatrix} dv, \quad (2.7.19)
\end{aligned}$$

where $\mathcal{T}$ *denotes the transport operator :* $\mathcal{T} = v \cdot \nabla_x - \nabla_x V \cdot \nabla_v$.

Let us write the Energy-Transport model (2.7.19) under the form of conservation laws. For any pair of functions $(A(t,x), C(t,x))$, we respectively denote by $n[A,C]$, $\mathcal{W}[A,C]$, $\Pi[A,C]$ and $\mathbb{Q}[A,C]$ the particle and energy densities, the pressure tensor and the heat flux tensor associated to A and C. They are given by

$$\begin{pmatrix} n[A,C] \\ \mathcal{W}[A,C] \end{pmatrix} = \int_{\mathbb{R}^3} \mathcal{M}[A,C] \begin{pmatrix} 1 \\ \frac{|v|^2}{2} \end{pmatrix} dv \quad (2.7.20)$$

and

$$\begin{pmatrix} \Pi[A,C] \\ \mathbb{Q}[A,C] \end{pmatrix} = \int_{\mathbb{R}^3} \begin{pmatrix} v \otimes v \\ \frac{|v|^2}{2} v \otimes v \end{pmatrix} \mathcal{M}[A,C] dv. \quad (2.7.21)$$

In addition, we will denote by $\Pi_{\vec{\Omega}_o}[A,C]$ and $\mathbb{Q}_{\vec{\Omega}_o}[A,C]$ the following tensors associated to A, C and $\vec{\Omega}_o$:

$$\begin{pmatrix} \Pi_{\vec{\Omega}_o}[A,C] \\ \mathbb{Q}_{\vec{\Omega}_o}[A,C] \end{pmatrix} = i \int_{\mathbb{R}^3} \begin{pmatrix} 1 \\ \frac{|v|^2}{2} \end{pmatrix} \left[(v \otimes \vec{\Omega}_o)(\vec{\sigma}), \mathcal{M}[A,C] \right] dv. \quad (2.7.22)$$

Lemma 2.7.3. *With notations* (2.7.20), (2.7.21) *and* (2.7.22), *the spin-vector Energy-Transport model* (2.7.19) *can be equivalently written*

$$\begin{aligned}
&\partial_t n + \nabla_x \cdot J^n = \\
&\quad \frac{i}{2} \int_{\mathbb{R}^3} \left[\vec{\Omega}_{ET} \cdot \vec{\sigma}, \mathcal{M}[A,C] \right] dv + \left(\int_{\mathbb{R}^3} \vec{\Omega}_o \times (\vec{\Omega}_o \times \vec{\mathcal{M}}^s[A,C]) dv \right) \cdot \vec{\sigma} + Q_{sf}(n) \quad (2.7.23)
\end{aligned}$$

$$\begin{aligned}
&\partial_t \mathcal{W} + \nabla_x \cdot J^w + J^n \cdot \nabla_x V = \\
&\frac{i}{2} \int_{\mathbb{R}^3} \left[\vec{\Omega}_{ET} \cdot \vec{\sigma}, \mathcal{M}[A,C] \right] \frac{|v|^2}{2} dv + \left(\int_{\mathbb{R}^3} \vec{\Omega}_o \times (\vec{\Omega}_o \times \vec{\mathcal{M}}^s[A,C]) \frac{|v|^2}{2} dv \right) \cdot \vec{\sigma} + Q_{sf}(\mathcal{W}). \quad (2.7.24)
\end{aligned}$$

The mass and energy fluxes are given by

$$J^n = -(\nabla_x \cdot \Pi + n\nabla_x V - \Pi_{\vec{\Omega}_o}) \tag{2.7.25}$$

$$J^w = -(\nabla_x \cdot \mathbb{Q} + \mathcal{W}\nabla_x V + \Pi\nabla_x V - \mathbb{Q}_{\vec{\Omega}_o}) \tag{2.7.26}$$

where Π, $\mathbb{Q}$, $\Pi_{\vec{\Omega}_o}$ *and* $\mathbb{Q}_{\vec{\Omega}_o}$ *are nonlinear functionals of* n *and* $\mathcal{W}$ *through* (2.7.21), (2.7.22) *and* (2.7.20). *Moreover, in the right hand side of the conservation equations* (2.7.23)-(2.7.24), *the effective field* $\vec{\Omega}_{ET}$ *is given by*

$$\vec{\Omega}_{ET} = \mathrm{div}_x(v \otimes \vec{\Omega}_o) - \nabla_x V \cdot \nabla_v \vec{\Omega}_o + \vec{\Omega}_e$$

and $\vec{\mathcal{M}}^s[A, C]$ *is the spin part of* $\mathcal{M}[A, C]$,

$$\vec{\mathcal{M}}^s[A, C] = \mathcal{M}[A, C] - \frac{1}{2} tr\left(\mathcal{M}[A, C]\right) I_2.$$

Remark 2.7.4. *The model* (2.7.23)-(2.7.24) *is constituted of two continuity equations on the density and the energy coupled via the maxwellian* $\mathcal{M}[A, C]$ *with additional rotational and relaxation terms as in the drift diffusion case. The first term of the right side of* (2.7.23) *(or* (2.7.24)*) describes the precession of the spin vector part of* $\mathcal{M}[A, C]$ *around the effective field* $\vec{\Omega}_{ET}$. *The other terms are relaxation terms.*

We discuss now an important property satisfied by the Energy-Transport model (2.7.23)-(2.7.24) : the entropy dissipation. This property is a direct consequence of our derivation, thanks to the entropy dissipation inequality satisfied by the collision operator (2.7.18). More precisely, we define the entropy by

$$\begin{aligned} \mathcal{S}(n, \mathcal{W}) &= \int_{\mathbb{R}^6} \langle \mathcal{M}[A, C], \log(\mathcal{M}[A, C]) - I_2 \rangle_2 dxdv \\ &= \int_{\mathbb{R}^6} \left\langle \mathcal{M}[A, C], A + C\frac{|v|^2}{2} - I_2 \right\rangle_2 dxdv \\ &= \int_{\mathbb{R}^3} (\langle A, n \rangle_2 + \langle C, \mathcal{W} \rangle_2 - tr(n)) dx \end{aligned} \tag{2.7.27}$$

where (A, C) and $(n, \mathcal{W})$ are related through (2.7.20). The function $\mathcal{S}$ is a strictly convex functional of $(n, \mathcal{W})$ and we have :

Lemma 2.7.5. *Let* $(n, \mathcal{W})$ *solves the Energy-Transport model given by the previous lemma. Then, the fluid entropy* $\mathcal{S}(n, \mathcal{W})$ *is a decreasing function of time*

$$\frac{d}{dt}\mathcal{S}(n, \mathcal{W}) \leq 0. \tag{2.7.28}$$

Proof of Theorem 2.7.2. We present now the formal derivation of (2.7.19). We assume that $F^\varepsilon \to F_0$ as $\varepsilon \to 0$ in a space of smooth functions. Multiplying

(2.5.2) by ε^2 and letting $\varepsilon \to 0$, one obtains $Q(F_0) = 0$. This implies that there exist $(A(t,x), C(t,x))$ such that $F_0 = \exp(A + C\frac{|v|^2}{2})$. Now, we introduce the following (Chapman-Enskog) expansion

$$F^\varepsilon = \mathcal{M}_{F^\varepsilon} + \varepsilon F_1^\varepsilon, \tag{2.7.29}$$

where $\mathcal{M}_{F^\varepsilon}$ is the maxwellian associated to F^ε. Thus, we have

$$F_1^\varepsilon = -\frac{1}{\varepsilon} Q(F^\varepsilon). \tag{2.7.30}$$

Inserting this expression into (2.5.2), we get

$$F_1^\varepsilon = -\varepsilon \partial_t F^\varepsilon - \mathcal{T} F^\varepsilon + \frac{i\varepsilon}{2}[\vec{\Omega}^\varepsilon \cdot \vec{\sigma}, F^\varepsilon] + \varepsilon Q_{sf}(F^\varepsilon).$$

Therefore, as $\varepsilon \to 0$, $F_1^\varepsilon \to F_1$ such that

$$F_1 = -\mathcal{T} F_0 + \frac{i}{2}[\vec{\Omega}_o \cdot \vec{\sigma}, F_0]. \tag{2.7.31}$$

Next, multiplying (2.5.2) by $\begin{pmatrix} 1 \\ \frac{|v|^2}{2} \end{pmatrix}$ and using the conservation properties (2.7.11), we get

$$\partial_t \int_{\mathbb{R}^3} F^\varepsilon \begin{pmatrix} 1 \\ \frac{|v|^2}{2} \end{pmatrix} dv + \frac{1}{\varepsilon} \int_{\mathbb{R}^3} \mathcal{T} F^\varepsilon \begin{pmatrix} 1 \\ \frac{|v|^2}{2} \end{pmatrix} dv = \frac{i}{2} \int_{\mathbb{R}^3} [\vec{\Omega}^\varepsilon \cdot \vec{\sigma}, F^\varepsilon] \begin{pmatrix} 1 \\ \frac{|v|^2}{2} \end{pmatrix} dv + \int_{\mathbb{R}^3} Q_{sf}(F^\varepsilon) \begin{pmatrix} 1 \\ \frac{|v|^2}{2} \end{pmatrix} dv$$

Now, using (2.7.29) and the fact that $\int_{\mathbb{R}^3} \mathcal{T}\mathcal{M}_{F^\varepsilon} \begin{pmatrix} 1 \\ \frac{|v|^2}{2} \end{pmatrix} dv = 0$ and $\int_{\mathbb{R}^3} [\vec{\Omega}_o \cdot \vec{\sigma}, \mathcal{M}_{F^\varepsilon}] \begin{pmatrix} 1 \\ \frac{|v|^2}{2} \end{pmatrix} dv = 0$ since $\mathcal{T}\mathcal{M}_{F^\varepsilon}$ and $\vec{\Omega}_o$ are odd vectors with respect to v, one obtains

$$\partial_t \int_{\mathbb{R}^3} F^\varepsilon \begin{pmatrix} 1 \\ \frac{|v|^2}{2} \end{pmatrix} dv + \int_{\mathbb{R}^3} \mathcal{T} F_1^\varepsilon \begin{pmatrix} 1 \\ \frac{|v|^2}{2} \end{pmatrix} dv = \frac{i}{2} \int_{\mathbb{R}^3} [\vec{\Omega}_o \cdot \vec{\sigma}, F_1^\varepsilon] \begin{pmatrix} 1 \\ \frac{|v|^2}{2} \end{pmatrix} dv + \frac{i}{2} \int_{\mathbb{R}^3} [\vec{\Omega}_e \cdot \vec{\sigma}, F^\varepsilon] \begin{pmatrix} 1 \\ \frac{|v|^2}{2} \end{pmatrix} dv + \int_{\mathbb{R}^3} Q_{sf}(F^\varepsilon) \begin{pmatrix} 1 \\ \frac{|v|^2}{2} \end{pmatrix} dv.$$

This gives when $\varepsilon \to 0$

$$\partial_t \int_{\mathbb{R}^3} F_0 \begin{pmatrix} 1 \\ \frac{|v|^2}{2} \end{pmatrix} dv + \int_{\mathbb{R}^3} \mathcal{T} F_1 \begin{pmatrix} 1 \\ \frac{|v|^2}{2} \end{pmatrix} dv = \frac{i}{2} \int_{\mathbb{R}^3} [\vec{\Omega}_o \cdot \vec{\sigma}, F_1] \begin{pmatrix} 1 \\ \frac{|v|^2}{2} \end{pmatrix} dv + \frac{i}{2} \int_{\mathbb{R}^3} [\vec{\Omega}_e \cdot \vec{\sigma}, F_0] \begin{pmatrix} 1 \\ \frac{|v|^2}{2} \end{pmatrix} dv + \int_{\mathbb{R}^3} Q_{sf}(F_0) \begin{pmatrix} 1 \\ \frac{|v|^2}{2} \end{pmatrix} dv.$$

Finally, inserting the expressions of F_0 and F_1 into the last equation leads to (2.7.19).

Proof of Lemma 2.7.5. We multiply (2.5.2) by $\log(F^\varepsilon)$, integrate with respect to x and v

$$\int_{\mathbb{R}^6}\langle\partial_t F^\varepsilon,\log F^\varepsilon\rangle_2 dxdv+\frac{1}{\varepsilon}\int_{\mathbb{R}^6}\langle\mathcal{T}F^\varepsilon,\log F^\varepsilon\rangle_2 dxdv=\frac{1}{\varepsilon^2}\int_{\mathbb{R}^6}\langle Q(F^\varepsilon),\log F^\varepsilon\rangle_2 dxdv$$
$$+\int_{\mathbb{R}^6}\langle\frac{i}{2}[\vec{\Omega}^\varepsilon\cdot\vec{\sigma},F^\varepsilon],\log F^\varepsilon\rangle_2 dxdv+\int_{\mathbb{R}^6}\langle Q_{sf}(F^\varepsilon),\log F^\varepsilon\rangle_2 dxdv. \quad (2.7.32)$$

We have

$$\begin{aligned}\frac{d}{dt}\int_{\mathbb{R}^6}\langle F^\varepsilon,\log F^\varepsilon-I_2\rangle_2 dxdv &= \frac{d}{dt}\int_{\mathbb{R}^6} tr(F^\varepsilon\cdot(\log F^\varepsilon-I_2))dxdv\\ &= \frac{d}{dt}\int_{\mathbb{R}^6} tr(h(F^\varepsilon))dxdv\end{aligned}$$

where $h=x(logx-1)$. In other side we have

$$\frac{d}{dt}tr(h(F^\varepsilon))=\delta_F(trh(.))|_{F^\varepsilon}\cdot\partial_t F^\varepsilon=tr(h'(F^\varepsilon)\cdot\partial_t F^\varepsilon)$$

where $\delta_F(tr(h(.)))$ denotes the Gâteaux derivative of $tr(h(.))$ (see also [18] for more details). We deduce that

$$\frac{d}{dt}tr(h(F^\varepsilon))=tr(\log F^\varepsilon\cdot\partial_t F^\varepsilon)=\langle\partial_t F^\varepsilon,\log F^\varepsilon\rangle_2.$$

Therefore,

$$\int_{\mathbb{R}^6}\langle\partial_t F^\varepsilon,\log F^\varepsilon\rangle_2 dxdv=\frac{d}{dt}\int_{\mathbb{R}^6}\langle F^\varepsilon,\log F^\varepsilon-I_2\rangle_2 dxdv.$$

A similar computations give

$$\int_{\mathbb{R}^6}\langle\mathcal{T}F^\varepsilon,\log F^\varepsilon\rangle_2 dxdv=\int_{\mathbb{R}^6}\mathcal{T}(\langle F^\varepsilon,\log F^\varepsilon-I_2\rangle_2)dxdv=0.$$

Moreover, we have

$$\begin{aligned}\int_{\mathbb{R}^6}\langle\frac{i}{2}[\vec{\Omega}^\varepsilon\cdot\vec{\sigma},F^\varepsilon],\log F^\varepsilon\rangle_2 dxdv &= -\int_{\mathbb{R}^6}\langle(\vec{\Omega}^\varepsilon\times\vec{f}_s^\varepsilon)\cdot\vec{\sigma},\log F^\varepsilon\rangle_2 dxdv\\ &= -2(\vec{\Omega}^\varepsilon\times\vec{f}_s^\varepsilon)\cdot\vec{g}_s^\varepsilon,\end{aligned}$$

where $\vec{f}_s^\varepsilon$ is the spin part of F^ε and $\vec{g}_s^\varepsilon$ the spin part of $log(F^\varepsilon)$. With (2.7.15), $\vec{g}_s^\varepsilon$ is parallel to $\vec{f}_s^\varepsilon$ and we conclude that

$$\int_{\mathbb{R}^6}\langle\frac{i}{2}[\vec{\Omega}^\varepsilon\cdot\vec{\sigma},F^\varepsilon],\log F^\varepsilon\rangle_2 dxdv=0.$$

In other side, using the entropy decay property of Q (2.7.18), the first term of the right hand side of (2.7.32) is negative. In addition, the third term of the right hand side of (2.7.32) is also negative. Indeed, we have

$$\left\langle tr(F^\varepsilon) - 2F^\varepsilon, \log\left(\frac{tr(F^\varepsilon)}{2}\right) I_2 \right\rangle_2 = -2\log\left(\frac{tr(F^\varepsilon)}{2}\right) tr(\vec{f}_s^{\,\varepsilon} \cdot \vec{\sigma}) = 0.$$

Then,

$$\begin{aligned}
\int_{\mathbb{R}^6} \langle Q_{sf}(F^\varepsilon), \log F^\varepsilon\rangle_2 dxdv &= \frac{1}{\tau_{sf}} \int_{\mathbb{R}^6} \langle tr(F^\varepsilon) - 2F^\varepsilon, \log F^\varepsilon\rangle_2 dxdv \\
&= \frac{1}{\tau_{sf}} \int_{\mathbb{R}^6} \left\langle tr(F^\varepsilon) - 2F^\varepsilon, \log F^\varepsilon - \log\left(\frac{tr(F^\varepsilon)}{2}\right)\right\rangle_2 dxdv \\
&= \frac{1}{\tau_{sf}} \int_{\mathbb{R}^6} \langle tr(F^\varepsilon) - 2F^\varepsilon, \log(2F^\varepsilon) - \log(tr(F^\varepsilon))\rangle_2 \, dxdv \\
&\leq 0 \qquad \text{(in view of (2.7.16))}.
\end{aligned}$$

As a conclusion, the solution of (2.5.2) with (2.7.14) satisfies

$$\frac{d}{dt} \int_{\mathbb{R}^6} \langle F^\varepsilon, \log F^\varepsilon - I_2\rangle_2 dxdv \leq 0.$$

To complete the proof, we pass to the limit $\varepsilon \to 0$. This ends the proof of the lemma since F^ε converges to $F_0 = \exp(A + C\frac{|v|^2}{2})$ where (A, C) is the solution of the spin-vector Energy-Transport model (2.7.19).

2.7.2 Drift-Diffusion with Fermi-Dirac statistics

The nonlinear BGK approximation of the collision operator for Fermi-Dirac statistics, when we consider a Boltzmann equation with scalar distribution function f, takes the form

$$Q(f) = \int_{\mathbb{R}^3} \sigma(v, v') \left[\mathcal{M}(v) f(v')(1 - f(v)) - \mathcal{M}(v') f(v)(1 - f(v'))\right] dv' \qquad (2.7.33)$$

where $\mathcal{M}$ is given by (2.1.5). We refer to [27] for the study of such operator. We list in the following lemma the main properties satisfied by (2.7.33).

Lemma 2.7.6. *Assume that the cross-section verifies Assumption 2.2.1. Let* $A = \{f \in L^1(\mathbb{R}^3)\,;\, 0 < f < 1 \text{ a.e.}\}$ *be the set of admissible functions. Then,*

1. *the operator* Q *given by* (2.7.33) *is a bounded operator on* A *in* $L^1(\mathbb{R}^3)$.
2. *For any* $f \in A$, *we have the following entropy inequality*

$$H(f) = \int_{\mathbb{R}^3} Q(f) \log\left(\frac{f}{(1-f)M_V}\right) dv \leq 0, \qquad (2.7.34)$$

where M_V is the maxwellian associated to the potential V given by

$$M_V := \frac{1}{(2\pi)^{\frac{3}{2}}} e^{-\frac{1}{2}|v|^2 - V}.$$

.

3. *The following statements are equivalent :*

   (i) $f \in A$ *and* $H(f) = 0$

   (ii) $f \in A$ *and* $Q(f) = 0$

   (iii) *there exists* $\mu \in \mathbb{R}$ *such that* $f(v) = (1 + e^{\frac{|v|^2}{2} - \mu})^{-1}$.

Inspired from the scalar case, we consider the following space of admissible functions

$$\mathcal{A} = \{F \in L^1(\mathbb{R}^3; \mathcal{H}_2(\mathbb{C}))\,; \quad 0 \prec F(v) \prec I_2 \; a.e.v\} \tag{2.7.35}$$

when, for two hermitian matrices A and B, the relation $A \prec B$ means that $(B - A)$ is a positive defined matrix. We will construct a collision operator Q_{FD} with 2×2 hermitian matrix value admitting the following properties inspired also from the scalar case :

1. Q_{FD} preserves the mass : $\int_{\mathbb{R}^3} Q_{FD} dv = 0$.
2. For every $F \in \mathcal{A}$, Q admits the following entropy inequality

$$H(F) = \int_{\mathbb{R}^3} Q_{FD}(F) \log(F(I_2 - F)^{-1} M_V^{-1}) dv \leq 0$$

3. $H(F) = 0 \Leftrightarrow Q_{FD}(F) = 0 \Leftrightarrow F = \mathcal{M}_F$.
   Here $\mathcal{M}_F$ denotes the maxwellian associated to F with the Fermi-Dirac statistics given by

$$\mathcal{M}_F = \left(I_2 + e^{\frac{|v|^2}{2} - \Pi} \right)^{-1} \tag{2.7.36}$$

   where Π is a unique matrix belonging to $\mathcal{H}_2(\mathbb{C})$ such that

$$\int_{\mathbb{R}^3} \mathcal{M}_F dv = \int_{\mathbb{R}^3} F dv. \tag{2.7.37}$$

We set as for the Energy-Transport case

$$Q_{FD}(F) = \mathcal{M}_F - F. \tag{2.7.38}$$

The maxwellian (2.7.36) with (2.7.37) can also be seen as the solution of an entropy minimization problem. When the only conserved moment is the density or the mass ; the convenient entropy concept is the relative entropy. It is given for Fermi-Dirac statistics by

$$h_{FD}(F) = F \left(\log F + \frac{|v|^2}{2} + V \right) + (I_2 - F) \log (I_2 - F)\,. \tag{2.7.39}$$

For any $F \in \mathcal{A}$ fixed, the solution of

$$\min_{G\in\mathcal{A}} \left\{ tr(h_{FD}(G))/ \quad \int_{\mathbb{R}^3} G dv = \int_{\mathbb{R}^3} F dv \right\}$$

is nothing but $\mathcal{M}_F$ given by (2.7.36)-(2.7.37). Besides, one can verify, by direct computations using decomposition of the matrices into charge and spin parts, that problem (2.7.36)-(2.7.37) is well posed and admits a unique solution. This is the aim of the following lemma and proposition where their proofs are left to the reader.

Lemma 2.7.7. *Let $\Pi = \pi_c I + \vec{\pi}_s \cdot \vec{\sigma} \in \mathcal{H}_2(\mathbb{C})$ and $F \in L^1(\mathbb{R}^3, \mathcal{H}_2^+(\mathbb{C}))$, then $\mathcal{M}_F$ defined by* (2.7.36) *belongs to $\mathcal{A}$. In addition, we have*

$$\mathcal{M}_F = \alpha_c I_2 + \vec{\alpha}_s \cdot \vec{\sigma} \tag{2.7.40}$$

such that $\alpha_c = FD(\pi_c), \vec{\alpha}_s = 0$ if $\vec{\pi}_s = 0$ and if $\vec{\pi}_s \neq 0$, we have

$$\alpha_c = \frac{1}{2}(FD(\pi_c + |\vec{\pi}_s|) + FD(\pi_c - |\vec{\pi}_s|)) \tag{2.7.41}$$

$$\vec{\alpha}_s = \frac{1}{2}(FD(\pi_c + |\vec{\pi}_s|) - FD(\pi_c - |\vec{\pi}_s|))\frac{\vec{\pi}_s}{|\vec{\pi}_s|}. \tag{2.7.42}$$

The function $FD(.)$ on $\mathbb{R}$ denotes the Fermi-Dirac distribution given by

$$FD(\phi) = \left(1 + e^{\frac{|v|^2}{2} - \phi}\right)^{-1}, \quad \forall \phi \in \mathbb{R}. \tag{2.7.43}$$

Proposition 2.7.8. *Let $F = F(v) \in L^1(\mathbb{R}^3, \mathcal{H}_2^+(\mathbb{C}))$. Then, there exists a unique 2×2 hermitian matrix Π independent of v satisfying* (2.7.37). *In addition, if we write $\Pi = \pi_c I_2 + \vec{\pi}_s \cdot \vec{\sigma}$ and $\rho := \int_{\mathbb{R}^3} F(v) dv = \rho_c I_2 + \vec{\rho}_s \cdot \vec{\sigma}$, then* (2.7.37) *is equivalent to*

$$\begin{cases} \displaystyle\int_{\mathbb{R}^3} FD(\pi_c + |\vec{\pi}_s|)(v) dv = \rho_c + |\vec{\rho}_s| \\ \displaystyle\int_{\mathbb{R}^3} FD(\pi_c - |\vec{\pi}_s|)(v) dv = \rho_c - |\vec{\rho}_s| \\ \text{and} \quad \dfrac{\vec{\pi}_s}{|\vec{\pi}_s|} = \dfrac{\vec{\rho}_s}{|\vec{\rho}_s|} \quad \text{if } \vec{\rho}_s \neq 0, \end{cases} \tag{2.7.44}$$

where FD is given by (2.7.43).

The newt proposition summarizes the main properties of the collision operator (2.7.38).

Proposition 2.7.9. *The operator Q_{FD} defined by* (2.7.38), (2.7.36) *and* (2.7.37) *satisfies the following properties.*

1. *Q_{FD} is bounded on $L^1(\mathbb{R}^3;\mathcal{H}_2^+(\mathbb{C}))$ i.e. there exists a constant C such that for all $F \in L^1(\mathbb{R}^3;\mathcal{H}_2^+(\mathbb{C}))$*

$$\|Q_{FD}(F)\|_{L^1(\mathbb{R}^3;\mathcal{H}_2^+(\mathbb{C}))} \leq C\|F\|_{L^1(\mathbb{R}^3;\mathcal{H}_2^+(\mathbb{C}))}. \tag{2.7.45}$$

2. *For all $F \in \mathcal{A}$, we have the following H-Theorem (or entropy decay)*

$$\mathcal{H}(F) := \int_{\mathbb{R}^3} Q_{FD}(F) : \overline{\left[\log(F(I_2 - F)^{-1}M_V^{-1})\right]} \leq 0. \tag{2.7.46}$$

3. *The following statements are equivalent*

   (i) *$F \in \mathcal{A}$ and $\mathcal{H}(F) = 0$.*

   (ii) *$F \in \mathcal{A}$ and $Q_{FD}(F) = 0$.*

   (iii) *there exists $\Pi \in \mathcal{H}_2(\mathbb{C})$ such that $F = \left(I_2 + e^{\frac{|v|^2}{2}-\Pi}\right)^{-1}$.*

Proof. 1. For any $\Pi \in \mathcal{H}_2(\mathbb{C})$, the matrix $\mathcal{M}_F$ given by (2.7.40), (2.7.41), (2.7.42) satisfies

$$\begin{aligned}
\|\mathcal{M}_F\|_2^2 &= (\alpha_c I_2 + \vec{\alpha}_s\cdot\vec{\sigma}) : \overline{(\alpha_c I_2 + \vec{\alpha}_s\cdot\vec{\sigma})} = 2(\alpha_c^2 + |\vec{\alpha}_s|^2)\\
&= FD(\pi_c + |\vec{\pi}_s|)^2 + FD(\pi_c - |\vec{\pi}_s|)^2\\
&\leq [FD(\pi_c + |\vec{\pi}_s|) + FD(\pi_c - |\vec{\pi}_s|)]^2.
\end{aligned}$$

Let $F \in L^1(\mathbb{R}^3;\mathcal{H}_2^+(\mathbb{C}))$ and let Π be the solution of (2.7.37). Then, in view of (2.7.44), we have

$$\begin{aligned}
\int_{\mathbb{R}^3}\|\mathcal{M}_F\|_2 dv &\leq \int_{\mathbb{R}^3} FD(\pi_c + |\pi_s|)dv + \int_{\mathbb{R}^3} FD(\pi_c - |\pi_s|)dv\\
&\leq \rho_c = |\int_{\mathbb{R}^3} f_c dv| \leq \int_{\mathbb{R}^3}|f_c|dv \leq \int_{\mathbb{R}^3}\|F\|_2 dv.
\end{aligned}$$

Thus, $\displaystyle\int_{\mathbb{R}^3}\|Q_{FD}(F)\|_2 \leq \int_{\mathbb{R}^3}\|\mathcal{M}_F\|_2 dv + \int_{\mathbb{R}^3}\|F\|_2 dv \leq 2\int_{\mathbb{R}^3}\|F\|_2 dv.$

2. For all $F \in \mathcal{A}$, it is simple to verify that $F(I_2 - F)^{-1}$ belongs to $\mathcal{H}_2^+(\mathbb{C})$ and F commutate with $(I_2 - F)^{-1}$. Then, $\log(F(I_2 - F)^{-1})$ is well defined and $\log(F(I_2 - F)^{-1}) = \log(F) - \log(I_2 - F)$. Let now Π be the solution of (2.7.37). Then, we have

$$\mathcal{M}_F(I_2 - \mathcal{M}_F)^{-1}M_V^{-1} = (2\pi)^{\frac{3}{2}}e^{\Pi+V}.$$

Indeed,

$$\begin{aligned}
\mathcal{M}_F(I_2 - \mathcal{M}_F)^{-1} &= \left(I_2 + e^{\frac{|v|^2}{2}-\Pi}\right)^{-1}(I_2 - \mathcal{M}_F)^{-1} = \left[(I_2 - \mathcal{M}_F)(I_2 + e^{\frac{|v|^2}{2}-\Pi})\right]^{-1}\\
&= \left(I_2 + e^{\frac{|v|^2}{2}-\Pi} - I_2\right)^{-1} = e^{\frac{-|v|^2}{2}}e^{\Pi} = (2\pi)^{\frac{3}{2}}M_V e^{\Pi+V}.
\end{aligned}$$

Therefore,

$$\log(\mathcal{M}_F(I_2-\mathcal{M}_F)^{-1}M_V^{-1}) = \frac{3}{2}\log(2\pi)I_2 + \Pi + V.$$

Since Π, V are independent of v and $\int_{\mathbb{R}^3} Q_{FD}(F)dv = 0$ then,

$$\begin{aligned}
\mathcal{H}(F) &= \int_{\mathbb{R}^3} Q_{FD}(F) : \overline{(\log(F(I_2-F)^{-1}M_V^{-1}) - \frac{3}{2}\log(2\pi)I_2 - \Pi - V)} \\
&= \int_{\mathbb{R}^3} Q_{FD}(F) : (\overline{\log(F(I_2-F)^{-1}M_V^{-1})} - \overline{\log(\mathcal{M}_F(I_2-\mathcal{M}_F)^{-1}M_V^{-1})}) \\
&= \int_{\mathbb{R}^3} (\mathcal{M}_F - F) : \left[\overline{\log(F) - \log(\mathcal{M}_F)} + \overline{\log(I_2-\mathcal{M}_F) - \log(I_2-F)}\right].
\end{aligned}$$

In view of (2.7.16), $\int_{\mathbb{R}^3} (\mathcal{M}_F - F) : \overline{(\log(F) - \log(\mathcal{M}_F))} \leq 0$ and

$$\begin{aligned}
&\int_{\mathbb{R}^3} (\mathcal{M}_F - F) : \overline{(\log(I_2-\mathcal{M}_F) - \log(I_2-F))} \\
&\qquad = \int_{\mathbb{R}^3} [(I_2-F) - (I_2-\mathcal{M}_F)] : \overline{(\log(I_2-\mathcal{M}_F) - \log(I_2-F))} \leq 0.
\end{aligned}$$

We deduce that $\mathcal{H}(F) \leq 0, \forall F \in \mathcal{A}$.
3. These equivalences are obvious using (2.7.17).

■

We state now the main results of this subsection where their proofs are similar to those presented in the last subsection.

Theorem 2.7.10. *Let F^ε be the solution of* (2.5.2)-(2.1.2) *with the collision operator Q_{FD} given by* (2.7.38). *Then, formally, $F^\varepsilon \to F_0$ as $\varepsilon \to 0$, where $F_0(t,x,v) = \left(I_2 + e^{\frac{|v|^2}{2} - \Pi(t,x)}\right)^{-1}$ and Π is solution of*

$$\begin{aligned}
\partial_t n[\Pi] + \nabla \cdot J = \frac{i}{2}\int_{\mathbb{R}^3} &\left[\vec{\Omega}_{FD}\cdot\vec{\sigma}, \left(I_2 + e^{\frac{|v|^2}{2} - \Pi(t,x)}\right)^{-1}\right] dv \\
&+ \left(\int_{\mathbb{R}^3} \vec{\Omega}_o \times (\vec{\Omega}_o \times \vec{F}_o^s)dv\right)\cdot\vec{\sigma} + Q_{sf}(n[\Pi]), \quad (2.7.47)
\end{aligned}$$

where the mass flux J is given by

$$J = -\nabla\cdot\mathbb{D}[\Pi] - \nabla_x V n[\Pi] + \mathbb{D}_{\vec{\Omega}_o}[\Pi]. \quad (2.7.48)$$

The density $n[\Pi]$, $\mathbb{D}[\Pi]$ and $\mathbb{D}_{\vec{\Omega}_o}[\Pi]$ are nonlinear functionals of Π given by

$$n[\Pi] = \int_{\mathbb{R}^3} \left(I_2 + e^{\frac{|v|^2}{2} - \Pi(t,x)}\right)^{-1} dv, \quad (2.7.49)$$

$$\mathbb{D}[\Pi] = \int_{\mathbb{R}^3} (v \otimes v) \left(I_2 + e^{\frac{|v|^2}{2} - \Pi(t,x)} \right)^{-1} dv,$$

and

$$\mathbb{D}_{\vec{\Omega}_o}[\Pi] = i \int_{\mathbb{R}^3} \left[(v \otimes \vec{\Omega}_o)(\vec{\sigma}), \left(I_2 + e^{\frac{|v|^2}{2} - \Pi(t,x)} \right)^{-1} \right] dv.$$

The Fermi-Dirac effective field $\vec{\Omega}_{FD}$ is similar to the one obtained in the derivation of energy transport model. It is given by

$$\vec{\Omega}_{FD} = \mathrm{div}_x(v \otimes \vec{\Omega}_o) - \nabla_x V \cdot \nabla_v \vec{\Omega}_o + \vec{\Omega}_e.$$

Finally, the $\vec{F}_0^s$ is the spin part of $F_0 = \left(I_2 + e^{\frac{|v|^2}{2} - \Pi(t,x)} \right)^{-1}$.

The entropy function is now defined by, where $F_0 = \left(I_2 + e^{\frac{|v|^2}{2} - \Pi} \right)^{-1}$ and $n = \int_{\mathbb{R}^3} F_0 dv$,

$$\begin{aligned}
\tilde{\mathcal{S}}(n) &= \int_{\mathbb{R}^6} \langle F_0, \log(F_0(I_2 - F_0)^{-1} M_V^{-1}) \rangle_2 dxdv + \int_{\mathbb{R}^6} tr(\log(I_2 - F_0)) dxdv \\
&= \int_{\mathbb{R}^6} \langle F_0, \frac{3}{2} \log(2\pi) I_2 + \Pi + V \rangle_2 dxdv + \int_{\mathbb{R}^6} tr(\log(I_2 - F_0)) dxdv \\
&= \int_{\mathbb{R}^3} \left(\frac{3}{2} \log(2\pi) tr(n) + \langle n, \Pi + V \rangle_2 \right) dx + \int_{\mathbb{R}^6} tr(\log(I_2 - F_0)) dxdv.
\end{aligned}$$

Proposition 2.7.11. *Let Π and $n := n[\Pi]$ solve the Drift-Diffusion system* (2.7.47)-(2.7.48)*. Then, the Fermi-Dirac fluid entropy $\tilde{\mathcal{S}}$ satisfies*

$$\frac{d}{dt} \tilde{\mathcal{S}}(n) \leq \int_{\mathbb{R}^3} \partial_t V tr(n) dx. \tag{2.7.50}$$

If the potential V is independent of time, then $\tilde{\mathcal{S}}(n)$ is a decreasing function of time

$$\frac{d}{dt} \tilde{\mathcal{S}}(n) \leq 0.$$

References

[1] C. Bardos, F. Golse, and D. Levermore, *Fluid dynamic limits of kinetic equations. I. Formal derivations*, J. Statist. Phys., 63 (1991), pp. 323–344.

[2] N. Ben Abdallah and P. Degond, *On a hierarchy of macroscopic models for semiconductors*, J. Math. Phys., 37 (1996), pp. 3306–3333.

[3] N. Ben Abdallah, P. Degond, and S. Génieys, *An Energy-Transport model derived from the Boltzmann equation of semiconductors*, J. Stat. Phys., 84 (1996), pp. 205–231.

[4] N. Ben Abdallah, S. Desvillettes, and S. Génieys, *On the convergence of the Boltzmann for the semiconductors toward the energy transport model*, J. Stat. Phys., 98 (2000), pp. 835–870.

[5] J. A. Bittencourt, *Fundamentals of plasma physics*, Pergamon Press, Oxford, 1986.

[6] F. Bouchut, F. Golse, and M. Pulvirenti, *Kinetic equations and asymptotic theory*, B. perthame, L. Desvillettes Eds, Series in Appl. Math., bf 4, Gauthier-Villars (2000).

[7] A. Bournel, *Magnéto-électronique dans des dispositifs à semiconducteurs*, Ann. Phys. Fr, 25 (2000), pp. 1–167.

[8] A. Bournel, V. Delmouly, P. Dollfus, G. Tremblay, and P. Hesto, *Theoretical and experimental considerations on the spin field effect transistor*, Physica E, 10 (2001), pp. 86–90.

[9] A. Bournel, P. Dollfus, E. Cassan, and P. Hesto, *Monte Carlo study of spin relaxation in AlGaAs/GaAs quantum wells*, Applied Physics Letters, 77 (2000), pp. 2346–2348.

[10] Y. A. Bychkov and E. I. Rashba, *Oscillatory effects and the magnetic susceptibility of carriers in inversion layers*, Journal of Physics C : Solid State Physics, 17 (1984), pp. 6039–6045.

[11] S. Datta and B. Das, *Electronic analog of the electro-optic modulator*, Applied Physics Letters, 56 (1990), pp. 665–667.

[12] P. Degond, *Mathematical modelling of microelectronics semiconductor devices*, in Some current topics on nonlinear conservation laws, vol. 15 of AMS/IP Stud. Adv. Math., Amer. Math. Soc., Providence, RI, 2000, pp. 77–110.

[13] P. Degond, G. Gallego, and F. Méhats, *Entropic discretization of a quantum drift-diffusion model*, SIAM J. Numer. Anal., 43 (2005), pp. 1828–1849.

[14] P. Degond, C. D. Levermore, and C. Schmeiser, *A note on the energy-transport limit of the semiconductor Boltzmann equation*, in Transport in transition regimes (Minneapolis, MN, 2000), vol. 135 of IMA Vol. Math. Appl., Springer, New York, 2004, pp. 137–153.

[15] P. Degond, F. Méhats, and C. Ringhofer, *Quantum hydrodynamic models derived from the entropy principle*, Contemp. Math. 371, Amer. Math. Soc., Providence RI (2005).

[16] ——, *Quantum energy-transport and drift-diffusion models*, J. Stat. Phys., 118 (2005), pp. 625–667.

[17] P. Degond and C. Ringhofer, *A note on binary quantum collision operators conserving mass, momentum and energy*, C. R. Acad. Sci. Paris, 336 (2003), pp. Ser I, 587–628.

[18] ——, *Quantum moment hydrodynamics and the entropy principle*, J. Stat. Phys., 112 (2003), pp. 587–628.

[19] P. Degond and C. Schmeiser, *Macroscopic models for semiconductor heterostructures*, J. Math. Phys., 39 (1998), pp. 4634–4663.

[20] G. Dresselhaus, *Spin-orbit coupling effects in zinc blende structures*, Phys. Rev., 100 (1955), pp. 580–586.

[21] R. J. Elliott, *Theory of the effect of spin-orbit coupling on magnetic resonance in some semiconductors*, Phys. Rev., 96 (1954), pp. 266–279.

[22] A. Fert, A. Friederich, and al, *Giant magnetoresistance of (001)fe/(001)cr magnetic superlattices*, Phys. Rev. Lett., 61 (1988), pp. 2472–2475.

[23] G. Fishman and G. Lampel, *Spin relaxation of photoelectrons in p-type gallium arsenide*, Phys. Rev. B, 16 (1977), pp. 820–831.

[24] G. Gallego and F. Méhats, *On Quantum Hydrodynamic and Quantum Energy Transport Models*, Commun. Math. Sci., 5 (2007), pp. 887–908.

[25] I. Gasser and R. Natalini, *The energy transport and the drift diffusion equations as relaxation limits of the hydrodynamic model for semiconductors*, Quart. Appl. Math., 57 (1999), pp. 269–282.

[26] F. Golse and D. Levermore, *Stokes-Fourier and acoustic limits for the Boltzmann equations : Convergence proofs*, Comm. Pure Appl. Math., 55 (2002), pp. 336–393.

[27] F. Golse and F. Poupaud, *Limite fluide des équations de Boltzmann des semi-conducteurs pour une statistique de Fermi-Dirac*, Asymptotic Anal., 6 (1992), pp. 135–160.

[28] F. Golse and L. Saint-Raymond, *Hydrodynamics limit for the Boltzmann equation*, Lecture Porto Ercole, (2004).

[29] ——, *The Navier-Stokes limit of the Boltzmann equation for bounded collision kernels*, Invent Math., 155 (2004), pp. 81–161.

[30] L. D. Landau and E. M. Lifshitz, *Quantum Mechanics*, Pergamon Press, Oxford, 1991.

[31] C. D. Levermore, *Moment closure hierarchies for kinetic theories*, J. Stat. Phys., 83 (1996), pp. 1021–1065.

[32] P. A. Markowich, C. A. Ringhofer, and C. Schmeiser, *Semiconductor equations*, Springer-Verlag, Vienna, 1990.

[33] M. S. Mock, *Analysis of mathematical models of semiconductor devices*, vol. 3 of Advances in Numerical Computation Series, Boole Press, Dún Laoghaire, 1983.

[34] A. Pazy, *Semigroups of linear operators and applications to partial differential equations*, vol. 44 of Applied Mathematical Sciences, Springer-Verlag, New York, 1983.

[35] Y. Pershin, S. Saikin, and V. Privman, *Semiclassical transport models for semiconductor spintronics*, Electrochem. Soc. Proc., 2004-13 (2005), pp. 183–205.

[36] Y. V. Pershin and V. Privman, *Focusing of spin polarization in semiconductors by inhomogeneous doping*, Phys. Rev. Lett., 90 (2003), p. 256602.

[37] F. Poupaud, *Diffusion approximation of the linear semiconductor Boltzmann equation : analysis of boundary layers*, Asymptotic Anal., 4 (1991), pp. 293–317.

[38] Y. Qi and S. Zhang, *Spin diffusion at finite electric and magnetic fields*, Phys. Rev. B, 67 (2003), p. 052407.

[39] Y. P. Raizer, *Gas Discharge Physics*, Springer, Berlin, 1997.

[40] M. Reed and B. Simon, *Methods of modern mathematical physics.*, Academic Press, New York, second ed., 1975. Functional analysis.

[41] S. Saikin, *A drift-diffusion model for spin-polarized transport in a two-dimensional non-degenerate electron gas controlled by spin orbit interaction*, Journal of Physics : Condensed Matter, 16 (2004), pp. 5071–5081.

[42] S. Saikin, Y. Pershin, and V. Privman, *Modelling for semiconductor spintronics*, IEE Proceedings Circuits, Devices and Systems, 152 (2005), pp. 366–376.

[43] C. Schmeiser and A. Zwirchmayr, *Elastic and drift-diffusion limits of electron-phonon interaction in semiconductors*, Math. Models Methods Appl. Sci., 8 (1998), pp. 37–53.

[44] T. Valet and A. Fert, *Theory of the perpendicular magnetoresistance in magnetic multilayers*, Phys. Rev. B, 48 (1993), pp. 7099–7113.

[45] C. Villani, *Limite hydrodynamiques de l'équation de Boltzmann*, Séminaire Bourbaki, 53ème année, no 893 (2000–2001).

[46] Z. G. Yu and M. E. Flatté, *Electric-field dependent spin diffusion and spin injection into semiconductors*, Phys. Rev. B, 66 (2002), p. 201202.

[47] Z. G. Yu and M. E. Flatté, *Spin diffusion and injection in semiconductor structures : electric field effects*, Phys. Rev. B, 66 (2002), p. 235302.

[48] I. Zutic, J. Fabian, and S. Das Sarma, *Spin-Polarized Transport in Inhomogeneous Magnetic Semiconductors : Theory of Magnetic/Nonmagnetic $p-n$ Junctions*, Phys. Rev. Lett., 88 (2002), p. 066603.

[49] I. Zutic, J. Fabian, and S. D. Sarma, *Spintronics : Fundamentals and applications*, Reviews of Modern Physics, 76 (2004), p. 323.

Chapter 3

Numerical Applications

Abstract

The purpose of this chapter is to somewhere validate numerically the models derived in the previous chapters. Two numerical applications are carried out. The first one concerns the simulation of transistor with spin rotation effect (spin-FET). Following the work of [6, 22], a subband drift-diffusion Schrödinger-Poisson model with spin rotation and relaxation effects is derived and used for the simulation. The second application is a well known effect in semiconductor spintronics : the accumulation of spin polarization density at the interface between two semi-conductor regions with different doping levels [18, 17]. This phenomena is illustrated using two-component drift-diffusion Poisson model. Moreover, we show the action of the Rashba spin-orbit coupling on this spin accumulation effect by means of spin vector drift-diffusion Poisson model.

3.1 Modelling and numerical implementation of spin-FET

3.1.1 Introduction

Recently, the spin-related properties of charge carries in semiconductors have generated a huge attention leading to proposition of new magnetoelectronics devices. The Rashba term in the spin-orbit coupling [11] appearing in a quantum well under electric field along the growth direction makes feasible the control of electron spin orientation through the confining electric field. This mechanism leads to the concept of the spin Field Effect Transistor, the spin-FET [14].

The spin-FET is a High Mobility Transistor (HEMT) in which the source and drain contacts are ferromagnetics. A HEMT transistor is composed of a channel which is an active region connected to two electrodes called the source and drain. It is based on the formation of electron confined gas in the channel at the heterointerface between different semiconductor heterostructures. The confinement in the channel is commanded by a Schottky gate. The source and drain are high doped regions and play the role of two small reservoirs. Apply at the electrodes a drain-source potential, V_{DS}, a drain current can be established.

The idea of spin-FET, due to Datta and Das [14], consists in replacing the source and drain by ferromagnetic contacts. The source then acts as polarizer and injects a spin polarized current. In the channel, the control of electron spin orientation is possible by the applied gate potential through the Rashba spin-orbit coupling. The drain plays the role of selector. It collects preferentially electrons with spin orientation depending on its magnetic moment.

The device considered here is a double gate MOSFET represented by Figure 3.1. We do not take a ferromagnetic contacts at the source and drain. We assume that a spin polarized current is injected from the source to the channel. The object is to show numerically the action of the gate voltage (via the Rashba coupling) on the spin dynamics in 1DEG. To this aim, we take a two dimension device in the (xz) plane. We assume that the particles are confined in the z direction and the transport is allowed in the x direction. The Rashba spin precession vector is then oriented in the y direction (perpendicular to device plane (xz)) and does not change direction. The aim of the simulation is to illustrate the efficiency of the gate control of the spin orientation in this case.

The results presented here are well known in semiconductor spintronics. See for example [8] for the study of 1DEG. However, when taking a two dimensional channel with width equal to W in the y direction, the situation is more complicated. Indeed, in two-dimensional electron gas, the Rashba effective field direction depends

strongly on v (or on the wave vector). Then, the electron/crystal scattering randomize the Rashba effective field direction. So, during the motion of one electron, its spin orientation becomes progressively incoherent. The spin polarization of the electron population may be thus fast relaxed (by the D'yakonov-Perel relaxation mechanism). Using Monte Carlo technique, A. Bournel and al study the gate induced spin precession in 2DEG [8, 9, 10]. They studied the influence of the width W on the spin diffusion length L_s or spin relaxation length induced by the interactions. It is shown that the D'yakonov-Perel spin relaxation mechanism tends to vanish (or to disappear as in the 1DEG case) when the channel width decreases. They prove that it is sufficient to take W less than 100 nm at the room temperature to have a spin relaxation length exceeding $1\mu m$. In this case, one obtains an efficient gate-controlled spin precession in the channel as in the one dimensional case presented here. For this, the spin orientation injected by the source contact has to be perpendicular to the source/channel interface. We refer also to [20, 21] for the study of gate-induced spin precession in 2DEGs. We don't study here the 2D channel case. The study of spin transport properties in 2DEG will be the subject of future works.

The model used for the simulation is a coupled quantum classical model. In the confinement direction, the length scale is of the order of the electron de Broglie wavelength and a quantum models have to be adapted in this direction. However the length scale in the transport direction is much bigger and a classical transport model can be used. This gives rise to the subband theory [1, 2, 15]. The subband models are the subject of many recent works. In [3], as mentioned in the first chapter of this thesis, a partially quantum/kinetic subband model is derived by a partially semi-classical limit from a full quantum model. A rigorous analysis of the limit model (Vlasov Schrödinger-Poisson model) is then investigated in [4]. We refer also to [7, 22, 5], for the derivation and study of quantum/fluid type models. The next subsection is dedicated to give more precise description on the subband quantum/drift-diffusion model.

3.1.2 A coupled quantum/drift diffusion model with spin-orbit effect

In this part, we will derive a macroscopic subband model by performing a diffusion limit of the Boltzmann Schrödinger system with spin-orbit term. We adapt the work of [22]. Assume that the quantum effects take place in one direction of the space denoted by z, $z \in [0,1]$, and in the other directions, $x \in \mathbb{R}^d$, the particles move classically. At a time $t > 0$ and a position $(x,z) \in \mathbb{R}^d \times [0,1]$, the density of the system is given by

$$N^{\varepsilon}(t,x,z)=\sum_{n\geqslant 1}(\int_{\mathbb{R}^d}F_n^{\varepsilon}(t,x,v)dv)|\chi_n(t,x,z)|^2. \tag{3.1.1}$$

The unknowns of the problem are $(\epsilon_n,\chi_n,F_n^{\varepsilon})_{n\geqslant 1}$. The subbands are characterized by the complete set, $(\epsilon_n,\chi_n)_n$, of the eigenelements of the one dimensional Schrödinger operator $-\frac{1}{2}\frac{d^2}{dz^2}+V$ with homogeneous Dirichlet data. More precisely, the sequence $(\epsilon_n(t,x),\chi_n(t,x,.))_n$ verifies

$$\left\{\begin{array}{l} -\frac{1}{2}\frac{d^2}{dz^2}\chi_n+V\chi_n=\epsilon_n\chi_n,\\ \chi_n(t,x,.)\in H_0^1(0,1),\quad \displaystyle\int_0^1\chi_n\chi_m=\delta_{nm}.\end{array}\right. \tag{3.1.2}$$

The potential $V(t,x,z)$ is supposed to be given and regular function (see Assumption 3.1.2). Generally, V is not given but satisfies the Poisson equation if one accounts the electrostatic forces. For each subband, the distribution function, $F_n^{\varepsilon}(t,x,v)\in\mathcal{H}_2^+(\mathbb{C})$, satisfies the following scaled spinor Boltzmann equation

$$\partial_t F_n^{\varepsilon}+\frac{1}{\varepsilon}(v.\nabla_x F_n^{\varepsilon}-\nabla_x\epsilon_n.\nabla_v F_n^{\varepsilon})=\frac{1}{\varepsilon^2}Q(F^{\varepsilon})_n+\frac{i}{2}[\Omega_n^{\varepsilon}.\vec{\sigma},F_n^{\varepsilon}], \tag{3.1.3}$$

where

$$\Omega_n^{\varepsilon}(t,x,v)=\frac{1}{\varepsilon}\Omega_n^o(t,x,v)+\Omega_n^e(t,x,v) \tag{3.1.4}$$

such that Ω_n^o, Ω_n^e are respectively odd and even functions with respect to v satisfying Assumption 3.1.3. Here, the collision operator takes the form

$$Q(F)_n=\sum_{n'}\int_{\mathbb{R}^2}\sigma_{nn'}(v,v')\{\mathcal{M}_n(v)F_{n'}(v')-\mathcal{M}_{n'}(v')F_n(v)\}dv' \tag{3.1.5}$$

which accounts the transition between the subbands. The normalized Maxwellian $\mathcal{M}_n$ is given by

$$\mathcal{M}_n(v)=\frac{1}{(2\pi)^{\frac{d}{2}}\mathcal{Z}}e^{-(\frac{1}{2}|v|^2+\epsilon_n)} \tag{3.1.6}$$

where $\mathcal{Z}$ is the repartition function

$$\mathcal{Z}(t,x)=\sum_n e^{-\epsilon_n(t,x)}. \tag{3.1.7}$$

Initially, we will take

$$F_n^{\varepsilon}(0,x,v)=F_{in,n}(x,v). \tag{3.1.8}$$

We fix as in the previous chapter the following assumptions on the cross-section, the potential and the effective field.

Assumption 3.1.1. *The cross-section is assumed to be symmetric and bounded from above and below. Namely,*

$$\exists \alpha_1, \alpha_2 > 0, \quad 0 < \alpha_1 \leq \sigma_{nn'}(v, v') \leq \alpha_2, \quad \forall n, n' \geq 1, \forall v \in \mathbb{R}^d, \forall v' \in \mathbb{R}^d.$$

Assumption 3.1.2. *For any fixed $T > 0$, $(t, x, z) \mapsto V(t, x, z)$ is a real non negative function belonging to $C^1([0, T], W^{1,\infty}(\mathbb{R}^d \times (0, 1)))$.*

Assumption 3.1.3. *For any $T > 0$, $(\Omega_n^o)_{n\in\mathbb{N}^*}$, $(\Omega_n^e)_{n\in\mathbb{N}^*} \subset C^1([0, T] \times \mathbb{R}_x^d \times \mathbb{R}_v^d, \mathbb{R}^3)$ are two sequences of respectively odd and even functions. In addition, there exists $(C_n)_n \in \ell^1(\mathbb{R}^+)$ and $m \in \mathbb{N}$ such that*

$$|\Omega_n^{o(e)}| + \sum_{\eta\in\{x_i,v_i\}} |\partial_\eta \Omega_n^{o(e)}| \leq C_n(1 + |v|)^m. \tag{3.1.9}$$

We will denote by $\ell^1(\mathbb{L}^2_{\mathcal{M}})$ the space given by

$$\ell^1(\mathbb{L}^2_{\mathcal{M}}) = \left\{ (F_n)_{n\geq 1} \subset \mathbb{L}^2_{\mathcal{M}} / \quad \sum_{n\geq 1} \int_{\mathbb{R}^d} \frac{\|F_n\|_2^2}{\mathcal{M}_n} dv < +\infty \right\}.$$

It is simple to show that the collision operator (3.1.5) is a linear, self-adjoint and nonpositive operator on $\ell^1(\mathbb{L}^2_{\mathcal{M}})$ satisfying

1. $\sum_{n\geq 1} \int_{\mathbb{R}^d} Q(F)_n(v)dv = 0$,
2. $Ker(Q) = \{F \in \ell^1(\mathbb{L}^2_{\mathcal{M}}),$ such that $\exists N \in \mathcal{H}_2^+(\mathbb{C}), F_n(v) = N\mathcal{M}_n(v), \forall n \geq 1\}$,
3. $\mathcal{R}(Q) = Ker(Q)^\perp = \left\{ F = (F_n)_n \in \ell^1(\mathbb{L}^2_{\mathcal{M}}),$ such that $\sum_n \int_{\mathbb{R}^d} F_n(v)dv = \begin{pmatrix} 0 & 0 \\ 0 & 0 \end{pmatrix} \right\}$,
4. $-\sum_{n\geq 1} \langle Q(F)_n, F_n\rangle_{\mathcal{M}} \geq \alpha_1 \sum_{n\geq 1} \|F_n - \mathcal{P}(F)_n\|_{\mathcal{M}}$, when $\mathcal{P}$ is the orthogonale projection on $Ker(Q)$.

The matrices, $(\mathbb{D}_i)_{i=1..4}$, appearing in the general drift diffusion model derived in Section 6 of the previous chapter are defined in this case as follows.

Proposition 3.1.4. *Let $\mathbb{D}_1$, $\mathbb{D}_2$, $\mathbb{D}_3$ and $\mathbb{D}_4$ be the matrices defined respectively by*

$$\begin{aligned} \mathbb{D}_1 &= \sum_n \int_{\mathbb{R}^d} (\theta_{1,n}(v) \otimes v)dv \in M_{dd}(\mathbb{R}) \qquad , \mathbb{D}_2 = \sum_n \int_{\mathbb{R}^d} (v \otimes \theta_{2,n}(v))dv \in M_{d3}(\mathbb{R}), \\ \mathbb{D}_3 &= \sum_n \int_{\mathbb{R}^d} (\Omega_n^o(v) \otimes \theta_{1,n}(v))dv \in M_{3d}(\mathbb{R}) \quad , \mathbb{D}_4 = \sum_n \int_{\mathbb{R}^d} (\theta_{2,n}(v) \otimes \Omega_n^o(v))dv \in M_{33}(\mathbb{R}) \end{aligned} \tag{3.1.10}$$

where θ_1, θ_2 are respectively the unique solutions of

$$-Q(\theta_1 Id)_n = v\mathcal{M}_n(v)Id, \quad \sum_n \int_{\mathbb{R}^d} \theta_{1,n}(v)dv = 0, \tag{3.1.11}$$

$$-Q(\theta_2 Id)_n = \Omega_n^o \mathcal{M}_n(v)Id, \quad \sum_n \int_{\mathbb{R}^d} \theta_{2,n}(v)dv = 0. \tag{3.1.12}$$

Then, The matrices $\mathbb{D}_1$ and $\mathbb{D}_4$ are symmetric positive definite and ${}^t\mathbb{D}_3 = \mathbb{D}_2$.

Passing to the limit $\varepsilon \to 0$, we get an hybrid Drift-Diffusion Schrödinger system. Namely, applying the same ideas as in the previous chapter, the following results hold.

Theorem 3.1.5. *Let $T > 0$, $(F_{in,n})_n \in \ell^1(\mathbb{L}^2_{\mathcal{M}}(dxdv))$ and assume that Assumptions 3.1.1, 3.1.2 and 3.1.3 hold. Then, for all $\varepsilon > 0$, the model (3.1.3)...(3.1.8) admits a unique weak solution $(F^\varepsilon_n)_n \in C^0([0,T];\ell^1(\mathbb{L}^2_{\mathcal{M}}(dxdv)))$. In addition, there exists $N_s \in L^2([0,T]\times\mathbb{R}^d,\mathcal{H}^+_2(\mathbb{C}))$ such that $F^\varepsilon_n \rightharpoonup \dfrac{N_s(t,x)}{\mathcal{Z}(t,x)}\mathcal{M}_n(t,x,v)$ weak $\star$ in $L^\infty([0,T],\ell^1(\mathbb{L}^2_{\mathcal{M}}(dxdv)))$ and the surface density $N^\varepsilon_s := \sum\limits_{n\geq 1}\int_{\mathbb{R}^d} F^\varepsilon_n(t,x,v)dv$ converges weakly to N_s in $L^2([0,T]\times\mathbb{R}^d,\mathcal{H}^+_2(\mathbb{C}))$. If we decompose the density matrix N_s into a spin independent and a spin dependent parts : $N_s = \dfrac{n_c}{2}I_2 + \vec{n}_s.\vec{\sigma}$ then, the charge density n_c and the spin density $\vec{n}_s$ satisfy*

$$\begin{cases} \partial_t n_c - \mathrm{div}_x(\mathbb{D}_1(\nabla_x n_c + \nabla_x V_s n_c)) = 0, \\ \\ \partial_t \vec{n}_s - \mathrm{div}_x(\mathbb{D}_1\cdot(\nabla_x\otimes\vec{n}_s + \nabla_x V_s\otimes\vec{n}_s) + 2(\mathbb{D}^k_2\times\vec{n}_s)_{k=1,2,3}) = \\ \qquad\qquad -\Omega\times\vec{n}_s + (\mathbb{D}_4 - tr\mathbb{D}_4)(\vec{n}_s) - 2\dfrac{\vec{n}_s}{\tau_{sf}}, \\ \\ N_s(0,x) = N_{in} := \sum\limits_{n\geq 1}\int_{\mathbb{R}^d} F_{in,n}(x,v)dv, \end{cases} \tag{3.1.13}$$

$$\text{with } \Omega = \mathrm{div}_x\mathbb{D}_2 - \mathbb{D}_3(\nabla_x V_s) + H_e,\ H_e(t,x) = \sum_n \int_{\mathbb{R}^d}\Omega^e_n(t,x,v)\mathcal{M}_n(t,x,v)dv. \tag{3.1.14}$$

The potential V_s is given by

$$V_s = -Log(\sum_n e^{-\epsilon_n}).$$

Furthermore, the model (3.1.13) satisfies the maximum principle. i.e. if initially $N_{in} \in L^2(\mathbb{R}^d,\mathcal{H}^+_2(\mathbb{C}))$ then, $N_s(t,x)$ is an Hermitian positive matrix for all $t\in[0,T]$ and $x\in\mathbb{R}^d$.

Remark 3.1.6. *The total density $N^\varepsilon(t,x,z)$ given by (4.5.3) converges weakly to N in $L^2([0,T]\times\mathbb{R}^d_x\times[0,1]_z,\mathcal{H}^+_2(\mathbb{C}))$ such that*

$$N(t,x,z) = \frac{N_s(t,x)}{\mathcal{Z}(t,x)}\sum_n e^{-\epsilon_n(t,x)}|\chi_n(t,x,z)|^2$$

and $N_s(t,x) = \displaystyle\int_0^1 N(t,x,z)dz$ is the surface density satisfying (3.1.13).

3.1.3 Setting of the problem and numerical results

For the application, we will take the Rashba spin-orbit effect. The Rashba effective field in the subband kinetic/quantum model is given in $2DEG$ by

$$\Omega_n^o = \alpha_n(t,x)(-v_2, v_1, 0), \tag{3.1.15}$$

where

$$\alpha_n(t,x) = \int_0^1 \partial_z V(t,x,z)|\chi_n(t,x,z)|^2 dz. \tag{3.1.16}$$

See the first chapter. In the example considered here, the transport takes place in one dimension and the subband Rashba spin-orbit effect is then characterized by the following effective field

$$\Omega_n^o(t,x,v) = \alpha_n(t,x)ve_y, \quad \forall (t,x,v) \in \mathbb{R}^+ \times \mathbb{R}^2_{x,v}. \tag{3.1.17}$$

We denote by (e_x, e_y, e_z) an orthonormal basis of the space with e_x and e_z are respectively the unit vectors of the transport direction x and the confinement direction z. We suppose in addition, for simplicity, that the cross-section $\sigma_{n,n'}(v,v')$ is a constant independent of n, n', v, v' and let $\tau > 0$ be the relaxation time such that $\sigma_{nn'}(v,v') = \dfrac{1}{\tau}$, for all n, n', v, v'. Then, θ_1 and θ_2 can be explicitly computed

$$\theta_{1,n} = \tau v \mathcal{M}_n(v), \quad \theta_{2,n} = \tau \Omega_n^o(v)\mathcal{M}_n(v). \tag{3.1.18}$$

In this case, the matrices $\mathbb{D}_1$, $\mathbb{D}_2$, $\mathbb{D}_3$ and $\mathbb{D}_4$ are equal to

$$\mathbb{D}_1 = \tau Id,\ \mathbb{D}_2 = {}^t\mathbb{D}_3 = \tau \sum_n \int_{\mathbb{R}^d} (v \otimes \Omega_n^o(v))\mathcal{M}_n(v)dv,\ \mathbb{D}_4 = \tau \sum_n \int_{\mathbb{R}^d} (\Omega_n^o \otimes \Omega_n^o)\mathcal{M}_n dv.$$

Thus, for $d = 1$ and Ω_n^o given by (3.1.17), we have

$$\mathbb{D}_1 = \tau Id, \quad \mathbb{D}_3 = {}^t\mathbb{D}_2 = \tau C_1 e_y \qquad \text{where} \quad C_1 = \frac{1}{\mathcal{Z}} \sum_n \alpha_n e^{-\boldsymbol{\epsilon}_n} \tag{3.1.19}$$

and

$$\mathbb{D}_4 - tr\mathbb{D}_4 = -\tau C_2 \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix} \qquad \text{where} \quad C_2 = \frac{1}{\mathcal{Z}} \sum_n \alpha_n^2 e^{-\boldsymbol{\epsilon}_n}. \tag{3.1.20}$$

Let us now summarize the complete stationary Drift Diffusion Schrödinger Poisson model written with the physical constants used for the simulation. We assume that the device occupies a $2D$ domain denoted by $[0, L] \times [0, \ell]$. At a position $(x, z) \in [0, L] \times [0, \ell]$, the total density matrix for Boltzmann statistics is

$$N(t,x,z) = \frac{N_s(t,x)}{\mathcal{Z}(t,x)} \sum_{n=1}^{\infty} e^{-\beta \boldsymbol{\epsilon}_n(t,x)} |\chi_n(t,x,z)|^2, \tag{3.1.21}$$

where $\beta = \dfrac{1}{k_B T}$, k_B is the Boltzmann constant and T denotes the temperature. The complete set of eigenfunctions and eigenvalues $(\chi_n, \epsilon_n)_{n\geq 1}$ satisfies

$$\begin{cases} -\dfrac{\hbar^2}{2m_*}\dfrac{d^2}{dz^2}\chi_n + (V + V_c)\chi_n = \epsilon_n \chi_n, \\ \chi_n(t,x,.) \in H_0^1(0,\ell), \quad \displaystyle\int_0^\ell \chi_n \chi_n' = \delta_{nn'}, \end{cases} \tag{3.1.22}$$

where $\hbar$ is the planck constant, m_* is the effective mass and V_c is a given potential barrier between the silicon and the oxyde in the nanotransistor (see Fig. 3.1). The electrostatic potential is given by $U = \frac{V}{e}$ where e is the elementary charge and satisfies the Poisson equation

$$-\Delta_{x,z} V = \frac{e}{\varepsilon_r \varepsilon_0}(tr(N) - N_D) \tag{3.1.23}$$

where ε_r is the relative permittivity, ε_0 the permittivity constant of the vacuum and N_D is the doping density which is equal to $N^+ \in \mathbb{R}^+$ in the drain and the source and $N^- \in \mathbb{R}^+$ in the channel. Writing the surface matrix density, N_s, as : $N_s(t,x) = \dfrac{n_c(t,x)}{2} I_2 + \vec{n}_s(t,x)\cdot\vec{\sigma}$, n_c and $\vec{n}_s$ satisfy the following stationary drift diffusion equations

$$\begin{cases} -\mathrm{div}_x(j_c) = 0, \quad j_c = \mathbb{D}(\partial_x n_c + \beta \partial_x V_s n_c), \\ -\mathrm{div}_x(\vec{j_s}) = -\mathbb{D}(\partial_x C_1 - \partial_x V_s C_1) e_y \times \vec{n}_s - \mathbb{D} C_2 \vec{n}_s^{\perp}, \\ \vec{j_s} = \mathbb{D}(\partial_x \vec{n}_s + \beta \partial_x V_s \vec{n}_s + 2C_1(e_y \times \vec{n}_s)), \end{cases} \tag{3.1.24}$$

where $\mathbb{D}$ is the diffusion constant $\mathbb{D} = \mu k_B T$ for a constant mobility μ and

$$V_s = -k_B T \log\left(\sum_{k=1}^{+\infty} e^{-\beta \epsilon_k}\right). \tag{3.1.25}$$

The functions C_1, C_2 are given in (3.1.19) and (3.1.20) and $\vec{n}_s^{\perp}$ is the part of $\vec{n}_s$ in the (ox, oz) plane perpendicular to the Rashba effective field (or to e_y) :

$$\vec{n}_s^{\perp} = \vec{n}_s - (\vec{n}_s \cdot e_y) e_y.$$

Remark that the total charge density appearing in the right hand side of (3.1.23) is given by

$$tr(N)(t,x,z) = \frac{n_c(t,x)}{\mathcal{Z}(t,x)} \sum_{n=1}^{\infty} e^{-\beta \epsilon_{n(t,x)}} |\chi_n(t,x,z)|^2. \tag{3.1.26}$$

Description of the scheme. To solve numerically the model (3.1.22)-(3.1.26), A finite element method with Gummel iterations is used [16]. We give here a brief

description of the algorithm. We refer to [6, 19] for more details. We mesh the domain by $N_x \times N_z$, $(x_i, z_j)_{1\leq i\leq N_x, 1\leq j\leq N_z}$, nodes.

We begin by resolving the 2D Schrodinger-Poisson system when there is no applied voltage. The boundary conditions used are as follows. At the source and the drain, the potential does not depend on the transport direction, we take $V(x = 0, z) = V(x = L, z) = V_b$ with $V_b(z)$ is the solution of $1D$ Schrödinger-Poisson system in the z direction. The surface density at the source and the drain is taken equal to $N^+ \times \ell_{Si}$. For $z = 0$ or $z = \ell$, we take a Dirichlet boundary condition on the gate contacts, $V(x, z = 0) = V(x, z = l) = V_{gs}$.

When a drain source voltage, V_{DS}, is applied, we resolve the Schrödinger-Poisson system coupled to the charge Drift Diffusion equation (the first equation of (3.1.24)) by Gummel iterations starting from the obtained potential in the first step and incrementing by $0.02V$. For the drift diffusion equation a Dirichlet conditions are used at $x = 0$ and $x = L$. For the potential we impose Dirichlet boundary conditions at the Gate and at the source and the Drain contacts : $V(x = 0, z) = V_b(z)$, $V(x = L, z) = V_b(z) + V_{DS}$.

The Gummel iterations can be summarized as follows. For a given potential, V_{old}, a diagonalization of the one dimensional Schrödinger operator (3.1.22) gives N_x sets of eigenfunctions $\{\chi_k(x_i, z)\}_{i=1,..N_x}$ and eigenvalues $\{\epsilon_k(x_i)\}$. The effective potential V_s is then computed from (3.1.25). This allows to obtain the surface charge density n_c by solving the first drift diffusion equation of (3.1.24) and then to compute a new potential V_{new} thanks to the resolution of (3.1.23) with (3.1.26). We repeat these steps until the difference $\|V_{new} - V_{old}\|_{L^\infty}$ be sufficiently small. Noting that the Poisson equation is resolved by implementing a quasi-Newton method [12].

Finally the spin part of the drift diffusion model (3.1.24) is resolved using Dirichlet boundary conditions. We assume that at $x = 0$ or $x = L$, the vectors $\vec{n}_s(x = 0)$ and $\vec{n}_s(x = L)$ are in the plane of the domain ((xz) plane). Then, the spin vector density $\vec{n}_s$ remains in this plane or it has no component in the y direction (parallel to e_y) and its perpendicular part, $\vec{n}_s^\perp$ (in the (xz) plane) solves

$$\begin{cases} -\mathrm{div}_x(\vec{j}_s^\perp) = -\mathbb{D}\big(C_2\vec{n}_s^\perp - (\partial_x C_1 - \partial_x V_s C_1)\mathcal{I}(\vec{n}_s^\perp)\big), \\ \\ \vec{j}_s^\perp = \mathbb{D}\big(\partial_x\vec{n}_s^\perp + \beta\partial_x V_s\vec{n}_s^\perp + 2C_1\mathcal{I}(\vec{n}_s^\perp)\big) \end{cases}$$

with $\mathcal{I} = \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix}$, $\vec{n}_s^\perp \in \mathbb{R}^2 \equiv \mathbb{C}$. We resolve this equation in $\mathbb{C}$, in which $\mathcal{I}$ is the pur imaginary unit.

Numerical results. The geometry of the device is given by Figure 3.1. We summarize in Table 3.1 the main values used in the simulation. We assume that the electrons are injected into the domain with spin vector density along the x-axis.

FIG. 3.1 – Schematic of the modeled device.

TAB. 3.1 – Table of the main values used.

Paramètre	Valeur	Longueur	Valeur
N^+	$10^{26} cm^{-3}$	L_S	5 nm
N^-	$10^{21} cm^{-3}$	L_C	20 nm
U_c	3 ev	L_D	5 nm
$\varepsilon_r(SiO_2)$	3.9	L_{ox}	2nm
$\varepsilon_r(Si)$	11.7	L_{Si}	6 nm

More precisely, we take $\vec{n}_s(x=0) = (n_c(x=0), 0)$. This means that the injected current in the device is supposed 100% spin polarized. Recall that the density spin polarization in this case is equal to $\frac{|\vec{n}_s(x=0)|}{n_c(x=0)} = 1$. We present in Figure 3.2 the sinus of the angle between $\vec{n}_s^{\perp}$ and the x-axis for different values of the gate potential V_{gs} and for drain source voltage $V_{DS} = 0.1V$. Figure 3.2 shows that the spin orientation rotates in the (xz) plane with an angular frequency proportional to the gate voltage. This shows also that the spin vector orientation reaching the drain contact can be controlled by V_{gs}.

FIG. 3.2 – The sinus of the angle (α) between the the density vector $\vec{n}_s^{\perp}$ and the x-axis for different values of the gate potential denoted by V_{gs} and for $V_{DS} = 0.1V$.

FIG. 3.3 – $I - V_{gs}$ characteristics for the device for $V_{DS} = 0.1V$. At the left, the charge current in a standard HEMT is represented. At the right, we plot the spin current density at the drain in spin-FET with spin selective drain in the direction parallel to x.

In Figure 3.3, we plot the current-voltage $(I-V_{gs})$ characteristics for $V_{DS} = 0.1V$.

In standard MOSFET, the current (or charge current given by the first equation of (3.1.24)) increases with the gate potential (left). The diffusion constant is given by the Einstein relation : $\mathbb{D} = \mu k_B T$ where $\mu = 0.12 m^2 V^{-1} s^{-1}$ and $T = 300K$. However, if we assume that the drain is a selective contact of electron spin. The magnitude of the drain current depends then on the orientation of the spin of the electrons reaching the drain with respect to the orientation of the magnetic moment of this contact. We consider a drain contact which selects spins parallel to the x direction. The x-part of the spin drain current as function of V_{gs} is illustrated in Figure 3.3 (right). It is not any more an increasing function. It oscillates with respect to the gate voltage V_{gs}. If the spin density reached the drain contact is oriented parallel to the x axis, the drain's current is important. In the other case, the current in the device is weak.

3.2 Spin accumulation in inhomogeneous semiconductor interfaces

The accumulation of electron spin polarization density at an interface separating two semiconductor regions with different doping levels is a well known effect in spintronics. We refer to [18, 17, 13] in which this effect was studied using two-component type models. In this section, some numerical results illustrating the propagation of spin polarization density through a boundary between two different doped semiconductor regions will be presented and interpreted. Two kind of transport models are used : two-component and spin vector Drift-Diffusion models coupled with the Poisson equation for self-consistent forces.

3.2.1 Presentation of the system

The geometry of the system under consideration is represented by figure 3.4. We consider in dimension one, two semi-conductor layers with doping densities N_1 and N_2 respectively such that $N_2 \geq N_1$. Supposing that a spin-polarized electrons are injected in the left semiconductor, under influence of the electric field, the spin polarized current is driven toward the second higher doped region. It was found that, see [18], the electron spin polarization density is accumulated near the interface between the two regions and becomes more pronounced when N_2 increases. To illustrate this

FIG. 3.4 – Schematic of the system under investigation : spin-polarized electrons are injected in the first semiconductor (S_1, N_1) with doping N_1 and transported under the action of the electric field in the x direction toward another N_2 doped semiconductor region (S_2, N_2).

phenomena, we begin by using a self consistent two-component drift-diffusion model

$$\begin{cases} \partial_t n_{\uparrow(\downarrow)} - \mathrm{div}_x j_{\uparrow(\downarrow)} = \dfrac{n_{\uparrow(\downarrow)} - n_{\downarrow(\uparrow)}}{\tau_{sf}}, \\ j_{\uparrow(\downarrow)} = D\left(\nabla_x n_{\uparrow(\downarrow)} + \dfrac{e}{k_B T}\nabla_x V n_{\uparrow(\downarrow)}\right), \\ -\Delta_x V = \dfrac{e}{\varepsilon_r \varepsilon_0}(n - N_i). \end{cases} \tag{3.2.1}$$

We assume that the system lies on the interval $I = [-10x_0, 10x_0]$ with x_0 is the scale of the transport direction x. For the numerical simulation we will take $x_0 = 1.37 \times 10^{-7} m$ in the sequel. The boundary between the two regions is supposed at point $b \in I$. The spin-up and spin-down densities, $n_\uparrow(t,x)$ and $n_\downarrow(t,x)$, satisfy the 2-component drift-diffusion system (3.2.1) with spin-flip collision term. The constant τ_{sf} is the spin-flip relaxation time and D is the diffusion constant. We denote by V the electrostatic potential satisfying the Poisson equation in which $n(t,x) = n_\uparrow(t,x) + n_\downarrow(t,x)$ is the total density of the particles (or the charge density) and $N_i(x)$ is the doping function

$$N_i(x) = \begin{cases} N_1 & \text{if } x < b, \\ N_2 & \text{if } x > b. \end{cases} \tag{3.2.2}$$

3.2.2 Numerical results

We have solved numerically system (3.2.1) using finite elements method with Gummel iterations and taking Dirichlet boundary conditions for the potential and the densities. The results presented here are representative for the general idea of

FIG. 3.5 – Electric field profil near the boundary, $E = -\partial_x V$, for $\frac{N_2}{N_1} = 5$.

the spin accumulation in inhomogeneous semiconductor interfaces. The values used for the different parameters are : $x_0 = 1.37 \times 10^{-7} m$, $b = -0.8 \times 10^{-7}$, $N_1 = 10^{21} m^{-3}$, $T = 300K$. Figure 3.5 shows the electric field profile ($E = -\partial_x V$) near the boundary in the case when $N_2 = 5N_1$. A peak is formed at the boundary due to the electrons diffusing from the highly doped right region to the less doped left region. Let us now present the evolution of the spin polarization density $p(t, x)$ defined by

$$p(t, x) = n_\uparrow(t, x) - n_\downarrow(t, x).$$

Figure 3.6 shows the evolution of $p(t, x)$ for different values of N_2 with respect to N_1. The initial spin-polarization (at $t = 0$) is represented by the dashed lines. In each of the different cases presented, $p(t, x)$ is plotted for different instances ; it converges when t increases to an equilibrium profile. In the case $N_2 = N_1$, no accumulation of spin-polarization is present at the boundary and p decreases exponentially to zero. However, when N_2 is greater than N_1 (we give in Figure 3.6 three cases : $N_2 = 5N_1$, $N_2 = 10N_1$ and $N_2 = 20N_1$), we see that a peak of spin polarization is formed near the boundary in the right region and becomes more pronounced when N_2 increases.

3.2.3 Spin accumulation and Rashba spin-orbit effect

The aim of this subsection is to study numerically the effect of the spin-orbit interaction on the spin accumulation in inhomogeneous semiconductor interfaces.

FIG. 3.6 – The evolution of the spin-polarization density for different values of N_2 with respect to N_1. In each case, the dashed line is the initial spin-polarization profile (at $t = 0$). The continuum curves represent the spin-polarization density for different instances.

We will use the spin vector drift-diffusion model derived in the previous chapter coupled with the Poisson equation. Let us write this model in the case of relaxation time approximation and with one dimensional Rashba spin-orbit effect where the effective field is given by

$$\Omega = \alpha v e_y$$

such that α is the order of the Rashba interaction and e_y is the unit vector of the y direction (perpendicular to the transport direction x). This effective field can appear for example if an electric field is applied along the z direction. The model is the following

$$\begin{cases} \partial_t n_c - \mathrm{div}_x(D(\partial_x n_c + \beta \partial_x V n_c)) = 0, \\ \partial_t \vec{N}_s - \mathrm{div}_x(D(\partial_x \vec{N}_s + \beta \partial_x V \vec{N}_s + 2\alpha e_y \times \vec{N}_s)) = \\ \qquad\qquad \alpha\beta D \partial_x V (e_y \times \vec{N}_s) - \alpha^2 D \vec{N}_s^{\perp} - \dfrac{2\vec{N}_s}{\tau_{sf}}, \\ -\Delta_x V = \dfrac{e}{\varepsilon_r \varepsilon_0}(n_c - N_i), \end{cases} \tag{3.2.3}$$

where $\beta = \dfrac{e}{k_B T}$ and D is the diffusion constant. We recall that n_c is the charge density and $\vec{N}_s$ is the spin-vector density where $\|\vec{N}_s\|$ represents the polarization density (or $n_\uparrow - n_\downarrow$ in the 2-component description). We denoted in the second equation by $\vec{N}_s^{\perp}$ the perpendicular part of $\vec{N}_s$ with respect to the effective field direction (or e_y direction). We have plotted in figure 3.7 the polarization density profile (i.e. the equilibrium profile of $\|N(t,x)\|$ when t increases) for different values of the spin-orbit coefficient (α). Figure 3.7 shows the variation of the spin accumulation at the boundary with respect to α. Let us mentioned the presence of oscillation effect of the spin accumulation due to the rotational and relaxation effects induced by the Rashba interactions.

FIG. 3.7 – The polarization profile as a function of the transport direction x and the coefficient of the Rashba spin-orbit coupling α.

References

[1] T. ANDO, A. B. FOWLER, AND F. STERN, *Electronic properties of two-dimensional electron systems*, Rev. Mod. Phys., 54 (1982), p. 437.

[2] G. BASTARD, *Wave mechanics applied to semiconductor heterostructures*, Les éditions de Physique, 1996.

[3] N. BEN ABDALLAH AND F. MÉHATS, *Semiclassical analysis of the Schrödinger equation with a partially confining potential*, J. Math. Pures Appl. (9), 84 (2005), pp. 580–614.

[4] N. BEN ABDALLAH AND F. MÉHATS, *On a Vlasov-Schrödinger-Poisson Model* , Comm. Partial Differential Equations, 29 (2004), pp. 173–206.

[5] N. BEN ABDALLAH, F. MÉHATS, AND C. NEGULESCU, *Adiabatic quantum-fluid transport models*, Comm. Math. Sci., 4 (2006), pp. 621–650.

[6] N. BEN ABDALLAH, F. MÉHATS, P. PIETRA, AND N. VAUCHELET, *A drift-diffusion subband model for the simulation of the Double-Gate MOSFET* , IEEE-NANO 2005, Conference on Nanotechnology, Nagoya.

[7] N. BEN ABDALLAH, F. MÉHATS, AND N. VAUCHELET, *Analysis of a Drift-Diffusion-Schrödinger-Poisson model*, C. R. Acad. Sci. Paris, Ser. I 335, pp. 1007–1012.

[8] A. BOURNEL, *Magnéto-électronique dans des dispositifs à semiconducteurs*, Ann. Phys. Fr, 25 (2000), pp. 1–167.

[9] A. Bournel, V. Delmouly, P. Dollfus, G. Tremblay, and P. Hesto, *Theoretical and experimental considerations on the spin field effect transistor*, Physica E, 10 (2001), pp. 86–90.

[10] A. Bournel, P. Dollfus, E. Cassan, and P. Hesto, *Monte Carlo study of spin relaxation in AlGaAs/GaAs quantum wells*, Applied Physics Letters, 77 (2000), pp. 2346–2348.

[11] Y. A. Bychkov and E. I. Rashba, *Oscillatory effects and the magnetic susceptibility of carriers in inversion layers*, Journal of Physics C : Solid State Physics, 17 (1984), pp. 6039–6045.

[12] P. Caussignac, B. Zimmermann, and R. Ferro, *Finite element approximation of electrostatic potential in one-dimensional multilayer structures with quantized electronic charge*, Computing, 45 (1990), pp. 251–264.

[13] D. Csontos and S. E. Ulloa, *Spin injection and accumulation in inhomogeneous semiconductors*, Physica E, 32 (2006), pp. 412–415.

[14] S. Datta and B. Das, *Electronic analog of the electro-optic modulator*, Applied Physics Letters, 56 (1990), pp. 665–667.

[15] J. H. Davies, *The physiscs of low dimensional semiconductors*, Cambrifge Univ. press, 1998.

[16] H. K. Gummel, *A self-consistent iterative scheme for one dimensional steady state transistor calculations*, IEEE Trans. On Elec. Dev., 11 (1964), p. 455.

[17] Y. V. Pershin, *Accumulation of electron spin polarization at semiconductor interfaces*, Phys. Rev. B, 68 (2003), p. 233309.

[18] Y. V. Pershin and V. Privman, *Focusing of Spin Polarization in Semiconductors by Inhomogeneous Doping*, Phys. Rev. Lett., 90 (2003), p. 256602.

[19] P. Pietra and N. Vauchelet, *Modeling and simulation of the diffusive transport in a nanoscale Double-Gate MOSFET* , submitted.

[20] S. Saikin, Y. Pershin, and V. Privman, *Modelling for semiconductor spintronics*, IEE Proceedings Circuits, Devices and Systems, 152 (2005), pp. 366–376.

[21] S. Saikin, M. Shen, and M.-C. Cheng, *Study of spin-polarized transport properties for spin-FET design optimization*, IEEE Trans. Nanotechnology, 3 (2004), pp. 173–179.

[22] N. Vauchelet, *Modélisation mathématique du transport diffusif de charges partiellement quantiques*, Thesis, Université Paul Sabatier-Toulouse III, (2006).

Part II

Diffusion and high magnetic fields

Chapter 4

Diffusion and guiding center approximation for particle transport in strong magnetic fields

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Abstract

The diffusion limit of the linear Boltzmann equation with a strong magnetic field is performed. The Larmor radius is supposed to be much smaller than the mean free path. The limiting equation is shown to be a diffusion equation in the parallel direction while in the orthogonal direction, the guiding center motion is obtained. The diffusion constant in the parallel direction is obtained through the study of a new collision operator obtained by averages of the original one. Moreover, a correction to the guiding center motion is derived.

Keywords. Diffusion limit, guiding-center approximation, high magnetic field.

4.1 Introduction

The motion of charged particles under the action of a strong magnetic field is an important phenomena encountered in artificial and natural plasmas (Tokamakas, ionospheric plasmas, etc). In the presence of constant magnetic field $\vec{B}$, a charged particle (electron in our case) of mass m and charge q with velocity v follow a helical trajectory around magnetic field line. The gyration radius of the particles, called Larmor radius r_L, is inversely proportional to the magnitude of the magnetic field ($r_L = \frac{mv}{qB}$). This means that when the magnetic field becomes large, the particles get trapped along the direction of $\vec{B}$. In addition, when an electric field $\vec{E}$ is applied, the particles experience a drift of the instantaneous centers of Larmor circles, called in the literature the guiding center motion, in the direction perpendicular to both the electric and magnetic fields. The velocity of this drift is given by the following formula

$$v_{drift} = \frac{\vec{E} \times \vec{B}}{B^2}.$$

Direct simulations of Vlasov or Boltzmann equations in the presence of such large magnetic fields requires the numerical resolutions of the small position and time scales induced by the gyration along the magnetic field. Hence, the question of deriving approximate models, numerically less expensive, is of great importance. Various models have been developed to this aim like the "guiding-center" and the gyrokinetic models. The guiding center approximation consists in averaging the motion over the gyroperiod when supposing B goes to $+\infty$ ($r_L \to 0$) [26] and the gyrokinetic approximation is a generalization of the guiding center one in the case of kinetic equations. For a complete physical review, we refer for instance to [27, 15, 28, 31]. Mathematically speaking, homogenization techniques were used in [19, 20] by E. Frénod and E. Sonnendrücker to justify the high magnetic field limit of Vlasov and Vlasov-Poisson systems. It is proven in [19] that the tridimensional guiding center approximation leads to a one-dimensional kinetic model in the direction of the magnetic field. The drift phenomenon perpendicular to the magnetic field is rigourously obtained in [20] for the two dimensional Vlasov equation on a sufficiently long time scale. Other asymptotic regimes of the Vlasov equation with strong magnetic fields are studied [21, 18, 22, 16, 17]. The gyrokinetic approximation of the Vlasov-Poisson system has also been intensively studied by F. Golse and L. Saint-Raymond for the two and tridimensional motions in various asymptotic regimes [24, 33, 25, 34].

In all the above references, the transport is assumed to be ballistic, which means that particles do not suffer any collision during their motion. We are here interested in regimes were collisions are important and we propose to study the interplay between the fluid limit induced by collisions and the high frequency gyrations around

the magnetic field. To simplify the study, we shall only consider collisions with a thermal bath at a given temperature. In this case, the diffusion limit of the obtained Boltzmann equation leads to the so-called drift diffusion equation. The question of deriving diffusions equations from the Boltzmann equation has been widely studied during the last three decades in the context of radiative transfer [5, 6, 35, 1, 7], in semiconductors and plasmas [32, 23, 30, 2, 3, 4, 8, 9, 10] and many other contexts that we do not mention here. In the presence of a magnetic field, an important quantity to be considered is the gyroperiod measuring the time that a particle of mass m with charge q and submitted to the constant magnetic field B makes a 2π rotation around this field ($T_c = 2\pi m/qB$). When the gyroperiod is much larger than the relaxation time, then the magnetic field effect disappear in the diffusion limit as will be seen later on. When T_c is of the same order of magnitude as the relaxation time, the diffusion matrix has an antisymmetric component, generated by the magnetic field (this has been proven for collision with walls by P. Degond & al [8, 11, 14]). Formal results for binary gas mixtures can also be found in [29, 12, 13, 9]. We shall consider in this paper the situation where the gyroperiod is much smaller than the relaxation time. In that case, one expects that the diffusion matrix is obtained through the analysis of an averaged collision operator. Also, the high frequency oscillations only occur in the direction perpendicular to the magnetic field while parallel velocity stay unaffected. Therefore, the behaviours of the solutions in these directions are expected to be different. We shall show in this paper that the transport is diffusive along the magnetic field, while it is dominated by the guiding center drift in the orthogonal direction. The diffusion coefficient in the parallel direction will be obtained by averaging the collision cross section around the magnetic field.

The outline of the paper is as follows. In the next section, we introduce the scaling, notations and state the main results. The proofs rely on the study of the operator accounting for collisions and gyration around the magnetic field. The analysis of this operator is done in Section 3. Section 4 is devoted to the asymptotics of this operator when the scaled gyration period tends to zero. It is shown that this limit is well described by a collision operator with a cross section averaged around the magnetic field. This result is then used in Section 5 in order to prove the main results of the paper. Some concluding remarks are listed in the last section of the paper.

4.2 Setting of the problem and main results

The problem we are interested in is a singular perturbation of the three dimensional Boltzmann equation with a constant large magnetic field. The position variable

is denoted by $\mathbf{r} = (x, y, z)$, the velocity variable is denoted $\mathbf{v} = (v_x, v_y, v_z)$. The magnetic field is assumed to be constant and parallel to the z axis. We shall denote by $\mathbf{r}_\perp = (x, y)$ and $\mathbf{v}_\perp = (v_x, v_y)$, the orthogonal variables. The distribution function is a solution of the following singularly perturbed Boltzmann equation

$$\begin{cases} \dfrac{\partial f^{\varepsilon\eta}}{\partial t} + \dfrac{\mathcal{T}_z f^{\varepsilon\eta}}{\varepsilon} + \dfrac{\mathcal{T}_\perp f^{\varepsilon\eta}}{\varepsilon\eta} + \dfrac{(\mathbf{v} \times \mathbf{e}_z)}{\varepsilon^2\eta^2} \cdot \nabla_{\mathbf{v}} f^{\varepsilon\eta} = \dfrac{Q(f^{\varepsilon\eta})}{\varepsilon^2} \\ f^{\varepsilon\eta}(t = 0) = f_0(\mathbf{r}, \mathbf{v}), \end{cases} \tag{4.2.1}$$

where $\mathcal{T}_\perp$ and $\mathcal{T}_z$ are the respectively perpendicular and parallel parts of the transport operator

$$\mathcal{T}_\perp = \mathbf{v}_\perp \cdot \nabla_{\mathbf{r}_\perp} + \mathbf{E}_\perp \cdot \nabla_{\mathbf{v}_\perp}, \quad \mathcal{T}_z = v_z \partial_z + E_z \partial_{v_z}.$$

The collision operator is given by

$$Q(f)(\mathbf{v}) = \int_{\mathbb{R}^3} \sigma(\mathbf{v}, \mathbf{v}')[\mathcal{M}(\mathbf{v}) f(\mathbf{v}') - \mathcal{M}(\mathbf{v}') f(\mathbf{v})] d\mathbf{v}'. \tag{4.2.2}$$

The function $\mathcal{M}$ is the normalized Maxwellian :

$$\mathcal{M}(\mathbf{v}) = \frac{1}{(2\pi)^{\frac{3}{2}}} e^{-\frac{1}{2}|\mathbf{v}|^2}, \tag{4.2.3}$$

and the cross section σ is symmetric and bounded from below and above by two positive constants. The parameter ε is intended to go to zero and represents the scaled mean free path. The scaled magnetic field is given by $\frac{\mathbf{e}_z}{\varepsilon\eta^2}$, while $\mathbf{E} = \begin{pmatrix} \mathbf{E}_\perp \\ \mathrm{E}_z \end{pmatrix}$ is the scaled electric field. The gyroperiod is $\varepsilon\eta^2$ and we shall consider the situation where η and ε go to zero simultaneously and the situation where ε tends to zero for η given then η tends to zero. Since the magnetic field strongly confines the motion of the particles in the perpendicular direction (x, y), we have rescaled this direction with the prefactor η. This is why the orthogonal operator $\mathcal{T}_\perp$ comes with a different scaling from the parallel one $\mathcal{T}_z$. By doing so, we shall obtain a non trivial motion in the orthogonal direction (guiding center).

4.2.1 Scaling

In this subsection, we shall explain the hypotheses that lead to the scaled Boltzmann equation (4.2.1). In particular, we highlight the differences of the position scales in the parallel and perpendicular directions (with respect to the magnetic field). The starting point is the diffusion scaling in the absence of a magnetic field. The unscaled Boltzmann equation in this case reads

$$\partial_t F + V \cdot \nabla_X F + \frac{q \nabla_X \Phi}{m} \cdot \nabla_V F = \mathbf{Q}(F)$$

where (t, X, V) are the physical time position and velocity variables, while Φ is the electrostatic potential, e is the elementary charge and m the mass of the electron (to fix the ideas, we consider electrons). The collision operator $\mathbf{Q}$ has the form

$$\mathbf{Q}(F) = \int \Sigma(V, V')[M_T(V)F(V') - M_T(V')F(V)]\, dV',$$

Σ is the transition rate and M_T is the Maxwellian at the temperature T

$$M_T(V) = (\frac{2\pi K_B T}{m})^{-3/2} \exp(-\frac{mv^2}{2K_B T}),$$

K_B being the Boltzmann constant. The thermal energy and velocity are respectively defined by

$$U_{th} = K_B T, \quad V_{th} = \sqrt{\frac{K_B T}{m}}.$$

The electrostatic energy is assumed to be of the order of the thermal energy and varies over a macroscopic length scale L :

$$q\Phi(X) = U_{th}\phi(\frac{X}{L}).$$

The transition rate Σ is the inverse of a time. The typical value of this time, the scattering time, is denoted by τ_s. So we write

$$\Sigma(V, V') == \frac{1}{\tau_s}\sigma(\frac{V}{V_{th}}, \frac{V'}{V_{th}})$$

where σ is its scaled version assumed to be of order 1. The mean free path L_s will be defined as the distance that a thermal electron crosses during the scattering time τ_s

$$L_s = V_{th}\tau_s.$$

This distance is assumed to be much smaller than the macroscopic distance L and we shall denote it by

$$\varepsilon = \frac{L_s}{L}.$$

The only thing left to know is the macroscopic time scale. Since the kernel of the collision operator is generated by the Maxwellian which carries no flux, one has to go to the diffusion scaling and define the macroscopic time τ_m by

$$\frac{\tau_s}{\tau_m} = (\frac{L_s}{L})^2 = \varepsilon^2.$$

Using $(\tau_m, L, V_{th}, U_{th})$ as units for time, position, velocity and energy, the Boltzman equation can be written

$$\partial_t f + \frac{1}{\varepsilon}(\mathbf{v} \cdot \nabla_{\mathbf{r}} f - \nabla_{\mathbf{r}}\phi \cdot \nabla_{\mathbf{v}} f) = \frac{Q(f)}{\varepsilon^2},$$

where Q is the scaled Boltzmann operator (4.2.2).

Let us now look at the effect of a large magnetic field $\mathcal{B} = B\mathbf{e}_z$. The scaled Boltzmann equation contains the additional term $-\frac{q}{m}(V \times \mathcal{B}) \cdot \nabla_{\mathcal{V}} \mathcal{F}$. An electron submitted to this magnetic field spins around it following the equation

$$m\frac{dV}{dt} = -qV \times \mathcal{B}.$$

The period of this precession, called the cyclotron period is given by

$$\tau_c = \frac{m}{qB}.$$

We shall assume that this period is much smaller than the scattering time and we write

$$\tau_c = \eta^2 \tau_s.$$

Of course the motion along the magnetic field stays unchanged and we shall not change the length scale in this direction. In the orthogonal direction however, the combined action of the electric field and the magnetic field results in the drift of the guiding center (the electron motion is a rotation around a center which is now drifting under the action of the electric field). The velocity of this drift is given by

$$V_c = \frac{E \times \mathcal{B}}{B^2}.$$

Its order of magnitude is then given by

$$V_c = \frac{E_\perp}{B},$$

wher $E_\perp$ is the perpendicular component of the electric field.

The last hypothesis that we make is the potential Φ varies in the orthogonal direction on a lengthscale $L_\perp$ which is not equal to the parallel lengthscale L. Moreover, $L_\perp$ is such that the guiding center moves during the macroscopic time by a distance of the order of $L_\perp$ itself. In other words, we want

$$E_\perp = \frac{U_{th}}{qL_\perp}, \quad V_c \tau_m = L_\perp.$$

Replacing the thermal energy by its expression given above in this section, we find after straightforward computations that

$$L_\perp^2 = \frac{\tau_m U_{th}}{qB} = \eta^2 L^2.$$

Now rescaling the orthogonal position variable by $L_\perp$, we obtain the Boltzmann equation (4.2.1).

Remark 4.2.1. From the scaling hypotheses, we see that between two successive collisions, the electron precesses a large number of times around the magnetic field. Therefore, one might expect that the collision cross section will be averaged along these precessions. On the other hand, since the orthogonal lengthscale has been designed in order to see the guiding center drift, the limiting equation should exhibit this term. Finally, since the parallel motion to the magnetic field does not feel the magnetic field, one is entitled to expect a non vanishing diffusion in this direction. This is exactly what we shall prove in this paper : drift in the orthogonal direction, finite diffusion in the parallel direction governed by a collision operator averaged over precessions around the magnetic field.

4.2.2 Notations

The analysis of the limit $\varepsilon \to 0$ naturally leads to the study of the operator

$$Q^\eta = Q - \frac{(\mathbf{v} \times \mathbf{e}_z)}{\eta^2} \cdot \nabla_{\mathbf{v}}, \tag{4.2.4}$$

while the limit $\eta \to 0$, involves the cylindrical averaging around the vector $\mathbf{e}_z$. To this aim, we denote by $\mathcal{R}(\tau)$ the rotation around $\mathbf{e}_z$ with angle τ which is the multiplication operator by the following matrix

$$\mathcal{R}(\tau) = \begin{pmatrix} \cos\tau & \sin\tau & 0 \\ -\sin\tau & \cos\tau & 0 \\ 0 & 0 & 1 \end{pmatrix}. \tag{4.2.5}$$

The cylindrical average of a function $h = h(\mathbf{v})$ is defined by

$$\mathcal{A}(h)(\mathbf{v}) := \overline{h}(\mathbf{v}) = \frac{1}{2\pi} \int_0^{2\pi} h(\mathcal{R}(\tau)\mathbf{v})\, d\tau. \tag{4.2.6}$$

It is clear that $\mathcal{A}$ is the orthogonal projector (in the L^2 sense) on the set of cylindrically invariant functions. We also define the partial average

$$\mathcal{A}_\tau(h)(\mathbf{v}) := \overline{h}_\tau(\mathbf{v}) = \frac{1}{2\pi} \int_0^{\tau} h(\mathcal{R}(s)\mathbf{v})\, ds. \tag{4.2.7}$$

We shall moreover define the averaged function $\overline{\sigma}$ and the symmetric average $\overline{\overline{\sigma}}$ by

$$\overline{\sigma}(\mathbf{v}, \mathbf{v}') = \frac{1}{2\pi} \int_0^{2\pi} \sigma\left(\mathcal{R}(\tau)\mathbf{v}, \mathbf{v}'\right)\, d\tau$$

$$\overline{\overline{\sigma}}\left(\mathbf{v}, \mathbf{v}'\right) = \frac{1}{4\pi^2} \int_0^{2\pi} \int_0^{2\pi} \sigma\left(\mathcal{R}(\tau)\mathbf{v}, \mathcal{R}(\tau')\mathbf{v}'\right)\, d\tau d\tau' = \frac{1}{2\pi} \int_0^{2\pi} \overline{\sigma}\left(\mathbf{v}, \mathcal{R}(\tau')\mathbf{v}'\right)\, d\tau',$$

and the corresponding collision operators

$$\overline{Q}(f)(\mathbf{v}) = \int_{\mathbb{R}^3} \overline{\sigma}(\mathbf{v},\mathbf{v}')[\mathcal{M}(\mathbf{v})f(\mathbf{v}') - \mathcal{M}(\mathbf{v}')f(\mathbf{v})]d\mathbf{v}', \tag{4.2.8}$$

$$\overline{\overline{Q}}(f)(\mathbf{v}) = \int_{\mathbb{R}^3} \overline{\overline{\sigma}}(\mathbf{v},\mathbf{v}')[\mathcal{M}(\mathbf{v})f(\mathbf{v}') - \mathcal{M}(\mathbf{v}')f(\mathbf{v})]d\mathbf{v}'. \tag{4.2.9}$$

We define the functional spaces

$$L^2_{\mathcal{M}} = \left\{ f = f(\mathbf{v}) \,/\, \int_{\mathbb{R}^3} \frac{|f(\mathbf{v})|^2}{\mathcal{M}(\mathbf{v})} d\mathbf{v} < +\infty \right\}, \tag{4.2.10}$$

and its cylindrically symmetric subspace

$$\overline{L}^2_{\mathcal{M}} = \{ f \in L^2_{\mathcal{M}} / \quad f(\mathcal{R}(\tau)\mathbf{v}) = f(\mathbf{v}), \quad \forall \tau \in [0, 2\pi] \}. \tag{4.2.11}$$

We also define the space

$$\mathcal{H}^2_{\mathcal{M}} = \{ f \in L^2_{\mathcal{M}}, \quad \text{such that, } \partial^\alpha f \in L^2_{\mathcal{M}}, \quad \text{for } |\alpha| \leq 2 \}. \tag{4.2.12}$$

We shall make the following hypotheses

Assumption 4.2.2. *The cross-section σ belongs to $W^{2,\infty}(\mathbb{R}^6)$ and is supposed to be symmetric and bounded from above and below :*

$$\exists \alpha_1, \alpha_2 > 0, \quad 0 < \alpha_1 \leq \sigma(\mathbf{v},\mathbf{v}') = \sigma(\mathbf{v}',\mathbf{v}) \leq \alpha_2, \quad \forall (\mathbf{v},\mathbf{v}') \in \mathbb{R}^6. \tag{4.2.13}$$

Assumption 4.2.3. *There exists a potential $V(t,\mathbf{r})$ in $C^1(\mathbb{R}^+; W^{1,\infty}(\mathbb{R}^3))$, such that $\mathbf{E} = -\nabla_{\mathbf{r}} V$.*

We finally define the space

$$L^2_{\mathcal{M}_V} = \left\{ f = f(\mathbf{r},\mathbf{v}) \,/\, \int_{\mathbb{R}^6} \frac{|f(\mathbf{r},\mathbf{v})|^2}{\mathcal{M}(\mathbf{v})\mathrm{e}^{-V(\mathbf{r})}} d\mathbf{v} < +\infty \right\}. \tag{4.2.14}$$

4.2.3 Main results

The main results of this paper are summarized in the following two theorems. The first one deals with the limit $\varepsilon \to 0$ while $\eta > 0$ is kept fixed.

Theorem 4.2.4. *Let $\eta > 0$ be fixed. Let $T \in \mathbb{R}^*_+$ and assume that the initial data of (4.2.1), f_0, belongs to $L^2_{\mathcal{M}_V}$. Then, with Assumptions 4.2.2 and 4.2.3, the problem (4.2.1) has a unique weak solution in $C^0([0,T], L^2_{\mathcal{M}_V})$. Moreover, the sequence $(f^{\varepsilon\eta})_\varepsilon$ converges weakly to $\rho_\eta(t,\mathbf{r})\mathcal{M}(\mathbf{v})$ in $L^\infty((0,T); L^2_{\mathcal{M}_V}))$ weak $\star$ where ρ_η satisfies*

$$\partial_t \rho_\eta - \mathrm{div}(\mathbb{D}^\eta(\nabla\rho_\eta - \rho_\eta \mathbf{E})) = 0 \tag{4.2.15}$$

and the diffusion matrix $\mathbb{D}^\eta$ *is given by the formula*

$$\mathbb{D}^\eta = \int \begin{pmatrix} \frac{1}{\eta}\mathbf{v}_\perp \\ v_z \end{pmatrix} \otimes \begin{pmatrix} \eta \mathbf{X}_\perp^\eta \\ X_z^\eta \end{pmatrix} d\mathbf{v},$$

$\mathbf{X}^\eta = \begin{pmatrix} \mathbf{X}_\perp^\eta \\ X_z^\eta \end{pmatrix}$ *being the only solution of (4.3.7).*

Remark 4.2.5. In the relaxation time case $\sigma(\mathbf{v}, \mathbf{v}') = \frac{1}{\tau}$, the matrix $\mathbb{D}^\eta$ can be computed explicitly :

$$\mathbb{D}^\eta = \tau \begin{pmatrix} \frac{\eta^2}{\tau^2+\eta^4} & \frac{\tau}{\tau^2+\eta^4} & 0 \\ -\frac{\tau}{\tau^2+\eta^4} & \frac{\eta^2}{\tau^2+\eta^4} & 0 \\ 0 & 0 & 1 \end{pmatrix}.$$

In the limit $\eta \to 0$, the upper 2 x 2 block of the matrix reduces to the antisymmetric matrix $\mathcal{I} = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}$, whereas its symmetric part is of order η^2. The following proposition shows that these features are still valid in the case of a non constant scattering section σ.

Proposition 4.2.6. *Writing* $\mathbf{X}^\eta = \begin{pmatrix} \mathbf{X}_\perp^\eta \\ \mathrm{X}_z^\eta \end{pmatrix}$, *we have the following expansions in* $\mathcal{H}^2_{\mathcal{M}}$ *as* η *tends to zero*

$$\mathrm{X}_z^\eta = \mathrm{X}_z^{(0)} + \eta^2 \mathrm{X}_z^{(1)} + \mathcal{O}(\eta^4),$$
$$\mathbf{X}_\perp^\eta = \mathbf{X}_\perp^{(0)} + \eta^2 \mathbf{X}_\perp^{(1)} + \mathcal{O}(\eta^4).$$

The diffusion matrix $\mathbb{D}^\eta$ *is a definite positive matrix. Its symmetric and antisymmetric parts,* $\mathbb{D}_s^\eta$ *and* $\mathbb{D}_{as}^\eta$, *have respectively the following expansions*

$$\mathbb{D}_s^\eta = \begin{pmatrix} \eta^2 \int \mathbf{v}_\perp \otimes \mathbf{X}_\perp^{(1)} d\mathbf{v} & 0 \\ 0 & D_z \end{pmatrix} + \eta^3 \mathbb{D}_{z\perp}^{(1)} + \mathcal{O}(\eta^4),$$

$$\mathbb{D}_{as}^\eta = \begin{pmatrix} 0 & 1 & 0 \\ -1 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix} + \eta \mathbb{D}_{z\perp}^{(0)} + \mathcal{O}(\eta^4)$$

where $D_z = \int v_z X_z^{(0)} \, d\mathbf{v}$ *and*

$$\mathbb{D}_{z\perp}^{(0)} = \int \begin{pmatrix} \mathbf{0} \\ v_z \end{pmatrix} \otimes \begin{pmatrix} \mathbf{X}_\perp^{(0)} \\ 0 \end{pmatrix} d\mathbf{v} - \int \begin{pmatrix} \mathbf{X}_\perp^{(0)} \\ 0 \end{pmatrix} \otimes \begin{pmatrix} \mathbf{0} \\ v_z \end{pmatrix} d\mathbf{v}$$

$$\mathbb{D}_{z\perp}^{(1)} = \int \begin{pmatrix} \mathbf{X}_\perp^{(1)} \\ 0 \end{pmatrix} \otimes \begin{pmatrix} \mathbf{0} \\ v_z \end{pmatrix} d\mathbf{v} + \int \begin{pmatrix} \mathbf{0} \\ v_z \end{pmatrix} \otimes \begin{pmatrix} \mathbf{X}_\perp^{(1)} \\ 0 \end{pmatrix} d\mathbf{v}.$$

Remark 4.2.7. The above theorem shows that the diffusion is of order $\mathcal{O}(1)$ in the parallel direction while it scales like η^2 in the orthogonal one, exactly like in the relaxation time coefficient. The antisymmetric part of the diffusion matrix acts essentially on the orthogonal direction and leads to the guiding center motion. However, the above formula shows a correction of order η of the guiding center motion, which is due to collisions. Indeed, it is readily seen that for any three dimensional vector $\mathbf{Z}$

$$-\mathbb{D}^{\eta}_{as}\mathbf{Z} = \mathbf{u}^{\eta} \times \mathbf{Z} + \mathcal{O}(\eta^4)$$

where

$$\mathbf{u}^{\eta} = \begin{pmatrix} -\eta \int X^{(0)}_y v_z d\mathbf{v} \\ \eta \int X^{(0)}_x v_z d\mathbf{v} \\ 1 \end{pmatrix},$$

and $(X^{(0)}_x, X^{(0)}_y)$ are the components of $\mathbf{X}^{(0)}_{\perp}$. This leads to

$$-\nabla \cdot (\mathbb{D}^{\eta}_{as}(\nabla_{\mathbf{r}}\rho_{\eta} - \rho_{\eta}\mathbf{E})) = \nabla \cdot (\rho_{\eta} E \times \mathbf{u}^{\eta}) + \mathcal{O}(\eta^4).$$

Theorem 4.2.8. *Under the same hypotheses as for Theorem 4.2.4, we now let ε and η simultaneously and independently tend to zero (there is no assumption on the relative scale between ε and η). In this case, the sequence $(f^{\varepsilon\eta})_{\varepsilon\eta}$ of weak solutions of (4.2.1) converges weakly to $\rho(t,\mathbf{r})\mathcal{M}(\mathbf{v})$ in $L^{\infty}([0,T], L^2_{\mathcal{M}_V})$ weak *, where ρ is the solution of*

$$\begin{cases} \partial_t \rho + \partial_z \mathrm{J}_z + \nabla \cdot (\rho \mathbf{E} \times \mathbf{e}_z) = 0 \\ \rho(0,\mathbf{r}) = \displaystyle\int_{\mathbb{R}^3} f_0(\mathbf{r},\mathbf{v})\, d\mathbf{v}. \end{cases} \tag{4.2.16}$$

The parallel current density, J_z is given by

$$\mathrm{J}_z = -D_z(\partial_z \rho - E_z \rho),$$

where D_z is the diffusion constant given by

$$D_z = \int_{\mathbb{R}^3} \mathrm{X}^{(0)}_z v_z d\mathbf{v}, \tag{4.2.17}$$

and $\mathrm{X}^{(0)}_z$ is the zero-th order term of X^{η}_z (defined by (4.4.7)).

4.3 Analysis of the operator Q^{η}

Let us consider the space $L^2_{\mathcal{M}}$ introduced in (4.2.10) and define the scalar product on this space by

$$\langle f, g \rangle_{\mathcal{M}} = \int_{\mathbb{R}^3} \frac{fg}{\mathcal{M}} d\mathbf{v}.$$

Let $D(Q^\eta)$ be defined by

$$D = D(Q^\eta) := \{f \in L^2_{\mathcal{M}} / \, (\mathbf{v} \times \mathbf{e}_z) \cdot \nabla_{\mathbf{v}} f \in L^2_{\mathcal{M}}\}. \tag{4.3.1}$$

We have the following result.

Proposition 4.3.1. *The operator Q^η given by (4.2.4) with domain D defined by (4.3.1) satisfies the following properties.*

1. *For any $f \in D$, we have $\int_{\mathbb{R}^3} Q^\eta(f) d\mathbf{v} = 0$ (mass conservation).*
2. *$(-Q^\eta, D)$ is a maximal monotone operator.*
3. *The kernel of Q^η is the real line spanned by the Maxwellian :*

$$Ker(Q^\eta) = \{f \in L^2_{\mathcal{M}} / \, \exists \alpha \in \mathbb{R} \text{ such that } f(\mathbf{v}) = \alpha \mathcal{M}(\mathbf{v})\}.$$

4. *Let $\mathcal{P}$ be the orthogonal projection on $KerQ^\eta$. The following coercivity inequality holds for any function $f \in D$*

$$-\langle Q^\eta(f), f\rangle_{\mathcal{M}} \geq \alpha_1 \|f - \mathcal{P}(f)\|^2_{\mathcal{M}}. \tag{4.3.2}$$

   where $\alpha_1 > 0$ is the lower bound of σ (4.2.13).

5. *The range of Q^η, denoted by $Im(Q^\eta)$, is the set of functions $g \in L^2_{\mathcal{M}}$ satisfying the solvability condition : $\int_{\mathbb{R}^3} g(\mathbf{v}) d\mathbf{v} = 0$. In addition, for all $g \in Im(Q^\eta)$ there exists a unique function $f \in D$ satisfying both $Q^\eta(f) = g$ and $\int_{\mathbb{R}^3} f(\mathbf{v}) d\mathbf{v} = 0$.*

Proof. First of all, we recall that the operator Q satisfies all items of Proposition 4.3.1 (by substituting D by $L^2_{\mathcal{M}}$). Now Items 1., 3. and 4. of the Proposition follow immediately from these properties since we have $\int_{\mathbb{R}^3} (\mathbf{e}_z \times \mathbf{v}) \cdot \nabla_{\mathbf{v}}(f) d\mathbf{v} = \int_{\mathbb{R}^3} \mathrm{div}_{\mathbf{v}}[(\mathbf{e}_z \times \mathbf{v}) f] d\mathbf{v} = 0$ and $\langle (\mathbf{e}_z \times v) \cdot \nabla_v f, f\rangle_{\mathcal{M}} = 0$. In order to prove Item 2., we need to prove that $I - Q^\eta$ is one-to-one from D to $L^2_{\mathcal{M}}$. In order to do so, we rewrite the equation $f - Q^\eta(f) = g$ under the following form

$$\frac{1}{\eta^2}(\mathbf{v} \times \mathbf{e}_z) \cdot \nabla_{\mathbf{v}} f + (1 + \nu(\mathbf{v})) f = Q^+(f) + g,$$

where we have written

$$Q(f) = Q^+(f) - \nu f, \tag{4.3.3}$$

$$Q^+(f) = (\int_{\mathbb{R}^3} \sigma(\mathbf{v}, \mathbf{v}') f(\mathbf{v}') d\mathbf{v}') \mathcal{M}(\mathbf{v}) \tag{4.3.4}$$

$$\nu(\mathbf{v}) = \int_{\mathbb{R}^3} \sigma(\mathbf{v}, \mathbf{v}') \mathcal{M}(\mathbf{v}') d\mathbf{v}'. \tag{4.3.5}$$

The characteristics of the equation are defined by

$$\left\{ \begin{array}{rl} \dfrac{d\mathbf{v}}{dt} & = \dfrac{1}{\eta^2}(\mathbf{v}\times\mathbf{e}_z) \\ \mathbf{v}|_{t=0} & = \mathbf{v}_0 \end{array} \right.$$

whose solution is $\mathbf{v}(t) = \mathcal{R}(\dfrac{t}{\eta^2})\mathbf{v}_0$. The solution of the equation can then be defined by integration over the characteristics and finally leads to $f = \mathcal{F}(Q^+(f)+g)$ where

$$\begin{aligned} \mathcal{F}(h)(\mathbf{v}) =& \frac{\eta^2}{B_\eta(\mathbf{v})}\int_0^{2\pi} h(\mathcal{R}(\tau)\mathbf{v})e^{\eta^2\int_0^\tau(1+\nu(\mathcal{R}(s)v))ds}d\tau, \\ B_\eta(v) =& e^{\eta^2\int_0^{2\pi}(1+\nu(\mathcal{R}(s)v))\,ds} - 1. \end{aligned}$$

A fixed point argument leads to the existence and uniqueness of $f \in L^2_{\mathcal{M}}$ solving the equation $f - Q^\eta(f) = g$ in the distributional sense. Since Q is a bounded operator on $L^2_{\mathcal{M}}$, we immediately obtain that $(\mathbf{v}\times\mathbf{e}_z)\cdot\nabla_{\mathbf{v}} f \in L^2_{\mathcal{M}}$ so that the constructed solution is in the domain D of the operator Q^η. Let us now prove item 5. Consider $g \in L^2_{\mathcal{M}}$ such that $\displaystyle\int_{\mathbb{R}^3} g(v)d\mathbf{v} = 0$. From the maximal monotonicity of Q^η, for each $\lambda > 0$, $\lambda Id - Q^\eta$ is surjective. Therefore, for all $\lambda > 0$, there exists $f_\lambda \in D(Q^\eta)$ satisfying

$$\lambda f_\lambda - Q^\eta(f_\lambda) = g. \tag{4.3.6}$$

Integrating this equation with respect to $\mathbf{v}$ gives $\lambda\displaystyle\int_{\mathbb{R}^3} f_\lambda d\mathbf{v} = \int_{\mathbb{R}^3} g d\mathbf{v} = 0$ and with (4.3.2) we get $-\langle Q^\eta(f_\lambda), f_\lambda\rangle_{\mathcal{M}} \geq \alpha_1\|f_\lambda\|^2_{\mathcal{M}}$. Taking the scalar product of (4.3.6) with f_λ in $L^2_{\mathcal{M}}$, one obtains

$$\lambda\|f_\lambda\|_{\mathcal{M}} + \alpha_1\|f_\lambda\|_{\mathcal{M}} \leq \|g\|_{\mathcal{M}}.$$

This implies that $(f_\lambda)_{\lambda>0}$ is bounded in $L^2_{\mathcal{M}}$. Up to an extraction of a subsequence, there exists $f \in L^2_{\mathcal{M}}$ such that (f_λ) converges weakly to f. By passing to the limit $\lambda \to 0$ in the weak form of equation (4.3.6), we get

$$\frac{1}{\eta^2}(\mathbf{v}\times\mathbf{e}_z)\cdot\nabla_v f - Q(f) = g \quad \text{in } D'(\mathbb{R}^3).$$

In addition, $Q(f)$ and g belong to $L^2_{\mathcal{M}}$, then $(\mathbf{v}\times\mathbf{e}_z)\cdot\nabla_{\mathbf{v}} f \in L^2_{\mathcal{M}}$ and then $f \in D(Q^\eta)$. Of course $\int_{\mathbb{R}^3} f d\mathbf{v} = 0$ since this is true for f_λ. Now if there is another solution of $-Q(\cdot) = g$ with zero velocity average, the difference of this solution with f is in the kernel of Q^η and has a zero average. It is necessarily equal to zero.

■

The following corollary is a direct consequence of Proposition 4.3.1.

Corollary 4.3.2. *For all $\eta > 0$, there exists a unique $\mathbf{X}_\eta = \begin{pmatrix} \mathbf{X}_\perp^\eta \\ \mathrm{X}_z^\eta \end{pmatrix}$ in $(D(Q^\eta))^3$ satisfying*

$$-Q^\eta(\mathbf{X}^\eta) = \begin{pmatrix} \frac{1}{\eta^2}\mathbf{v}_\perp \\ v_z \end{pmatrix} \mathcal{M}(\mathbf{v}) \quad \textit{and} \quad \int_{\mathbb{R}^3} \mathbf{X}^\eta(\mathbf{v}) d\mathbf{v} = 0 \tag{4.3.7}$$

and from the coercivity inequality (4.3.2), $(\mathrm{X}_z^\eta)_\eta$ *and* $(\eta^2 \mathbf{X}_\perp^\eta)_\eta$ *are bounded sequences in* $L^2_{\mathcal{M}}$. *Namely, we have the following a priori estimates*

$$\|\mathrm{X}_z^\eta\|_{\mathcal{M}} + \|\eta^2 \mathbf{X}_\perp^\eta\|_{\mathcal{M}} \leq \frac{1}{\alpha_1} \|\mathbf{v}\mathcal{M}\|_{\mathcal{M}}. \tag{4.3.8}$$

The following proposition allows to reformulate the problem $Q^\eta(f) = -g$ by using the characteristics.

Proposition 4.3.3. *For all $g \in Im(Q^\eta)$, we have the following equivalence*

$$-Q^\eta(f) = g \Leftrightarrow f - L_\eta(Q^+(f)) = L_\eta(g) \tag{4.3.9}$$

where Q^+ is given by (4.3.4) *and L_η is the operator on $L^2_{\mathcal{M}}$ given by the expression :*

$$L_\eta(f) = \frac{\eta^2}{C_\eta(v)} \int_0^{2\pi} f(\mathcal{R}(\tau)v) e^{\eta^2 \int_0^\tau \nu(\mathcal{R}(s)v)ds} d\tau, \quad C_\eta(v) = e^{\eta^2 \int_0^{2\pi} \nu(\mathcal{R}(s)v)ds} - 1. \tag{4.3.10}$$

Proof. Let $(S^\eta, D(S^\eta))$ be the unbounded operator on $L^2_{\mathcal{M}}$ defined by

$$D(S^\eta) = \{f \in L^2_{\mathcal{M}} \,/\, (\mathbf{v} \times \mathbf{e}_z) \cdot \nabla_{\mathbf{v}} f \in L^2_{\mathcal{M}}\} \tag{4.3.11}$$

$$S^\eta(f) = \frac{1}{\eta^2}(\mathbf{v} \times \mathbf{e}_z) \cdot \nabla_{\mathbf{v}} f + \nu(\mathbf{v}) f \quad \forall f \in D(S^\eta). \tag{4.3.12}$$

With the decomposition (4.3.3), we have $Q^\eta = Q^+ - S^\eta$. Proceeding as in the proof of Proposition 4.3.1 (replacing $\nu + 1$ by ν), we show that S^η is invertible and its inverse is nothing but L_η. The equation $-Q^\eta(f) = g$ is equivalent to $f - (S^\eta)^{-1}(Q^+(f)) = (S^\eta)^{-1}(g)$ which concludes the proof. ■

Lemma 4.3.4. *For all $f \in L^1_{loc}(\mathbb{R}^3)$, we have :*

$$|L_\eta(f)| \leq \frac{\eta^2}{e^{2\pi\alpha_1\eta^2} - 1} \int_0^{2\pi} |f(\mathcal{R}(\tau)v)| e^{\alpha_2 \eta^2 \tau} d\tau. \tag{4.3.13}$$

Proof. This estimate follows immediately from the definition of L_η (4.3.10) using Assumption 4.2.2. ■

Proposition 4.3.5. *Under Assumption 4.2.2, the solution* $\mathbf{X}^\eta$ *of* (4.3.7) *belongs to* $(\mathcal{H}^2_{\mathcal{M}}(\mathbb{R}^3))^3$ *and* $\mathbf{X}^\eta$ *and all its derivatives with respect to* v *of order less than or equal* 2 *(up to dividing by the Maxwellian) are polynomially increasing when* $|v|$ *goes to* $+\infty$*. Namely, we have*

$$|\mathbf{X}^\eta(\mathbf{v})| \leq Q_1^\eta(|\mathbf{v}|)\mathcal{M}(\mathbf{v}), \tag{4.3.14}$$

$$|\partial^\alpha \mathbf{X}^\eta(\mathbf{v})| \leq Q_3^\eta(|\mathbf{v}|)\mathcal{M}(\mathbf{v}), \tag{4.3.15}$$

for all $\alpha = (\alpha_1, \alpha_2) \in \mathbb{N}^2$ *with* $\alpha_1 + \alpha_2 \leq 2$ *and where* $\partial^\alpha := \sum_{i,j=1}^{3} \partial_{\mathbf{v}_i}^{\alpha_1} \partial_{\mathbf{v}_j}^{\alpha_2}$*. Here,* Q_1^η *and* Q_3^η *are two polynomials of degrees* 1 *and* 3 *respectively (depending on* η*).*

Proof. From (4.3.9), we deduce the identity

$$\mathbf{X}^\eta = L_\eta(\mathbf{v}^\eta \mathcal{M}) + L_\eta(Q^+(\mathbf{X}^\eta)),$$

where

$$\mathbf{v}^\eta = \begin{pmatrix} \dfrac{1}{\eta^2}\mathbf{v}_\perp \\ v_z \end{pmatrix}.$$

Moreover, we have $|Q^+(\mathbf{X}^\eta)| \leq \alpha_2(\int_{\mathbb{R}^3} \mathbf{X}^\eta(\mathbf{v}')d\mathbf{v}')\mathcal{M}(\mathbf{v}) \leq c_0\mathcal{M}(\mathbf{v})$ and with (4.3.13) one obtains (4.3.14). Estimate (4.3.15) follows by derivation of the above equation with respect to v and by using the fact that the cross-section $\sigma(v, v')$ belongs to $W^{2,\infty}(\mathbb{R}^6)$.

■

4.4 Expansion of $\mathbf{X}^\eta$ with respect to η

A rigourous expansion of $\mathbf{X}_\eta$ around $\eta = 0$ will be carried out in this section. Corollary 4.3.2 provides us with bounds of order $\mathcal{O}(1)$ for X_z^η and of order $\mathcal{O}(\frac{1}{\eta^2})$ for $\mathrm{X}_\perp^\eta$. We shall prove in this section that $\mathbf{X}_\perp^\eta$ is actually bounded in $\mathcal{H}^2_{\mathcal{M}}$. This is due to the fast precession around the axis $\mathbf{e}_z$ generated by the differential term $\frac{1}{\eta^2}(\mathbf{v} \times \mathbf{e}_z) \cdot \nabla_{\mathbf{v}}$. Filtering out these oscillations is done through the reformulation (4.3.9) of the equation satisfied by $\mathbf{X}^\eta$. Moreover, we shall expand $\mathbf{X}^\eta$ in powers of η^2 up to the first order.

Definition 4.4.1. *Let* $\overline{Q}$ *be the operator on* $L^2_{\mathcal{M}}$ *defined by* (4.2.8) *and let* $\overline{\overline{Q}}$ *the one defined on* $\overline{L}^2_{\mathcal{M}}$ *by* (4.2.9)*. Then,* $\overline{Q}$ *restricted to* $\overline{L}^2_{\mathcal{M}}$ *coincides with* $\overline{\overline{Q}}$*.*

We now list the properties of $\overline{\overline{Q}}$ which are completely inherited from those of Q.

Proposition 4.4.2 (***Properties of*** $\overline{\overline{Q}}$). *The operator* $\overline{\overline{Q}}$ *is a bounded operator on* $\overline{L}^2_{\mathcal{M}}$ *equipped with the* $L^2_{\mathcal{M}}$ *scalar product. It satisfies the following properties whose proof are immediate and are left to the reader.*

1. *For all* $f \in \overline{L}^2_{\mathcal{M}}$, *we have* $\overline{\overline{Q}}(f) = \overline{Q}(f) = \overline{Q(f)}$.
2. $-\overline{\overline{Q}}$ *is a bounded, symmetric, non-negative operator on* $\overline{L}^2_{\mathcal{M}}$.
3. *The null set of* $\overline{\overline{Q}}$ *is given by*
$$N(\overline{\overline{Q}}) = \{n\mathcal{M}(\mathbf{v}), n \in \mathbb{R}\}.$$
4. *Let* $\mathcal{P} : \overline{L}^2_{\mathcal{M}} \to N(\overline{\overline{Q}})$ *be the orthogonal projection on* $N(\overline{\overline{Q}})$, *the following coercivity inequality holds,*
$$-\langle\overline{\overline{Q}}(f), f\rangle_{\mathcal{M}} \geq \alpha_1\|f - \mathcal{P}(f)\|^2_{\mathcal{M}}.$$
i.e $-\overline{\overline{Q}}$ *is coercive on* $N(\overline{\overline{Q}})^\perp$.
5. *The range of* $\overline{\overline{Q}}$ *in* $\overline{L}^2_{\mathcal{M}}$ *is given by*
$$Im(\overline{\overline{Q}}) = N(\overline{Q})^\perp = \left\{f \in \overline{L}^2_{\mathcal{M}} / \int_{\mathbf{v}} f d\mathbf{v} = 0\right\} = Im(Q) \cap \overline{L}^2_{\mathcal{M}}.$$

In the sequel, we shall also need the properties of $\overline{Q}$ considered on the whole space $L^2_{\mathcal{M}}$ (whereas $\overline{\overline{Q}}$ is restricted to cylindrically symmetric functions). Some of the properties of $\overline{Q}$ are inherited from those of Q but some of these properties like the symmetry are lost. The following proposition summarizes these properties.

Proposition 4.4.3 (***Properties of*** $\overline{Q}$). *The operator* $\overline{Q}$ *is a bounded operator. It satisfies the following properties.*

1. *The null set of* $\overline{Q}$ *is*
$$N(\overline{Q}) = N(Q) = \{n\mathcal{M}(v), n \in \mathbb{R}\}.$$
2. *The range of* $\overline{Q}$ *in* $L^2_{\mathcal{M}}$ *is the following set*
$$Im(\overline{Q}) = \left\{g \in L^2_{\mathcal{M}} / \int_{\mathbb{R}^3} \frac{\nu g}{\overline{\nu}} d\mathbf{v} = 0\right\}. \tag{4.4.1}$$
3. *For each* $g \in Im(\overline{Q})$, *there exists a unique function* $f \in L^2_{\mathcal{M}}$ *satisfying* $\int_{\mathbb{R}^3} f d\mathbf{v} = 0$ *such that* $\overline{Q}(f) = g$. *The solution can be written* $f = \overline{f} + \dfrac{\overline{g} - g}{\overline{\nu}}$ *where the isotropic part of* f, $\overline{f} = \mathcal{A}(f)$, *verifies*
$$\overline{\overline{Q}}(\overline{f}) = \overline{g} + \overline{Q}^+(\frac{g - \overline{g}}{\overline{\nu}}), \tag{4.4.2}$$
and where we have denoted $\overline{Q} = \overline{Q}^+ - \overline{\nu}$. *In addition, there exists a constant* $C > 0$ *independent of* g *(and* f*) such that*
$$\|f\|_{\mathcal{M}} \leq C\|g\|_{\mathcal{M}}. \tag{4.4.3}$$

Proof. Let us begin with item 1. It is clear that if f is Maxwellian, it is in the kernel of $\overline{Q}$. Let now $f \in N(\overline{Q})$. We have $\overline{Q}^+(f) - \overline{\nu} f = 0$. Since the Maxwellian is cylindrically symmetric, it is readily seen that $\overline{Q}^+(f)$ is always cylindrically symmetric. Therefore, $f = \frac{1}{\overline{\nu}}\overline{Q}^+(f)$, is cylindrically symmetric and thus

$$\overline{\overline{Q}}(f) = \overline{Q}(f) = 0.$$

In view of Proposition 4.4.2, f is proportional to the maxwellian.

In order to prove items 2. and 3., we consider $g \in Im(\overline{Q})$, and $f \in L^2_{\mathcal{M}}$ such that $\overline{Q}(f) = g$. Decomposing f and g as $f = \overline{f} + h_f$ (resp. $g = \overline{g} + h_g$) where $\overline{h_f} = \overline{h_g} = 0$, we have

$$\overline{Q}(\overline{f}) + \overline{Q}^+(h_f) - \overline{g} = h_g + \overline{\nu} h_f.$$

The left hand side of the above equality is cylindrically symmetric, whereas cylindrical averages of the right hand side vanish. Therefore, both are equal to zero. We deduce that

$$h_f = -\frac{h_g}{\overline{\nu}} = \frac{\overline{g} - g}{\overline{\nu}},$$

whereas $\overline{f}$ satisfies

$$\overline{Q}(\overline{f}) = \overline{g} - \overline{Q}^+(h_f)$$

which can be rewritten $\overline{\overline{Q}}(\overline{f}) = \overline{g} - \overline{Q}^+(\frac{\overline{g}-g}{\overline{\nu}})$ and also

$$\overline{\overline{Q}}(\overline{f} + \frac{\overline{g}}{\overline{\nu}}) = \overline{Q}^+(\frac{g}{\overline{\nu}}).$$

This equation has a solution if and only if the right hand side has zero velocity average (see Proposition 4.4.2). A straightforward computation shows that this is equivalent to the condition $\displaystyle\int_{\mathbb{R}^3} \frac{\nu g}{\overline{\nu}} d\mathbf{v} = 0$. Let us finally show estimate (4.4.3). Remark first that for any $f \in L^2_{\mathcal{M}}$ with $f = \overline{f} + h_f$ and $\overline{h_f} = 0$, we have $\|f\|^2_{\mathcal{M}} = \|\overline{f}\|^2_{\mathcal{M}} + \|h_f\|^2_{\mathcal{M}}$ and then $\|\overline{f}\|_{\mathcal{M}} \leq \|f\|_{\mathcal{M}}$. Besides, equation (4.4.2) is posed on $\overline{L}^2_{\mathcal{M}}$ then, from the coercivity of $-\overline{\overline{Q}}$ on $N(\overline{\overline{Q}})^\perp$ (see Proposition 4.4.2), there exists a constant $C_1 > 0$ such that

$$\|\overline{f}\|_{\mathcal{M}} \leq C_1(\|\overline{g} + \overline{Q^+}(\frac{g-\overline{g}}{\overline{\nu}})\|_{\mathcal{M}}) \leq C_1(\|g\|_{\mathcal{M}} + \|Q^+(\frac{g-\overline{g}}{\overline{\nu}})\|_{\mathcal{M}}) \leq C_1'\|g\|_{\mathcal{M}}.$$

In addition, since $h_f = \dfrac{\overline{g} - g}{\overline{\nu}}$ and with (4.2.13), there exists $C_2 > 0$ such that $\|h_f\|_{\mathcal{M}} \leq C_2\|g\|_{\mathcal{M}}$ and estimate (4.4.3) holds.

■

Definition 4.4.4. *We define the gyration operator $\mathcal{G}$ by $\mathcal{G}(f) = (\mathbf{v} \times \mathbf{e}_z) \cdot \nabla_{\mathbf{v}} f$, with domain D.*

The kernel of this operator is nothing but the set of cylindrically symmetric functions. It is clear that its range is contained in the set of $L^2_{\mathcal{M}}$ functions which have zero cylindrical averages. The following lemma shows that both sets coincide.

Lemma 4.4.5. *Let $g \in L^2_{\mathcal{M}}$ with zero cylindrical average ($\mathcal{A}(g) = 0$). Then, the set of solutions of the equation*

$$\mathcal{G}(f) = g, \tag{4.4.4}$$

in nonempty. Any solution f can be written

$$f = f_1 + \mathcal{A}_1(g)$$

where f_1 si an arbitrary cylindrically symmetric function (which means that $\mathcal{A}(f_1) = f_1$) and the average operator $\mathcal{A}_1$ is defined by

$$\mathcal{A}_1(g) = \frac{1}{\overline{\nu}(\mathbf{v})} \int_0^{2\pi} g(\mathcal{R}(\tau)v)\overline{\nu_\tau} d\tau = \frac{1}{2\pi\overline{\nu}} \int_0^{2\pi} g(\mathcal{R}(\tau)v) \int_0^{\tau} \nu(\mathcal{R}(s)v)\, ds\, d\tau. \tag{4.4.5}$$

Moreover, we have

$$\mathcal{A}(\nu\mathcal{A}_1(g)) = 0.$$

Proof. Let us consider the problem

$$\mathcal{G}(f_\eta) + \eta^2 \nu f_\eta = g.$$

This problem has a unique solution f_η defined by

$$\begin{aligned} f_\eta = \frac{1}{\eta^2} L_\eta(g) &= \frac{1}{C_\eta(v)} \int_0^{2\pi} g(\mathcal{R}(\tau)v) e^{\eta^2 \int_0^\tau \nu(\mathcal{R}(s)v)ds} d\tau \\ &= \frac{1}{C_\eta(v)} \int_0^{2\pi} g(\mathcal{R}(\tau)v)[e^{\eta^2 \int_0^\tau \nu(\mathcal{R}(s)v)ds} - 1] d\tau \end{aligned}$$

where

$$C_\eta(v) = e^{\eta^2 \int_0^{2\pi} \nu(\mathcal{R}(s)v)ds} - 1 = e^{2\pi\eta^2\overline{\nu}} - 1.$$

Passing to the limit $\eta \to 0$, we find that f_η converges almost everywhere towards $\mathcal{A}_1(g)$. Moreover $\mathcal{A}(\eta^2\nu f_\eta) = \mathcal{A}(g) = 0$, which proves after passing to the limit $\eta \to 0$ that $\mathcal{A}(\nu\mathcal{A}_1(g)) = 0$. Of course, any other solution of the equation $\mathcal{G}(f) = g$ is obtained by adding an arbitrary cylindrically symmetric function.

■

Let us now consider the problem

$$\left\{ \begin{array}{lcl} \mathcal{G}(f) & = & g \\ \mathcal{A}(Q(f)) & = & h. \end{array} \right. \tag{4.4.6}$$

It is clear that the above system does not have a solution unless $\mathcal{A}(g) = 0$ and $h \in \overline{L}^2_{\mathcal{M}}$ with $\int_{\mathbb{R}^3} h\, d\mathbf{v} = 0$. The proposition below shows that these conditions are sufficient and gives the general solution of the problem.

Proposition 4.4.6. *Let g and h be in $L^2_{\mathcal{M}}$ such that $\mathcal{A}(g) = 0$, $\mathcal{A}(h) = h$ and $\int h\, d\mathbf{v} = 0$. Then the problem (4.4.6) has a unique solution up to a Maxwellian (the Maxwellian is the only solution of the homogeneous problem). The unique solution f which has zero average is given by*

$$f = f_1 + \mathcal{A}_1(g)$$

$$\overline{Q}(f) = -\overline{\nu}\mathcal{A}_1(g) + h$$

with f_1 is an arbitrary cylindrically symmetric function. Moreover, the mapping $(g, h) \mapsto f$ is linear and continuous both on $L^2_{\mathcal{M}}$ and $H^2_{\mathcal{M}}$, i.e.

$$\|f\|_{L^2_{\mathcal{M}}} \leq C(\|h\|_{L^2_{\mathcal{M}}} + \|g\|_{L^2_{\mathcal{M}}}), \quad \|f\|_{H^2_{\mathcal{M}}} \leq C(\|h\|_{H^2_{\mathcal{M}}} + \|g\|_{H^2_{\mathcal{M}}}).$$

Proof. First of all, Lemma 4.4.5 shows that $f = f_1 + \mathcal{A}_1(g)$. Besides, we have

$$\overline{Q}(f) = \mathcal{A}(Q(f)) + \mathcal{A}(\nu f) - \overline{\nu} f.$$

Since f_1 is cylindrically symmetric, then $\mathcal{A}(\nu f_1) - \overline{\nu} f_1 = 0$, which leads, thanks to the identity $\mathcal{A}(\nu \mathcal{A}_1(g)) = 0$, to $\overline{Q}(f) = -\overline{\nu}\mathcal{A}_1(g) + h$. It is now enough, in view of the solvability condition (4.4.1) to check that $\int \frac{\nu}{\overline{\nu}}(-\overline{\nu}\mathcal{A}_1(g) + h) d\mathbf{v} = 0$, which is readily seen.

■

4.4.1 Expansion of X^η_z

The idea is to make a Hilbert expansion of X^η_z in powers of η^2 :

$$\mathrm{X}^\eta_z = \sum_i \eta^{2i} \mathrm{X}^{(i)}_z.$$

We have the following equations

$$\begin{aligned}
\mathcal{G}(\mathrm{X}^{(0)}_z) &= 0, \\
\mathcal{G}(\mathrm{X}^{(1)}_z) &= Q(\mathrm{X}^{(0)}_z) + v_z \mathcal{M}, \\
\mathcal{G}(\mathrm{X}^{(i+1)}_z) &= Q(\mathrm{X}^{(i)}_z), \quad i \geq 1,
\end{aligned}$$

where we have taken advantage of the fact that $\mathcal{A}(v_z\mathcal{M}) = v_z\mathcal{M}$. The solvability conditions become

$$\mathcal{A}(Q(\mathrm{X}^{(0)}_z) + v_z\mathcal{M}) = 0$$

$$\mathcal{A}(Q(\mathrm{X}^{(i)}_z)) = 0, \quad i \geq 1.$$

Therefore, the terms of the expansion can be successively computed by solving the problems

$$\begin{cases} \mathcal{G}(\mathrm{X}_z^{(0)}) &= 0 \\ \mathcal{A}(Q(\mathrm{X}_z^{(0)})) &= -v_z\mathcal{M} \end{cases}$$

$$\begin{cases} \mathcal{G}(\mathrm{X}_z^{(1)}) &= Q(\mathrm{X}_z^{(0)}) + v_z\mathcal{M} \\ \mathcal{A}(Q(\mathrm{X}_z^{(1)})) &= 0 \end{cases}$$

$$\begin{cases} \mathcal{G}(\mathrm{X}_z^{(i+1)}) &= Q(\mathrm{X}_z^{(i)}) \\ \mathcal{A}(Q(\mathrm{X}_z^{(i+1)})) &= 0. \end{cases}$$

From Proposition 4.4.6, we deduce that $\mathrm{X}_z^{(i)}$ are uniquely determined by the above equations and are in $H^2_{\mathcal{M}}$.

Proposition 4.4.7. *Let $\mathbf{X}^\eta$ be defined by* (4.3.7)*. The function $\mathrm{X}_z^{(0)}$ is uniquely determined by*

$$-\overline{\overline{Q}}(\mathrm{X}_z^{(0)}) = v_z\mathcal{M}, \quad \int_{\mathbb{R}^3} \mathrm{X}_z^{(0)}(\mathbf{v})d\mathbf{v} = 0 \tag{4.4.7}$$

and $\mathrm{X}_z^{(1)}$ is the unique solution in $L^2_{\mathcal{M}}$ of

$$-\overline{Q}(\mathrm{X}_z^{(1)}) = \overline{\nu}\mathcal{A}_1(Q(\mathrm{X}_z^{(0)}) + v_z\mathcal{M}) = \overline{\nu}\mathcal{A}_1(Q(\mathrm{X}_z^{(0)}) - \overline{\overline{Q}}(\mathrm{X}_z^{(0)})), \quad \int_{\mathbb{R}^3} \mathrm{X}_z^{(1)}(\mathbf{v})d\mathbf{v} = 0 \tag{4.4.8}$$

where $\mathcal{A}_1$ is the averaging operator defined by (4.4.5)*. Then the following expansion holds in the strong topology of $\mathcal{H}^2_{\mathcal{M}}$*

$$\mathrm{X}_z^\eta = \mathrm{X}_z^{(0)} + \eta^2\mathrm{X}_z^{(1)} + \mathcal{O}(\eta^4). \tag{4.4.9}$$

Proof. We write

$$\mathrm{X}_z^\eta = \mathrm{X}_z^{(0)} + \eta^2\mathrm{X}_z^{(1)} + \eta^4 r^\eta.$$

From the definitions of $\mathrm{X}_z^{(i)}$, it is readily seen that

$$\mathcal{G}(r^\eta) = \eta^2 Q(r^\eta) + Q(\mathrm{X}_z^{(1)})$$

$$\mathcal{A}(Q(r^\eta)) = 0.$$

Hence, we have that

$$\overline{Q}(r^\eta) = -\overline{\nu}\mathcal{A}_1(\eta^2 Q(r^\eta) + Q(\mathrm{X}_z^{(1)})).$$

Using estimate (4.4.3), we obtain for some constant $C > 0$ independent of η

$$\|r^\eta\|_{L^2_{\mathcal{M}}} \leq C(\eta^2\|r^\eta\|_{L^2_{\mathcal{M}}} + \|\mathrm{X}_z^{(1)}\|_{L^2_{\mathcal{M}}})$$

which shows the boundedness of r^η in $L^2_{\mathcal{M}}$. Differentiating the above identity with respect to the velocity variable, on can show simply the boundedness of r^η in $\mathcal{H}^2_{\mathcal{M}}$. ∎

4.4.2 Expansion of $\mathbf{X}_\eta^\perp$

In this subsection, we expand the orthogonal part of $\mathbf{X}^\eta$. We follow the same steps as for X_z^η and write the equations satisfied by the formal expansion of $\mathbf{X}_\perp^\eta$. Namely, we have

$$\begin{aligned}
\mathcal{G}(\mathbf{X}_\perp^{(0)}) &= \mathbf{v}_\perp\mathcal{M},\\
\mathcal{G}(\mathbf{X}_\perp^{(1)}) &= Q(\mathbf{X}_\perp^{(0)}),\\
\mathcal{G}(\mathbf{X}_\perp^{(i+1)}) &= Q(\mathbf{X}_\perp^{(i)}), \quad i \geq 1.
\end{aligned}$$

As for X_z^η, the above system can be reformulated as follows

$$\left\{\begin{array}{lcl} \mathcal{G}(\mathbf{X}_\perp^{(0)}) & = & \mathbf{v}_\perp\mathcal{M} \\ \mathcal{A}(Q(\mathbf{X}_\perp^{(0)})) & = & 0 \end{array}\right.$$

$$\left\{\begin{array}{lcl} \mathcal{G}(\mathbf{X}_\perp^{(1)}) & = & Q(\mathbf{X}_\perp^{(0)}) \\ \mathcal{A}(Q(\mathbf{X}_\perp^{(1)})) & = & 0 \end{array}\right.$$

$$\left\{\begin{array}{lcl} \mathcal{G}(\mathbf{X}_\perp^{(i+1)}) & = & Q(\mathbf{X}_\perp^{(i)}) \\ \mathcal{A}(Q(\mathbf{X}_\perp^{(i+1)})) & = & 0. \end{array}\right.$$

Proposition 4.4.8. *The expansion*

$$\mathbf{X}_\perp^\eta = \mathbf{X}_\perp^{(0)} + \eta^2\mathbf{X}_\perp^{(1)} + \mathcal{O}(\eta^4),$$

holds true in $\mathcal{H}^2_{\mathcal{M}}$. *Morever,* $\mathbf{X}_\perp^{(0)}$ *satisfies*

$$\mathbf{X}_\perp^{(0)} - \mathcal{A}(\mathbf{X}_\perp^{(0)}) = -\mathcal{I}(\mathbf{v}_\perp\mathcal{M}),$$

with $\mathcal{I} = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}$.

The proof of this proposition is identical to that of Proposition 4.4.7 and is skipped. The only thing which has to be checked is the expression of the anisotropic part of $\mathbf{X}_\perp^{(0)}$ which can be deduced from the identities

$$-\mathbf{v}_\perp\mathcal{M} = \mathcal{G}(\mathcal{I}(\mathbf{v}_\perp\mathcal{M})), \quad \mathcal{A}(\mathcal{I}(\mathbf{v}_\perp\mathcal{M})) = 0.$$

4.5 Proof of the main theorems

We begin this section by making precise the definition of weak solutions of the Boltzmann equation and give quite standard a priori estimates on this solution. For the moment, ε and η are arbitrary and all the constants are, unless specified, independent of these parameters.

Definition 4.5.1. *Let $T \in \mathbb{R}_+^*$, a function $f^{\varepsilon\eta} \in L^1_{loc}([0,T]\times\mathbb{R}^6)$ is called weak solution of (4.2.1) if it satisfies*

$$-\int_0^T\int_{\mathbb{R}^6} f^{\varepsilon\eta}\left[\partial_t\psi + \frac{\mathcal{T}_z\psi}{\varepsilon} + \frac{\mathcal{T}_\perp\psi}{\varepsilon\eta}\right]dtd\mathbf{r}d\mathbf{v} - \frac{1}{\varepsilon^2\eta^2}\int_0^T\int_{\mathbb{R}^6} f^{\varepsilon\eta}\mathcal{G}(\psi)dtd\mathbf{r}d\mathbf{v}$$
$$= \frac{1}{\varepsilon^2}\int_0^T\int_{\mathbb{R}^6} Q(f^{\varepsilon\eta})\psi dtd\mathbf{r}d\mathbf{v} + \int_{\mathbb{R}^6} f_0(x,v)\psi(0,x,v)d\mathbf{r}d\mathbf{v}, \quad (4.5.1)$$

for all $\psi \in C_c^1([0,T)\times\mathbb{R}^6)$.

Theorem 4.5.2. *Assume that $f_0 \in L^2_{\mathcal{M}_V}(d\mathbf{r}d\mathbf{v})$. Then, $\forall\varepsilon,\eta > 0$ and $\forall T \in \mathbb{R}_+^*$, there exists a unique weak solution $f^{\varepsilon\eta} \in C^0([0,T], L^2_{\mathcal{M}_V}(d\mathbf{r}d\mathbf{v}))$ of (4.2.1). In addition, the following mass conservation equation holds*

$$\partial_t\rho^{\varepsilon\eta} + \mathrm{div}_{\mathbf{r}}\mathbf{J}^{\varepsilon\eta} = 0 \quad (4.5.2)$$

where

$$\rho^{\varepsilon\eta}(t,x) = \int_{\mathbb{R}^3} f^{\varepsilon\eta}d\mathbf{v}, \quad \mathrm{J}_z^{\varepsilon\eta} = \frac{1}{\varepsilon}\int_{\mathbb{R}^3} v_z f^{\varepsilon\eta}d\mathbf{v}, \quad \mathbf{J}_\perp^{\varepsilon\eta} = \frac{1}{\varepsilon\eta}\int_{\mathbb{R}^3}\mathbf{v}_\perp f^{\varepsilon\eta}d\mathbf{v}, \quad (4.5.3)$$

and there exists a constant $C > 0$ independent of ε and η such that

$$\|f^{\varepsilon\eta}(t)\|_{L^2_{\mathcal{M}}(d\mathbf{r}d\mathbf{v})} \le C \qquad \forall t \in [0,T], \quad (4.5.4)$$

$$\|f^{\varepsilon\eta} - \rho^{\varepsilon\eta}\mathcal{M}\|_{L^2([0,T],L^2_{\mathcal{M}}(d\mathbf{r}d\mathbf{v}))} \le C\varepsilon. \quad (4.5.5)$$

An immediate consequence of the integrability properties of the function $f^{\varepsilon\eta}$, with respect to $\mathbf{v}$ is that the weak formulation (4.5.1) is satisfied by test functions which are not necessarily compactly supported in velocity. More precisely, we have

Corollary 4.5.3. *Let $f^{\varepsilon\eta}$ be the solution exhibited in Theorem 4.5.2. Then the weak formulation (4.5.1) is satisfied by test functions lying in the set*

$$\mathcal{T} = \{\psi(t,\mathbf{r},\mathbf{v}) \in C^1([0,T)\times\mathbb{R}^6) \text{ compactly supported w.r.t. } t \text{ and } \mathbf{r} \text{ and}$$
$$\exists n \in \mathbb{N}, C \in \mathbb{R}_+, \quad |\nabla_{t,\mathbf{r},\mathbf{v}}\psi(t,\mathbf{r},\mathbf{v})| \le C(1+|\mathbf{v}|)^n\}. \quad (4.5.6)$$

We shall not prove this corollary which is straightforward. The proof of Theorem 4.5.2 is also classical (see for example [32]). We show here how the a priori estimates (4.5.4) and (4.5.5) can be obtained. We simply multiply the Boltzmann equation (4.2.1) by $\frac{f^{\varepsilon\eta}}{\mathcal{M}_V}$ and integrate with respect to $\mathbf{r}$ and $\mathbf{v}$. Straightforward computations show that this leads to the entropy inequality

$$\frac{d}{dt}\int \frac{(f^{\varepsilon\eta})^2}{2\mathcal{M}_V}\,d\mathbf{r}d\mathbf{v} - \int \partial_t V \frac{(f^{\varepsilon\eta})^2}{2\mathcal{M}_V}\,d\mathbf{r}d\mathbf{v}$$
$$= \frac{1}{\varepsilon^2}\int Q^\eta(f^{\varepsilon\eta})\frac{f^{\varepsilon\eta}}{\mathcal{M}_V}\,d\mathbf{r}d\mathbf{v} \leq -\frac{\alpha_1}{\varepsilon^2}\|f^{\varepsilon\eta} - \rho^{\varepsilon\eta}\mathcal{M}\|^2_{L^2_{\mathcal{M}_V}}.$$

Thanks to the boundedness of the potential V and its derivatives, estimate (4.5.4) follows by applying Gronwall Lemma and then the bound (4.5.5) follows immediately.

4.5.1 Proof of Theorem 4.2.4

In this section, we are interested in the limit $\varepsilon \to 0$, while η is fixed. To this aim, we follow the usual approach based on the moment method. Namely, thanks to estimates (4.5.4) and (4.5.5), the sequences $f^{\varepsilon\eta}, (\rho^{\varepsilon\eta}), (J_z^{\varepsilon\eta})$ and $(\mathbf{J}_\perp^{\varepsilon\eta})$ are bounded with respect to ε. One can find $\rho_\eta(t,x) \in L^2((0,T)\times\mathbb{R}^3)$ such that $\rho^{\varepsilon\eta}$ converges weakly to ρ_η in $L^2((0,T)\times\mathbb{R}^3)$ and $f^{\varepsilon\eta} \rightharpoonup \rho_\eta\mathcal{M}$ in $L^\infty(0,T;L^2_{\mathcal{M}}(\mathbb{R}^6))$. Similarly, $\mathbf{J}^{\varepsilon\eta}$ converges weakly to $\mathbf{J}^\eta$ in $L^2((0,T)\times\mathbb{R}^3)$. We have of course, the mass conservation equation

$$\partial_t\rho_\eta + \mathrm{div}_{\mathbf{r}}\mathbf{J}^\eta = 0.$$

Now the only thing left to show is to identify $\mathbf{J}^\eta$. The way to proceed for identifying $\mathbf{J}^\eta$ is standard (see for instance [1, 5, 35, 7, 32, 10, 2, 3, 4]). The Boltzmann equation can be rewritten

$$\varepsilon\frac{\partial f^{\varepsilon\eta}}{\partial t} + \mathcal{T}_z f^{\varepsilon\eta} + \frac{\mathcal{T}_\perp f^{\varepsilon\eta}}{\eta} = \frac{Q^\eta(f_{\varepsilon\eta})}{\varepsilon} \tag{4.5.7}$$

Let now $\mathbf{X}^{\eta*}$ be the solution of

$$Q^{\eta*}(\mathbf{X}^{\eta*}) = -\begin{pmatrix} \frac{1}{\eta^2}\mathbf{v}_\perp \\ v_z \end{pmatrix}\mathcal{M}(\mathbf{v}) \quad \text{and} \quad \int_{\mathbb{R}^3}\mathbf{X}^{\eta*}(\mathbf{v})d\mathbf{v} = 0,$$

where $Q^{\eta*} := (Q^\eta)^*$ is the adjoint in $L^2_{\mathcal{M}}$ of Q^η. It is readily seen that $Q^{\eta*}$ has the same expression as Q^η except that η^2 is replaced by $-\eta^2$. We then have the following result.

Corollary 4.5.4. *The following expansion holds in* $\mathcal{H}^2_{\mathcal{M}}$

$$\mathbf{X}_\perp^{\eta*} = -\mathbf{X}_\perp^{(0)} + \eta^2\mathbf{X}_\perp^{(1)} + \mathcal{O}(\eta^4) \quad ; \quad X_z^{\eta*} = X_z^{(0)} - \eta^2 X_z^{(1)} + \mathcal{O}(\eta^4).$$

We multiply (4.5.7) by $\dfrac{X_z^{\eta*}}{\mathcal{M}}$ and integrate w.r.t. $\mathbf{v}$. The right hand side of the obtained equation is nothing but

$$\frac{1}{\varepsilon}\int\frac{Q^\eta(f^{\varepsilon\eta})X_z^{\eta*}}{\mathcal{M}}d\mathbf{v} = \frac{1}{\varepsilon}\int\frac{Q^{\eta*}(X_z^{\eta*})f^{\varepsilon\eta}}{\mathcal{M}}d\mathbf{v} = -J_z^{\varepsilon\eta}.$$

Therefore

$$-J_z^{\varepsilon\eta} = \varepsilon\partial_t \int \frac{f^{\varepsilon\eta} X_z^{\eta*}}{\mathcal{M}}\, d\mathbf{v} + \int \frac{X_z^{\eta*}}{\mathcal{M}} \mathcal{T}_z f^{\varepsilon\eta} d\mathbf{v} + \frac{1}{\eta}\int \frac{X_z^{\eta*}}{\mathcal{M}} \mathcal{T}_\perp f^{\varepsilon\eta} d\mathbf{v}.$$

Thanks to the bounds (4.5.4) and (4.3.14), we can pass to the limit in the above equation as ε tends to zero and obtain

$$-J_z^{\eta} = \int \frac{X_z^{\eta*}}{\mathcal{M}} \mathcal{T}_z(\rho_\eta \mathcal{M}) d\mathbf{v} + \frac{1}{\eta}\int \frac{X_z^{\eta*}}{\mathcal{M}} \mathcal{T}_\perp(\rho_\eta \mathcal{M}) d\mathbf{v},$$

which leads to the expression

$$-J_z^{\eta} = [\int X_z^{\eta*} v_z d\mathbf{v}](\partial_z \rho_\eta + \rho_\eta \partial_z V) + \frac{1}{\eta}[\int X_z^{\eta*} \mathbf{v}_\perp d\mathbf{v}] \cdot (\nabla_{\mathbf{r}_\perp} \rho_\eta + \rho_\eta \nabla_{\mathbf{r}_\perp} V).$$

Multiplying the Boltzmann equation (4.5.7) by $\dfrac{\eta \mathbf{X}_\perp^{\eta*}}{\mathcal{M}}$ and proceeding analogously, we find out that

$$-\mathbf{J}_\perp^{\eta} = \eta[\int \mathbf{X}_\perp^{\eta*} v_z d\mathbf{v}](\partial_z \rho_\eta + \rho_\eta \partial_z V) + [\int \mathbf{X}_\perp^{\eta*} \otimes \mathbf{v}_\perp d\mathbf{v}](\nabla_{\mathbf{r}_\perp} \rho_\eta + \rho_\eta \nabla_{\mathbf{r}_\perp} V).$$

Using the property $\int X_z^{\eta*} v_z d\mathbf{v} = \int v_z X_z^{\eta} d\mathbf{v}$ as well as $\int X_z^{\eta*} \mathbf{v}_\perp d\mathbf{v} = \eta^2 \int v_z \mathbf{X}_\perp^{\eta} d\mathbf{v}$ and analogous formulae for the terms appearing in the expression of $\mathbf{J}_\perp^{\eta}$, we finally obtain the expression

$$\mathbf{J}^{\eta} = -\mathbb{D}^{\eta}(\nabla_{\mathbf{r}} \rho_\eta + \rho_\eta \nabla_r V)$$

where

$$\mathbb{D}^{\eta} = \int \begin{pmatrix} \eta \mathbf{X}_\perp^{\eta*} \\ X_z^{\eta*} \end{pmatrix} \otimes \begin{pmatrix} \frac{1}{\eta}\mathbf{v}_\perp \\ v_z \end{pmatrix} d\mathbf{v} = \int \begin{pmatrix} \frac{1}{\eta}\mathbf{v}_\perp \\ v_z \end{pmatrix} \otimes \begin{pmatrix} \eta \mathbf{X}_\perp^{\eta} \\ X_z^{\eta} \end{pmatrix} d\mathbf{v}.$$

One can then expand $\mathbb{D}^{\eta}$ as

$$\mathbb{D}^{\eta} = \mathbb{D}_\perp^{\eta} + \mathbb{D}_z^{\eta} + \eta \mathbb{D}_{z\perp}^{\eta}$$

where

$$\mathbb{D}_\perp^{\eta} = \int \begin{pmatrix} \mathbf{X}_\perp^{\eta*} \\ 0 \end{pmatrix} \otimes \begin{pmatrix} \mathbf{v}_\perp \\ 0 \end{pmatrix} d\mathbf{v} = \int \begin{pmatrix} \mathbf{v}_\perp \\ 0 \end{pmatrix} \otimes \begin{pmatrix} \mathbf{X}_\perp^{\eta} \\ 0 \end{pmatrix} d\mathbf{v},$$

$$D_z^{\eta} = \int \begin{pmatrix} \mathbf{0} \\ X_z^{\eta*} \end{pmatrix} \otimes \begin{pmatrix} \mathbf{0} \\ v_z \end{pmatrix} d\mathbf{v} = \int \begin{pmatrix} \mathbf{0} \\ v_z \end{pmatrix} \otimes \begin{pmatrix} \mathbf{0} \\ X_z^{\eta} \end{pmatrix} d\mathbf{v},$$

$$\mathbb{D}_{z\perp}^{\eta} = \int \begin{pmatrix} \mathbf{0} \\ v_z \end{pmatrix} \otimes \begin{pmatrix} \mathbf{X}_\perp^{\eta} \\ 0 \end{pmatrix} d\mathbf{v} + \int \begin{pmatrix} \mathbf{X}_\perp^{\eta*} \\ 0 \end{pmatrix} \otimes \begin{pmatrix} \mathbf{0} \\ v_z \end{pmatrix} d\mathbf{v}.$$

4.5.2 Proof of Proposition 4.2.6

Let us expand first $\mathbb{D}_\perp^\eta$. Following the expansion of $\mathbf{X}_\perp^{\eta*}$ and that of $\mathbf{X}_\perp^\eta$, we obtain that

$$\mathbb{D}_\perp^\eta = \mathbb{D}_\perp^{(0)} + \eta^2 \mathbb{D}_\perp^{(1)} + \mathcal{O}(\eta^4),$$

where

$$\mathbb{D}_\perp^{(0)} = -\int \begin{pmatrix} \mathbf{X}_\perp^{(0)} \\ 0 \end{pmatrix} \otimes \begin{pmatrix} \mathbf{v}_\perp \\ 0 \end{pmatrix} d\mathbf{v} = \int \begin{pmatrix} \mathbf{v}_\perp \\ 0 \end{pmatrix} \otimes \begin{pmatrix} \mathbf{X}_\perp^{(0)} \\ 0 \end{pmatrix} d\mathbf{v}$$

and

$$\mathbb{D}_\perp^{(1)} = \int \begin{pmatrix} \mathbf{X}_\perp^{(1)} \\ 0 \end{pmatrix} \otimes \begin{pmatrix} \mathbf{v}_\perp \\ 0 \end{pmatrix} d\mathbf{v} = \int \begin{pmatrix} \mathbf{v}_\perp \\ 0 \end{pmatrix} \otimes \begin{pmatrix} \mathbf{X}_\perp^{(1)} \\ 0 \end{pmatrix} d\mathbf{v}.$$

It is clear that $\mathbb{D}_\perp^{(0)}$ is antisymmetric while $\mathbb{D}_\perp^{(1)}$ is symmetric and we have

$$\mathbb{D}_\perp^{(0)} = -\int \begin{pmatrix} \mathbf{X}_\perp^{(0)} - \mathcal{A}(\mathbf{X}_\perp^{(0)}) \\ 0 \end{pmatrix} \otimes \begin{pmatrix} \mathbf{v}_\perp \\ 0 \end{pmatrix} d\mathbf{v}.$$

Since $\mathbf{X}_\perp^{(0)} - \mathcal{A}(\mathbf{X}_\perp^{(0)}) = -\mathcal{I}(\mathbf{v}_\perp \mathcal{M})$, we have

$$\begin{aligned} \mathbb{D}_\perp^{(0)} &= \begin{pmatrix} \int_{\mathbb{R}^3} \mathcal{I}(\mathbf{v}_\perp \mathcal{M}) \otimes \mathbf{v}_\perp dv & \mathbf{0} \\ \mathbf{0} & 0 \end{pmatrix} = \begin{pmatrix} \mathcal{I} \cdot \int_{\mathbb{R}^3} (\mathbf{v}_\perp \otimes \mathbf{v}_\perp) \mathcal{M} dv & \mathbf{0} \\ \mathbf{0} & 0 \end{pmatrix} \\ &= \begin{pmatrix} 0 & 1 & 0 \\ -1 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix} \end{aligned}$$

where we have noticed that $\displaystyle\int_{\mathbb{R}^3} \mathbf{v}_\perp \otimes \mathbf{v}_\perp \mathcal{M} d\mathbf{v}$ is nothing but the identity matrix on $\mathbb{R}^2$. Let us now expand $\mathbb{D}_z^\eta$. We have

$$\mathbb{D}_z^\eta = \mathbb{D}_z^{(0)} + \eta^2 \mathbb{D}_z^{(1)} + \mathcal{O}(\eta^4)$$

where

$$\mathbb{D}_z^{(0)} = D_z \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix}$$

which $D_z = \int v_z \mathbf{X}_z^{(0)} \, d\mathbf{v}$. Comparing the expansions of X_z^η and $X_z^{\eta*}$, we deduce that $\mathbb{D}_z^{(1)}$ is equal to zero. Let us now expand $\mathbb{D}_{z\perp}^\eta$. Of course we have

$$\mathbb{D}_{z\perp}^\eta = \mathbb{D}_{z\perp}^{(0)} + \eta^2 \mathbb{D}_{z\perp}^{(1)} + \mathcal{O}(\eta^4),$$

where

$$\mathbb{D}^{(0)}_{z\perp} = \int \begin{pmatrix} \mathbf{0} \\ v_z \end{pmatrix} \otimes \begin{pmatrix} \mathbf{X}^{(0)}_\perp \\ 0 \end{pmatrix} d\mathbf{v} - \int \begin{pmatrix} \mathbf{X}^{(0)}_\perp \\ 0 \end{pmatrix} \otimes \begin{pmatrix} \mathbf{0} \\ v_z \end{pmatrix} d\mathbf{v}$$

and

$$\mathbb{D}^{(1)}_{z\perp} = \int \begin{pmatrix} \mathbf{0} \\ v_z \end{pmatrix} \otimes \begin{pmatrix} \mathbf{X}^{(1)}_\perp \\ 0 \end{pmatrix} d\mathbf{v} + \int \begin{pmatrix} \mathbf{X}^{(1)}_\perp \\ 0 \end{pmatrix} \otimes \begin{pmatrix} \mathbf{0} \\ v_z \end{pmatrix} d\mathbf{v}.$$

We can now make explicit the expansion of $\mathbb{D}^\eta = \mathbb{D}^\eta_s + \mathbb{D}^\eta_{as}$ where the indices s and as stand for the symmetric and antisymmetric parts

$$\mathbb{D}^\eta_s = \begin{pmatrix} \eta^2 \int \mathbf{v}_\perp \otimes \mathbf{X}^{(1)}_\perp d\mathbf{v} & 0 \\ 0 & D_z \end{pmatrix} + \eta^3 \mathbb{D}^{(1)}_{z\perp} + \mathcal{O}(\eta^4)$$

$$\mathbb{D}^\eta_{as} = \begin{pmatrix} \mathcal{I} & \mathbf{0} \\ \mathbf{0} & 0 \end{pmatrix} + \eta \mathbb{D}^{(0)}_{z\perp} + \mathcal{O}(\eta^4).$$

4.5.3 Proof of Theorem 4.2.8

Lemma 4.5.5. *The density $\rho^{\varepsilon\eta}$ and the parallel current $J^{\varepsilon\eta}_z$ (4.5.3) are bounded in $L^2_{t,x}([0,T]\times\mathbb{R}^3)$ with respect to ε and η. In addition, there exist ρ and J_z in $L^2([0,T]\times\mathbb{R}^3)$ such that, up to extraction of subsequences, we have*

$$\begin{aligned} &\rho^{\varepsilon\eta} \rightharpoonup \rho \quad \textit{weakly in } L^2_{t,x} \\ &f^{\varepsilon\eta} \rightharpoonup \rho\mathcal{M} \quad \textit{in } L^\infty([0,T], L^2_{\mathcal{M}}(d\mathbf{r}d\mathbf{v})) \\ &\mathrm{J}^{\varepsilon\eta}_z \rightharpoonup \mathrm{J}_z \quad \textit{in } L^2_{t,x}. \end{aligned}$$

However, estimates (4.5.5) and (4.5.4) do not give a bound to $\mathbf{J}^{\varepsilon\eta}_\perp$ and are not sufficient to close the limit equation or to find relations between the corresponding limits of the current and the density. To deal with this lack of compactness, we have to filter out the oscillations generated by the magnetic field in the orthogonal direction.

Proposition 4.5.6. *Let $\mathbf{J}^{\varepsilon\eta}_\perp$ be the perpendicular part of the current given by* (4.5.3). *Then,*

$$\mathbf{J}^{\varepsilon\eta}_\perp \rightharpoonup \mathbf{J}_\perp \quad \textit{in } D'([0,T)\times\mathbb{R}^3)$$

with

$$\mathbf{J}_\perp = (\rho\mathbf{E}_\perp - \nabla_{\mathbf{r}_\perp}\rho)\times\mathbf{e}_z.$$

Proof. Multiplying (4.2.1) by $\dfrac{\eta\mathbf{X}^{\eta*}_\perp}{\mathcal{M}}$ and integrating with respect to $\mathbf{v}$, we get

$$-\mathbf{J}^{\varepsilon\eta}_\perp = \varepsilon\eta\partial_t \int_{\mathbb{R}^3} \frac{f^{\varepsilon\eta}\mathbf{X}^{\eta*}_\perp}{\mathcal{M}} d\mathbf{v} + \int_{\mathbb{R}^3} \mathcal{T}_\perp f^{\varepsilon\eta} \frac{\mathbf{X}^{\eta*}_\perp}{\mathcal{M}} d\mathbf{v} + \eta \int_{\mathbb{R}^3} \mathcal{T}_z f^{\varepsilon\eta} \frac{\mathbf{X}^{\eta*}_\perp}{\mathcal{M}} d\mathbf{v}.$$

More precisely, by taking a test function $\frac{\eta \mathbf{X}_\perp^{\eta *}}{\mathcal{M}}\phi(t,x)$ in the weak formulation (4.5.1), where $\phi(t,x) \in C_c^1([0,T)\times\mathbb{R}^3)$ we have

$$\begin{aligned}
&\int_0^T \int_{\mathbb{R}^3} \mathbf{J}_\perp^{\varepsilon\eta}(t,x)\phi(t,x)dtdx \\
= \;& \varepsilon\eta \int_0^T \int_{\mathbb{R}^6} f^{\varepsilon\eta}\frac{\mathbf{X}_\perp^{\eta *}}{\mathcal{M}}\partial_t\phi dtd\mathbf{r}d\mathbf{v} + \int_0^T \int_{\mathbb{R}^6} f^{\varepsilon\eta}\mathcal{T}_\perp(\frac{\mathbf{X}_\perp^{\eta *}\phi}{\mathcal{M}})dtd\mathbf{r}d\mathbf{v} \\
& +\eta \int_0^T \int_{\mathbb{R}^6} f^{\varepsilon\eta}\mathcal{T}_z(\frac{\mathbf{X}_\perp^{\eta *}\phi}{\mathcal{M}})dtd\mathbf{r}d\mathbf{v} + \varepsilon\eta \int_{\mathbb{R}^6} f_0(x,v)\frac{\mathbf{X}_\perp^{\eta *}}{\mathcal{M}}\phi(0,x)dxd\mathbf{v}.
\end{aligned}$$

In view of Corollary 4.5.4, $\mathbf{X}_\perp^{\eta *} \to -\mathbf{X}_\perp^{(0)}$ strongly in $\mathcal{H}^2_{\mathcal{M}}$ while $(f^{\varepsilon\eta})$ converges to $\rho\mathcal{M}$ weakly $L^2(0,T,L^2_{\mathcal{M}}(d\mathbf{r}d\mathbf{v}))$. Therefore, we can pass to the limit in the above formula and get

$$\begin{aligned}
\lim_{\varepsilon,\eta\to 0}\int_0^T \int_{\mathbb{R}^3} \mathbf{J}_\perp^{\varepsilon\eta}(t,x)\phi(t,x)dtdx &= -\int_0^T \int_{\mathbb{R}^6} \rho\mathcal{M}\mathcal{T}_\perp(\frac{\mathbf{X}_\perp^{(0)}\phi}{\mathcal{M}})d\mathbf{r}d\mathbf{v}dt \\
&= \int_0^T \int_{\mathbb{R}^3} \rho\mathcal{I}(\nabla_{\mathbf{r}_\perp}\phi - \nabla_{\mathbf{r}_\perp}V\phi)d\mathbf{r}\,dt,
\end{aligned}$$

where

$$\mathcal{I} = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix} = -\int_{\mathbb{R}^3} \mathbf{X}_\perp^{(0)} \otimes \mathbf{v}_\perp \, d\mathbf{v}.$$

This concludes the proof of the proposition.

■

The only thing left to do is to give the expression of the limiting parallel current. To this aim, we use the test function $\frac{\mathrm{X}_z^{\eta *}}{\mathcal{M}}\phi(t,x)$ in the weak formulation where ϕ is a regular compactly supported function

$$\begin{aligned}
&\int_0^T \int_{\mathbb{R}^3} J_z^{\varepsilon\eta}(t,x)\phi(t,x)dtdx \\
= \;& \int_0^T \int_{\mathbb{R}^6} f^{\varepsilon\eta}\mathcal{T}_z(\frac{\mathrm{X}_z^{\eta *}\phi}{\mathcal{M}})dtd\mathbf{r}d\mathbf{v} + \varepsilon\int_{\mathbb{R}^6} f_0(x,v)\frac{\mathrm{X}_z^{\eta *}}{\mathcal{M}}\phi(0,x)dxd\mathbf{v}. \\
& +\varepsilon \int_0^T \int_{\mathbb{R}^6} f^{\varepsilon\eta}\frac{\mathrm{X}_z^{\eta *}}{\mathcal{M}}\partial_t\phi dtd\mathbf{r}d\mathbf{v} + \frac{1}{\eta}\int_0^T \int_{\mathbb{R}^6} f^{\varepsilon\eta}\mathcal{T}_\perp(\frac{\mathrm{X}_z^{\eta *}\phi}{\mathcal{M}})dtd\mathbf{r}d\mathbf{v}.
\end{aligned} \tag{4.5.8}$$

The first term of the right hand side converges as ε and η tend to zero towards

$$\int_0^T \int_{\mathbb{R}^6} \rho\mathcal{M}\mathcal{T}_z(\frac{\mathrm{X}_z^{(0)}\phi}{\mathcal{M}})dtd\mathbf{r}d\mathbf{v} = \int_0^T \int_{\mathbb{R}^3} \rho D_z(\partial_z\phi - \phi\partial_z V)\,dtd\mathbf{r}.$$

The second and third terms obviously tend to zero. The following lemma shows that the last term of (4.5.8) converges to zero.

Lemma 4.5.7. *Let $\phi(t,\mathbf{r})$ be a compactly supported C^2 function. Then, we have*

$$\lim_{\varepsilon,\eta\to 0}\frac{1}{\eta}\int_0^T\int_{\mathbb{R}^6} f^{\varepsilon\eta}\mathcal{T}_\perp(\frac{\mathrm{X}_z^{\eta *}\phi}{\mathcal{M}})dtd\mathbf{r}d\mathbf{v}=0.$$

Proof. Since we have $\mathrm{X}_z^{\eta *}=\mathrm{X}_z^{(0)}+\mathcal{O}(\eta^2)$ in $\mathcal{H}^2_{\mathcal{M}}$ strong, we can replace $\mathrm{X}_z^{\eta *}$ by $\mathrm{X}_z^{(0)}$. Now, we remark that $\mathrm{X}_z^{(0)}$ is cylindrically symmetric so that

$$\mathcal{A}(\mathcal{T}_\perp(\frac{\mathrm{X}_z^{(0)}\phi}{\mathcal{M}}))=0.$$

Therefore, one can find a test function $\psi(t,x,v)$ in the set $\mathcal{T}$ such that

$$\mathcal{T}_\perp(\frac{\mathrm{X}_z^{(0)}\phi}{\mathcal{M}})=\mathcal{G}(\psi).$$

The fact that ψ lies in $\mathcal{T}$ comes from the formula $\psi=\mathcal{A}_1(\mathcal{T}_\perp(\frac{\mathrm{X}_z^{(0)}\phi}{\mathcal{M}}))$. Using this function ψ in the weak formulation, we obtain

$$\frac{1}{\eta}\int_0^T\int_{\mathbb{R}^6} f^{\varepsilon\eta}\mathcal{T}_\perp(\frac{\mathrm{X}_z^{(0)}\phi}{\mathcal{M}})dtd\mathbf{r}d\mathbf{v}=\frac{1}{\eta}\int_0^T\int_{\mathbb{R}^6} f^{\varepsilon\eta}\mathcal{G}(\psi)dtd\mathbf{r}d\mathbf{v}.$$

Using the weak formulation (4.5.1), the right hand side of the above identity can be immediately estimated as $\mathcal{O}(\varepsilon)$, which tends to zero as ε and η tend to zero.

■

4.6 Concluding remarks

We have proven in this paper that the diffusion limit of the Boltzmann equation with an ultrastrong magnetic field leads to a diffusion equation in the parallel direction and a guiding center motion in the orthogonal one. The proof has been done for the linear Boltzmann equation and in the case of a constant magnetic field and involved the analysis of the operator involving collisions and gyrations around the electrostatic field. If the magnetic field has a constant direction but smoothly varies in position and time while staying away from zero, the analysis can be carried out without difficulty and the results can be generalized. A more difficult problem appear if one couples the Boltzmann equation to the scaled Poisson equation or when the collision operator has nonlinear features. In this case, the method used in this paper might not be sufficient and the use of double scale limits might be necessary as it is for gyrokinetic limits.

References

[1] C. Bardos, R. Santos, and R. Sentis, *Diffusion approximation and computation of the critical size of a transport operator*, Trans. Amer. Math. Soc., 284 (1984), pp. 617–649.

[2] N. Ben Abdallah and P. Degond, *On a hierarchy of macroscopic models for semiconductors*, J. Math. Phys., 37 (1996), pp. 3306–3333.

[3] N. Ben Abdallah, P. Degond, and S. Génieys, *An energy-transport model for semiconductors derived from the boltzmann equation*, J. Stat. Phys., 84 (1996), pp. 205–231.

[4] N. Ben Abdallah, L. Desvillettes, and S. Génieys, *On the convergence of the boltzmann equation for semiconductors towards an energy-transport model*, J. Stat. Phys., 98 (2000), pp. 835–870.

[5] A. Bensoussan, J.-L. Lions, and G. Papanicolaou, *Asympototic study of periodic structures*, North Holland, Amsterdam, 1978.

[6] ——, *Boundary layers and homogenization of transport processes*, J. Pub. Res. Inst. Math. Sci Kyoto, 15 (1979), pp. 53–157.

[7] R. Dautray and J.-L. Lions, *Analyse mathématique et calcul numérique pour les sciences et les techniques*, vol. 9, Evolution : numérique, transport INSTN : Collection Enseignement of Applied Mathematical Sciences, Masson, Paris, 1988.

[8] P. Degond, *A model of near-wall conductivity and its application to plasma thrusters*, SIAM J. Appl. Math., 58 (1998), pp. 1138–1162 (electronic).

[9] P. Degond, *Asymptotic continuum models for plasmas and disparate mass gaseous binary mixtures*, Material Substructures in Complex Bodies, Elsevier, (2007).

[10] P. Degond, T. Goudon, and F. Poupaud, *Diffusion limit for non homogeneous and non micro-reversible processes*, Indiana University Math. J., 49 (2000), pp. 1175–1198.

[11] P. Degond, V. Latocha, S. Mancini, and A. Mellet, *Diffusion dynamics of an electron gas confined between two plates*, Methods Appl. Anal., 9 (2002), pp. 127–150.

[12] P. Degond and B. Lucquin-Desreux, *The asymptotics of collision operators for two species of particles of disparate masses*, Math. Models Methods Appl. Sci., 6 (1996), pp. 405–436.

[13] P. Degond and B. Lucquin-Desreux, *Transport coefficients of plasmas and disparate mass binary gases*, Transport Theory Statist. Phys., 25 (1996), pp. 595–633.

[14] P. Degond and S. Mancini, *Diffusion driven by collisions with the boundary*, Asymptot. Anal., 27 (2001), pp. 47–73.

[15] D. H. E. Dubin, J. A. Krommes, C. Oberman, and W. W. Lee, *Nonlinear gyrokinetic equations*, Physics of Fluids, 26 (1983), pp. 3524–3535.

[16] E. Frénod, *Application of the averaging method to the gyrokinetic plasma*, Asymptot. Anal., 46 (2006), pp. 1–28.

[17] E. Frenod and K. Hamdache, *Homogenisation of transport kinetic equations with oscillating potentials*, Proc. Roy. Soc. Edinburgh Sect. A, 126 (1996), pp. 1247–1275.

[18] E. Frénod, P.-A. Raviart, and E. Sonnendrücker, *Two-scale expansion of a singularly perturbed convection equation*, J. Math. Pures Appl. (9), 80 (2001), pp. 815–843.

[19] E. Frénod and E. Sonnendrücker, *Homogenization of the Vlasov equation and of the Vlasov-Poisson system with a strong external magnetic field*, Asymptot. Anal., 18 (1998), pp. 193–213.

[20] E. Frénod and E. Sonnendrücker, *Long time behavior of the two-dimensional Vlasov equation with a strong external magnetic field*, Math. Models Methods Appl. Sci., 10 (2000), pp. 539–553.

[21] E. Frénod and E. Sonnendrücker, *The finite Larmor radius approximation*, SIAM J. Math. Anal., 32 (2001), pp. 1227–1247 (electronic).

[22] E. Frénod and F. Watbled, *The Vlasov equation with strong magnetic field and oscillating electric field as a model for isotop resonant separation*, Electron. J. Differential Equations, (2002, No. 06), p. 20 (electronic).

[23] F. Golse and F. Poupaud, *Limite fluide des équations de Boltzmann des semi-conducteurs pour une statistique de Fermi-Dirac*, Asymptotic Anal., 6 (1992), pp. 135–160.

[24] F. Golse and L. Saint-Raymond, *The Vlasov-Poisson system with strong magnetic field*, J. Math. Pures Appl. (9), 78 (1999), pp. 791–817.

[25] F. Golse and L. Saint-Raymond, *The Vlasov-Poisson system with strong magnetic field in quasineutral regime*, Math. Models Methods Appl. Sci., 13 (2003), pp. 661–714.

[26] H. Grad, *The guiding center plasma*, in Proc. Sympos. Appl. Math., Vol. XVIII, Amer. Math. Soc., Providence, R.I., 1967, pp. 162–248.

[27] W. W. Lee, *Gyrokinetic approach in particle simulation*, Physics of Fluids, 26 (1983), pp. 556–562.

[28] R. G. Littlejohn, *Hamiltonian formulation of guiding center motion*, Phys. Fluids, 24 (1981), pp. 1730–1749.

[29] B. Lucquin-Desreux, *Diffusion of electrons by multicharged ions*, Math. Models Methods Appl. Sci., 10 (2000), pp. 409–440.

[30] P. A. Markowich, C. A. Ringhofer, and C. Schmeiser, *Semiconductor equations*, Springer-Verlag, Vienna, 1990.

[31] T. G. Northrop, *The guiding center approximation to charged particle motion*, Annals of Physics, 15 (1961), pp. 79–101.

[32] F. Poupaud, *Diffusion approximation of the linear semiconductor Boltzmann equation : analysis of boundary layers*, Asymptotic Anal., 4 (1991), pp. 293–317.

[33] L. Saint-Raymond, *The gyrokinetic approximation for the Vlasov-Poisson system*, Math. Models Methods Appl. Sci., 10 (2000), pp. 1305–1332.

[34] L. Saint-Raymond, *Control of large velocities in the two-dimensional gyrokinetic approximation*, J. Math. Pures Appl. (9), 81 (2002), pp. 379–399.

[35] R. Sentis, *Approximation and homogenization of a transport process*, SIAM J. Appl. Math., 39 (1980), pp. 134–141.

Part III

Confinement

Chapter 5

High density limit of the stationary one dimensional Schrödinger-Poisson system

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Abstract

The stationary one dimensional Schrödinger–Poisson system on a bounded interval is considered in the limit of a small Debye length (or small temperature). Electrons are supposed to be in a mixed state with the Boltzmann statistics. Using various reformulations of the system as convex minimization problems, we show that only the first energy level is asymptotically occupied. The electrostatic potential is shown to converge towards a boundary layer potential with a profile computed by means of a half space Schrödinger–Poisson system.

Keywords. convex minimization, min-max theorem, concentration-compactness principle, boundary layer.

5.1 Introduction and main results

5.1.1 Introduction

The Schrödinger–Poisson system is one of the most used models for quantum transport of charged particles in semiconductors as well as for quantum chemistry problems [3, 5, 8, 13, 14, 15, 18, 19, 20, 22, 21, 23, 30]. It describes the quantum motion of an ensemble of electrons submitted to and interacting with an electrostatic potential. The electron ensemble might be completely confined or in interaction with reservoirs. In the latter case, one speaks about open systems for which the particles are described by means of the scattering states of the Schrödinger Hamiltonian corresponding to the electrostatic potential which is in turn coupled to electron particle density through the electrostatic interaction. This leads to nonlinear partial differential equations whose analysis involves scattering theory techniques and limiting absorption theorems [23, 4, 3] and in which the repulsive character of the electrostatic interaction plays an important role in the analysis (it provides the necessary a priori estimates for solving the problem).

For closed systems, the particles are described thanks to the eigenstates and eigenenergies of the Schrödinger Hamiltonian. The electron density is the superposition of the densities of the eigenstates with an occupation number decreasingly depending on their eigenenergy. The coupling is again obtained through the Poisson equation modeling the electrostatic interaction. This problem was reformulated by Nier [20, 22, 21] as a minimization of a convex function (whose unknown is the electrostatic potential) which allows us to prove existence and uniqueness results. In [15], one can find generalizations including local contributions to the potential and which can be included in the functional to be minimized. This short review partially covers stationary problems. For evolution problems, an extended bibliography is available, and we refer the reader to the books of Markowich, Ringhofer, and Schmeiser [19] and Cazenave [10] for references.

In this paper we are interested in a singularly perturbed version of the Schrödinger–Poisson system which arises from the description of the so-called two dimensional electron gases [1, 11]. The electrons, in such systems, are strongly confined in one direction, at the interface between two material, and are free to move in the two remaining ones. In [6], the analysis of the Schrödinger equation of strongly confined electrons in one direction is performed. The confined direction is called z and the confining potential is assumed to be given and scaled as $\frac{1}{\varepsilon^2}V_c(\frac{z}{\varepsilon})$, where ε is a small parameter. Approximate models for the transport direction (orthogonal to z) derived heuristically in the previous works [26, 27, 25] are then analyzed in [6, 24]. The aim of the present work is to somehow justify the scaling $\frac{1}{\varepsilon^2}V_c(\frac{z}{\varepsilon})$ by the

analysis of the self-consistent Schrödinger–Poisson system in the z direction. This is why we shall forget about the transport issues in the orthogonal direction and assume that the considered system is invariant with respect to it. The parameter ε in the present work is linked to the scaled Debye length as shall be explained later. The analysis relies on the minimization formulation of the problem leading to a singularly perturbed functional. After a rescaling argument, we are led to the analysis of a half space Schrödinger–Poisson system in which only the first eigenstate is occupied. Additional estimates are obtained thanks to reformulation of the single state Schrödinger–Poisson system as another minimization problem whose unknown is the first eigenfunction (and not the potential). This formulation is used in quantum chemistry [9].

Let us now come to the precise description of the problem and the results. The system is one dimensional and occupies the interval $[0,1]$. The electrostatic energy is given by $V_\varepsilon(z)$. It satisfies the following one dimensional stationary Schrödinger–Poisson system :

$$\begin{cases} -\dfrac{d^2\varphi_p}{dz^2} + V\varphi_p = \mathcal{E}_p\varphi_p, \qquad z \in [0,1], \\ \varphi_p \in H^1(0,1), \quad \varphi_p(0) = 0, \quad \varphi_p(1) = 0, \quad \displaystyle\int_0^1 \varphi_p\varphi_q = \delta_{pq}, \\ -\varepsilon^3\dfrac{d^2V}{dz^2} = \dfrac{1}{\mathcal{Z}}\displaystyle\sum_{p=1}^{+\infty} e^{-\mathcal{E}_p}|\varphi_p|^2, \quad \mathcal{Z} = \displaystyle\sum_{p=1}^{+\infty} e^{-\mathcal{E}_p}, \\ V(0) = 0, \quad \dfrac{dV}{dz}(1) = 0. \end{cases} \tag{5.1.1}$$

The dimensionless parameter ε is a small parameter which is devoted to tending to zero. The choice of the third power is done for notational convenience as shall be understood later. This parameter is related to the Debye length and shall be explicitly given by the rescaling of the Schrödinger–Poisson system (5.1.19) (see subsection 1.3). The eigenvalues of the Schrödinger operator $(\mathcal{E}_p)_p$ are the energy levels in the potential well. The sum in the right-hand side of the Poisson equation includes all eigenvalues of the Schrödinger operator. In the limit $\varepsilon \to 0$, one expects that the wave functions concentrate at $z = 0$. The boundary condition for the potential at $z = 1$ is physically justified in some physical situations such as in bulk materials. However, a Dirichlet condition is more commonly used in such problems. The analysis can be carried out in that case with the cost of technical complexity since a new boundary layer at $z = 1$ will appear and the eigenvalues will have asymptotically a double multiplicity. For simplicity, we do not consider this case. Since the density is very high in the limit $\varepsilon \to 0^+$, the Boltzmann statistics should be replaced by the Fermi–Dirac ones. The analysis can be done in this case with the cost of technical complications. More detailed comments about this are given in

the last section of this paper. In order to analyze the boundary layer, we make the change of variables

$$\varphi_p(z) = \frac{1}{\sqrt{\varepsilon}}\psi_p\left(\frac{z}{\varepsilon}\right), \quad \mathcal{E}_p = \frac{1}{\varepsilon^2}E_p, \quad V(z) = \frac{1}{\varepsilon^2}U\left(\frac{z}{\varepsilon}\right), \quad \xi = \frac{z}{\varepsilon}. \tag{5.1.2}$$

Then, U verifies $-\frac{d^2U}{d\xi^2} = \frac{1}{\tilde{\mathcal{Z}}}\sum_{p=1}^{+\infty} e^{\frac{-E_p}{\varepsilon^2}}|\psi_p|^2$ with $\tilde{\mathcal{Z}} = \sum_{p=1}^{+\infty} e^{\frac{-E_p}{\varepsilon^2}}$. Since there is a uniform gap with respect to ε between E_1 and E_p for $p \geq 2$ (see Lemma 5.4.4), the terms $e^{\frac{-E_p}{\varepsilon^2}}$ with $p \geq 2$ are expected to be negligible when compared to the first one ($p = 1$). Therefore, it is natural to expect the solution of (5.1.1) to be asymptotically close to the solution of the following Schrödinger–Poisson system in which only the first energy level is taken into account :

$$\begin{cases} -\dfrac{d^2\tilde{\varphi}_1}{dz^2} + \tilde{V}\tilde{\varphi}_1 = \tilde{\mathcal{E}}_1\tilde{\varphi}_1, \qquad z \in [0,1], \\ \tilde{\mathcal{E}}_1 = \displaystyle\inf_{\varphi \in H_0^1(0,1),\, \|\varphi\|_{L^2}=1} \left\{ \int_0^1 |\varphi'|^2 + \int_0^1 \tilde{V}\varphi^2 \right\}, \\ -\varepsilon^3 \dfrac{d^2\tilde{V}}{dz^2} = |\tilde{\varphi}_1|^2, \\ \tilde{V}(0) = 0, \quad \dfrac{d\tilde{V}}{dz}(1) = 0. \end{cases} \tag{5.1.3}$$

Moreover, when ε goes to zero, we will prove that the electrostatic potential, $\tilde{V}_\varepsilon$, solution of (5.1.3) converges towards a boundary layer potential with profile, U_0, solution of the following half line problem :

$$\begin{cases} -\dfrac{d^2\psi_1}{d\xi^2} + U\psi_1 = E_1\psi_1, \qquad \xi \in [0, +\infty[, \\ E_1 = \displaystyle\inf_{\psi \in H_0^1(\mathbb{R}^+),\, \|\psi\|_{L^2}=1} \left\{ \int_0^{+\infty} |\psi'|^2 + \int_0^{+\infty} U\psi^2 \right\}, \\ -\dfrac{d^2U}{d\xi^2} = |\psi_1|^2, \\ U(0) = 0, \quad \dfrac{dU}{d\xi} \in L^2(\mathbb{R}^+). \end{cases} \tag{5.1.4}$$

5.1.2 Main results

In this paper, a rigourous analysis and comparison of the systems presented above will be provided. Namely, (5.1.1) and (5.1.3) are posed on a bounded domain. The one dimensional Schrödinger–Poisson system on a bounded interval was studied by Nier in [20]. Each of these systems can be reformulated as a minimization problem (see section 2 for details). However, the limit problem (5.1.4) is posed on an unbounded domain. Our first result deals with the study of (5.1.4). We also prove that it can be formulated as a minimization problem.

Theorem 5.1.1. *Let $J_0(.)$ be the energy functional defined on $\dot{H}_0^1(\mathbb{R}^+)$ (given by (5.1.22)) by*

$$J_0(U) = \frac{1}{2}\int_0^{+\infty} |U'|^2 - E_1^\infty[U], \tag{5.1.5}$$

where $E_1^\infty[U]$ is the fundamental mode of the Schrödinger operator given by (5.3.1). The limit problem (5.1.4) has a unique solution $(U_0, E_{1,0}, \psi_{1,0})$, and U_0 satisfies the following minimization problem :

$$J_0(U_0) = \inf_{U\in\dot{H}_0^1(\mathbb{R}^+)} J_0(U). \tag{5.1.6}$$

The comparison of the systems presented above is established by our second main theorem.

Theorem 5.1.2. *Let V_ε, $\tilde{V}_\varepsilon$, and U_0 be the potentials satisfying problems (5.1.1), (5.1.3), and (5.1.4), respectively. Then the following estimates hold :*

$$\|V_\varepsilon - \tilde{V}_\varepsilon\|_{H^1(0,1)} = \mathcal{O}(e^{-\frac{c}{\varepsilon^2}}) \tag{5.1.7}$$

and

$$\left\|\tilde{V}_\varepsilon - \frac{1}{\varepsilon^2}U_0\left(\frac{\cdot}{\varepsilon}\right)\right\|_{H^1(0,1)} = \mathcal{O}(e^{-\frac{c}{\varepsilon}}), \tag{5.1.8}$$

where c is a general strictly positive constant independent of ε.

The paper is organized as follows. In the next subsection, we present some remarks on the scaling giving model (5.1.1), and we end this section by fixing some notation and definitions. In section 5.2, we recall the spectral properties of the Schrödinger operator on a bounded domain and state the optimization problems corresponding to (5.1.1) and (5.1.3) (or more precisely to the intermediate systems (5.1.10) and (5.1.11)). Section 5.3 is devoted to the analysis of the limit problem (5.1.4) posed on the half line (proof of Theorem 5.1.1). We will first study the properties of the fundamental mode of the Schrödinger operator (Proposition 5.3.2). The limit problem leads us to the study of a minimization problem posed on an unbounded domain. This will be done by means of the concentration-compactness principle introduced by Lions in [17]. Estimates (5.1.7) and (5.1.8) are proved in section 5.4. Some comments concerning the Fermi–Dirac statistics, the choice of the boundary conditions, and the problems of the multidimensional case are given in section 5.5. Finally, Appendix A.1.1 is devoted to the proof of Lemma 5.3.4.

First, let us make this remark.

Remark 5.1.3. *To prove (5.1.7)–(5.1.8), we use the scaled versions of (5.1.1) and (5.1.3) when applying the changes of variables (5.1.2) and*

$$\tilde{\varphi}_1(z) = \frac{1}{\sqrt{\varepsilon}}\tilde{\psi}_1\left(\frac{z}{\varepsilon}\right), \quad \tilde{\mathcal{E}}_1 = \frac{1}{\varepsilon^2}\tilde{E}_1, \quad \tilde{V}(z) = \frac{1}{\varepsilon^2}\tilde{U}\left(\frac{z}{\varepsilon}\right), \quad \xi = \frac{z}{\varepsilon}. \tag{5.1.9}$$

Then the intermediate Schrödinger–Poisson models write

$$\begin{cases} -\dfrac{d^2\psi_p}{d\xi^2} + U\psi_p = E_p\psi_p, \qquad \xi \in \left[0, \dfrac{1}{\varepsilon}\right], \\ \psi_p \in H^1\left(0, \dfrac{1}{\varepsilon}\right), \quad \psi_p(0) = 0, \quad \psi_p\left(\dfrac{1}{\varepsilon}\right) = 0, \quad \displaystyle\int_0^{\frac{1}{\varepsilon}} \psi_p\psi_q = \delta_{pq}, \\ -\dfrac{d^2U}{d\xi^2} = \dfrac{1}{\tilde{\mathcal{Z}}} \displaystyle\sum_{p=1}^{+\infty} e^{\frac{-E_p}{\varepsilon^2}} |\psi_p|^2, \quad \tilde{\mathcal{Z}} = \displaystyle\sum_{p=1}^{+\infty} e^{\frac{-E_p}{\varepsilon^2}}, \\ U(0) = 0, \quad \dfrac{dU}{d\xi}\left(\dfrac{1}{\varepsilon}\right) = 0 \end{cases} \tag{5.1.10}$$

and

$$\begin{cases} -\dfrac{d^2\tilde{\psi}_1}{d\xi^2} + \tilde{U}\tilde{\psi}_1 = \tilde{E}_1\tilde{\psi}_1, \qquad \xi \in \left[0, \dfrac{1}{\varepsilon}\right], \\ \tilde{E}_1 = \displaystyle\inf_{\psi \in H_0^1(0, \frac{1}{\varepsilon}),\, \|\psi\|_{L^2}=1} \left\{ \int_0^{\frac{1}{\varepsilon}} |\psi'|^2 + \int_0^{\frac{1}{\varepsilon}} \tilde{U}\psi^2 \right\}, \\ -\dfrac{d^2\tilde{U}}{d\xi^2} = |\tilde{\psi}_1|^2, \\ \tilde{U}(0) = 0, \quad \dfrac{d\tilde{U}}{d\xi}\left(\dfrac{1}{\varepsilon}\right) = 0. \end{cases} \tag{5.1.11}$$

Remark that it is natural to expect (5.1.11) *to be close, when* ε *goes to zero, to the limit problem* (5.1.4) *posed on* $[0, +\infty)$.

5.1.3 Remark on the scaling

Here we show how the system (5.1.1) can be obtained by a rescaling of the Schrödinger–Poisson system written with the physical dimensional variables. Indeed, let $(\chi_p(Z), \Lambda_p)$ be the eigenfunctions and the eigenenergies of the one dimensional Schrödinger operator (the confinement operator) $-\frac{\hbar^2}{2m}\frac{d^2}{dZ^2} + W$ with homogeneous Dirichlet data :

$$-\frac{\hbar^2}{2m}\frac{d^2\chi_p}{dZ^2} + W\chi_p = \Lambda_p\chi_p, \tag{5.1.12}$$

where $\hbar$ is the Planck constant and m denotes the effective mass of the electrons in the crystal. The $(\chi_p)_p$ is an orthonormal basis of $L^2(0, L)$. The variable Z belongs to $[0, L]$, where L is the typical length of the confinement. Denoting by n the electronic density, this can be written

$$n(Z) = \sum_{p=1}^{+\infty} n_p |\chi_p(Z)|^2. \tag{5.1.13}$$

In this formula, $|\chi_p(Z)|^2$ is the probability of presence at point Z of an electron in the pth state. Using Boltzmann statistics, the occupation factor n_p is given by

$$n_p = \frac{N_s}{\mathcal{Z}} \exp\left(-\frac{\Lambda_p}{k_B T}\right), \quad \mathcal{Z} = \sum_{q=1}^{+\infty} \exp\left(-\frac{\Lambda_q}{k_B T}\right), \tag{5.1.14}$$

where k_B is the Boltzmann constant, T denotes the temperature, and N_s is the surface density assumed to be given. With this notation we have $\int_0^L n(Z)\, dZ = N_s$, which means that the total number of electrons in the interval $[0, L]$ (per unit surface in the two remaining spatial directions) is given. The electrostatic potential W and the electron density n are coupled through the Poisson equation :

$$-\frac{d^2 W}{dZ^2} = \frac{q^2}{\varepsilon_0 \varepsilon_r} n \tag{5.1.15}$$

with boundary conditions

$$W(0) = 0, \quad \frac{dW}{dZ}(L) = 0. \tag{5.1.16}$$

In (5.1.15), the constant q is the elementary electric charge and ε_0, ε_r are, respectively, the permittivity of the vacuum and the relative permittivity of the material.

Let us rescale the problem (5.1.12)–(5.1.16) by noticing that

$$z = \frac{Z}{L} \in [0, 1], \quad W(Z) = (k_B T) V\left(\frac{Z}{L}\right), \quad \Lambda_p = (k_B T)\mathcal{E}_p, \quad \chi_p(Z) = \frac{1}{\sqrt{L}} \varphi_p\left(\frac{Z}{L}\right). \tag{5.1.17}$$

We assume that $\frac{\hbar^2}{2mL^2}$ is of the same order of the thermal energy $(k_B T)$. In order to simplify the mathematical presentation, we suppose that

$$\frac{\hbar^2}{2mL^2} = k_B T. \tag{5.1.18}$$

By inserting (5.1.17) into the system (5.1.12)–(5.1.16), we obtain, after straightforward computation, the system (5.1.1) in which ε is related to the scaled Debye length :

$$\varepsilon^3 = \left(\frac{\lambda_D}{L}\right)^2, \quad \lambda_D = \sqrt{\frac{k_B T \varepsilon_0 \varepsilon_r}{q^2 N}}, \tag{5.1.19}$$

where $N = \frac{N_s}{L}$ is the average volume density of electrons.

5.1.4 Notation and definitions

We summarize in this subsection the different variables and notation used in this paper.

– For the Schrödinger–Poisson problems posed on $[0,1]$, z denotes the space variable, V denotes the potential variable, and $(\mathcal{E},\varphi)$ represents any eigenvalue and the corresponding eigenfunction of the Schrödinger operator. For systems posed on $[0,\frac{1}{\varepsilon}]$ or on $\mathbb{R}^+$, we use ξ, U, and (E,ψ) as variables. The same notation with $\tilde{}$, i.e., $(\tilde{V},\tilde{\mathcal{E}},\tilde{\varphi})$ or $(\tilde{U},\tilde{E},\tilde{\psi})$, is used for the variables of Schrödinger–Poisson systems in which only the first eigenstate is taken into account.

– For any real valued function $V \in L^2(0,L)$, where $L>0$ is given ($L=1$ or $\frac{1}{\varepsilon}$ here), we denote by $H[V]$ the Dirichlet–Schrödinger operator

$$H[V] = -\frac{d^2}{dx^2} + V(x) \quad (x = z \text{ or } \xi \text{ here}) \tag{5.1.20}$$

defined on the domain $D(H[V]) = H^2(0,L) \cap H_0^1(0,L)$. In addition, the sequence of eigenenergies and eigenfunctions of $H[V]$ will be denoted by $(E_p[V],\psi_p[V])_{p\in\mathbb{N}^*}$. We give in the next section the main properties satisfied by the functions $V \mapsto E_p[V]$ and $V \mapsto \psi_p[V]$ for any $p \in \mathbb{N}^*$.

– The potentials satisfying (5.1.1) and (5.1.3) are denoted by V_ε and $\tilde{V}_\varepsilon$. In addition, $(\mathcal{E}_{p,\varepsilon},\varphi_{p,\varepsilon})$ and $(\tilde{\mathcal{E}}_{p,\varepsilon},\tilde{\varphi}_{p,\varepsilon})$, with $p \in \mathbb{N}^*$, represent the corresponding energy couples of $H[V_\varepsilon]$ and $H[\tilde{V}_\varepsilon]$, respectively. In other words, $\mathcal{E}_{p,\varepsilon} := E_p[V_\varepsilon]$, $\varphi_{p,\varepsilon} := \psi_p[V_\varepsilon]$, $\tilde{\mathcal{E}}_{p,\varepsilon} := E_p[\tilde{V}_\varepsilon]$, and $\tilde{\varphi}_{p,\varepsilon} := \psi_p[\tilde{V}_\varepsilon]$. Similarly, the solutions of (5.1.10) and (5.1.11) will be denoted, respectively, by $(U_\varepsilon,E_{p,\varepsilon},\psi_{p,\varepsilon})$ and $(\tilde{U}_\varepsilon,\tilde{E}_{p,\varepsilon},\tilde{\psi}_{p,\varepsilon})$. Finally, we fix $(U_0,E_{1,0},\psi_{1,0})$ to denote the solution of the limit problem (5.1.4).

Let us now define some spaces which will be used throughout this paper.

Definition 5.1.4. (i) *For $L>0$, we define*

$$H^{1,0}(0,L) = \left\{U \in H^1(0,L),\, U(0)=0\right\}. \tag{5.1.21}$$

(ii) *The space $\dot{H}_0^1(\mathbb{R}^+)$ is defined as follows :*

$$\dot{H}_0^1(\mathbb{R}^+) = \left\{U \in L^2_{loc}(\mathbb{R}^+),\, U' \in L^2(\mathbb{R}^+),\, U(0)=0, \text{ and } U \geq 0\right\}. \tag{5.1.22}$$

(iii) *For any $0<L\leq+\infty$, we shall denote by S_L the set of normalized functions of $H_0^1(0,L)$ with respect to the L^2-norm*

$$S_L = \left\{\varphi \in H_0^1(0,L),\, \int_0^L \varphi^2 = 1\right\}. \tag{5.1.23}$$

Here $H_0^1(0,L)$ is the space of H^1-functions vanishing on 0 and L, and when $L=+\infty$

$$H_0^1(\mathbb{R}^+) = \left\{\psi \in H^1(\mathbb{R}^+),\, \psi(0)=0\right\}.$$

5.2 Schrödinger–Poisson system on a bounded domain

We begin this part by recalling some basic properties satisfied by the eigenvalues and the eigenfunctions of the one dimensional Schrödinger operator (5.1.20). These properties are standard and can be found in [16, 20, 28, 29]. The operator $H[V]$ is self-adjoint, is bounded from below, and has compact resolvent. There exists a strictly increasing sequence $(E_p[V])_p$ of real numbers tending to $+\infty$ and an orthonormal basis of $L^2(0,L)$, $(\psi_p[V])_p$, such that $\psi_p[V] \in D(H[V])$ and

$$H[V]\psi_p[V] = E_p[V]\psi_p[V]. \tag{5.2.1}$$

For $V = 0$, we have by a simple calculation

$$E_p[0] = \frac{\pi^2 p^2}{L^2}, \quad \psi_p[0](x) = \sqrt{\frac{2}{L}} \sin\left(\frac{p\pi x}{L}\right). \tag{5.2.2}$$

The eigenvalues $E_p[V]$ are simple and satisfy the following characterization (min-max principle) [29] :

$$E_p[V] = \min_{V_p \in \mathbb{V}_p(D(H[V]))} \max_{\varphi \in V_p,\, \varphi \neq 0} \frac{(H[V]\varphi, \varphi)_{L^2}}{\|\varphi\|^2_{L^2}}, \tag{5.2.3}$$

where $\mathbb{V}_p\left(D(H[V])\right)$ is the set of the subspaces of $D(H[V])$ with dimension equal to p, and $(.,.)$ denotes the scalar product in L^2. In view of the min-max formula (5.2.3), one can verify that for any $p \in \mathbb{N}^*$, $E_p[.]$ is an increasing function, which means that

$$E_p[V] \leq E_p[W] \quad \text{if } V \leq W \text{ a.e.}$$

Moreover, we have the Lipschitz property, for any real valued functions V, W in $L^\infty(0,L)$,

$$|E_p[V] - E_p[W]| \leq \|V - W\|_{L^\infty(0,L)}. \tag{5.2.4}$$

Besides, one can prove the following lemma [20].

Lemma 5.2.1. *For any $p \in \mathbb{N}^*$, the maps*

$$E_p[.] : L^2(0,L) \longrightarrow \mathbb{R}, \quad \psi_p[.] : L^\infty(0,L) \longrightarrow L^1(0,L)$$

are Gâteaux differentiable, and their derivatives are given, respectively, by

$$\begin{aligned} dE_p[V].W &= \int_0^L |\psi_p[V]|^2 W dx \quad \textit{and} \\ d\psi_p[V].W &= \sum_{q \neq p} \frac{1}{E_p[V] - E_q[V]} \left(\int_0^L W \psi_p \psi_q dx \right) \psi_q \end{aligned} \tag{5.2.5}$$

for any $V, W \in L^\infty(0,L)$.

Using the spectral properties of the Schrödinger operator, one can prove the following proposition. For details on the proof see [20].

Proposition 5.2.2. *The systems* (5.1.10) *and* (5.1.11) *are well posed. They are equivalent, respectively, to the following minimization problems :*

$$J_\varepsilon(U_\varepsilon) = \inf_{U\in H^{1,0}(0,M_\varepsilon)} J_\varepsilon(U) \tag{5.2.6}$$

and

$$\tilde{J}_\varepsilon(\tilde{U}_\varepsilon) = \inf_{U\in H^{1,0}(0,M_\varepsilon)} \tilde{J}_\varepsilon(U), \tag{5.2.7}$$

where $M_\varepsilon = \frac{1}{\varepsilon}$. *The energy functionals* J_ε *and* $\tilde{J}_\varepsilon$ *are given by*

$$J_\varepsilon(U) = \frac{1}{2}\int_0^{M_\varepsilon} |U'|^2 + \varepsilon^2 \log\left(\sum_{p=1}^{+\infty} e^{-\frac{E_p[U]}{\varepsilon^2}}\right) \tag{5.2.8}$$

and

$$\tilde{J}_\varepsilon(U) = \frac{1}{2}\int_0^{M_\varepsilon} |U'|^2 - E_1[U]. \tag{5.2.9}$$

Each one of problems (5.2.6) *and* (5.2.7) *admits a unique solution.*

Remark 5.2.3. *One can similarly study the systems* (5.1.1) *and* (5.1.3) *and prove that each one is equivalent to an optimization problem.*

5.3 Analysis of the limit problem (5.1.4)

The aim of this part is to study the well-posedness of the limit problem (5.1.4) posed on the half line. Namely, this part is concerned with the proof of Theorem 5.1.1. We begin with the study of the fundamental mode, $E_1^\infty[.]$, of the Schrödinger operator. Its main properties are listed in Proposition 5.3.2.

5.3.1 Properties of the fundamental mode of the Schrödinger operator on $[0, +\infty)$

We begin by defining the fundamental mode.

Definition 5.3.1. *For any real and positive function* $U \in L^1_{loc}(\mathbb{R}^+)$, *the fundamental mode of the Schrödinger operator is*

$$E_1^\infty[U] = \inf_{\psi\in S_\infty} J_U(\psi), \tag{5.3.1}$$

where for any $\psi \in S_\infty$ *(defined by* (5.1.23)*) we have*

$$J_U(\psi) = \int_0^{+\infty} |\psi'|^2 + \int_0^{+\infty} U\psi^2. \tag{5.3.2}$$

One difficulty due to the unboundedness of the interval $[0,+\infty)$ is that $E_1^\infty[.]$ might not be an eigenvalue but only the lower bound of the essential spectrum. The following proposition gives some properties of $E_1^\infty[.]$ and some sufficient conditions on the potential for which $E_1^\infty[.]$ is an eigenvalue.

Proposition 5.3.2. *1. The map $U \mapsto E_1^\infty[U]$ is a continuous, concave, and increasing function with values in $\overline{\mathbb{R}^+} := [0,+\infty]$ satisfying*

$$E_1^\infty[U] \leq \limsup_{\xi\to+\infty} U(\xi). \tag{5.3.3}$$

2. If $U \in L^1_{loc}(\mathbb{R}^+)$, $U \geq 0$ such that $E_1^\infty[U] < \liminf_{\xi\to+\infty} U(\xi)$, then $E_1^\infty[U]$ is reached by a unique positive function $\psi_1[U]$, which means that there exists a unique positive function $\psi_1[U] \in S_\infty$ such that $E_1^\infty[U] = J_U(\psi_1[U])$. In addition, we have

$$\frac{dE_1^\infty}{dU}[U].W = \int_0^{+\infty} |\psi_1[U]|^2 W d\xi \tag{5.3.4}$$

for any function W in $L_0^\infty(\mathbb{R}^+)$, the space of bounded functions with compact support on $\mathbb{R}^+$.

3. Let $U \in L^1_{loc}(\mathbb{R}^+)$ be a positive function such that $\lim_{\xi\to+\infty} U(\xi)$ exists, $U \leq \lim_{\xi\to+\infty} U(\xi)$, and $E_1^\infty[U] = \lim_{\xi\to+\infty} U(\xi)$. Then we have

$$\frac{dE_1^\infty}{dU}[U].W = 0$$

for any $W \in L_0^\infty(\mathbb{R}^+)$.

4. Let α be an arbitrary positive constant. Then we have

$$E_1^\infty[\alpha\sqrt{\xi}] = \alpha^{\frac{4}{5}} E_1^\infty[\sqrt{\xi}]. \tag{5.3.5}$$

Remark 5.3.3. *There is quite a difference between the third case of this proposition, where $E_1^\infty[U] = \lim_{\xi\to+\infty} U(\xi)$, and the second case, which includes $E_1^\infty[U] < \lim_{\xi\to+\infty} U(\xi)$. This result is natural and can be interpreted as follows. The classically allowed region for a particle with energy E is the set $\mathcal{A} = \{\xi \in [0,+\infty);\, U(\xi) \leq E\}$. In the case $E \geq U(\xi)$ on $[0,+\infty)$, the set $\mathcal{A}$ extends to $+\infty$ so that there is no bound state, while in the case $E < \lim_{\xi\to+\infty} U(\xi)$ the set $\mathcal{A}$ is bounded and E is a bounded state energy.*

Lemma 5.3.4. *Let $U \in \dot{H}^1_0(\mathbb{R}^+)$ such that $E_1^\infty[U] < \liminf_{+\infty} U$. Then all minimizing sequences $(\psi_n)_n$ of problem (5.3.1) are relatively compact in $L^2(\mathbb{R}^+)$.*

This lemma is needed for the proof of the second point of Proposition 5.3.2. It is proved in Appendix A.1.1. The proof is based on the concentration-compactness principle.

Proof of Proposition 5.3.2. 1. Remark first that for any positive function U, $E_1^\infty[U]$ exists and belongs to $\overline{\mathbb{R}^+}$. It is easy to check, from the definition of $E_1^\infty[.]$, that it is a continuous, concave, and increasing function. To prove inequality (5.3.3), let $\psi \in S_\infty$ be fixed and set $\psi_\delta = \sqrt{\delta}\psi(\delta\xi)$ for any real positive δ. Then $\psi_\delta \in S_\infty$, and since $E_1^\infty[U]$ verifies (5.3.1), we have

$$E_1^\infty[U] \leq J_U(\psi_\delta). \tag{5.3.6}$$

Moreover, we have $J_U(\psi_\delta) = \delta^2 \int_0^{+\infty} |\psi'(\xi)|^2 d\xi + \int_0^{+\infty} U(\frac{\xi}{\delta})\psi^2(\xi)d\xi$. Then

$$\limsup_{\delta\to 0} J_U(\psi_\delta) \leq \int_0^{+\infty} \limsup_{\delta\to 0} U\left(\frac{\xi}{\delta}\right)\psi^2(\xi)d\xi \leq \limsup_{\xi\to+\infty} U(\xi).$$

Taking the $\limsup_{\delta\to 0}$ of (5.3.6), one obtains inequality (5.3.3).

2. Let $(\psi_n)_n$ be a minimizing sequence of $E_1^\infty[U]$; i.e., $\psi_n \in S_\infty$ for any $n \in \mathbb{N}^*$ and $J_U(\psi_n) \to_{n\to+\infty} E_1^\infty[U]$. The sequence $(\psi_n)_n$ is bounded in $H_0^1(\mathbb{R}^+)$, there exist a function $\psi \in H_0^1(\mathbb{R}^+)$ and a subsequence also denoted (ψ_n) such that (ψ_n) converges weakly to ψ in $H_0^1(\mathbb{R}^+)$, and since $J_U(.)$ is weakly lower semicontinuous (it is strictly convex and lower semicontinuous) we have $J_U(\psi) \leq \liminf_{n\to+\infty} J_U(\psi_n)$. Then

$$J_U(\psi) \leq E_1^\infty[U]. \tag{5.3.7}$$

Besides, the hypothesis $E_1^\infty[U] < \liminf_{+\infty} U$ implies that the sequence $(\psi_n)_n$ is relatively compact in $L^2(\mathbb{R}^+)$ (see Lemma 5.3.4). Then, up to an extraction of subsequence, $(\psi_n)_n$ converges strongly to ψ in $L^2(\mathbb{R}^+)$. Since $\|\psi_n\|^2_{L^2(\mathbb{R}^+)} = 1$, for all n, we have $\|\psi\|^2_{L^2(\mathbb{R}^+)} = 1$, and then ψ belongs to S_∞. Therefore, in view of the definition of $E_1^\infty[U]$ (5.3.1), $E_1^\infty[U] \leq J_U(\psi)$ and with (5.3.7) we have $E_1^\infty[U] = J_U(\psi)$. Let us now show that $E_1^\infty[U]$ is a simple eigenvalue and the corresponding eigenfunction has a constant sign. Indeed, let ψ_1 and ψ_2 be two minimizers of $J_U(.)$ on S_∞, i.e., $\psi_1, \psi_2 \in S_\infty$, such that $E_1^\infty[U] = J_U(\psi_1) = J_U(\psi_2)$, and let $\phi = \sqrt{\frac{\psi_1^2}{2} + \frac{\psi_2^2}{2}}$. The function ϕ belongs to S_∞, and we have

$$J_U(\phi) = \frac{1}{2}J_U(\psi_1)+\frac{1}{2}J_U(\psi_2)-\int_0^{+\infty}\left|\frac{\psi_1\psi_2' - \psi_2\psi_1'}{2\phi}\right|^2 = E_1^\infty[U]-\int_0^{+\infty}\left|\frac{\psi_1\psi_2' - \psi_2\psi_1'}{2\phi}\right|^2.$$

Since $E_1^\infty[U] \leq J_U(\phi)$ ($\phi \in S_\infty$), we get $\int_0^{+\infty}\left|\frac{\psi_1\psi_2'-\psi_2\psi_1'}{2\phi}\right|^2 = 0$, which implies that ψ_1 and ψ_2 are proportional, and so $E_1^\infty[U]$ is simple. In particular, ψ and $|\psi|$ are two minimizers of $E_1^\infty[U]$; they are then proportional, and since $\int_0^{+\infty}|\psi|^2 = 1$ we conclude that $\psi = \pm|\psi|$. We then choose $\psi_1[U] = |\psi|$, which is positive. This is the unique positive eigenfunction corresponding to $E_1^\infty[U]$. To end the proof of the second point of Proposition 5.3.2, let W be a compactly supported bounded function ($W \in L_0^\infty(\mathbb{R}^+)$) and remark that for a small real t we have $E_1^\infty[U +$

$tW] \leq E_1^\infty[U] + |t|\|W\|_\infty < \liminf_{\xi\to+\infty} U(\xi)$. In addition, since $W \in L_0^\infty$, we have $\liminf_{\xi\to+\infty} U = \liminf_{\xi\to+\infty}(U(\xi) + tW(\xi))$. Then, for any small real t, we have $E_1^\infty[U + tW] < \lim_{\xi\to+\infty}(U(\xi) + tW(\xi))$. Therefore, for all bounded and compactly supported functions W and for all $t \in \mathbb{R}$ small, $E_1^\infty[U + tW]$ is an eigenvalue. Let ψ_t be the corresponding positive eigenfunction. We have

$$E_1^\infty[U + tW] = \int_0^{+\infty} |\psi_t'|^2 d\xi + \int_0^{+\infty} (U + tW)|\psi_t|^2 d\xi \geq E_1^\infty[U] + t\int_0^{+\infty} W|\psi_t|^2 d\xi.$$

Similarly, one has

$$E_1^\infty[U] \geq E_1^\infty[U + tW] - t\int_0^{+\infty} W|\psi_1[U]|^2 d\xi.$$

Then, if t is a small nonnegative real (without loss of generality), one can write

$$\int_0^{+\infty} W|\psi_t|^2 d\xi \leq \frac{E_1^\infty[U + tW] - E_1^\infty[U]}{t} \leq \int_0^{+\infty} W|\psi_1[U]|^2 d\xi. \tag{5.3.8}$$

Besides, since $(\psi_t)_t$ is bounded in $H_0^1(\mathbb{R}^+)$, there exists a positive function $\psi_0 \in H_0^1$ such that ψ_t converges weakly to ψ_0, when $t \to 0^+$, in $H_{loc}^1(\mathbb{R}^+)$ and strongly in $L_{loc}^2(\mathbb{R}^+)$. By passing to the limit $t \to 0^+$ in

$$-\psi_t'' + (U + tW)\psi_t = E_1^\infty[U + tW]\psi_t$$

we obtain

$$-\psi_0'' + U\psi_0 = E_1^\infty[U]\psi_0 \quad \text{in } \mathcal{D}'(0, +\infty).$$

Since ψ_0 is positive, we deduce that $\psi_0 = \psi_1[U]$. Finally, to obtain (5.3.4) we just have to take the limit $t \to 0^+$ of (5.3.8).

3. Remark first that, since $E_1^\infty[.]$ is a nondecreasing real function, we have for $t \geq 0$

$$\frac{E_1^\infty[U - t|W|] - E_1^\infty[U]}{t} \leq \frac{E_1^\infty[U + tW] - E_1^\infty[U]}{t} \leq \frac{E_1^\infty[U + t|W|] - E_1^\infty[U]}{t}.$$

Therefore, it is sufficient to prove $\frac{dE_1^\infty}{dU}[U].W = 0$ for $W \geq 0$ and $W \leq 0$ (the general case can be deduced by passing to the limit $t \to 0^+$ in the above inequalities).

(i) Let $W \in L_0^\infty(\mathbb{R}^+)$ and $W \geq 0$. Then we have $E_1^\infty[U] \leq E_1^\infty[U + tW]$. Besides, by (5.3.3), we have $E_1^\infty[U + tW] \leq \lim_{\xi\to+\infty}(U(\xi) + tW(\xi)) = \lim_{\xi\to+\infty} U(\xi) = E_1^\infty[U]$. Then, for all $W \geq 0$ in L_0^∞, $E_1^\infty[U + tW] = E_1^\infty[U]$, and the result is proved in this case.

(ii) Let $W \in L_0^\infty(\mathbb{R}^+)$, let $W \leq 0$, and let $(t_n)_{n\in\mathbb{N}}$ be a sequence decreasing towards 0^+. The sequence $(E_1^\infty[U+t_nW])_n$ is increasing and satisfies $E_1^\infty[U+t_nW] \leq$

$\lim_{+\infty} U = E_1^\infty[U]$ for all $n \in \mathbb{N}$. Therefore, either it is stationary in the vicinity of $+\infty$ and in that case $\frac{dE_1^\infty}{dU}[U].W = 0$, or it satisfies

$$E_1^\infty[U + t_n W] < \lim_{+\infty} U \quad \forall n \in \mathbb{N}. \tag{5.3.9}$$

In the latter case, $E_1^\infty[U + t_n W]$ is an eigenvalue and there exists a sequence $(\psi_n) \in S_\infty$, $\psi_n \geq 0$, such that

$$E_1^\infty[U + t_n W] = J_{U+t_n W}(\psi_n) = \inf_{\psi \in S_\infty} J_{U+t_n W}(\psi).$$

Besides, we have $E_1^\infty[U + t_n W] \geq E_1^\infty[U] + t_n \int_0^{+\infty} W\psi_n^2 d\xi$ and

$$\left| \frac{E_1^\infty[U + t_n W] - E_1^\infty[U]}{t_n} \right| \leq -\int_0^{+\infty} W\psi_n^2 d\xi. \tag{5.3.10}$$

The sequence $(\psi_n)_n$ being bounded in $H_0^1(\mathbb{R}^+)$, one can find a positive function $\psi \in H_0^1(\mathbb{R}^+)$ and a subsequence of $(\psi_n)_n$ also denoted by $(\psi_n)_n$ such that ψ_n converges weakly to ψ in $H_{loc}^1(\mathbb{R}^+)$ and strongly in $L_{loc}^2(\mathbb{R}^+)$. In addition ψ satisfies, in the sense of distributions,

$$-\psi'' + U\psi = E_1^\infty[U]\psi = \lim_{+\infty}(U)\psi.$$

This implies that $\psi'' = (U - \lim_{+\infty} U)\psi \leq 0$ with $\psi \in H_0^1(\mathbb{R}^+)$. We deduce that $\psi = 0$ a.e., and we get the result by passing to the limit in (5.3.10), W being compactly supported.

4. Let us now verify the identity (5.3.5). Since the potential $(\alpha\sqrt{\xi})$ tends to $+\infty$ when ξ goes to $+\infty$, $E_1^\infty[\alpha\sqrt{\xi}]$ is reached by a positive function $\psi \in S_\infty$:

$$-\psi''(\xi) + (\alpha\sqrt{\xi})\psi = E_1^\infty[\alpha\sqrt{\xi}]\psi.$$

Setting $\xi = \alpha^\beta \zeta$ and $\overline{\psi}(\zeta) = \sqrt{\alpha^\beta}\psi(\alpha^\beta\zeta)$ for an arbitrary constant β, we get

$$-\frac{1}{\alpha^{2\beta}}\overline{\psi}''(\zeta) + \alpha^{1+\frac{\beta}{2}}\sqrt{\zeta}\overline{\psi}(\zeta) = E_1^\infty[\alpha\sqrt{\xi}]\overline{\psi}(\zeta).$$

By choosing β such that $-2\beta = 1 + \frac{\beta}{2}$, so that $\beta = \frac{-2}{5}$, we obtain

$$-\overline{\psi}''(\zeta) + \sqrt{\zeta}\overline{\psi}(\zeta) = \alpha^{\frac{-4}{5}} E_1^\infty[\alpha\sqrt{\xi}]\overline{\psi}(\zeta),$$

which implies that $E_1^\infty[\alpha\sqrt{\xi}] = \alpha^{\frac{4}{5}} E_1^\infty[\sqrt{\xi}]$. The proof of Proposition 5.3.2 is achieved.

5.3.2 Proof of Theorem 5.1.1

In what follows, we will show that (5.1.6) admits a unique solution verifying (5.1.4). Indeed, the functional $J_0(.)$ is obviously continuous and strictly convex on $\dot{H}^1_0(\mathbb{R}^+)$. To prove the existence of a unique $U_0 \in \dot{H}^1_0(\mathbb{R}^+)$ satisfying (5.1.6), it remains to verify that $J_0(.)$ is coercive on $\dot{H}^1_0(\mathbb{R}^+)$. For this let $U \in \dot{H}^1_0(\mathbb{R}^+)$ and write $U(\xi) = \int_0^\xi U'(t)dt$. This implies that $U(\xi) \leq \|U'\|_{L^2}\sqrt{\xi}$, and since $E_1^\infty[.]$ is an increasing function one has $E_1^\infty[U] \leq E_1^\infty[\|U'\|_{L^2}\sqrt{\xi}]$. Applying (5.3.5) with $\alpha = \|U'\|_{L^2}$ we get $E_1^\infty[U] \leq \|U'\|_{L^2}^{\frac{4}{5}} E_1^\infty[\sqrt{\xi}]$, and finally we have

$$J_0(U) \geq \frac{1}{2}\|U'\|_{L^2}^2 - E_1^\infty[\sqrt{\xi}].\|U'\|_{L^2}^{\frac{4}{5}} \xrightarrow[\|U\|_{H^1}\to+\infty]{} +\infty.$$

Let us now prove that U_0 is a solution of the limit problem (5.1.4). Namely, we have to check that $E_1^\infty[U_0]$ is an eigenvalue. To this aim, we first write the Euler–Lagrange equation for U_0 :

$$-U_0'' = \frac{dE_1^\infty}{dU}[U_0] \geq 0. \tag{5.3.11}$$

Therefore, U_0 is a concave function belonging to $\dot{H}^1_0(\mathbb{R}^+)$. It is thus a continuous, increasing, and positive function on $\mathbb{R}^+$, and $\lim_{+\infty} U_0$ exists in $\overline{\mathbb{R}}$. It now remains to check that $E_1^\infty[U_0] < \lim_{+\infty} U_0$, which will ensure that $E_1^\infty[U_0] := E_{1,0}$ is an eigenvalue with unique positive eigenfunction $\psi_{1,0} \in S_\infty$ (see point two of Proposition 5.3.2). We proceed by contradiction and assume that $E_1^\infty[U_0] = \lim_{+\infty} U_0$. Applying the third point of Proposition 5.3.2, one obtains $\frac{dE_1^\infty}{dU}[U_0] = 0$. In view of (5.3.11) and the fact that U_0 is a concave positive function in $\dot{H}^1_0(\mathbb{R}^+)$, we deduce that $U_0 = 0$ and $\min_{U\in\dot{H}^1_0(\mathbb{R}^+)} J_0(U) = 0$. But a simple rescaling argument shows that J_0 takes negative values, and so its minimum is negative. To prove this claim, we fix a potential U in $\dot{H}^1_0(\mathbb{R}^+)$ such that $\int_0^{+\infty} |U'|^2 = 1$, $\lim_{+\infty} U = +\infty$ and let $\psi_1 \in S_\infty$ be the eigenfunction corresponding to $E_1^\infty[U]$. For $\varepsilon > 0$, setting $U^\varepsilon(\xi) = \varepsilon^2 U(\varepsilon\xi)$ and $\psi_1^\varepsilon(\xi) = \sqrt{\varepsilon}\psi_1(\varepsilon\xi)$, we have

$$-\frac{d^2\psi_1^\varepsilon}{d\xi^2} + U^\varepsilon\psi_1^\varepsilon(\xi) = \varepsilon^2 E_1^\infty[U]\psi_1^\varepsilon(\xi),$$

which implies that $E_1^\infty[U^\varepsilon] = \varepsilon^2 E_1^\infty[U]$. After straightforward computations, we finally obtain

$$\begin{aligned} J_0(U^\varepsilon) = \frac{1}{2}\int_0^{+\infty} \left|\frac{dU^\varepsilon}{d\xi}\right|^2 d\xi - E_1^\infty[U^\varepsilon] &= \frac{\varepsilon^5}{2}\int_0^{+\infty} |U'|^2 d\xi - \varepsilon^2 E_1^\infty[U] \\ &= -\varepsilon^2 E_1^\infty[U]\left(1 - \frac{\varepsilon^3}{2E_1^\infty[U]}\right), \end{aligned}$$

which is negative for ε small enough. The proof of Theorem 5.1.1 is complete.

5.4 Convergence analysis

The various models presented in the first section of this work are all well posed. In this section, we shall estimate the difference between their solutions in terms of ε. Namely, we have to prove estimates (5.1.7) and (5.1.8). The following lemma will be useful.

Lemma 5.4.1. *Let $(U_0, E_{1,0}, \psi_{1,0})$ be the solution of the limit problem* (5.1.4)*. There exist $a, b \in \mathbb{R}^+$ independent of ε such that for all ε small we have*

$$\|\psi_{1,0}\|_{L^2(M_\varepsilon,+\infty)} \leq a e^{-bM_\varepsilon} \tag{5.4.1}$$

with $M_\varepsilon = \frac{1}{\varepsilon}$.

Proof. We have $-\psi''_{1,0} + U_0\psi_{1,0} = E_{1,0}\psi_{1,0}$ such that $\psi_{1,0} \geq 0$, $\psi_{1,0}(\xi) \to_{\xi\to+\infty} 0$ ($\psi_{1,0} \in H^1_0(\mathbb{R}^+)$), $E_{1,0} < \lim_{+\infty} U_0$, and U_0 increases to its limit at $+\infty$. Then one can find two nonnegative constants c and δ independent of ε such that for all ε small enough we have

$$-\psi''_{1,0}(\xi) \leq -\delta\psi_{1,0}(\xi) \quad \text{for } \xi \in [M_\varepsilon, +\infty[$$

and $\psi_{1,0}(M_\varepsilon) \leq ce^{-\sqrt{\delta}M_\varepsilon}$. Let $S(\xi) = ce^{-\sqrt{\delta}\xi}$ and $\psi = \psi_{1,0} - S$. Then we have $S'' = \delta S$ and

$$-\psi''(\xi) + \delta\psi(\xi) \leq 0, \qquad \xi \in [M_\varepsilon, +\infty[\tag{5.4.2}$$

with

$$\psi(M_\varepsilon) \leq 0 \quad \text{and} \quad \psi(+\infty) = 0.$$

By the maximum principle, one deduces that $\psi \leq 0$ on $[M_\varepsilon, +\infty[$. Thus

$$\psi_{1,0}(\xi) \leq ce^{-\sqrt{\delta}\xi} \quad \text{on } [M_\varepsilon, +\infty[,$$

which yields estimate (5.4.1). ■

We begin by proving the second estimate (5.1.8) of Theorem 5.1.2. For this we will compare (see Proposition 5.4.3) the potentials U_0 and $\tilde{U}_\varepsilon$ solutions of (5.1.6) and (5.2.7), respectively. This will be done thanks to an idea consisting of the reformulation of the problems (5.1.4) and (5.1.11) as minimization problems whose unknown is the first eigenfunction. This is the subject of the following remark.

Remark 5.4.2. *For $\phi \in S_{M_\varepsilon}$ (see Definition* 5.1.4*), where $M_\varepsilon = \frac{1}{\varepsilon}$, let us set*

$$A_\varepsilon(\phi) = \int_0^{M_\varepsilon} |\phi'(\xi)|^2 d\xi + \frac{1}{2}\int_0^{M_\varepsilon}\int_0^{M_\varepsilon} \phi^2(\xi)\phi^2(\zeta)\min(\xi,\zeta)d\xi d\zeta \tag{5.4.3}$$

and for $\phi \in S_\infty$

$$A_0(\phi) = \int_0^{+\infty} |\phi'(\xi)|^2 d\xi + \frac{1}{2}\int_0^{+\infty}\int_0^{+\infty} \phi^2(\xi)\phi^2(\zeta)\min(\xi,\zeta)d\xi d\zeta. \tag{5.4.4}$$

The functional A_ε satisfies $A_\varepsilon(|\phi|) = A_\varepsilon(\phi)$ and the convexity property

$$A_\varepsilon\left(\sqrt{t\phi_1^2 + (1-t)\phi_2^2}\right) \leq tA_\varepsilon(\phi_1) + (1-t)A_\varepsilon(\phi_2)$$

for $t \in (0,1)$, the inequality being strict if $|\phi_1|$ and $|\phi_2|$ are not proportional (these properties are also satisfied by A_0). The functionals are obvious weakly lower semicontinuous on their domain of definition, in such a way that the minimization problems

$$A_\varepsilon(\phi_\varepsilon) = \min_{\phi \in H_0^1(0,M_\varepsilon),\, \|\phi\|_{L^2}=1} A_\varepsilon(\phi) \tag{5.4.5}$$

and

$$A_0(\phi_0) = \min_{\phi \in H_0^1(\mathbb{R}^+),\, \|\phi\|_{L^2}=1} A_0(\phi) \tag{5.4.6}$$

have unique positive solutions. The problems (5.4.5) *and* (5.4.6) *are equivalent, respectively, to* (5.1.11) *and* (5.1.4)*. Indeed, the functions ϕ_ε and ϕ_0 satisfy*

$$-\phi_\varepsilon'' + U(\phi_\varepsilon)\phi_\varepsilon = \mu_\varepsilon\phi_\varepsilon \quad \text{on } [0, M_\varepsilon],$$

$$-\phi_0'' + U(\phi_0)\phi_0 = \mu_0\phi_0 \quad \text{on } \mathbb{R}^+,$$

where μ_ε (respectively, μ_0) is the Lagrange multiplicator associated with the constraint $\|\phi\|_{L^2} = 1$ and $U(\phi_\varepsilon)$, $U(\phi_0)$ denote, respectively,

$$U(\phi_\varepsilon)(\xi) = \int_0^{M_\varepsilon} |\phi_\varepsilon(\zeta)|^2 \min(\xi,\zeta)d\zeta, \quad U(\phi_0)(\xi) = \int_0^{+\infty} |\phi_0(\zeta)|^2 \min(\xi,\zeta)d\zeta.$$

In addition, since ϕ_ε and ϕ_0 are positive and the function $K(\xi,\zeta) = \min(\xi,\zeta)$ is the kernel corresponding to the Laplacian in dimension one, we have

$$(U(\phi_\varepsilon), \mu_\varepsilon, \phi_\varepsilon) = (\tilde{U}_\varepsilon, \tilde{E}_{1,\varepsilon}, \tilde{\psi}_{1,\varepsilon}) \quad \text{and} \quad (U(\phi_0), \mu_0, \phi_0) = (U_0, E_{1,0}, \psi_{1,0}).$$

Proposition 5.4.3. *The solutions U_0 and $\tilde{U}_\varepsilon$ of* (5.1.6) *and* (5.2.7)*, respectively, verify the following estimate :*

$$\left\| \frac{d}{d\xi}(\tilde{U}_\varepsilon - U_0) \right\|^2_{L^2(0,M_\varepsilon)} = \mathcal{O}(e^{-\frac{c}{\varepsilon}}), \tag{5.4.7}$$

where c is a strictly positive constant independent of ε and $M_\varepsilon = \frac{1}{\varepsilon}$. This yields estimate (5.1.8)*.*

Proof. We start by comparing $A_0(\psi_{1,0})$ and $A_\varepsilon(\tilde{\psi}_{1,\varepsilon})$. Let $\chi_\varepsilon \in \mathcal{D}(0,+\infty)$ be such that $\chi_\varepsilon(\xi) = 1$ on $[0, M_\varepsilon - 1]$, $\chi_\varepsilon(\xi) = 0$ on $[M_\varepsilon, +\infty[$, and $0 \leq \chi_\varepsilon \leq 1$. The function $\chi_\varepsilon.\psi_{1,0}|_{(0,M_\varepsilon)}$ belongs to $H_0^1(0,M_\varepsilon)$, and for ε small we have $\|\chi_\varepsilon.\psi_{1,0}\|_{L^2(0,M_\varepsilon)} \neq 0$. Let $\beta_\varepsilon = \|\chi_\varepsilon.\psi_{1,0}\|_{L^2(0,M_\varepsilon)}$. Then we have $\frac{1}{\beta_\varepsilon}\chi_\varepsilon.\psi_{1,0} \in S_{M_\varepsilon}$ and, with (5.4.1), $\beta_\varepsilon =$

$1+O(e^{-\frac{c}{\varepsilon}})$. Then, in view of Remark 5.4.2, the following inequalities can be straightforwardly justified :

$$A_\varepsilon(\tilde{\psi}_{1,\varepsilon}) \leq A_\varepsilon\left(\frac{1}{\beta_\varepsilon}\chi_\varepsilon.\psi_{1,0}\right) \leq A_\varepsilon(\psi_{1,0}) + \mathcal{O}(e^{-\frac{c}{\varepsilon}}) \leq A_0(\psi_{1,0}) + \mathcal{O}(e^{-\frac{c}{\varepsilon}}),$$

where c is a strictly positive constant independent of ε. Besides, we have

$$A_0(\psi_{1,0}) \leq A_0(\tilde{\psi}_{1,\varepsilon}) = A_\varepsilon(\tilde{\psi}_{1,\varepsilon}).$$

Here and in what follows, we still denote by $\tilde{\psi}_{1,\varepsilon}$ the extension of $\tilde{\psi}_{1,\varepsilon}$ by zero on $[M_\varepsilon, +\infty[$ when it is taken as a function on $\mathbb{R}^+$. Consequently, we have

$$|A_\varepsilon(\tilde{\psi}_{1,\varepsilon}) - A_0(\psi_{1,0})| = A_\varepsilon(\tilde{\psi}_{1,\varepsilon}) - A_0(\psi_{1,0}) = \mathcal{O}(e^{-\frac{c}{\varepsilon}}). \tag{5.4.8}$$

Furthermore, A_0 is uniformly convex on S_∞ and $\psi_{1,0}$ realizes its minimum. Then one can find a constant $c_0 > 0$ independent of ε such that

$$\|\psi_{1,0} - \tilde{\psi}_{1,\varepsilon}\|^2_{H^1(\mathbb{R}^+)} \leq c_0|A_0(\psi_{1,0}) - A_0(\tilde{\psi}_{1,\varepsilon})|.$$

In addition, since $A_0(\tilde{\psi}_{1,\varepsilon}) = A_\varepsilon(\tilde{\psi}_{1,\varepsilon})$ and with (5.4.8), one deduces that

$$\|\psi_{1,0} - \tilde{\psi}_{1,\varepsilon}\|^2_{H^1(\mathbb{R}^+)} = \mathcal{O}(e^{-\frac{c}{\varepsilon}}). \tag{5.4.9}$$

The potential $U_0 - \tilde{U}_\varepsilon$ satisfies

$$-\frac{d^2}{d\xi^2}(U_0 - \tilde{U}_\varepsilon)(\xi) = |\psi_{1,0}(\xi)|^2 - |\tilde{\psi}_{1,\varepsilon}(\xi)|^2 \quad \text{on } [0, M_\varepsilon].$$

Then, multiplying this equation by $U_0 - \tilde{U}_\varepsilon$, one obtains after integration by parts

$$\begin{aligned}\left\|\frac{d}{d\xi}(U_0 - \tilde{U}_\varepsilon)\right\|^2_{L^2(0,M_\varepsilon)} &\leq \frac{dU_0}{d\xi}(M_\varepsilon)(U_0(M_\varepsilon) - \tilde{U}_\varepsilon(M_\varepsilon)) \\ &\quad + \sup_{\xi\in[0,M_\varepsilon]}(|U_0(\xi) - \tilde{U}_\varepsilon(\xi)|)\int_0^{M_\varepsilon}(|\psi_{1,0}|^2 - |\tilde{\psi}_{1,\varepsilon}|^2)d\xi.\end{aligned}$$

Moreover, in view of Remark 5.4.2, we have, for every $\xi \in [0, M_\varepsilon]$,

$$\begin{aligned}(U_0 - \tilde{U}_\varepsilon)(\xi) &= \int_0^{M_\varepsilon}(|\psi_{1,0}|^2 - |\tilde{\psi}_{1,\varepsilon}|^2)(\zeta)\min(\xi,\zeta)d\zeta + \int_{M_\varepsilon}^{+\infty}|\psi_{1,0}|^2\min(\xi,\zeta)d\zeta \\ &\leq M_\varepsilon\left(\int_0^{M_\varepsilon}(|\psi_{1,0}|^2 - |\tilde{\psi}_{1,\varepsilon}|^2)(\zeta)d\zeta + \int_{M_\varepsilon}^{+\infty}|\psi_{1,0}|^2(\zeta)d\zeta\right)\end{aligned}$$

and $\frac{dU_0}{d\xi}(M_\varepsilon) = -\int_{M_\varepsilon}^{+\infty}\frac{d^2U_0}{d\xi^2}(\xi)d\xi = \int_{M_\varepsilon}^{+\infty}|\psi_{1,0}|^2d\xi$. Then

$$\begin{aligned}\left\|\frac{d}{d\xi}(U_0 - \tilde{U}_\varepsilon)\right\|^2_{L^2(0,M_\varepsilon)} &\leq M_\varepsilon\left(\int_0^{M_\varepsilon}(|\psi_{1,0}|^2 - |\tilde{\psi}_{1,\varepsilon}|^2)(\zeta)d\zeta + \int_{M_\varepsilon}^{+\infty}|\psi_{1,0}|^2(\zeta)d\zeta\right)^2 \\ &\leq 2M_\varepsilon\left(\|\psi_{1,0} - \tilde{\psi}_{1,\varepsilon}\|^2_{L^2(0,M_\varepsilon)} + \|\psi_{1,0}\|^4_{L^2(M_\varepsilon,+\infty)}\right),\end{aligned}$$

and with (5.4.9) and (5.4.1) one obtains (5.4.7). Moreover, with the change of variable $\tilde{V}_\varepsilon(.) = \frac{1}{\varepsilon^2}\tilde{U}_\varepsilon(\frac{\cdot}{\varepsilon})$ one deduces that

$$\left\| \frac{d}{d\xi}\left(\tilde{V}_\varepsilon - \frac{1}{\varepsilon^2}\tilde{U}_0\left(\frac{\cdot}{\varepsilon}\right)\right)\right\|^2_{L^2(0,1)} = \frac{1}{\varepsilon^5}\left\|\frac{d}{d\xi}(\tilde{U}_\varepsilon - U_0)\right\|^2_{L^2(0,M_\varepsilon)} = \mathcal{O}(e^{-\frac{c}{\varepsilon}}),$$

and then estimate (5.1.8) holds. ■

Let us now give the following result, which shows the existence of a uniform gap between the first eigenvalue $\tilde{E}_{1,\varepsilon} := E_1[\tilde{U}_\varepsilon]$ and the others $E_p[\tilde{U}_\varepsilon]$.

Lemma 5.4.4. *There exists a constant $G > 0$, independent of ε, such that*

$$E_p[\tilde{U}_\varepsilon] - \tilde{E}_{1,\varepsilon} \geq G \quad \forall p \geq 2. \tag{5.4.10}$$

Proof. Since $(E_p[\tilde{U}_\varepsilon])_{p\geq 1}$ is an increasing sequence, it is sufficient to show (5.4.10) only for $p = 2$. We argue by contradiction and suppose that $|E_2[\tilde{U}_\varepsilon] - \tilde{E}_{1,\varepsilon}| \to 0$ as ε goes to zero. In view of Remark 5.4.2, we have $\tilde{E}_{1,\varepsilon} = A_\varepsilon(\tilde{\psi}_{1,\varepsilon})$ and $E_{1,0} = A_0(\psi_{1,0})$. Then, with (5.4.8), $|\tilde{E}_{1,\varepsilon} - E_{1,0}| = \mathcal{O}(e^{-\frac{c}{\varepsilon}})$. We deduce that $E_2[\tilde{U}_\varepsilon]$ and $\tilde{E}_{1,\varepsilon}$ converge to $E_{1,0}$ when $\varepsilon \to 0$. Then the eigenfunctions $\psi_2[\tilde{U}_\varepsilon]$ and $\tilde{\psi}_{1,\varepsilon}$, corresponding, respectively, to $E_2[\tilde{U}_\varepsilon]$ and $\tilde{E}_{1,\varepsilon}$, prolonged by zero on $[\frac{1}{\varepsilon}, +\infty)$, are bounded in $H^1_0(\mathbb{R}^+)$ with respect to ε. There exists ψ_1 (respectively, ψ_2) $\in H^1_0(\mathbb{R}^+)$ such that $\tilde{\psi}_{1,\varepsilon}$ (respectively, $\psi_2[\tilde{U}_\varepsilon]$) converges weakly in $H^1_{loc}(\mathbb{R}^+)$ to ψ_1 (respectively, ψ_2). By passing to the limit $\varepsilon \to 0^+$ in $\mathcal{D}'(0, +\infty)$, in the equations

$$-\tilde{\psi}''_{1,\varepsilon} + \tilde{U}_\varepsilon\tilde{\psi}_{1,\varepsilon} = \tilde{E}_{1,\varepsilon}\tilde{\psi}_{1,\varepsilon},$$

$$-(\psi_2[\tilde{U}_\varepsilon])'' + \tilde{U}_\varepsilon\psi_2[\tilde{U}_\varepsilon] = E_2[\tilde{U}_\varepsilon]\psi_2[\tilde{U}_\varepsilon]$$

one deduces that ψ_1 and ψ_2 are two eigenfunctions corresponding to $E_{1,0}$. In addition, we have

$$\begin{aligned}
|J_{U_0}(\tilde{\psi}_{1,\varepsilon}) - E_{1,0}| &= \left|\int_0^{+\infty} |\tilde{\psi}'_{1,\varepsilon}|^2 + \int_0^{+\infty} U_0|\tilde{\psi}_{1,\varepsilon}|^2 - E_{1,0}\right| \\
&= \left|\int_0^{M_\varepsilon} |\tilde{\psi}'_{1,\varepsilon}|^2 + \int_0^{M_\varepsilon} \tilde{U}_\varepsilon|\tilde{\psi}_{1,\varepsilon}|^2 - E_{1,0} + \int_0^{+\infty} (U_0 - \tilde{U}_\varepsilon)|\tilde{\psi}_{1,\varepsilon}|^2\right| \\
&\leq |\tilde{E}_{1,\varepsilon} - E_{1,0}| + \sup_{[0,M_\varepsilon]}(|U_0 - \tilde{U}_\varepsilon|) \underset{\varepsilon\to 0}{\longrightarrow} 0.
\end{aligned}$$

Then $(\tilde{\psi}_{1,\varepsilon})$ (and similarly $(\psi_2[\tilde{U}_\varepsilon])$) is a minimizing sequence of "$E_{1,0} = \inf_{\psi\in S_\infty} J_{U_0}(\psi)$." Moreover, since $E_{1,0} < \lim_{+\infty} U_0$ (see the proof of Theorem 5.1.1) and applying Lemma 5.3.4, $(\tilde{\psi}_{1,\varepsilon})$ and $(\psi_2[\tilde{U}_\varepsilon])$ (up to extraction of subsequences) converge strongly in $L^2(\mathbb{R}^+)$. Thus, since $\tilde{\psi}_{1,\varepsilon}$ and $\psi_2[\tilde{U}_\varepsilon]$ are two normalized and orthogonal functions in $L^2(\mathbb{R}^+)$ for any $\varepsilon > 0$, we deduce that their limits when $\varepsilon \to 0$, ψ_1 and ψ_2, which are two eigenfunctions of $E_{1,0}$, are also normalized and orthogonal in $L^2(\mathbb{R}^+)$. This contradicts the fact that $E_{1,0}$ is a simple eigenvalue. ■

Proposition 5.4.5. *The potentials U_ε and $\tilde{U}_\varepsilon$ solutions of* (5.1.10) *and* (5.1.11) *verify that*

$$\|U_\varepsilon - \tilde{U}_\varepsilon\|_{H^1(0,M_\varepsilon)} = \mathcal{O}(e^{-\frac{c}{\varepsilon^2}}), \tag{5.4.11}$$

where c is a strictly positive constant independent of ε. This gives estimate (5.1.7).

Proof. Recall first that U_ε and $\tilde{U}_\varepsilon$ verify, respectively, (5.2.6) and (5.2.7). To prove estimate (5.4.11), it is sufficient to compare the energies $J_\varepsilon(U_\varepsilon)$ and $J_\varepsilon(\tilde{U}_\varepsilon)$ because we have

$$\|U_\varepsilon - \tilde{U}_\varepsilon\|^2_{H^1(0,M_\varepsilon)} \leq c_0 |J_\varepsilon(U_\varepsilon) - J_\varepsilon(\tilde{U}_\varepsilon)|, \tag{5.4.12}$$

where c_0 is independent of ε. A straightforward comparison gives the following inequalities :

$$\tilde{J}_\varepsilon(\tilde{U}_\varepsilon) \leq \tilde{J}_\varepsilon(U_\varepsilon) \leq J_\varepsilon(U_\varepsilon) \leq J_\varepsilon(\tilde{U}_\varepsilon). \tag{5.4.13}$$

Besides, we have $\tilde{U}_\varepsilon \geq 0$, and $E_p[.]$ is an increasing function ; then $E_p[\tilde{U}_\varepsilon] \geq E_p[0] = \varepsilon^2 p^2 \pi^2$. Moreover, since $\tilde{E}_{1,\varepsilon}$ converges to $E_{1,0}$, which is then finite, there exists a constant $c_1 > 0$ independent of ε such that

$$E_p[\tilde{U}_\varepsilon] - \tilde{E}_{1,\varepsilon} \geq \varepsilon^2 p^2 \pi^2 - c_1. \tag{5.4.14}$$

Combining (5.4.10) and (5.4.14), one finds $c_2 > 0$ and $c_3 > 0$ independent of ε such that

$$E_p[\tilde{U}_\varepsilon] - \tilde{E}_{1,\varepsilon} \geq c_2 \varepsilon^2 p^2 \pi^2 + c_3 \quad \forall p \geq 2.$$

This implies that

$$\sum_{p \geq 2} e^{-\frac{E_p[\tilde{U}_\varepsilon] - E_1[\tilde{U}_\varepsilon]}{\varepsilon^2}} = \mathcal{O}(e^{-\frac{c_3}{\varepsilon^2}}),$$

and since

$$J_\varepsilon(\tilde{U}_\varepsilon) = \tilde{J}_\varepsilon(\tilde{U}_\varepsilon) + \varepsilon^2 \log\left(1 + \sum_{p \geq 2} e^{-\frac{E_p[\tilde{U}_\varepsilon] - E_1[\tilde{U}_\varepsilon]}{\varepsilon^2}}\right),$$

we obtain

$$J_\varepsilon(\tilde{U}_\varepsilon) = \tilde{J}_\varepsilon(\tilde{U}_\varepsilon) + \mathcal{O}(\varepsilon^2 e^{-\frac{c_3}{\varepsilon^2}}),$$

which leads to (5.4.11) in view of (5.4.12) and (5.4.13). ■

5.5 Comments

5.5.1 Fermi–Dirac statistics

It is more natural to consider Fermi–Dirac statistics in the high density limit ($\varepsilon \to 0$). Here we give some remarks and elements on the limit in this case. The scaled occupation factor of the pth state with Fermi–Dirac statistics is given by

$$n_p^{FD} = f_{FD}(\mathcal{E}_p - \mathcal{E}_F),$$

where $\mathcal{E}_F$ is the Fermi level and f_{FD} is the Fermi–Dirac distribution

$$f_{FD}(u) = \log(1 + e^{-u}), \tag{5.5.1}$$

The scaled Boltzmann distribution function, however, is given by $f_B(u) = e^{-u}$. The Poisson equation in model (5.1.1) can be written as follows :

$$-\frac{d^2V}{d\xi^2} = \sum_{p=1}^{+\infty} f_{B(FD)}(\mathcal{E}_p - \mathcal{E}_F)|\varphi_p|^2$$

under the following constraint on the Fermi energy :

$$\sum_{p=1}^{+\infty} f_{B(FD)}(\mathcal{E}_p - \mathcal{E}_F) = \frac{1}{\varepsilon^3}. \tag{5.5.2}$$

In the Boltzmann case, one can explicitly solve (5.5.2) with respect to $\mathcal{E}_F$, and we have

$$e^{\mathcal{E}_F} = \frac{1}{\varepsilon^3 \sum_{p=1}^{+\infty} e^{-\mathcal{E}_p}},$$

which yields (5.1.1). The first remark we give in the Fermi–Dirac case is that $e^{\mathcal{E}_F}$ cannot be expressed explicitly in terms of $e^{-\mathcal{E}_p}$. The analysis of the limit can, however, be extended to this case but with technical complications that we have avoided in the Boltzmann statistics case. When applying the change of variables (5.1.2) and $\mathcal{E}_F = \frac{1}{\varepsilon^2}\epsilon_F$ the intermediate problem (5.1.10) becomes in the Fermi–Dirac statistics case

$$\begin{cases} -\dfrac{d^2\psi_p}{d\xi^2} + U\psi_p = E_p\psi_p, \qquad \xi \in \left[0, \dfrac{1}{\varepsilon}\right], \\ \psi_p \in H^1\left(0, \dfrac{1}{\varepsilon}\right), \quad \psi_p(0) = 0, \quad \psi_p\left(\dfrac{1}{\varepsilon}\right) = 0, \quad \displaystyle\int_0^{\frac{1}{\varepsilon}} \psi_p\psi_q = \delta_{pq}, \\ -\dfrac{d^2U}{d\xi^2} = \varepsilon^3 \displaystyle\sum_{p=1}^{+\infty} f_{FD}\left(\dfrac{E_p - \epsilon_F}{\varepsilon^2}\right)|\psi_p|^2, \quad \displaystyle\sum_{p=1}^{+\infty} f_{FD}\left(\dfrac{E_p - \epsilon_F}{\varepsilon^2}\right) = \dfrac{1}{\varepsilon^3}, \\ U(0) = 0, \quad \dfrac{dU}{d\xi}\left(\dfrac{1}{\varepsilon}\right) = 0. \end{cases} \tag{5.5.3}$$

Since f_{FD} is a regular, positive, and decreasing function on $\mathbb{R}$, the Schrödinger–Poisson system in a bounded domain in the Fermi–Dirac case is well posed and can also be expressed as an optimization problem ; see the work of Nier [20] in the unidimensional case and [21] in higher dimensions. More precisely, (5.5.3) is equivalent to

$$J_\varepsilon(U_\varepsilon) = \inf_{U \in H^{1,0}(0, \frac{1}{\varepsilon})} J_\varepsilon(U), \tag{5.5.4}$$

where

$$J_\varepsilon(U) = \frac{1}{2}\int_0^{\frac{1}{\varepsilon}} |U'|^2 - \varepsilon^3 \sum_{p=1}^{+\infty} \left[f_{FD}\left(\frac{E_p[U]-\epsilon_F[U]}{\varepsilon^2}\right)\epsilon_F[U] - \varepsilon^2 \int_{\frac{E_p[U]-\epsilon_F[U]}{\varepsilon^2}}^{+\infty} f_{FD}(u)du \right]. \tag{5.5.5}$$

Replacing $f_{FD}(.)$ by $f_B(u) = e^{-u}$, $J_\varepsilon(.)$ is nothing else but the functional (5.2.8) modulo a constant independent of the variable U. The uniform gap showed in Lemma 5.4.4 remains correct. Then, as in the proof of Proposition 5.4.5, there are two constants $c_1 > 0$ and $c_2 > 0$ such that

$$(E_p - \epsilon_F) - (E_1 - \epsilon_F) \geq c_1 \varepsilon^2 p^2 \pi^2 + c_2 \quad \forall p \geq 2.$$

Since f_{FD} is a decreasing function and $\log(1+u) \sim u$ when $u \to 0^+$, then for all $p \geq 2$

$$\begin{aligned}\log\left(1 + e^{-\frac{E_p-\epsilon_F}{\varepsilon^2}}\right) &\leq \log\left(1 + e^{-\frac{c_2}{\varepsilon^2}} e^{-c_1 p^2\pi^2} e^{-\frac{E_1-\epsilon_F}{\varepsilon^2}}\right) \leq c e^{-\frac{c_2}{\varepsilon^2}} e^{-c_1 p^2\pi^2} e^{-\frac{E_1-\epsilon_F}{\varepsilon^2}} \\ &\leq c e^{-\frac{c_2}{\varepsilon^2}} e^{-c_1 p^2\pi^2} \log\left(1 + e^{-\frac{E_1-\epsilon_F}{\varepsilon^2}}\right),\end{aligned}$$

where $c > 0$ is a general constant independent of ε. This implies that

$$\frac{\sum_{p\geq 2} \log\left(1 + e^{-\frac{E_p-\epsilon_F}{\varepsilon^2}}\right)}{\log\left(1 + e^{-\frac{E_1-\epsilon_F}{\varepsilon^2}}\right)} \leq c \left(\sum_{p\geq 2} e^{-c_1 p^2\pi^2}\right) e^{-\frac{c_2}{\varepsilon^2}}.$$

Thus, a formal analysis shows that, asymptotically when $\varepsilon \to 0$, (5.5.3) is close to a Schrödinger–Poisson system with only the first energy level. However, the rigorous analysis of the limit, $\varepsilon \to 0$, of (5.5.4)–(5.5.5) is more technically complicated than the Boltzmann case for which the functional J_ε has an explicit expression given by (5.2.8).

5.5.2 Boundary conditions and higher dimension

The choice of Neumann boundary condition at $z = 1$ can be justified for modulation doping devices (see [2]) for which $z = 1$ is in the bulk of the semiconductor and the hypothesis of a vanishing electric field is justified. This hypothesis also makes the analysis simple because the boundary layer in the limit $\varepsilon \to 0^+$ is located at $z = 0$. If V satisfies Dirichlet boundary conditions, then another boundary layer takes place at $z = 1$. The analysis can probably be extended to this case, but the first eigenvalue will have asymptotically a multiplicity 2. The multidimensional problem is more complicated, where the location of the electrons in the boundary layer may depend on the geometry of the boundary. Such problems have been noticed for the Schrödinger equation with a magnetic field by [7, 12] and are beyond the scope of our work.

References

[1] T. Ando, A. B. Fowler, and F. Stern, *Electronic properties of two-dimensional electron systems*, Rev. Mod. Phys., 54, 2 (1982), p. 437.

[2] G. Bastard, *Wave mechanics applied to semiconductor heterostructures*, Les éditions de physiques, 1996.

[3] N. Ben Abdallah, *On a multidimensional Schrödinger-Poisson scattering model for semiconductors*, J. Math. Phys., 41.

[4] N. Ben Abdallah, P. Degond, and P. Markowich, *On a One-Dimensional Schrödinger-Poisson Scattering Model*, ZAMP, 48 (1997), pp. 35–55.

[5] N. Ben Abdallah and F. Méhats, *On a Vlasov-Schrödinger-Poisson model*, Comm. Partial Differential Equations, 29 (2004), pp. 173–206.

[6] N. Ben Abdallah, F. Méhats, and O. Pinaud, *Adiabatic approximation of the Schrödinger-Poisson system with a partial confinement*, SIAM J. Math. Anal., 36 (2004/2005), pp. 986–1013.

[7] V. Bonnaillie, *On the fundamental state energy for a Schrödinger operator with magnetic field in domains with corners*, Asymptotic Analysis, 41 (2005), pp. 215–258.

[8] F. Castella, *L^2 solutions to the Schrödinger-Poisson system : existence, uniqueness, and approximation*, Math. Models Methods Appl. Sci, 7 (1997), pp. 1051–1083.

[9] I. Catto, C. Le Bris, and P.-L. Lions, *Mathematical Theory of Thermodynamic Limits Thomas-Fermi Type Models*, Clarendon Press, Oxford, 1998.

[10] T. Cazenave, *Semilinear Schrödinger equations*, Courant Lecture Notes in Mathematics, 10. AMS, Providence RI (2003).

[11] J. Harris, C. T. Foxon, K. Barnham, D. Lacklison, J. Hewett, and C. White, *Two-dimensional electron gas strutures with mobilities in excess of* $3.10^6 cm^2 V^1 S^1$, J. Appl. Phys., 61 (1986), p. 1219.

[12] B. Helffer and A. Mohamed, *Semiclassical analysis for the ground state energy of a Schrödinger operator with magnetic wells*, J. Funct. Anal., 138 (1996), pp. 40–81.

[13] R. Illner, P. Zweifel, and H. Lange, *Global existence, Uniqueness and Asymptotic Behavior of Solutions of the Wigner-Poisson and Schrödinger-Poisson systems*, Math. Methods Appl. Sci, 17 (1994), pp. 349–376.

[14] H.-C. Kaiser and J. Rehberg, *On stationary Schrödinger-Poisson equations modelling an electron gas with reduced dimension*, Math. Meth. Appl. Sci, 20, Issue 15 (1997), pp. 1283–1312.

[15] ——, *About a stationary Schrödinger-Poisson system with Kohn-Sham potential in a bounded two- or three-dimensional domain*, Nonlinear Analysis, 41 (2000), pp. 33–72.

[16] T. Kato, *Perturbation Theory for Linear Operators*, Springer-Verlag, Berlin, Heidelberg, 1966.

[17] P. Lions, *The concentration-compactness principle in the Calculus of Variations. The locally compact case, part 1*, Ann. Inst. Henri Poincaré, analyse non linéaire, 1 (1984), pp. 109–145.

[18] P. A. Markowich, *Boltzmann distributed quantum steady states and their classical limit*, Forum Math, 6 (1994), pp. 1–33.

[19] P. A. Markowich, C. A. Ringhofer, and C. Schmeiser, *Semiconductor equations*, Springer-Verlag, Vienna, 1990.

[20] F. Nier, *A stationary Schrödinger-Poisson System Arising from the modelling of electronic devices*, Forum Math., 2 (1990), pp. 489–510.

[21] ——, *A variational formulation of Schrödinger-Poisson Systems in Dimension* $d \leq 3$, Comm. Partial Differential Equations, 18 (1993), pp. 1125–1147.

[22] ——, *Schrödinger-Poisson Systems in Dimension* $d \leq 3$ *:The Whole-space case*, Proc. Roy. Soc. Edinburgh Sect. A, 123 (1993), pp. 1179–1201.

[23] ——, *The dynamics of some quantum open systems with short-range nonlinearities*, Nonlinearity, 11 (1998), pp. 1127–1172.

[24] O. Pinaud, *Adiabatic approximation of the Schrödinger-Poisson system with a partial confinement : the stationnary case*, J. Math. Phys., 45 (2004), p. 2029.

[25] E. Polizzi, *Modélisation et simulation numériques du transport quantique balistique dans les nanostructures semi-conductrices*, PhD. Thesis, INSA, Toulouse, France, (2001).

[26] E. Polizzi and N. Ben Abdallah, *Self-consistent three dimensional model for quantum ballistic transport in open systems*, Phys. Rev B., 66 (2002), pp. 245301–245309.

[27] ——, *subband decomposition approach for the simulation of quantum electron transport in nanostructures*, J. Comp. Phys., 202 (2005), pp. 150–180.

[28] E. Poschel, J.and Trubowitz, *Inverse spectral theory*, Academic Press, 1987.

[29] M. Reed and B. Simon, *Methods of Modern Mathematical Physics*, Academic Press, New York, San Francisco and London.

[30] B. Vinter, *Subbands and charge control in a two-dimensional electron gas field effect transistor*, Appl. Phys. Lett., 44 (1987), p. 307.

Annexe A

A.1 Concentration-Compactness principle

A.1.1 Proof of Lemma 5.3.4

This appendix is devoted to the proof of Lemma 5.3.4. We will use the concentration-compactness principle. This principle is a general method introduced by Lions [17] to solve various minimizing problems posed on unbounded domains. It is shown that all minimizing sequences are relatively compact if and only if some strict subadditivity inequalities hold. The proof is based upon a lemma called the concentration-compactness lemma. For more details on the principle, we refer the reader to [17]. Let us begin by recalling the concentration-compactness lemma.

Lemma A.1.1 (concentration-compactness lemma)**.** *1. Let $(\rho_n)_{n\geq 1}$ be a sequence in $L^1(\mathbb{R})$ satisfying $\rho_n \geq 0$ in $\mathbb{R}$ and $\int_{\mathbb{R}} \rho_n dx = \lambda$ for a fixed $\lambda > 0$. Then there exists a subsequence $(\rho_{n_k})_{k\geq 1}$ satisfying one of the three following possibilities :*

(i) *(Compactness) : there exists $y_k \in \mathbb{R}$ such that*

$$\forall \varepsilon > 0, \quad \exists R < +\infty, \quad \int_{y_k + B_R} \rho_{n_k}(x)dx \geq \lambda - \varepsilon,$$

where $B_R = \{x \in \mathbb{R};\ |x| \leq R\}$.

(ii) *(Vanishing) :*

$$\lim_{k\to+\infty} \sup_{y\in\mathbb{R}} \int_{y+B_R} \rho_{n_k}(x)dx = 0.$$

(iii) *(Dichotomy) : There exists $\alpha \in]0, \lambda[$ such that for all $\varepsilon > 0$, there exist $k_0 \geq 1$ and $\rho_k^1, \rho_k^2 \in L^1_+(\mathbb{R})$ such that for $k \geq k_0$*

$$\|\rho_{n_k} - (\rho_k^1 + \rho_k^2)\|_{L^1} \leq \varepsilon, \quad \left|\int_{\mathbb{R}} \rho_k^1 dx - \alpha\right| \leq \varepsilon, \quad \left|\int_{\mathbb{R}} \rho_k^2 dx - (\lambda - \alpha)\right| \leq \varepsilon,$$

where ρ_k^1 has compact support and $\mathrm{dist}(\mathrm{supp}(\rho_k^1), \mathrm{supp}(\rho_k^2)) \to_k +\infty$.

2. If $\rho_n = |u_n|^2$ with u_n bounded in $H^1(\mathbb{R})$, there exists a subsequence (ρ_{n_k}) such that either compactness (i)*, vanishing* (ii)*, or dichotomy* (iii) *occurs as follows : there exists $\alpha \in]0, \lambda[$ such that for all $\varepsilon > 0$ there exist $k_0 \geq 1$, u_k^1, u_k^2 bounded in $H^1(\mathbb{R})$ satisfying for $k \geq k_0$*

$$\begin{cases} \|u_{n_k} - (u_k^1 + u_k^2)\|_{L^2} \leq \delta(\varepsilon) \xrightarrow[\varepsilon \to 0]{} 0, \\ \left| \displaystyle\int_{\mathbb{R}} |u_k^1|^2 dx - \alpha \right| \leq \varepsilon, \qquad \left| \displaystyle\int_{\mathbb{R}} |u_k^2|^2 dx - (\lambda - \alpha) \right| \leq \varepsilon, \\ \operatorname{dist}\left(\operatorname{supp}(u_k^1), \operatorname{supp}(u_k^2)\right) \xrightarrow[k \to +\infty]{} +\infty, \\ \liminf\limits_k \displaystyle\int_{\mathbb{R}} \{|\nabla u_{n_k}|^2 - |\nabla u_k^1|^2 - |\nabla u_k^2|^2\} dx \geq 0. \end{cases}$$

First, we need to give some notation. For $V \in \dot{H}_0^1(\mathbb{R}^+)$ and $\varepsilon \in \mathbb{R}^+$, we define

$$I_\varepsilon = \inf \left\{ J_V(\varphi), \quad \varphi \in H_0^1(\mathbb{R}^+), \quad \int_0^{+\infty} \varphi^2 = \varepsilon \right\}, \tag{A.1.1}$$

where $J_V(\varphi) = \int_0^{+\infty} |\varphi'|^2 + \int_0^{+\infty} V\varphi^2$, and

$$I_\varepsilon^\infty = \inf \left\{ J_\infty(\varphi), \quad \varphi \in H_0^1(\mathbb{R}^+), \quad \int_0^{+\infty} \varphi^2 = \varepsilon \right\}, \tag{A.1.2}$$

where $J_\infty(\varphi) = \int_0^{+\infty} |\varphi'|^2 + V^\infty \int_0^{+\infty} \varphi^2$ and $V^\infty = \liminf_{+\infty} V$.

Lemma A.1.2. *Let $V \in \dot{H}_0^1(\mathbb{R}^+)$ such that $E_1^\infty[V] < \liminf_{+\infty} V$. Then the following strict subadditivity inequality holds :*

$$I_\varepsilon < I_\alpha + I_{\varepsilon-\alpha}^\infty \quad \forall\, 0 < \alpha < \varepsilon. \tag{A.1.3}$$

Proof. Take $\varphi \in H_0^1(\mathbb{R}^+)$ such that $\int_0^{+\infty} \varphi^2 = \varepsilon$ and let $\psi = \frac{\sqrt{\alpha}}{\sqrt{\varepsilon}}\varphi$. Then $\psi \in H_0^1(\mathbb{R}^+)$, $\int_0^{+\infty} \psi^2 = \alpha$, and $J_V(\psi) = \frac{\alpha}{\varepsilon} J_V(\varphi)$. This implies that $\varepsilon I_\alpha \leq \alpha I_\varepsilon$ for any arbitrary $\alpha > 0$ and $\varepsilon > 0$. We also deduce that $\varepsilon I_\alpha = \alpha I_\varepsilon$ (and similarly $\varepsilon I_\alpha^\infty = \alpha I_\varepsilon^\infty$) for any $\varepsilon, \alpha > 0$. In particular, if $\alpha = 1$, $\varepsilon I_1 = I_\varepsilon$ (or $\varepsilon I_1^\infty = I_\varepsilon^\infty$) for any $\varepsilon > 0$. Moreover, by definition we have $I_1 = E_1^\infty[V] < V^\infty$. Then, for all $\varphi \in H_0^1(\mathbb{R}^+)$ such that $\int_0^{+\infty} \varphi^2 = 1$, we have $I_1 < \int_0^{+\infty} |\varphi'|^2 + V^\infty$. This implies that $I_1 < I_1^\infty$, and by multiplying by $(\varepsilon - \alpha)$, which is positive if $0 < \alpha < \varepsilon$, one obtains $\varepsilon I_1 - \alpha I_1 < (\varepsilon - \alpha) I_1^\infty$ and inequality (A.1.3) holds. ∎

Proof of Lemma 5.3.4. Applying the concentration-compactness lemma for $(\rho_n)_n$: $\rho_n(x) = |\psi_n(x)|^2$ on $\mathbb{R}^+$ and zero elsewhere, there exists a subsequence $(\rho_{n_k})_k$ satisfying one of the three cases given by Lemma A.1.1. If vanishing (ii) occurs, i.e., if

$$\lim_{k \to +\infty} \sup_{y \in \mathbb{R}} \int_{y + B_R} \rho_{n_k}(x) dx = 0 \quad \forall R \geq 0,$$

which implies that

$$\lim_{k\to+\infty}\sup_{y\in\mathbb{R}^+}\int_y^{y+R}|\psi_{n_k}(x)|^2dx=0\quad\forall R\geq 0,$$

then, for all $\varepsilon>0$ small enough, one can find a sequence $(R_k)_k$ of increasing positive real such that $\int_0^{R_k}|\psi_{n_k}(x)|^2dx\leq\varepsilon$ for all k. We have

$$\begin{aligned}\int_0^{+\infty}|\psi'_{n_k}|^2dx+\int_0^{+\infty}V\psi_{n_k}^2dx &= \int_0^{+\infty}|\psi'_{n_k}|^2dx+\int_0^{R_k}V\psi_{n_k}^2dx+\int_{R_k}^{+\infty}V\psi_{n_k}^2dx\\ &\geq \int_0^{+\infty}|\psi'_{n_k}|^2dx-\|V\|_\infty.\varepsilon+(V^\infty-\varepsilon)\int_{R_k}^{+\infty}\psi_{n_k}^2dx.\end{aligned}$$

This implies that there exists $\delta(\varepsilon)$, tending to zero when $\varepsilon\to 0$, such that

$$J_V(\psi_{n_k})\geq J_\infty(\psi_{n_k})-\delta(\varepsilon)\geq I_1^\infty-\delta(\varepsilon).$$

Now let k go to $+\infty$ and ε to zero. Then we obtain

$$I_1\geq I_1^\infty,$$

which contradicts the strict subadditivity inequality (A.1.3).

Now we assume that $(\rho_{n_k})_k$ verifies the dichotomy case; i.e., there exists $\alpha\in]0,1[$ such that for all $\varepsilon>0$ there exist $k_0\geq 1$, ψ_k^1,ψ_k^2 bounded in $H^1(\mathbb{R}^+)$ satisfying for $k\geq k_0$

$$\begin{cases}\|\psi_{n_k}-(\psi_k^1+\psi_k^2)\|_{L^2}\leq\delta(\varepsilon)\xrightarrow[\varepsilon\to 0]{}0,\\ \left|\displaystyle\int_0^{+\infty}|\psi_k^1(x)|^2dx-\alpha\right|\leq\varepsilon,\qquad\left|\int_0^{+\infty}|\psi_k^2(x)|^2dx-(1-\alpha)\right|\leq\varepsilon,\\ \operatorname{dist}\big(\operatorname{supp}(\psi_k^1),\operatorname{supp}(\psi_k^2)\big)\xrightarrow[k\to+\infty]{}+\infty,\\ \liminf_k\underbrace{\displaystyle\int_{\mathbb{R}^+}\{|\nabla\psi_{n_k}|^2-|\nabla\psi_k^1|^2-|\nabla\psi_k^2|^2\}dx}_{\gamma_k}\geq 0.\end{cases}$$

One can write (see [17])

$$\psi_{n_k}=\psi_k^1+\psi_k^2+\varphi_k,\quad\text{where}\quad\psi_k^1\psi_k^2=\psi_k^1\varphi_k=\psi_k^2\varphi_k=0\quad\text{a.e.},$$

and without loss of generality, we suppose that $\operatorname{supp}(\psi_k^2)\subset[R_k,+\infty[$, where R_k tends to $+\infty$ with k. This implies that

$$\begin{aligned}\int_0^{+\infty}V\psi_{n_k}^2&=\int_0^{+\infty}V|\psi_k^1|^2+\int_0^{+\infty}V|\psi_k^2|^2+\int_0^{+\infty}V|\varphi_k|^2\\ &\geq\int_0^{+\infty}V|\psi_k^1|^2+(V^\infty-\varepsilon)\int_0^{+\infty}|\psi_k^2|^2-\|V\|_\infty.\delta(\varepsilon)\end{aligned}$$

and

$$\int_0^{+\infty} |\psi'_{n_k}|^2 + \int_0^{+\infty} V\psi_{n_k}^2 \geq \int_0^{+\infty} |\psi'_{n_k}|^2 + \int_0^{+\infty} V|\psi_k^1|^2 + V^\infty \int_0^{+\infty} |\psi_k^2|^2 - \delta(\varepsilon).$$

Hence,

$$J_V(\psi_{n_k}) \geq \gamma_k + J_V(\psi_k^1) + J_\infty(\psi_k^2) - \delta(\varepsilon). \tag{A.1.4}$$

Besides, let $\alpha_k = \int_0^{+\infty} |\psi_k^1(x)|^2 dx$, $\beta_k = \int_0^{+\infty} |\psi_k^2(x)|^2 dx$. For all fixed $\varepsilon > 0$, the sequences $(\alpha_k)_k$ and $(\beta_k)_k$ are bounded in $\mathbb{R}^+$. There are subsequences, still denoted by $(\alpha_k)_k$ and $(\beta_k)_k$, which converge in $\mathbb{R}^+$ to α_ε and β_ε, respectively, where α_ε and β_ε belong to $\mathbb{R}^+$ such that

$$|\alpha_\varepsilon - \alpha| \leq \varepsilon \quad \text{and} \quad |\beta_\varepsilon - (1-\alpha)| \leq \varepsilon. \tag{A.1.5}$$

Inequality (A.1.4) yields

$$J_V(\psi_{n_k}) \geq \gamma_k + I_{\alpha_k} + I_{\beta_k}^\infty - \delta(\varepsilon).$$

Taking the $\liminf_k$ of the last inequality and letting ε tend to zero, we obtain in view of (A.1.5) and the fact that $\liminf_k \gamma_k \geq 0$

$$I_1 \geq I_\alpha + I_{1-\alpha}^\infty,$$

which contradicts the strict subadditivity inequality (A.1.3).

Consequently, the sequence $(\rho_{n_k})_k$ verifies the compactness case of the concentration-compactness lemma which yields straightforwardly that the minimizing sequence $(\psi_n)_n$ is relatively compact in $L^2(\mathbb{R}^+)$.

A.2 Pauli Matrices

Definition A.2.1. *The Pauli matrices are the three matrices σ_1, σ_2 and σ_3 defined by*

$$\sigma_1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \sigma_2 = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \quad \sigma_3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}. \tag{A.2.1}$$

These matrices satisfy the following properties

Lemma A.2.2. *1. We have the following equalities*

$$[\sigma_1, \sigma_2] = 2i\sigma_3, \quad [\sigma_2, \sigma_3] = 2i\sigma_1, \quad [\sigma_3, \sigma_1] = 2i\sigma_2 \text{ and } \quad [\sigma_i, \sigma_i] = 0.$$

which is equivalent to ($\vec{\sigma} \times \vec{\sigma} = ([\sigma_2, \sigma_3], [\sigma_3, \sigma_1], [\sigma_1, \sigma_2])$)

$$\vec{\sigma} \times \vec{\sigma} = 2i\vec{\sigma}.$$

In general, one has $[\vec{a} \cdot \vec{\sigma}, \vec{b} \cdot \vec{\sigma}] = 2i(\vec{a} \times \vec{b}) \cdot \vec{\sigma}$.

2. The contracted product of (σ_i) *give*

$$\sigma_i : \overline{\sigma}_j = 2\delta_{ij} \quad \textit{and} \quad (\vec{a}\cdot\vec{\sigma}) : \overline{(\vec{b}\cdot\vec{\sigma})} = 2\vec{a}\cdot\vec{b}.$$

3. $(\vec{a}\cdot\vec{\sigma})(\vec{b}\cdot\vec{\sigma}) = \vec{a}\cdot\vec{b}I + i(\vec{a}\times\vec{b})\cdot\vec{\sigma}.$

Summary. This thesis is decomposed into three parts. The main part is devoted to the study of spin polarized currents in semiconductor materials. An hierarchy of microscopic and macroscopic models are derived and analyzed. These models takes into account the spin relaxation and precession mechanisms acting on the spin dynamics in semiconductors. We have essentially two mechanisms : the spin-orbit coupling and the spin-flip interactions. We begin by presenting a semiclassical analysis (via the Wigner transformation) of the Schrödinger equation with spin-orbit hamiltonian. At kinetic level, the spinor Vlasov (or Boltzmann) equation is an equation of distribution function with 2×2 hermitian positive matrix value. Starting then from the spinor form of the Boltzmann equation with different spin-flip and non spin-flip collision operators and using diffusion asymptotic techniques, different continuum models are derived. We derive drift-diffusion, SHE and Energy-Transport models of two-components or spin-vector types with spin rotation and relaxation effects. Two numerical applications are then presented : the simulation of transistor with spin rotational effect and the study of spin accumulation effect in inhomogenous semiconductor interfaces.

In the second part, the diffusion limit of the linear Boltzmann equation with a strong magnetic field is performed. The Larmor radius is supposed to be much smaller than the mean free path. The limiting equation is shown to be a diffusion equation in the parallel direction while in the orthogonal direction, the guiding center motion is obtained. The diffusion constant in the parallel direction is obtained through the study of a new collision operator obtained by averages of the original one. Moreover, a correction to the guiding center motion is derived.

In the third part of this thesis, we are interested in the description of the confinement potential in two-dimensional electron gases. The stationary one dimensional Schrödinger–Poisson system on a bounded interval is considered in the limit of a small Debye length (or small temperature). Electrons are supposed to be in a mixed state with the Boltzmann statistics. Using various reformulations of the system as convex minimization problems, we show that only the first energy level is asymptotically occupied. The electrostatic potential is shown to converge towards a boundary layer potential with a profile computed by means of a half space Schrödinger–Poisson system.

Key words. *Semiclassical analysis, Wigner transformation, spin-orbit hamiltonian, spinor Boltzmann equation, micro-macro limit, diffusion limit, moment method, entropy minimization, drift-diffusion, SHE, Energy-Transport, two-component models, Spin-FET, finite elements, Gummel iterations, guiding-center approximation, high magnetic field, convex minimization, min-max theorem, concentration-compactness principle, boundary layer.*