Modélisation mathématique du transport diffusif de charges partiellement quantiques.

Nicolas Vauchelet

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Nicolas VAUCHELET

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le 24 novembre 2006 devant le jury composé de

Naoufel BEN ABDALLAH	Directeur de thèse	Université Paul Sabatier, Toulouse
Laurent DESVILLETTES	Rapporteur	ENS Cachan
Florian MEHATS	Directeur de thése	Université Rennes 1
Paola PIETRA	Examinateur	IMATI, Pavia, Italie
Jean-Michel ROQUEJOFFRE	Examinateur	Université Paul Sabatier, Toulouse
Giuseppe TOSCANI	Rapporteur	Université de Pavia, Italie

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Unité Mixte de Recherches CNRS - Université Paul Sabatier Toulouse 3 - INSA Toulouse

UMR 5640

UFR MIG, Université Paul Sabatier Toulouse 3, 118 route de Narbonne, 31062 TOULOUSE cédex, France

Tel: (33) (0)5 61 55 69 22 ; Fax: (33) (0)5 61 55 83 85 ; Mail: umrmip@mip.ups-tlse.fr

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Chapter 1

Introduction générale

Les travaux présentés dans ce mémoire de thèse concernent la modélisation, l'étude mathématique et l'analyse numérique du transport des particules chargées dans des dispositifs nanométriques à base de matériaux semiconducteurs. Depuis une cinquantaine d'année, un effort constant dans la miniaturisation des composants électroniques a été entrepris. Ces dispositifs peuvent être insérés en plus grand nombre dans les circuits intégrés ce qui améliore considérablement les performances des processeurs. Par ailleurs, ces composants deviennent plus fonctionnels, ont des temps de réponses plus courts et une consommation plus faible. De tels motivations justifient l'intérêt croissant pour les nanotechnologies.

Pour des échelles de grandeurs allant jusqu'au micron, une description purement classique du transport des particules chargées reste satisfaisante. A partir des années cinquante, de nombreux modèles mathématiques ont été introduits décrivant le transport des électrons (ou éventuellement des trous) en microélectronique. Ces modèles ne prennent pas du tout en compte les effets quantiques et occultent complétement la mécanique quantique dans leurs approches. Ils se contentent d'une description purement classique du transport des charges qui peut se hiérarchiser en différents modèles selon la précision de description des phénomènes physiques espérée. Au niveau cinétique, le mouvement est décrit par une grandeur statistique, la fonction de distribution $f(t, x, v)$, où $f(t, x, v)dxdv$ correspond au nombre de particules présentes à l'instant t dans un volume $dxdv$ de l'espace des phases autour du point position-vitesse (x, v). L'évolution de cette fonction est régit par des équations cinétiques comme l'équation de Vlasov s'il n'y a pas de collisions et l'équation de Boltzmann dans un cadre collisionnel [17, 21, 38, 61]. Les modèles cinétiques étant encore très coûteux numériquement, il est préférable de se tourner vers des modèles macroscopiques cependant moins précis car s'intéressant à des quantités moyennées en vitesse. Il s'agit alors d'une description fluide du mouvement.

Les modèles macroscopiques sont obtenus à partir d'un modèle cinétique par différents processus adaptés à des situations particulières. Avec une limite hydrodynamique, reposant sur la méthode des moments, on obtient des modèles hydrodynamiques comme les équations d'Euler et de Navier-Stokes [3, 17, 39, 41, 42, 46, 57, 62]. Suivant les changements d'échelles spatiales et temporelles effectués [10], une limite de diffusion permet d'obtenir une hiérarchie de modèles fluides parmi lesquels on trouve les modèles SHE (Spherical Harmonic Expansion) [18, 23], ET (Energy Transport) [11, 12, 25, 29] et de dérive-diffusion

[14, 15, 40, 49, 50, 56]. Ces différents modèles résultent des dominances des mécanismes collisionels. La limite de diffusion consiste à perturber la fonction de distribution solution de l'équation cinétique autour d'un équilibre thermodynamique local par un petit paramètre correspondant au rapport entre le libre parcours moyen des particules et la longueur macroscopique caractéristique. L'obtention rigoureuse de ces modèles fluides à partir des équations cinétiques a fait l'objet d'une intense recherche (en plus des travaux cités ci-dessus on rajoutera [4, 5, 26, 27, 43, 44, 47]) et certaines limites rigoureuses restent encore à établir.

Ces modèles restent valable en micro-électronique. Cependant les besoins grandissants des technologies de la communication et de l'information ont poussé les constructeurs à mettre au point des composants à des échelles nanométriques. Or lorsque la taille des dispositifs atteint des dimensions très petites ($<$100 nm), des phénomènes quantiques apparaissent comme les interférences, le confinement ou encore l'effet tunnel. Il devient alors nécessaire de considérer des modélisations tenant compte de ces phénomènes.

Plusieurs approches ont été entreprises dans le but de revenir à une description quantique du transport de charges. Une première voie consiste à considérer l'équation de Schrödinger (ou de Von Neumann). De nombreux résultats mathématiques sur l'étude de cette équation ont été obtenus ces dernières années (voir par exemple [2, 8, 19, 20, 31, 32]). Une modélisation complétement quantique du transport balistique des charges dans une nanostructure est alors obtenue en couplant cette équation avec l'équation de Poisson [7, 8, 24, 51, 52, 53, 54, 55]. Cependant, un tel modèle présente le gros désavantage de ne pas tenir compte des nombreuses collisions que rencontrent les particules lors du transport et se contente donc d'une description balistique du transport. De plus, il reste très coûteux à réaliser numériquement avec des conditions physiques réalistes.

D'autres stratégies consistant à utiliser les résultats bien connus sur le transport des particules chargées en microélectronique permettent de mettre au point des modèles quantiques prenant en compte les collisions des électrons avec les impuretés du réseau cristallin ou avec les phonons (pseudo-particules représentant les vibrations du réseau). Une approche consiste à incorporer des termes correctifs "quantiques" dans des modèles classiques. Ceci permet d'élaborer des modèles comme le modèle de density-gradient (ou dérive-diffusion quantique) et des modèles de l'hydrodynamique quantique [1, 35, 36, 37, 45]. Ces modèles exploitent une analogie entre l'équation de Schrödinger et le système d'Euler sans pression. En effet, l'amplitude et la phase de la fonction d'onde satisfaisant l'équation de Schrödinger sont solutions du système d'Euler sans pression dans lequel on a ajouté un terme correctif appelé potentiel de Bohm. Les modèles sus-nommés sont alors obtenus en ajoutant phénoménologiquement ce potentiel de Bohm aux modèles classiques correspondants. Ils sont bien établis pour des états purs mais dans des systèmes à plusieurs particules un problème de fermeture apparait. Récemment une stratégie reposant sur la méthode des moments a permis d'établir des modèles hydrodynamiques et de résoudre ce problème de fermeture via la définition d'équilibres locaux quantiques minimisant une entropie sous contraintes [26, 27, 28, 34].

Enfin, toujours dans l'optique d'utiliser les résultats bien maîtrisés sur les modèles classiques, une autre approche est d'utiliser des modèles couplés quantiques-classiques. Ainsi, en remarquant que les effets quantiques interviennent souvent dans des zones bien identifiées des dispositifs nanométriques, une méthode de couplage consiste à découper le domaine d'étude, à décrire chaque zone de ce domaine par un modèle classique ou quantique suivant le phénomène à observer et à coupler spatialement ces modèles par des conditions d'interface [7, 11, 24]. Cette méthode permet de réduire considérablement le coût numérique des simulations.

Dans cette thèse nous nous intéressons à une stratégie de couplage différente : le couplage directionnel. Dans la plupart des dispositifs électroniques à l'échelle nanométrique, les différentes directions d'espace ne jouent pas le même rôle. Le transport des charges s'effectue dans des directions privilégiées alors que le gaz que forment les particules est confiné dans la (ou les) autre(s) direction(s). Ainsi lorsque par exemple le transport des charges se concentre à l'interface entre deux matériaux différents (à l'interface Oxyde-Silicium d'un MOSFET par exemple), les dimensions caractéristiques du confinement deviennent très petites devant celles du transport. On se retrouve alors à étudier le transport de charges dans un gaz d'électrons bidimensionnel. Une modélisation quantique dans la direction transverse au transport est alors couplée à un modèle cinétique ou fluide dans les autres directions dites parallèles au mouvement.

Dans ce travail de thèse, nous nous intéressons à l'analyse mathématique et numérique de modèles couplés classiques-quantiques où le couplage est directionnel comme expliqué ci-dessus. Avant de montrer les résultats obtenus, nous présentons au prochain chapitre les modèles des sous-bandes utilisés et le couplage et rappelons la limite formelle de l'équation de Boltzmann des semiconducteurs vers l'équation de dérive-diffusion. Le mémoire de cette thèse est décomposé en trois grande parties :

- La première partie est consacrée à l'analyse mathématique d'un modèle dérive-diffusion-Schrödinger-Poisson, noté DDSP. Dans ce cas, le régime du transport est fluide et le système est alors décrit dans la direction de transport au moyen de l'équation de dérive-diffusion.

- La seconde partie concerne l'analyse mathématique de la limite diffusive du modèle des sous-bandes cinétique vers le modèle fluide analysé dans la première partie.

- Enfin la troisième partie présente des résultats de simulations numériques du système DDSP étudié dans la première partie, utilisé pour modéliser le transport dans des nanostructures à base de matériaux semiconducteurs.

Nous présentons maintenant le modèle DDSP qui est le thème central de cette étude. Lorsque les électrons sont extrêmement confinés, comme dans des dispositifs nanométriques à semiconducteurs, l'énergie devient partiellement quantifiée en niveau d'énergie. Ces niveaux d'énergie sont décrits par les éléments propres du Hamiltonien partiel dans la direction de confinement et sont usuellement appelés *sous-bandes* dans la littérature physique [6, 22, 30]. Pour fixer les notations, on nomme z **la direction de confinement** et x **la (ou les) directions de transport**. Les particules sont soumises dans le domaine d'étude à un potentiel $V(t,x,z)$ qui dépend de la variable temporelle t et des variables spatiales (x,z).

Dans la direction z, le confinement impose une quantification du système et donc le Hamiltonien partiel $-\frac{1}{2}\partial_z^2 + V$ doit avoir un spectre discret. On supposera ici que ce confinement se réalise par un mur infini en $z = 0$ et $z = 1$. La variable z est par conséquent bornée dans le domaine $(0, 1)$. (On peut aussi supposer que le confinement est du à un potentiel qui tend vers $+\infty$ quand z tend vers $+\infty$.) Les sous-bandes sont alors définies par :

$$\begin{cases} -\frac{1}{2}\,\partial_z^2\chi_k + V\chi_k = \epsilon_k\chi_k & (k \geq 1), \\ \chi_k(t,x,\cdot) \in H_0^1(0,1), & \int_0^1 \chi_k\,\chi_\ell\,dz = \delta_{k\ell}\,. \end{cases} \tag{1.0.1}$$

Dans ce système, t et x sont considérés comme des paramètres. Il s'agit d'un problème de Sturm-Liouville en dimension 1. Par conséquent, les valeurs propres $(\epsilon_k)_{k\geq 1}$ ne se croisent pas et forment une suite strictement croissante tendant vers $+\infty$ et les $(\chi_k)_{k\geq 1}$ réalisent une base orthonormées de $L^2(0, 1)$.

Pour connaître les quantités macroscopiques, il convient d'abord de déterminer le facteur d'occupation de chaque sous-bande $\rho_k(t, x)$. La densité des porteurs de charges sera alors donnée par :

$$N(t,x,z) = \sum_{k\geq 1} \rho_k(t,x)|\chi_k(t,x,z)|^2. \tag{1.0.2}$$

La connaissance de la densité permet alors de déterminer le potentiel électrostatique autoconsistant généré par les électrons eux-mêmes et calculé au moyen de l'équation de Poisson :

$$-\Delta_{x,z}V = N(t,x,z) = \sum_{k\geq 1} \rho_k(t,x)|\chi_k(t,x,z)|^2. \tag{1.0.3}$$

Dans la direction de transport x, les dimensions sont supposées telles qu'une description classique reste satisfaisante. Comme on l'a vu précédemment, on peut alors considérer plusieurs niveaux de description suivant le contexte physique : cinétique ou fluide. Les grandeurs macroscopiques déterminant le transport sont alors obtenues au moyen des équations de Vlasov, si on néglige les collisions, ou de Boltzmann au niveau cinétique et au niveau fluide grâce au système de dérive-diffusion. On se retrouve donc avec un système couplant l'une de ces trois équations avec le modèle des sous-bandes (1.0.1) et l'équation de Poisson (1.0.3).

Dans ce travail de thèse nous nous intéressons au transport dans des structures semi-conductrices pour lesquelles les collisions sont le principal mécanisme responsable du mouvement. Les équations de transport considérées vont donc être les équations de Boltzmann et de dérive-diffusion (le système Vlasov-Schrödinger-Poisson a été étudié en [13]). Nous avons donc analysé deux modèles : le modèle de dérive-diffusion-Schrödinger-Poisson, noté en abrégé DDSP, et le modèle de Boltzmann-Schrödinger-Poisson notamment sa limite de diffusion vers DDSP.

Pour le modèle DDSP, dans la direction de transport x, la densité surfacique notée N_s est calculée grâce à l'équation de dérive-diffusion. Il s'agit d'une équation de conservation pour la densité de particules dans laquelle la densité de courant est la somme de deux termes. L'un, appelé courant de dérive, est proportionnel à la densité de particules et aux forces électrostatiques. L'autre est le courant de diffusion et est proportionnel au gradient de la densité de particules [33, 49, 50]. Cette équation peut être dérivée de la théorie cinétique en effectuant une limite de diffusion, i.e. le libre parcours moyen devient très petit par rapport aux longueurs caractéristiques du système (voir [40, 56]). Elle s'écrit :

$$\partial_t N_s - \text{div}_x(\mathbb{D}(\nabla_x N_s + N_s \nabla_x V_s)) = 0, \tag{1.0.4}$$

où $\mathbb{D}$ est la matrice de diffusion qui contient les informations physiques des collisions. Cette équation est couplée au modèle des sous-bandes (1.0.1) et à l'équation de Poisson (1.0.3). Le couplage s'obtient grâce à la définition du potentiel effectif V_s qui garde la trace du confinement dans la direction transverse et à l'expression de la densité N. En effet, on verra au chapitre suivant que le potentiel effectif s'obtient lors de la limite diffusive et vaut :

$$V_s(t,x) = -\log \sum_{k\geq 1} e^{-\epsilon_k(t,x)}. \tag{1.0.5}$$

Par ailleurs, on a vu en (1.0.2) que la connaissance de la densité nécessitait la détermination du facteur d'occupation ρ_k. Le système étant à l'équilibre thermodynamique, ce facteur est donné par une fonction statistique de l'équillibre. Typiquement, si on dénote ϵ l'énergie, cette fonction est donnée par la distribution de Fermi-Dirac $1/(1+\exp(\frac{\epsilon-\epsilon_F}{k_B T})$ où k_B est la constante de Boltzmann, T la température du réseau et ϵ_F est le niveau de Fermi qui correspond à la séparation entre les états occupés et non-occupés à la température absolue 0 K. Cette statistique peut être approchée dans le cas $\epsilon - \epsilon_F >> k_B T$ par la statistique de Boltzmann : $\exp(\frac{\epsilon-\epsilon_F}{k_B T})$. Dans notre étude on considérera des statistiques de Boltzmann et on supposera pour simplifier l'écriture le système normalisé telle que $k_B T = 1$. La densité des particules s'écrit alors

$$N(t,x,z) = \sum_{k\geq 1} e^{\epsilon_F(t,x)-\epsilon_k(t,x)} |\chi_k(t,x,z)|^2.$$

En intégrant cette expression en z, on obtient une relation entre la densité surfacique et le niveau de Fermi :

$$N_s(t,x) = \int_0^1 N(t,x,z)\,dz = e^{\epsilon_F(t,x)} \sum_{k\geq 1} e^{-\epsilon_k(t,x)}.$$

Ce qui permet de réécrire la densité électronique sous la forme :

$$N(t,x,z) = N_s(t,x) \sum_{k=1}^{+\infty} \frac{e^{-\epsilon_k(t,x)}}{\sum_{\ell\geq 1} e^{-\epsilon_\ell(t,x)}} |\chi_k(t,x,z)|^2. \tag{1.0.6}$$

Le système dérive-diffusion-Schrödinger-Poisson étudié est alors le système d'équations (1.0.4)–(1.0.1)–(1.0.3) couplé grâce aux expressions (1.0.5) et (1.0.6).

La variable de transport x est supposée appartenir à un domaine borné régulier ω de $\mathbb{R}^2$. Le domaine d'étude total sera noté $\Omega = \omega \times (0,1) \subset \mathbb{R}^3$. Pour compléter ce système il faut alors imposer des conditions aux bords que nous considérerons de deux natures :

- des conditions de type Dirichlet :

$$\begin{cases} N_s(t,x) = N_b(x), \quad V(t,x,z) = V_b(x,z), & \text{pour } x \in \partial\omega, \quad z \in (0,1), \\ \partial_z V(t,x,0) = \partial_z V(t,x,1) = 0, & \text{pour } x \in \omega, \end{cases} \tag{1.0.7}$$

  où $\partial\omega$ est la frontière de ω.

- des conditions de type Neumann : dans ce cas la masse est conservée au cours du transport

$$\begin{cases} \partial_\nu N_s(t,x) = 0, \quad \partial_\nu V(t,x,z) = 0, & \text{pour } x \in \partial\omega, \quad z \in (0,1), \\ V(t,x,0) = V(t,x,1) = 0, & \text{pour } x \in \omega, \end{cases} \tag{1.0.8}$$

où $\nu(x)$ est la normale sortante en $x \in \partial\omega$.

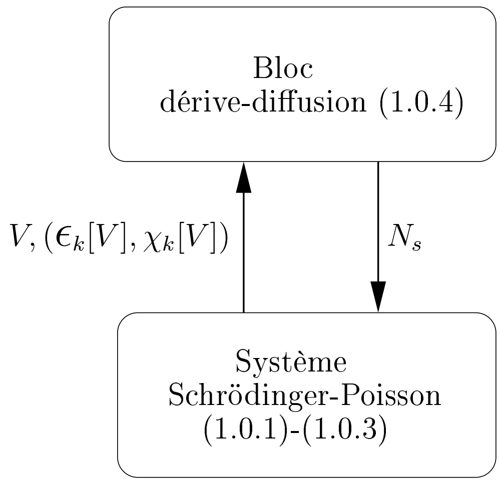

Figure 1.1: **Structure du système DDSP :** un bloc DD et un bloc quasistatique SP.

Par analogie avec le modèle classique dérive-diffusion-Poisson, ce système est structuré en deux blocs : un bloc dérive-diffusion et un bloc Schrödinger-Poisson quasistatique (voir Figure 1.1). Le bloc dérive-diffusion permet le calcul de la densité surfacique N_s en supposant le potentiel électrostatique V connu (et donc V_s aussi est connu grâce à (1.0.5)). Si N_s est déterminé, alors l'étude du bloc Schrödinger-Poisson permet de calculer le potentiel V et les éléments propres de l'Hamiltonien $(\epsilon_k, \chi_k)_{k\geq 1}$ qui seront alors obtenus par diagonalisation de l'Hamiltonien.

La principale difficulté soulevée par l'équation de dérive-diffusion (1.0.4) vient de la dépendance non linéaire du potentiel effectif V_s (1.0.5) de V. En effet, cette dépendance se fait via la définition des éléments propres de l'Hamiltonien. De même l'étude du système Schrödinger-Poisson requiert des estimations précises des éléments propres en fonction du potentiel électrostatique V. De telles estimations sont données en annexe de ce document. Le caractère bien posé de ce système est obtenu grâce à des techniques de minimisation de fonctionnelle développées par Nier [52, 53, 54]. Cependant suivant la donnée entrante du bloc Schrödinger-Poisson (qui est N_s pour DDSP mais qui peut être le facteur d'occupation ρ si le transport est considéré au niveau cinétique) et des estimations dont on dispose sur celle-ci, la fonctionnelle utilisée n'est plus la même et l'étude du système doit être adaptée aux estimations disponible. C'est pourquoi, aux chapitres 4, 5, 6 et 7, l'étude du système Schrödinger-Poisson est reprise à chaque fois dans un cadre différent.

Nous allons dans la suite de cette introduction détailler chacun des chapitres de cette thèse. Ces chapitres sont rédigés sous forme d'articles, le système d'équations considéré étant rappelé en début de chacun, de manière à ce que, pour faciliter la lecture, chacun puisse être lu indépendemment des autres.

Partie I : Existence, unicité et comportement en temps long

Le système classique dérive-diffusion-Poisson revisité *(Chapitre 3)*

Ce chapitre peut être considéré comme un chapitre d'introduction de la première partie. En effet, cette partie est consacrée à l'étude mathématique du modèle DDSP. Cependant au niveau purement classique, le transport des particules chargées dans des dispositifs à semiconducteurs ou à plasmas peut être modélisé par un système couplé dérive-diffusion-Poisson. L'objectif de ce chapitre est donc de présenter dans un cas plus simple les méthodes qui seront utiles par la suite dans le cas du modèle DDSP.

Le système de dérive-diffusion est très utilisé en microélectronique pour modéliser le transport des particules chargées dans des dispositifs à semiconducteurs ou à plasmas [49, 50]. Il s'agit d'une équation de conservation dans laquelle le courant est somme d'un courant de dérive proportionnel à la densité de particules N et aux forces électrostatiques et d'un courant de diffusion proportionnel au gradient de la densité de particules. Dans un domaine $\Omega \subset \mathbb{R}^3$, ce système s'écrit :

$$\partial_t N - \text{div}_x(\mathbb{D}(\nabla N + N\nabla V)) = 0, \qquad t \in \mathbb{R}^+,$$

où $\mathbb{D}$ est une matrice de diffusion qui contient les informations sur les collisions que subissent les particules. Le potentiel électrostatique est autoconsistant et est obtenu par l'équation de Poisson :

$$-\Delta V(t,x) = N(t,x).$$

Depuis Gajewski [33], de nombreux résultats sur l'existence, l'unicité et le comportement en temps long des solutions de ce système ont été établis. Mais généralement ils sont obtenus dans le cas où la matrice de diffusion $\mathbb{D}$ est supposée scalaire et constante. Dans la réalité, cette matrice n'est pas scalaire et est déterminée grâce aux coefficients de l'opérateur de collisions considéré au niveau cinétique. La dépendance de la matrice de diffusion en ces coefficients n'est pas très évidente et on supposera donc dans toute cette partie pour simplifier que $\mathbb{D}$ est connue et suffisamment régulière et que $\mathbb{D} \geq \alpha Id$.

En temps long on s'attend à ce que les solutions (N, V) convergent vers la solution (N_∞, V_∞) du système stationnaire :

$$-\text{div}\,(\mathbb{D}(\nabla N_\infty + N_\infty \nabla V_\infty)) = 0, \qquad -\Delta V_\infty = N_\infty.$$

Pour mener à bien l'étude de l'existence et du comportement en temps long des solutions, il convient de définir un cadre fonctionnel et donc d'avoir des estimations a priori sur les solutions. Une quantité primordiale pour ce genre de système est l'entropie relative définie par :

$$E(t) = \int_\Omega (N \log \frac{N}{N_\infty} + N_\infty - N)\, dx + \frac{1}{2}\int_\Omega |\nabla(V - V_\infty)|^2\, dx.$$

Alors l'estimation permettant d'avoir des bornes sur les quantités considérées est

$$E(t) + \alpha \int_0^t \int_\Omega e^{-V} \frac{|\nabla(Ne^V)|^2}{Ne^V}\, dxd\tau \leq E(0).$$

On voit alors clairement qu'avec des conditions initiales adéquates, on obtient une borne de la densité dans $L \log L$ et du potentiel dans H^1. Cependant, lorque la matrice de densité est supposée égale à l'identité, on obtient par simple multiplication de l'équation de dérive-diffusion par N et par intégration par parties une borne de N dans L^2. En prenant des conditions aux bords telles qu'on puisse utiliser la régularité elliptique de l'équation de Poisson, on obtient alors suffisamment de régularité pour montrer l'existence et l'unicité de solutions par un point fixe [49].

Dans le cas $L \log L$, l'analyse de l'existence requiert plus de travail. En effet, compte tenu du manque de régularité des solutions, il est coutume dans ce genre de problème de régulariser le système par un paramètre $\varepsilon > 0$ tel que formellement le système régularisé se réduit au système non régularisé pour $\varepsilon = 0$ et de prouver l'existence de solutions pour ce système régularisé. La dernière étape consiste alors à utiliser l'estimation d'entropie pour passer à la limite et montrer que les grandeurs macroscopiques convergent quand $\varepsilon \to 0$ vers des solutions de dérive-diffusion-Poisson. Avec cette méthode, on ne peut malheureusement pas établir l'unicité des solutions.

Par ailleurs dans ce chapitre, on s'intéresse aussi au comportement en temps long des solutions. Cette étude repose principalement sur l'entropie. Une technique répendue revient à montrer au moyen d'inégalités de type logarithmique Sobolev la décroissance exponentielle de l'entropie relative vers 0. Ceci permet d'avoir la convergence exponentielle du potentiel dans H^1 et au moyen des inégalités de Csizàr-Kullback de la densité dans L^1. Cependant ce traitement repose fortement sur le fait que la masse est conservée au cours du transport ce qui n'est pas le cas si on ne suppose plus les conditions aux bords conservatives. Nous avons donc envisagé une autre approche consistant à linéariser l'entropie relative. Cette méthode a aussi l'avantage d'obtenir plus de régularité sur les solutions étant donné que la linéarisation apporte une borne de la densité dans L^2 au bout d'un certains temps et non plus dans $L \log L$.

Tous ces résultats sont présentés dans ce chapitre en essayant de montrer les difficultés qu'entrainent la considération d'une matrice de diffusion non scalaire. Les techniques présentées seront utilisées dans les deux chapitres suivants lorsque les électrons sont confinés dans la direction transverse au transport.

Théorie L^2 pour le système DDSP *(Chapitre 4)*

Dans ce chapitre on s'intéresse au transport diffusif d'un gaz d'électrons confiné dans une nanostructure. La direction de confinement est notée $z \in (0, 1)$ tandis que le transport s'effectue dans un domaine borné régulier ω du plan $\mathbb{R}^2$. Dans cette première partie on suppose se trouver dans le régime diffusif donc le transport est déterminé grâce aux grandeurs macroscopiques comme la densité des particules. Le modèle considéré est donc le système DDSP introduit ci-dessus (1.0.4)–(1.0.1)–(1.0.3) complété avec les conditions aux bords de Dirichlet (1.0.7). Pour simplifier l'étude on ne considère que le cas où la matrice de diffusion est l'identité et les conditions aux bords sont choisies telles que l'on puisse utiliser la régularité elliptique du problème de Poisson.

On présente dans ce chapitre deux résultats distincts. Le premier concerne l'existence et l'unicité des solutions, le second leur comportement en temps long. De même que dans le cas dérive-diffusion-Poisson classique, le fait de considérer une matrice de diffusion égale à l'identité simplifie beaucoup l'étude. En effet, on peut obtenir directement par des intégrations par parties des estimations L^2 sur la densité (et donc H^2 sur le potentiel grâce à la régularité elliptique de l'équation de Poisson) et l'existence peut être obtenue grâce à un point fixe. La quantité primordiale permettant l'établissement des résultats est l'entropie relative de (ρ_k, V) par rapport à $(\underline{\rho_k}, \underline{V})$ définie par

$$\begin{aligned} W = & \sum_k \int_\omega (\rho_k \log(\rho_k/\underline{\rho_k}) - \rho_k + \underline{\rho_k})\, dx + \frac{1}{2} \iint_\Omega |\nabla_{x,z}(V - \underline{V})|^2 \, dxdz \\ & + \int_\omega \sum_k u\, e^{-\epsilon_k} \left(\epsilon_k[V] - \epsilon_k[\underline{V}] - \langle |\chi_k|^2 (V - \underline{V}) \rangle \right) dx, \end{aligned}$$

dans laquelle les quantités soulignées sont des prolongements réguliers au domaine d'étude des valeurs aux bords.

Par analogie avec le système dérive-diffusion-Poisson, il est judicieux de voir le système complet comme une équation de dérive-diffusion couplée avec le système Schrödinger-Poisson quasistatique (cf Figure 1.1). Une fois l'estimation d'entropie obtenue, la résolution est basée sur ce diagramme : il apparait donc que trois étapes seront nécessaires pour établir l'existence. La première étape est consacrée à l'étude du bloc dérive-diffusion en supposant le potentiel V (et donc l'énergie effective V_s) connu. La seconde étape s'intéresse au bloc quasistatique Schrödinger-Poisson en supposant la densité surfacique donnée. Enfin, l'existence est prouvée grâce à un point fixe sur la densité surfacique N_s. Une étude minutieuse des propriétés spectrales de l'Hamiltonien est alors nécessaire pour traiter les termes correctifs quantiques intervenant lors des calculs. Ces propriétés sont énoncées et pour certaines d'entre elles démontrées en annexe.

Cette résolution repose essentiellement sur deux points cruciaux : (i) le caractère bien posé du système Schrödinger-Poisson lorsque la densité N_s est donnée, (ii) l'estimation d'entropie permettant de construire une solution globale en temps.

La non-conservation de la masse oblige à considérer le traitement du comportement en temps long par le biais de la linéarisation de l'entropie relative par rapport aux solutions du système stationnaire. En adaptant alors les techniques du cas classique (présentées au chapitre 3), on montre alors la convergence exponentielle en temps long de la densité dans L^2 et du potentiel électrostatique dans H^1.

Théorie $L \log L$ pour DDSP pour un système isolé *(Chapitre 5)*

Le système DDSP considéré dans ce chapitre est le même modèle couplé quantique-classique qu'au chapitre précédent. Le couplage est donc directionnel et les effets quantiques sont transcrits via le modèle des sous-bandes. Les résultats présentés ici concernent l'existence et le comportement en temps long des solutions. Cependant, dans ce chapitre on ne considère plus que la matrice de diffusion soit scalaire et par soucis de complétude, on utilise des conditions aux bords de type Neumann sur la densité (1.0.8) (bien évidemment, en adaptant les démonstrations, les résultats restent valable avec les conditions aux bords du chapitre précédent).

La principale difficulté introduite par une matrice de diffusion distincte de l'identité est la perte de l'estimation dans L^2 de la densité (voir Proposition 4.2.3). Il ne reste alors que l'estimation d'entropie et donc il faut travailler avec une densité uniquement bornée dans $L \log L$ et un potentiel électrostatique dans H^1. Comme on l'a signalé ci-dessus, pour l'analyse de l'existence il convient de considérer le système comme une équation de dérive-diffusion couplé avec le système de Schrödinger-Poisson quasistatique par analogie avec le système de dérive-diffusion couplé avec Poisson.

Les propriétés du système Schrödinger-Poisson quasistatique sont bien connues [13, 52, 53, 54]. Dans ce cas un premier problème apparait par rapport au chapitre précédent : le second membre de l'équation de Poisson (1.0.3) est le produit d'une fonction dans $L \log L$ avec le carré d'une fonction qui ne peut pas être mieux que H^1. Il faut pouvoir donné un sens à ce produit. C'est ce qui est fait grâce aux inégalités de Young et de Trudinger (présentées en annexe) et à une étude précise de la dépendance des éléments spectraux de l'Hamiltonien vis à vis du potentiel. De plus, si on veut espérer obtenir un résultat d'existence au système complet dans ce cadre, il est nécessaire de pouvoir s'assurer de l'existence et de l'unicité d'une solution au système de Schrödinger-Poisson pour un facteur d'occupation donné dans $L \log L$. Il est donc primordial d'étudier minutieusement le système Schrödinger-Poisson quasistatique. Ensuite, l'existence pour le système complet est obtenu comme au chapitre 2 par une méthode de régularisation et de passage à la limite sur les solutions du système régularisé.

Le choix des conditions de Neumann sur la densité permet ici de bénéficier de la conservation de la masse. Par soucis de complétude, on présente ici l'étude du comportement en temps long au moyen des techniques basées sur les inégalités de Sobolev logarithmique.

Partie II : De Boltzmann vers DDSP

Le cas de la dimension 2 *(Chapitre 6)*

Ce chapitre présente deux résultats importants : un résultat d'existence de solutions à un modèle cinétique de sous-bandes et la limite de diffusion rigoureuse de ce modèle vers le modèle DDSP. Malheureusement, des difficultés techniques ne nous permettent pas d'obtenir de résultats d'existence dans le cas où le domaine d'étude total est en trois dimensions : nous considérons donc que le transport ne s'effectue que sur un segment de la droite réelle. Le cas d'un transport en 2D sera discuté au chapitre suivant.

On considère toujours un gaz d'électrons confiné dans une nanostructure où le confinement a lieu dans la direction z transverse au transport suivant x et est décrit par le modèle des sous-bandes. Le régime de transport considéré dans cette partie est le régime cinétique. Lorsque les porteurs de charges subissent des collisions, le transport est bien décrit par l'équation de Boltzmann. Cette équation donne l'évolution de la fonction de distribution $f_k(t,x,v)$ de la $k$ième sous-bande dans l'espace des phases $(x,v) \in (a,b) \times \mathbb{R}$.

On rappelle la signification physique de la fonction de distribution : $f_k(t,x,v)\,dxdv$ correspond au nombre de particules présentent dans la sous-bande k dans un petit volume $dxdv$ de l'espace des phases autour de la position (x,v). Cette fonction satisfait l'équation de Boltzmann :

$$\partial_t f_k(t,x,v) + \{\mathcal{H}_k, f_k\} = Q(f)_k, \qquad k \geq 1,$$

où $\{\cdot,\cdot\}$ est le crochet de Poisson défini par $\{g,h\} = \nabla_x h \cdot \nabla_v g - \nabla_x g \cdot \nabla_v h$. L'énergie du système dans la $k$ième sous-bande noté $\mathcal{H}_k$ est la somme de l'énergie cinétique et de l'énergie potentielle :

$$\mathcal{H}_k(t,x,v) = \frac{1}{2}v^2 + \epsilon_k(t,x),$$

où les ϵ_k sont définis en (1.0.1). L'opérateur de collisions prend en compte les intéractions entre les électrons et les phonons et s'écrit

$$Q(f)_k = \sum_{k'} \int_{\mathbb{R}} \alpha_{k,k'}(v,v')(\mathcal{M}_k(v) f_{k'}(v') - \mathcal{M}_{k'}(v') f_k(v))\,dv',$$

dans lequel la maxwellienne est définie par

$$\mathcal{M}_k(t,x,v) = \frac{1}{\sqrt{2\pi}\sum_k e^{-\epsilon_k(t,x)}}\ \exp(-\mathcal{H}_k(t,x,v)).$$

Le facteur d'occupation ρ_k de la $k$ième sous-bande vaut alors : $\rho_k(t,x) = \int_{\mathbb{R}} f_k(t,x,v)\,dv$. En reprenant l'expression de la densité dans le modèle des sous-bandes (1.0.2), on déduit

$$N(t,x,z) = \sum_{k\geq 1} \int_{\mathbb{R}} f_k(t,x,v) |\chi_k(t,x,z)|^2\,dv.$$

Lorsque les collisions deviennent nombreuses, le mouvement des particules entre dans un régime fluide. Le libre parcours moyen qui représente la distance entre deux collisions successives devient négligeable par rapport aux grandeurs caractéristiques du milieu. Mathématiquement, cela se traduit après un rescaling par l'apparition d'un paramètre η tendant vers 0 dans l'équation de Boltzmann :

$$\partial_t f_k^\eta(t,x,v) + \frac{1}{\eta}\{\mathcal{H}_k^\eta, f_k^\eta\} = \frac{1}{\eta^2} Q^\eta(f^\eta)_k. \tag{1.0.9}$$

Le couplage de cette équation avec le modèle des sous-bandes induit que le système de Schrödinger-Poisson dépend intrinsèquement du petit paramètre η :

$$\begin{cases} -\dfrac{1}{2}\,\partial_z^2 \chi_k^\eta + V^\eta \chi_k^\eta = \epsilon_k^\eta \chi_k^\eta \qquad (k \geq 1), \\ \chi_k^\eta(t,x,\cdot) \in H_0^1(0,1), \qquad \displaystyle\int_0^1 \chi_k^\eta\, \chi_\ell^\eta\,dz = \delta_{k\ell}\,, \end{cases} \tag{1.0.10}$$

$$-\Delta_{x,z} V^\eta = N^\eta(t,x,z) = \sum_{k\geq 1} \int_{\mathbb{R}} f_k^\eta(t,x) |\chi_k^\eta(t,x,z)|^2. \tag{1.0.11}$$

Nous présentons donc dans ce chapitre une étude du système couplé (1.0.9)–(1.0.11) que nous avons choisi de compléter par des conditions de réflexion spéculaire aux bords et en particulier de la convergence quand η tend vers 0 de ce système vers le modèle fluide DDSP analysé aux chapitres 4 et 5 de cette thèse. De même que dans la première partie, cette étude s'appuie sur les techniques utilisées dans le cas classique. La convergence du modèle Boltzmann-Poisson vers le système dérive-diffusion-Poisson a été montrée par Masmoudi et Tayeb [47]. Deux outils sont indispensables : les solutions renormalisées de Di Perna Lions et une estimation d'entropie. L'entropie du système est définie par :

$$W^\eta(t) = \sum_k \iint_{(a,b)\times\mathbb{R}} \left(f_k^\eta \log \frac{f_k^\eta}{M_k} - f_k^\eta + M_k \right) dxdv + \frac{1}{2} \iint_\Omega |\nabla_{x,z} V^\eta|^2 \, dxdz$$

et le taux de dissipation par :

$$\mathcal{R}^\eta(t) = \frac{1}{2} \sum_k \iint_{(a,b)\times\mathbb{R}} \left(\sqrt{f_k^\eta} - \sqrt{N_s^\eta \mathcal{M}_k^\eta} \right)^2 dxdv,$$

où $M_k = K \exp(-\frac{1}{2}(v^2+k^2))$ avec K un facteur de normalisation tel que $\sum_k \int_\mathbb{R} M_k \, dv = 1$. Alors, l'estimation d'entropie s'écrit :

$$0 \leq W^\eta(t) + \frac{\alpha_1}{2\eta^2} \int_0^t \mathcal{R}^\eta(s) \, ds \leq C, \tag{1.0.12}$$

où α_1 et C sont des constantes positives. On remarque qu'il ne s'agit pas d'une entropie relative et donc l'estimation obtenue ne donne qu'une borne sur la fonction de distribution et sur le potentiel. L'utilisation des solutions renormalisées apparaît donc naturellement compte tenu du peu de régularité que nous avons. Ainsi dans l'équation de Boltzmann le terme des forces électrostatiques n'est pas mieux que L^2 et donc son produit avec f_k^η qui est dans $L \log L$ n'a de sens que dans un concept de solutions renormalisées.

L'estimation d'entropie permet alors le passage à la limite faible sur des solutions renormalisées judicieuses de l'équation de Boltzmann en utilisant le théorème de Dunford-Pettis et les lemmes de moyenne. Formellement, il apparaît clairement avec (1.0.9) que la limite de la fonction de distribution f_k^η doit appartenir au noyau de l'opérateur de collision qui est engendré par les maxwelliennes. Et le taux de dissipation mesure la distance entre les fonctions de distribution et leurs équilibres. De plus, il est important d'établir clairement la dépendance du potentiel (et donc des éléments propres de l'Hamiltonien) vis à vis des facteurs d'occupation $(\rho_k)_{k\geq 1}$. Tous ces outils permettent alors de déterminer la limite des solutions renormalisées (f_k^η, V^η) du système (1.0.9)–(1.0.11).

Dans leur article [13], les auteurs ont démontré l'existence de solutions au système Vlasov-Schrödinger-Poisson uniquement sous l'hypothèse supplémentaire de données initiales petites. Sans cette hypothèse, l'unicité des solutions du système Schrödinger-Poisson n'est plus assurée. Par conséquent, l'existence des solutions au système Boltzmann-Schrödinger-Poisson (1.0.9)–(1.0.10)–(1.0.11) n'est établie que dans le cas où les données initiales sont supposées petites. Tout d'abord, on effectue une troncature et une régularisation. La régularisation a lieu sur le système de Schrödinger-Poisson pour avoir des estimations meilleures que H^1 sur le potentiel. La troncature de l'opérateur de collision permet d'obtenir une borne L^∞ de la fonction de distribution et l'existence au système régularisé par une méthode de point fixe comme en [13]. Il suffit alors de faire tendre les paramètres de régularisation vers 0 en utilisant des techniques similaires à la limite de diffusion. Malheureusement, dans le cas où le transport s'effectue dans un domaine borné du plan, les techniques employées n'assurent plus l'unicité des solutions au système de Schrödinger-Poisson et donc l'existence des solutions du système couplé ne peut pas être démontrée.

Le cas de la dimension 3 *(Chapitre 7)*

Comme on l'a précisé ci-dessus, l'existence des solutions au système (1.0.9)–(1.0.11) n'a pas pu être établie dans le cas où le transport s'effectue dans un domaine du plan $\mathbb{R}^2$. Cependant si on admet avoir construit une solution renormalisée comme cela a été effectué dans le chapitre précédent, il est possible de prouver la limite de diffusion du système (1.0.9)–(1.0.11) vers le modèle DDSP. En effet, cela revient à considérer que le paramètre de régularisation est η et on se rapproche donc des solutions, dont on suppose qu'elles existent, du système de dérive-diffusion-Schrödinger-Poisson. La démonstration de cette limite de diffusion fait l'objet de ce chapitre.

Les grandes idées de la démonstration sont similaires à celles du cas du transport monodimensionnel. Cependant, comme les injections de Sobolev donnent des estimations plus faibles, il convient d'utiliser pleinement toutes les informations fournies par l'estimation d'entropie (1.0.12). De la même manière qu'au chapitre 5, l'emploi judicieux des inégalités de Trudinger et de Young permet de mettre en dualité l'espace $L \log L$ avec le carré de fonctions dans H^1, ce qui utile compte tenu de la forme du membre de droite de l'équation de Poisson (1.0.11). Et les propriétés des éléments propres ont dues être perfectionnées (voir en annexe).

Partie III : Simulations numériques

Simulation d'un transistor double grille avec le modèle DDSP *(Chapitre 8)*

L'application la plus en vue des modélisations effectuées est leur utilisation à des fins numériques pour obtenir des simulations du transport dans des nanostructures. Le dispositif considéré ici est un nanotransistor de type MOSFET (Metal Oxid Semiconductor Field Effect Transistor) à deux grilles sur lesquelles un potentiel peut être appliqué. Les transistors à effet de champs sont composés d'un corps conducteur, appelé canal, connecté à deux électrodes. En appliquant aux électrodes un potentiel drain-source V_{DS}, un courant drain-source est établi.

Le MOSFET est un dispositif unipolaire, i.e. le courant est transporté par seulement un type de porteurs (les électrons). Le transistor est constitué d'un substrat semiconducteur (silicium Si) à l'intérieur duquel deux régions fortement dopées sont introduites (la source et le drain). Les grilles sont isolées de la région active par une couche d'oxyde SiO_2. Une représentation schématique du dispositif est présentée Figure 1.2.

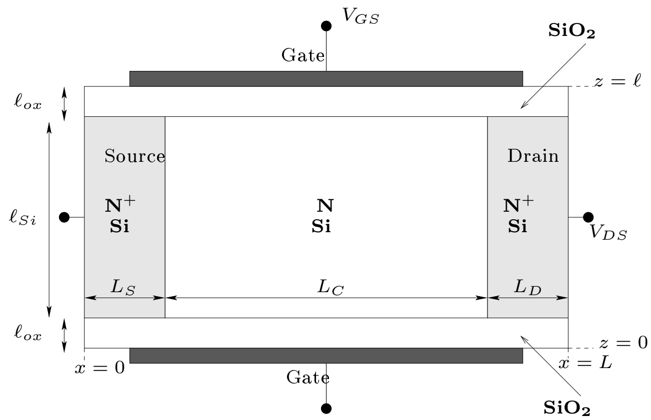

Figure 1.2: Représentation schématique du MOSFET à double grilles simulé numériquement. Le transport des électrons s'effectue dans le canal, la région active entre la source et le drain.

Une particularité du MOSFET est que le gaz d'électrons est confiné dans la direction z de telle manière que la dimension de l'espace de propagation est réduite. Des simulations numériques grâce à des modèles de type Schrödinger-Poisson ont été obtenues pour de tels dispositifs [51, 55]. Cependant les algorithmes, même accélérés, restent d'un coût numérique assez élevé. Dans ce chapitre nous utilisons le modèle couplé DDSP présenté dans la première partie de cette thèse pour la simulation numérique d'un Double-Gate MOSFET. On utilise une discrétisation par éléments finies et une itération de Gummel. Le modèle des sous-bandes présente l'avantage de réduire considérablement le coût de la simulation de l'équation de Schrödinger. En effet, il suffit juste dans ce cas de diagonaliser l'Hamiltonien sur chaque tranche verticale du maillage. Les résultats sont présentés dans le cas stationnaire.

Couplage de DDSP avec un modèle complétement quantique *(Chapitre 9)*

Ce dernier chapitre présente une modélisation hybride quantique classique du transport dans le nanotransistor présenté ci-dessus. La principale équation rendant compte des effets quantiques est l'équation de Schrödinger. Vu que ces effets sont principalement localisés dans le canal, il peut être judicieux de simuler cette zone par un modèle de type Schrödinger-Poisson et d'utiliser le modèle des sous-bandes DDSP pour la modélisation de la source et du drain. Il s'agit alors d'un couplage spatial. Une attention particulière est donc portée sur les conditions d'interface. Une représentation schématique du dispositif est donné Figure 1.3.

Le modèle utilisé dans la zone classique est celui simulé au chapitre précédent. Le modèle quantique est présenté en [51]. Il s'agit d'un modèle des sous-bandes pour le système de Schrödinger-Poisson. La fonction d'onde ψ solution de l'équation de Schrödinger peut alors se décomposer sur la base orthonormale formée par les vecteurs propres de

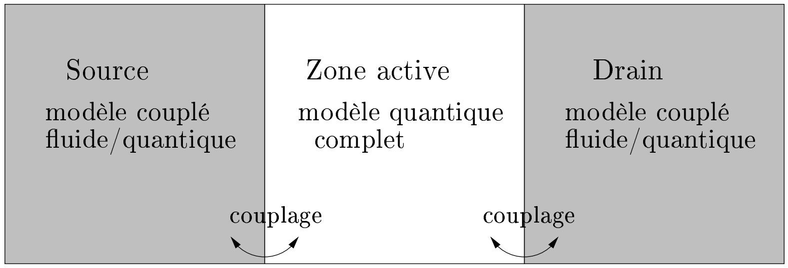

Figure 1.3: Représentation schématique des différentes zones de description du dispositif.

l'opérateur de Schrödinger $(\chi_k)_{k\geq 1}$ dans la direction z :

$$\psi(x,z) = \sum_{k\geq 1} \phi_k(x)\chi_k(x,z).$$

Le problème se trouve donc réduit aux équations satisfaites par les ϕ_k, fonctions ne dépendant que de x, solutions d'équations de Schrödinger projetées sur la direction de transport x. Cette méthode permet de réduire la dimensionnalité et donc le coût numérique de la simulation. De plus l'approximation WKB, qui consiste à chercher des solutions de l'équation de Schrödinger sous la forme $\phi(x) = \alpha(x)e^{\mathbf{i}S(x)/h}$, permet d'accélerer davantage l'algorithme de résolution. Le lecteur intéressé pourra se réferer à l'article cité pour un exposé détaillé de l'approximation WKB.

Une stratégie du couplage entre la zone quantique et la zone classique a été présentée en [7, 24]. Dans [7], l'auteur s'est intéressé au couplage entre l'équation de Boltzmann et l'équation de Schrödinger. En utilisant ces résultats, l'article [24] présente un couplage entre l'équation de dérive-diffusion et l'équation de Schrödinger. Nous nous proposons d'étendre ces résultats au modèle avec les sous-bandes. Aux interfaces, les électrons sont soit transmis, soit réfléchis sur une autre sous-bande. La zone active doit alors être connectée à la source et au drain par des conditions ouvertes aux bords qui tiennent compte de ces réflections et transmissions. Les conditions d'interface doivent alors rendre compte de la continuité du courant entre les deux zones.

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Chapter 2

Les modèles de sous-bandes, du microscopique au macroscopique

2.1 The modeling

In this chapter, we use the subband decomposition method to model the transport of a quasi bidimensional electron gas confined in a nanostructure. The main interest of such a modeling is to obtain numerical simulations of the transport of particles in nanostructures. It plays an important role in the determination of the limit size of the nanoscale MOSFETs as well as the design of new devices. In these ultimate size devices, electrons might be extremely confined in a direction. This direction will be referred to as the confinement direction and denoted by z. To simplify we assume that the confinement is realized by a infinite barrier at $z = 0$ and $z = 1$, which implies that the partial Hamiltonian in the z direction admits an infinite sequence of eigenvalues. The transport direction is denoted by x.

In a full quantum system, the ballistic transport is well modeled by a Schrödinger equation which can be coupled to a Poisson equation if we want to take into account the electrostatics interactions. A derivation of subband models from the linear Schrödinger equation was introduced in [3]. In this article, the potential V is assumed to be given and the x variable is assumed to be semiclassical. By introducing the parameter ε which represents the quotient between the characteristics length in the z and the x directions and after a rescaling, the transport is modeled by the following Schrödinger equation :

$$\mathbf{i}\varepsilon\partial_t\psi^\varepsilon = -\frac{\varepsilon^2}{2}\Delta_x\psi^\varepsilon - \frac{1}{2}\partial_z^2\psi^\varepsilon + V\psi^\varepsilon. \tag{2.1.1}$$

An important condition to allow a separation of the confinement and of the transport direction is that the time does not play the same role in the x and in the z directions. In fact the quantum effects are quasistatics with respect to time. If we take formally the limit $\varepsilon = 0$ in the above equation, we are naturally induced to consider the eigenspaces of the partial Hamiltonian in the z direction, usually called *subbands* in the physic literature

[1, 5, 6] :

$$\begin{cases} -\dfrac{1}{2}\,\partial_z^2\chi_k + V\chi_k = \epsilon_k\chi_k & (k \geq 1), \\ \chi_k(t,x,\cdot) \in H_0^1(0,1), & \displaystyle\int_0^1 \chi_k\,\chi_\ell\,dz = \delta_{k\ell}\,. \end{cases}$$

The eigenvectors $(\chi_k)_{k\geq 1}$ form a orthonormal basis of $L^2(0,1)$. We can decompose ψ^ε on this basis by writing $\psi^\varepsilon = \sum_k \phi_k^\varepsilon \chi_k$. The function ϕ_k^ε is then solution of a set of equations on the index k :

$$\mathbf{i}\varepsilon\partial_t\phi_k^\varepsilon = -\frac{\varepsilon^2}{2}\Delta_x\phi_k^\varepsilon + \epsilon_k\phi_k^\varepsilon + \sum_\ell r_{k,\ell}^\varepsilon.$$

These equations are coupled thanks to the remainders $r_{k\ell}^\varepsilon$. Using the Wigner transform [11] in the semiclassical variable x, Ben Abdallah and Méhats have proved in [3] that the Schrödinger equation (2.1.1) converges to the Vlasov-Schrödinger system :

$$\partial_t f_k + v\cdot\nabla_x f_k - \nabla_x\epsilon_k\cdot\nabla_v f_k = 0, \tag{2.1.2}$$

$$\begin{cases} -\dfrac{1}{2}\,\partial_z^2\chi_k + V\chi_k = \epsilon_k\chi_k & (k \geq 1), \\ \chi_k(t,x,\cdot) \in H_0^1(0,1), & \displaystyle\int_0^1 \chi_k\,\chi_\ell\,dz = \delta_{k\ell}\,. \end{cases} \tag{2.1.3}$$

We recover the decoupling at the limit of the transport equations on each subband. In fact the Wigner transform is a density matrix whose non diagonal terms vanish when taking the semiclassical limit $\varepsilon \to 0$.

The transport on each subband is governed by the force field $-\nabla_x\epsilon_k$. The density is obtained thanks to the identity :

$$N(t,x,z) = \sum_{k\geq 1}\left(\int_{\mathbb{R}^2} f_k(t,x,v)\,dv\right)|\chi_k(t,x,z)|^2.$$

We can take into account the electrostatic interactions by assuming that this system is coupled to the Poisson equation $-\Delta_{x,z}V = N$. Therefore we obtain the Vlasov-Schrödinger-Poisson system. (The rigorous semiclassical limit of the 3D Schrödinger-Poisson system to the Vlasov-Schrödinger-Poisson system is a work in progress). This system has been analyzed in [2]. The authors have shown that this system is well posed when the occupation factors of the kth subband for $k \geq 2$ are small enough and for boundary conditions which allow to use the elliptic regularity on the Poisson equation.

Thus we have constructed a coupled quantum-classical model for the ballistic transport of an electron gas confined in a nanostructure. The confinement is traduced thanks to the subband decomposition method. However, in semiconductors, collisions are very important and drive the carriers towards a diffusive regime. Getting inspiration from what we know for a classical motion, we can take into account collisions by heuristically introducing a collision operator in the transport equation and thus replacing the Vlasov equation by the Boltzmann equation for the semiconductors :

$$\partial_t f_k + v\cdot\nabla_x f_k - \nabla_x\epsilon_k\cdot\nabla_v f_k = Q(f)_k, \tag{2.1.4}$$

The collision operator Q can have different forms depending on statistics that we are looking at : Boltzmann or Fermi-Dirac. These forms are presented in the next section. Therefore a model for the transport at the kinetic regime can be the Boltzmann equation (2.1.4) coupled to the subband model (2.1.3) and the Poisson equation. In this approach, electrons are like point particles in the transport direction while they behave like waves in the transversal direction.

In the following of this chapter, we present the fomal diffusive limit of the Boltzmann equation (2.1.4) towards the drift-diffusion equation. For the sake of simplicity, we consider that the energy level ϵ_k are given. The formal derivation is presented for both Boltzmann and Fermi-Dirac statistics. For Boltzmann statistics, we obtain at the limit the drift-diffusion equation (1.0.4) presented in the introduction with the identity (1.0.5) for the effective potential. We refer to [9, 8] for a rigorous proof of this limit for a classical motion. An idea of a rigorous proof based on a Hilbert expansion is given in section 2.5. Moreover, we explain the changes when the semiconductor presents an anisotropy and different effective mass with respect to the directions.

2.2 Formal diffusive limit : Introduction

Let $\eta > 0$ be the scaled mean free path assumed to be small. We consider the Boltzmann equation for the subband model defined on the phase space $\mathbb{R}^2 \times \mathbb{R}^2$. The position x belongs to $\mathbb{R}^2$, the motion quantity $p \in \mathbb{R}^2$ and the time variable t is nonnegative. We consider that the temperature of the lattice T_L is normalized such that $k_B T_L = 1$, where k_B is the Boltzmann constant. Then, the distribution function of the electrons in each subband f_k^η satisfies :

$$\partial_t f_k^\eta + \frac{1}{\eta}\{\mathcal{H}_k, f_k^\eta\} = \frac{1}{\eta^2} Q(f^\eta)_k,$$

where $\{\cdot,\cdot\}$ is the Poisson bracket: $\{g,h\} = \nabla_x h \cdot \nabla_p g - \nabla_p h \cdot \nabla_x g$. Moreover $\mathcal{H}_k$ is the energy of the system in the kth subband

$$\mathcal{H}_k(t,x,p) = \frac{1}{2}\frac{p^2}{m} + \epsilon_k(t,x).$$

ϵ_k is the potential energy of the kth subband. m is the mass of the charge carriers. More explicitly, we can rewrite the Boltzmann equation :

$$\partial_t f_k^\eta + \frac{1}{\eta}\left(\frac{p}{m} \cdot \nabla_x f_k^\eta - \nabla_x \epsilon_k \cdot \nabla_p f_k^\eta\right) = \frac{1}{\eta^2} Q(f^\eta)_k, \quad (x,p) \in \mathbb{R}^2 \times \mathbb{R}^2. \tag{2.2.5}$$

Q is the collision operator. We consider two forms for this operator : for Boltzmann statistics and for Fermi-Dirac statistics. Q_B, the collision operator for Boltzmann statistics in the linear BGK approximation, reads in the following form:

$$Q_B(f)_k = \sum_{k'} \int_{\mathbb{R}^2} \alpha_{k,k'}(p,p')(\mathcal{M}_k(p) f_{k'}(p') - \mathcal{M}_{k'}(p') f_k(p))\, dp', \tag{2.2.6}$$

where the function $\mathcal{M}_k$ is the normalized Maxwellian

$$\mathcal{M}_k(t,x,p) = \frac{1}{2\pi\mathcal{Z}} e^{-\mathcal{H}_k(t,x,p)} \tag{2.2.7}$$

and where the repartition function $\mathcal{Z}$ is given by

$$\mathcal{Z}(t,x) = \sum_{k=1}^{+\infty} e^{-\epsilon_k(t,x)}.$$

For the Fermi-Dirac case the collision operator is given by :

$$Q_{FD}(f)_k = \sum_{k'} \int_{\mathbb{R}^2} \alpha_{k,k'}(p,p')(\mathcal{M}_k(p) f_{k'}(p')(1-f_k(p)) - \mathcal{M}_{k'}(p') f_k(p)(1-f_{k'}(p')))\, dp'.$$

Assumption 2.2.1 *The cross-section α is assumed to be symmetric and bounded from above and below :*

$$\exists\, \alpha_1, \alpha_2 > 0,\; 0 < \alpha_1 \le \alpha_{k,k'}(p,p') \le \alpha_2, \forall\, k,k' \ge 1,\; \forall\, p \in \mathbb{R}^2,\; \forall\, p' \in \mathbb{R}^2. \tag{2.2.8}$$

The initial and the boundary conditions are assumed to be given by :

$$f^\eta(0,x,p) = f^{in}(x,p) \ge 0. \tag{2.2.9}$$

For the sake of simplicity, we consider the transport on the whole space $\mathbb{R}^2$ with infinite boundary conditions.

Assumption 2.2.2 *We assume that ϵ_k is given for all $k \ge 1$ in $L^\infty((0,T), H^1(\mathbb{R}^2))$ and that $\partial_t \epsilon_k \in L^\infty((0,T)\times\mathbb{R}^2)$, that is*

$$\exists\, \mu > 0 \text{ such that } \forall\, (t,x) \in (0,T)\times\mathbb{R}^2,\; |\partial_t \epsilon_k| \le \mu. \tag{2.2.10}$$

Moreover, we suppose that $(\epsilon_k)_{k\ge1}$ is a nondecreasing sequence of positive functions satisfying

$$\exists\, C_0 > 0,\; \forall\, (t,x) \in (0,T)\times\mathbb{R}^2,\; \forall\, k \ge 1,\; |\epsilon_k(t,x) - \frac{1}{2}\pi^2 k^2| \le C_0,$$

such that we can give a sense to $\mathcal{Z}$ (4.1.2).

Remark 2.2.3 *Assumptions 2.2.2 are not really strong. In fact if ϵ_k is given by the subband model i.e. it is the kth eigenvalue of the stationary Schrödinger operator for an electrostatic potential V. Then all these estimates hold true with constants μ and C_0 depending on V (cf Appendix). It remains to obtain some regularity on the potential V, which is the main difficulty.*

2.3 Formal derivation for the Boltzmann case.

In this chapter, we only consider a simplified approach of the diffusive limit : we assume that the eigenenergies of the subband are given and satisfy Assumption 2.2.2. It is equivalent to consider that there is no coupling between the transport direction and the quantum confinement in the transverse direction. A rigorous study of this limit for the whole system is the subject of chapter 6 and 7.

2.3.1 Properties of the collision operator

Here we establish some well-known properties of the collision operator Q_B defined by (2.2.6). For this section, the time variable t and the position x are only parameters. For the clarity, we omit to write the dependency in t and x and only consider the dependency in p. To this aim, we define the weighted-space

$$L^2_{\mathcal{M}} = \{f = (f_k)_{k\geq 1} \text{ such that } \sum_k \int_{\mathbb{R}^2} \frac{f_k^2}{\mathcal{M}_k}\, dp < \infty\},$$

which is an Hilbert space with the scalar product

$$\langle f, g\rangle_{\mathcal{M}} = \sum_k \int_{\mathbb{R}^2} \frac{f_k g_k}{\mathcal{M}_k}\, dp.$$

Proposition 2.3.1 *We assume the cross-section* α *satisfy* (2.2.8). *Then the following properties hold for* Q_B *:*

(i) $\sum_k \int Q_B(f)_k\, dp = 0$.

(ii) Q_B *is a linear, selfadjoint and negative bounded operator on* $L^2_{\mathcal{M}}$.

(iii) Ker $Q_B = \{f \in L^2_{\mathcal{M}},$ *such that* $\exists\, N_s \in \mathbb{R}, f_k = N_s \mathcal{M}_k\}$.

(iv) If $\mathcal{P}$ *is the orthogonal projection on Ker* Q_B *with the scalar product* $\langle\cdot,\cdot\rangle_{\mathcal{M}}$*, then*

$$-\langle Q_B(f), f\rangle_{\mathcal{M}} \geq \alpha_1 \|f - \mathcal{P}(f)\|^2_{\mathcal{M}}. \tag{2.3.11}$$

Proof. (i) is obvious. For the sake of simplicity we will use the standard notation $f' = f(p')$. For (ii), we have:

$$\langle Q_B(f), g\rangle_{\mathcal{M}} = \sum_{k,k'} \int \alpha \mathcal{M}_k(p)\mathcal{M}_{k'}(p') \left(\frac{f_{k'}(p')}{\mathcal{M}_{k'}(p')} - \frac{f_k(p)}{\mathcal{M}_k(p)}\right) \frac{g_k(p)}{\mathcal{M}_k(p)}\, dpdp'.$$

With our assumption (2.2.8) and the fact that $(\sum \int |f_k|\, dp)^2 \leq \|f\|^2_{\mathcal{M}}$ we get

$$|\langle Q_B(f), g\rangle_{\mathcal{M}}| \leq C\|f\|_{\mathcal{M}}\|g\|_{\mathcal{M}},$$

for all f, g in $L^2_{\mathcal{M}}$. Thus Q_B is bounded. Moreover,

$$\langle Q_B(f), g\rangle_{\mathcal{M}} = -\frac{1}{2}\sum_{k,k'} \int \alpha_{k,k'} \mathcal{M}_k \mathcal{M}'_{k'} \left(\frac{f'_{k'}}{\mathcal{M}'_{k'}} - \frac{f_k}{\mathcal{M}_k}\right)\left(\frac{g'_{k'}}{\mathcal{M}'_{k'}} - \frac{g_k}{\mathcal{M}_k}\right) dpdp'.$$

This provides the selfadjointness and negativity of Q.

The inclusion $\supseteq$ in (iii) is obvious. If $f \in Ker\, Q_B$ then $\langle Q_B(f), f\rangle_{\mathcal{M}} = 0$. The previous identity implies $f_k = N_s \mathcal{M}_k$. Thus (iii) holds true.

$$(Ker Q_B)^{\perp} = \{f \in L^2_{\mathcal{M}} \text{ such that } \sum_k \int f_k\, dp = 0\} \tag{2.3.12}$$

We have,

$$\begin{aligned}\langle Q_B(f), f\rangle_{\mathcal{M}} &= \langle Q_B(f) - Q_B(\mathcal{P}(f)), f\rangle_{\mathcal{M}} = \langle f - \mathcal{P}(f), Q_B(f)\rangle_{\mathcal{M}} \\ &= \langle g, Q_B(g)\rangle_{\mathcal{M}},\end{aligned}$$

where we take $g = f - \mathcal{P}(f)$. Therefore,

$$-\langle Q_B(f), f\rangle_{\mathcal{M}} = \frac{1}{2}\sum_{k,k'}\int \alpha_{k,k'}\mathcal{M}_k\mathcal{M}'_{k'}\left(\frac{g'_{k'}}{\mathcal{M}'_{k'}} - \frac{g_k}{\mathcal{M}_k}\right)^2 dpdp'.$$

With (2.2.8) and since $g \in (Ker\, Q)^\perp$, we obtain

$$-\langle Q_B(f), f\rangle_{\mathcal{M}} \geq \alpha_1 \sum_k \left(\int_{\mathbb{R}}^2 \frac{g_k^2}{\mathcal{M}_k}\, dp\right) = \alpha_1\|f - \mathcal{P}(f)\|^2_{\mathcal{M}}.$$

□

Lemma 2.3.2 *$Im\, Q_B$ is a closed subset of $L^2_{\mathcal{M}}$.*

Proof. Let $(h_n)_{n\in\mathbb{N}} \in Im\, Q_B$ converging towards h in $L^2_{\mathcal{M}}$. $h_n = Q_B(f_n) = Q_B(g_n)$ where $g_n = f_n - P(f_n)$. From (2.3.11), we have :

$$\alpha_1\|g_n - g_m\|^2_{\mathcal{M}} \leq \|h_n - h_m\|_{\mathcal{M}}\|g_n - g_m\|_{\mathcal{M}}.$$

This provides that (g_n) is a Cauchy sequence in $L^2_{\mathcal{M}}$. Thus there exists $g \in L^2_{\mathcal{M}}$ such that $g_n \longrightarrow g$. By continuity of Q_B and uniqueness of the limit, $h = Q_B(g)$. □

Corollary 2.3.3 *Since Q_B is selfadjoint, we have $(Ker\, Q_B)^\perp = Im\, Q_B$.
Thus $Q_B(f) = h$ admits a solution in $L^2_{\mathcal{M}}$ iff $h \in (Ker\, Q_B)^\perp$. Moreover this solution is unique if we impose $f \in (Ker\, Q_B)^\perp$.*

Proposition 2.3.4 *There exists $\Theta \in (L^2_{\mathcal{M}})^2$ such that for all $k \geq 1$,*

$$Q_B(\Theta)_k = -\frac{p}{m}\mathcal{M}_k \quad and \quad \sum_k \int_{\mathbb{R}^2} \Theta_k\, dp = 0. \tag{2.3.13}$$

We define the diffusion matrix by

$$\mathbb{D} = \int \sum_k \Theta_k \otimes \frac{p}{m}\, dp. \tag{2.3.14}$$

Then $\mathbb{D}$ is a symmetric coercive matrix.

Proof. It is an easy consequence of Corollary 2.3.3. It remains to prove the symmetry and the coercivity of $\mathbb{D}$.

$$\mathbb{D}_{i,j} = \frac{1}{m}\int p_i \left(\sum_k \Theta_k\right)_j dp = -\sum_k \int \frac{(\Theta_k)_j Q_B(\Theta_k)_i}{\mathcal{M}_k}\, dp = -\langle \Theta_j, Q_B(\Theta_i)\rangle_{\mathcal{M}}.$$

The selfadjointness of Q_B provides that $\mathbb{D}$ is symmetric. Let $X \in \mathbb{R}^2$, we set $f_X = X_1\Theta_1 + X_2\Theta_2$,

$$\langle \mathbb{D}X, X\rangle_{\mathcal{M}} = \sum_{1\le i,j\le 2} \mathbb{D}_{i,j}X_iX_j = -\langle Q_B(f_X), f_X\rangle_{\mathcal{M}}.$$

Since $\Theta \in (Ker\, Q_B)^{\perp}$, we have $f_X \in (Ker\, Q_B)^{\perp}$. Using (2.3.11), we get :

$$\langle \mathbb{D}X, X\rangle_{\mathcal{M}} \ge \alpha_1 \|f_X\|^2_{\mathcal{M}}.$$

We conclude by showing that $X \mapsto \|f_X\|_{\mathcal{M}}$ is a norm on $\mathbb{R}^2$. But, by linearity of Q_B,

$$\sum_{i=1}^{2} X_i\Theta_i = 0 \Rightarrow \sum_{i=1}^{2} X_i Q_B(\Theta_i)_k = 0, \forall\, k \ge 1.$$

This implies that $\sum_i X_i p_i \mathcal{M}_k = 0$, $\forall\, k \ge 1$. Thus $X = 0$. □

Remark 2.3.5 PARTICULAR CASE WHEN α IS A CONSTANT

If we assume that for all k, k', p, p', $\alpha(k,p,k',p') = 1/\tau$ where τ is a relaxation time which can depend on some parameters like the time t and the position x. Then,

$$\mathbb{D} = \sum_k \int_{\mathbb{R}^2} \tau \mathcal{M}_k \frac{p}{m} \otimes \frac{p}{m}\, dp = \frac{\tau}{m^2} Id. \tag{2.3.15}$$

2.3.2 Asymptotic expansion for the diffusive limit

We will consider in this section the formal diffusive limit as $\eta \to 0$ of the Boltzmann equation (2.2.5). We will use an Hilbert expansion. First, let us recall an existence result for our problem which is a direct corollary of well-known existence results on the Boltzmann equation (see for instance [4], [7]).

Theorem 2.3.6 *For fixed $\eta > 0$, under Assumptions 2.2.1 and 2.2.2, the problem* (2.2.5)–(2.2.9) *admits a unique weak solution $f^\eta \in L^\infty_{loc}(\mathbb{R}^+, \ell^1(L^1(\mathbb{R}^2 \times \mathbb{R}^2)))$ and $f^\eta \ge 0$.*

Proposition 2.3.7 *Under Assumptions 2.2.8, if the solution f^η in Theorem 2.3.6 admits an Hilbert expansion with respect to η, $f^\eta = f^0 + \eta f^1 + \dots$. Then $f^0 = N_s\mathcal{M}$ and N_s is the solution of the drift-diffusion equation*

$$\partial_t N_s - \mathrm{div}_{\,x}(\mathbb{D}(\nabla_x N_s + N_s \nabla_x V_s)) = 0, \tag{2.3.16}$$

where the diffusion matrix $\mathbb{D}$ is defined in (2.3.14) *and with the initial condition defined by $N_s^{in} = \sum_k \int_{\mathbb{R}^2} f_k^{in}(x,p)\, dp$.*

Proof. Formally, we have:

$$Q_B(f^0)_k + \eta Q_B(f^1)_k + O(\eta^2) = \eta\left(\frac{p}{m}\cdot \nabla_x f_k^0 - \nabla_x \epsilon_k \cdot \nabla_p f_k^0\right) + O(\eta^2).$$

Therefore we get $f^0 \in Ker\, Q_B$. Thus, from 2.3.1 :

$$f_k^0 = N_s \mathcal{M}_k \ , \forall k \geq 1. \tag{2.3.17}$$

And f^1 exists iff

$$\frac{p}{m} \cdot \nabla_x f_k^0 - \nabla_x \epsilon_k \cdot \nabla_p f_k^0 \in (Ker\, Q_B)^\perp.$$

However,

$$\frac{p}{m} \cdot \nabla_x f_k^0 - \nabla_x \epsilon_k \cdot \nabla_p f_k^0 = \mathcal{M}_k \frac{p}{m} \cdot (\nabla_x N_s + N_s \nabla_x V_s),$$

where we denote $V_s = -\log(\sum_k e^{-\epsilon_k})$. We have obviously $\int p \mathcal{M}_k \, dp = 0$. We chose $\Theta \in L^2_M$ as in (2.3.13). Thus,

$$f^1 = -\Theta \cdot (\nabla_x N_s + N_s \nabla_x V_s). \tag{2.3.18}$$

We integrate (2.2.5) with respect to p and sum over k. Since $\int \nabla_p f_k^\eta \, dp = 0$,

$$\partial_t \int \sum_k f_k^\eta \, dp + \frac{1}{\eta} \int \sum_k \frac{p}{m} \cdot \nabla_x f_k^\eta \, dp = 0.$$

Moreover the second term can be written

$$\begin{aligned} \frac{1}{\eta} \int \frac{p}{m} \cdot \nabla_x f_k^\eta \, dp &= \frac{1}{\eta} \int \frac{p}{m} \cdot \nabla_x (N_s \mathcal{M}_k) \, dp + \int \frac{p}{m} \cdot \nabla_x f_k^1 \, dp + O(\eta) \\ &= -\text{div}_x \int (\Theta_k \otimes \frac{p}{m})(\nabla_x N_s + N_s \nabla_x V_s) \, dp + O(\eta), \end{aligned}$$

thanks to (2.3.18). We use the operator $\mathbb{D}$ defined in (2.3.14). By assuming that we can pass to the limit, we find the *drift-diffusion* equation :

$$\partial_t N_s - \text{div}_x (\mathbb{D} \cdot (\nabla_x N_s + N_s \nabla_x V_s)) = 0.$$

And we have $N_s = \sum_k \int f_k^0 \, dp$. Therefore we recover the initial condition $N_s(0, x) = N_s^{in} = \sum_k \int f_k^{in} \, dp$. □

2.4 The 3 valleys case

Our physical devices of interest are very small double-gate-MOSFETs of silicon structure. Due to anisotropic effects in silicon [10], the effective mass are not the same in each direction (x, y, z) : we note m_t^* the transverse effective mass and m_ℓ^* the longitudinal one. Also three different electrons configurations appear in the bandstructure : (m_t^*, m_t^*, m_ℓ^*), (m_t^*, m_ℓ^*, m_t^*) and (m_ℓ^*, m_t^*, m_t^*). In the following, we will consider the general configuration (m_x^*, m_y^*, m_z^*), where m_x^* (respectively m_y^* and m_z^*) corresponds to the effective mass in the x direction (respectively y and z direction).

The distribution function of the kth subband and the ith valley f_k^i $(i = 1, 2, 3)$ satisfies the following Boltzmann equation :

$$\eta \partial_t f_k^{i,\eta} + \frac{p_x}{m_x^*} \partial_x f_k^{i,\eta} + \frac{p_y}{m_y} \partial_y f_k^{i,\eta} - \partial_x \epsilon_k^i \partial_{p_x} f_k^{i,\eta} - \partial_y \epsilon_k^i \partial_{p_y} f_k^{i,\eta} = \frac{1}{\eta} Q_B(f^\eta)_k^i, \qquad (2.4.19)$$

with

$$Q_B(f)_k^i = \sum_{k',i'} \int_{\mathbb{R}^2} \alpha_{k,k'}^{i,i'}(v, v')(f_{k'}^{i'}(p')\mathcal{M}_k^i(p) - f_k^i(p)\mathcal{M}_{k'}^{i'}(p'))\, dp'.$$

This collision operator takes into account collisions between particles of the same valley and particles from other valleys. Of course, all the properties stated in Proposition 2.3.1 still hold. The function repartition is defined by

$$\mathcal{Z} = \sum_{k,i} \int e^{-(\frac{p_x^2}{2m_x^*} + \frac{p_y^2}{2m_y^*} + \epsilon_k^i)}\, dp. \qquad (2.4.20)$$

And the Maxwellian is now defined by

$$\mathcal{M}_k^i(p) = \frac{\exp\left(-(\frac{p_x^2}{2m_x^*} + \frac{p_y^2}{2m_y^*} + \epsilon_k^i)\right)}{\mathcal{Z}}. \qquad (2.4.21)$$

Proposition 2.4.1 *Let $f^\eta \in L^\infty([0,T], L^2_{\mathcal{M}})$ be a solution of the Boltzmann equation for the three valleys (2.4.19) coupled with the subband problem. Then, formally, as $\eta \to 0$ the solution f^η converges towards $N_s \mathcal{M}_k$, where N_s is the solution of a drift-diffusion equation coupled with the Schödinger-Poisson system :*

$$\partial_t N_s + \text{div}\, (\mathbb{D}(\nabla N_s + N_s \nabla V_s)) = 0,$$

$$-\frac{1}{2}\frac{d}{dz}\left(\frac{1}{m_t^*}\frac{d}{dz}\chi_k^t\right) + V\chi_k^t = \epsilon_k^t \chi_k^t, \qquad \chi_k^t \in H_0^1(0,1), \int_0^1 \chi_k^t \chi_{k'}^t\, dz = \delta_{kk'},$$

$$-\frac{1}{2}\frac{d}{dz}\left(\frac{1}{m_\ell^*}\frac{d}{dz}\chi_k^\ell\right) + V\chi_k^\ell = \epsilon_k^\ell \chi_k^\ell, \qquad \chi_k^\ell \in H_0^1(0,1), \int_0^1 \chi_k^\ell \chi_{k'}^\ell\, dz = \delta_{kk'},$$

$$-\Delta V = N = \frac{N_s}{\mathcal{Z}} \sum_k \left(e^{-\epsilon_k^\ell} |\chi_k^\ell|^2 + 2\sqrt{\frac{m_\ell^*}{m_t^*}} e^{-\epsilon_k^t} |\chi_k^t|^2 \right),$$

where

$$V_s = -\log \mathcal{Z}\ ; \qquad \mathcal{Z} = 2\pi m_t^* \left(\sum_k e^{-\epsilon_k^\ell} + 2\sqrt{\frac{m_\ell^*}{m_t^*}} \sum_k e^{-\epsilon_k^t} \right);$$

and $\mathbb{D}$ is a symmetric coercive matrix which will be determined in the proof.

Proof. As before, we assume that f^η admits a Hilbert development of the form : $f^\eta = f^0 + \eta f^1 + ...$ Then, by identifying the terms with respect to the power of η, we have

$$Q_B(f^0)_k^i = 0 \qquad \Longrightarrow \qquad f_k^{0,i} = N_s \mathcal{M}_k^i,$$

and

$$Q_B(f^1)^i_k = \frac{p_x}{m_x}\partial_x(N_s\mathcal{M}^i_k) + \frac{p_y}{m_y}\partial_y(N_s\mathcal{M}^i_k) - \partial_x\epsilon^i_k\partial_{p_x}f^i_k - \partial_y\epsilon^i_k\partial_{p_y}f^i_k.$$

We can prove as we have done in Proposition 2.3.1 and Corollary 2.3.3 that there exists a function $\Theta^i \in L^2_{\mathcal{M}^i}$ such that $Q(\Theta_x)^i_k = \frac{p_x}{m_x}\mathcal{M}^i_k$ and $Q(\Theta_y)^i_k = \frac{p_y}{m_y}\mathcal{M}^i_k$. Therefore,

$$f_{1,i} = (\nabla_{x,y}N_s + N_s\nabla_{x,y}(-\log\mathcal{Z}))\Theta^i_k.$$

We define the diffusion matrix (symmetric and coercive) by

$$\mathbb{D} = \sum_{k,i}\iint \Theta^i_k \otimes \frac{p}{m}\,dp,$$

where $\frac{p}{m} = (\frac{p_x}{m_x^*}, \frac{p_y}{m_y^*})$. Integrating equation (2.4.19) and passing to the limit $\eta \to 0$, we get :

$$\partial_t N_s + \text{div}_{\,x,y}(\mathbb{D}(\nabla_{x,y}N_s + N_s\nabla_{x,y}(-\log\mathcal{Z}))) = 0,$$

and

$$\mathcal{Z} = \sum_{k,i}\iint e^{-\frac{p^2}{2m}}\,dp e^{-\epsilon^i_k} = 2\pi\sum_{k,i}\sqrt{m_x^*m_y^*}e^{-\epsilon^i_k}.$$

Since we have three configurations possible for the silicon (m_t^*, m_t^*, m_ℓ^*), (m_t^*, m_ℓ^*, m_t^*) and (m_ℓ^*, m_t^*, m_t^*), we have

$$\mathcal{Z} = 2\pi(m_t^*\sum_k e^{-\epsilon^1_k} + \sqrt{m_t^*m_\ell^*}\sum_k e^{-\epsilon^2_k} + \sqrt{m_t^*m_\ell^*}\sum_k e^{-\epsilon^3_k}).$$

The eigenenergies ϵ^i_k of the kth subband and the ith valley are the eigenvalues of the Hamiltonian in the z direction. Thus, these quantities only depends on the effective mass in the z direction :

$$-\frac{1}{2}\frac{d}{dz}\left(\frac{1}{m_z^*}\frac{d}{dz}\chi^i_k\right) + V\chi^i_k = \epsilon^i_k\chi^i_k.$$

And the electrostatic potential is given by the Poisson equation

$$-\Delta V = N = \sum_{k,i}\int N_s\mathcal{M}^i_k(p)|\chi^i_k|^2\,dp,$$

where N is the density of charge carriers for the whole system. We have two configurations in which $m_z^* = m_t^*$, thus the eigensystem is $(\epsilon^t_k, \chi^t_k)_{k\geq 1}$. And there is one configuration where $m_z^* = m_\ell^*$, the eigensystem is then $(\epsilon^\ell_k, \chi^\ell_k)_{k\geq 1}$. Thus we have,

$$\mathcal{Z} = 2\pi m_t^*\left(\sum_k e^{-\epsilon^\ell_k} + 2\sqrt{\frac{m_\ell^*}{m_t^*}}\sum_k e^{-\epsilon^t_k}\right).$$

And the density satisfy

$$N = \frac{N_s}{\mathcal{Z}}\sum_k\left(e^{-\epsilon^\ell_k}|\chi^\ell_k|^2 + 2\sqrt{\frac{m_\ell^*}{m_t^*}}e^{-\epsilon^t_k}|\chi^t_k|^2\right).$$

□

2.5 A convergence proof of the derivation

In this section we will briefly give an idea of a rigorous proof of the diffusive limit of the Boltzmann equation (2.2.5) towards the drift-diffusion equation (2.3.16). The main result is the following theorem :

Theorem 2.5.1 *Let $T > 0$. We assume that Assumptions 2.2.1 and 2.2.2 hold. Let $(f_k^\eta)_{k\geq 1}$ be a solution of the Boltzmann equation (2.2.5)–(2.2.9). Then N_s^η defined by $N_s^\eta := \sum_k \int f_k^\eta \, dp$ converges weakly towards $N_s \in L^2([0,T]\times\mathbb{R}^2)$ solution of the drift-diffusion equation :*

$$\partial_t N_s - \operatorname{div}_x(\mathbb{D}\cdot(\nabla_x N_s + N_s \nabla_x V_s)) = 0,$$

where $V_s = -\log(\sum_k e^{-\epsilon_k})$, with the initial data $N_s^{in}(x) = \sum_k \int f_k^{in}(x,p)\, dp$

For the proof of this result, we first need to define the function $M_k = \dfrac{1}{2\pi} e^{-\frac{p^2}{2m}-\epsilon_k}$ which is such that

$$\frac{p}{m}\cdot\nabla_x M_k - \nabla_x \epsilon_k \cdot \nabla_p M_k = 0.$$

The key point is to obtain uniform estimates with respect to η. To this aim, we will use assumption (2.2.10). Let us first define a functional framework.

Definition 2.5.2 *Let $T > 0$, we consider the Banach spaces $X = L^\infty([0,T], L^2_{M(t)})$, and $Y = L^2([0,T], L^2_{M^{-1}(t)})$*

Lemma 2.5.3 *Assume $f_0 \in \ell^1(L^1_{x,p}) \cap L^2_{\mathcal{M}(t=0)}$. Then the unique solution f^η of the Boltzmann equation (2.2.5) in $L^\infty([0,T], \ell^1(L^1_{x,p}))$ is in X.*

Moreover, f^η is bounded in X independently of η.

Proof. If we assume that all the functions are regular enough to justify all calculations, we can multiply (2.2.5) by $f_k^\eta/\mathcal{M}_k$, and integrate, we get,

$$\frac{d}{dt}\sum_k \iint \frac{(f_k^\eta)^2}{2M_k}\, dxdp - \sum_k \iint \partial_t \epsilon_k \frac{(f_k^\eta)^2}{2M_k}\, dxdp = \frac{1}{\eta^2}\sum_p \iint Q_B(f_k^\eta)\frac{f_k^\eta}{M_k}\, dxdp. \quad (2.5.22)$$

From assumption (2.2.10), there exists $\mu \geq 0$ such that $\forall\, t \in [0,T]$, $\forall\, x \in \mathbb{R}^2$, $|\partial_t \epsilon_k| \leq \mu$. We define the quantities :

$$X^\eta(t) = \sum_k \iint \frac{(f_k^\eta)^2}{2\mathcal{M}_k}\, dxdp \quad \text{and} \quad S^\eta(t) = -\sum_k \iint Q_B(f_k^\eta)\frac{f_k^\eta}{\eta^2 \mathcal{M}_k}\, dxdp. \quad (2.5.23)$$

S^η is the term of entropy production. Since Q_B is negative, $\forall t \in [0,T]$, $S^\eta(t) \geq 0$. From (2.5.22),

$$\frac{dX^\eta}{dt} - \mu X^\eta \leq -S^\eta. \quad (2.5.24)$$

To justify all calculations, we regularized the problem and consider f_R a solution of the regularized, truncated problem, $f_R \in \mathcal{D}([0,T]\times\mathbb{R}^2\times\mathbb{R}^2)$. Thus f_R satisfies (2.5.22) and

$$\frac{d}{dt}\sum_k \iint \frac{f_R^2}{2\mathcal{M}_k}\,dxdp \le \mu \sum_k \iint \frac{f_R^2}{2\mathcal{M}_k}\,dxdp.$$

Thus, f_R is bounded in X independently of R. We can then extract a subsequence converging towards a function $g \in X$ in $X - weak^*$. We know moreover that f_R satisfies the Cauchy criterion in $L^\infty([0,T],\ell^1(L^1_{x,p}))$ as a solution of the truncated problem thus converges strongly towards f in this space. By uniqueness of the *weak** limit, $g = f$ a.e.

□

Lemma 2.5.4 *Up to an extraction, there exists $f^0 \in X$ and $N_s \in L^2([0,T]\times\mathbb{R}^2)$ such that:*

(i) $f^\eta \longrightarrow f^0$ in $X - weak^*$.

(ii) $N_s^\eta \longrightarrow N_s$ in $L^2_{t,x} - weak$.

(iii) If we define the current by

$$J^\eta = \frac{1}{\eta}\sum_{k\ge1}\int \frac{p}{m} f_k^\eta\,dp, \tag{2.5.25}$$

then

$$J^\eta \to J^0 = \frac{1}{\eta}\sum_{k\ge1}\int \frac{p}{m} f_k^0\,dp \qquad in\ L^2_{t,x} - weak.$$

Moreover, $f_k^0 = N_s\mathcal{M}_k$ a.e. for all $k \ge 1$.

Proof. We integrate (2.5.24) between 0 and t, for all $t \in [0,T]$,

$$X^\eta(t) - \mu\int_0^t X^\eta(s)\,ds + \int_0^t S^\eta(s)\,ds \le X_0.$$

Thus, there exists a constant $C > 0$ such that:

$$0 \le \int_0^T S^\eta(s)ds \le C \tag{2.5.26}$$

If $\mathcal{P}$ defined the orthogonal projection on $Ker\,Q_B$, then $\exists\, N^\eta(t,x) \in \mathbb{R}$ such that $\mathcal{P}(f^\eta)_k = N^\eta\mathcal{M}_k$ and $f^\eta - \mathcal{P}(f^\eta) \in (Ker\,Q_B)^\perp$. Thus $\sum_k \int (f_k^\eta - \mathcal{P}(f^\eta)_k)\,dp = 0$, which provides

$$N^\eta(t,x) = \sum_k \int f_k^\eta\,dp = N_s^\eta. \tag{2.5.27}$$

From (iv) of Proposition 2.3.1 and (2.5.26), we obtain the bound

$$\sum_k \int_0^T \iint \frac{(f_k^\eta - N_s^\eta\mathcal{M}_k)^2}{M_k}\,dtdxdp \le c\eta^2. \tag{2.5.28}$$

We verify easily that $\|f^\eta\|_X$ is bounded. Thus we can extract a subsequence satisfying (i). Then, from (2.5.28), we have

$$\sum_k \int_0^T \iint \frac{(N_s^\eta \mathcal{M}_k)^2}{M_k}\, dtdxdp = \sum_k \int_0^T \iint \left(\frac{N_s^\eta}{\mathcal{Z}}\right)^2 M_k\, dtdxdp \leq C$$

It provides that $\|N_s^\eta/\mathcal{Z}\|_Y$ is bounded. Thus, up to an extraction, for all $\phi \in L_t^2 L_{M^{-1}}^2$,

$$\sum_k \int_0^T \iint \frac{N_s^\eta}{\mathcal{Z}} M_k \phi_k\, dpdxdt \longrightarrow \sum_k \int_0^T \iint \rho^0 M_k \phi_k\, dpdxdt. \tag{2.5.29}$$

If we define $N_s := \rho^0 \mathcal{Z} \in L^2([0,T]\times\mathbb{R}^2)$, and if we chose $\xi \in L^2([0,T]\times\mathbb{R}^2)$ and define $\phi_k(t,x,p) = \xi(t,x)$, for all $k \geq 1$, (we verify easily that $\phi \in L_t^2 L_{M^{-1}}^2$ for such a ξ) we deduce

$$\int_0^T \int_{\mathbb{R}^2} N_s^\eta \xi\, dxdt \longrightarrow \int_0^T \int_{\mathbb{R}^2} N_s \xi\, dxdt.$$

This proves the point (ii). Moreover, we set for all $\psi \in L_t^\infty L_M^2$, $\phi = \psi/M \in L_t^2 L_{M^{-1}}^2$ in (2.5.29). Then, $N_s^\eta M_k/\mathcal{Z} = N_s^\eta \mathcal{M}_k \longrightarrow \rho^0 M_k$ in $X - weak^*$. From (2.5.28), f_k^η and $N_s^\eta \mathcal{M}_k$ have the same weak limit. Thus,

$$\forall\, k \geq 1, \quad f_k^0 = N_s \mathcal{M}_k \ \text{ a.e.} \tag{2.5.30}$$

Now, we have with a Cauchy-Schwarz inequality

$$\begin{aligned} J^\eta &= \frac{1}{\eta}\sum_{k\geq 1}\int \frac{p}{m}(f_k^\eta - N_s^\eta \mathcal{M}_k)\, dp \\ &\leq \left(\sum_{k\geq 1}\int \frac{p^2}{m^2} M_k\, dp\right)^{1/2} \left(\sum_{k\geq 1}\int \frac{(f_k^\eta - N_s^\eta \mathcal{M}_k)^2}{\eta^2 M_k}\, dp\right)^{1/2}. \end{aligned}$$

With (2.5.28) we deduce that J^η is bounded in $L_{t,x}^2$. Thus we can extract a subsequence converging towards J^0 in $L_{t,x}^2$-weak. □

Proof of Theorem 2.5.1 : We consider the transport equation :

$$\eta \partial_t f_k^\eta + \frac{p}{m} \cdot \nabla_x f_k^\eta - \nabla_x \epsilon_k \cdot \nabla_p f_k^\eta = \frac{Q_B(f^\eta)_k}{\eta}. \tag{2.5.31}$$

After an integration, we find the conservation equation :

$$\partial_t N_s^\eta + \text{div}_{\,x} J^\eta = 0, \tag{2.5.32}$$

where the current is in (2.5.25). To have an expression of the current J^η, we remark that if we consider the function Θ defined in 2.3.14, the selfadjointness of Q_B shows

$$\sum_k \int \frac{\Theta_k Q_B(f^\eta)_k}{\eta^2 \mathcal{M}_k}\, dp = -\frac{1}{\eta} J^\eta. \tag{2.5.33}$$

Thus, multiplying (2.5.31) by $\Theta_k/\mathcal{M}_k$, integrating with respect to p and summing over k, we obtain :

$$-J^\eta = \sum_k \int \frac{\Theta_k}{\mathcal{M}_k}(\frac{p}{m}\cdot\nabla_x f_k^\eta - \nabla_x\epsilon_k\cdot\nabla_p f_k^\eta + \eta\partial_t f_k^\eta)\,dp.$$

Assuming we can pass to the limit formally, with (2.5.30) we find

$$-J^0 = \sum_k \int \Theta_k(\frac{p}{m}\cdot(\nabla_x N_s - N_s\nabla_x(\log\mathcal{Z})))\,dp = \mathbb{D}\cdot(\nabla_x N_s + N_s\nabla_x V_s). \qquad (2.5.34)$$

To establish the rigorous limit as $\eta\to 0$, we use the weak formulation of (2.5.31) and (2.5.32) : for all $\phi\in C^1([0,T]\times\mathbb{R}^2)$ compactly supported and all $\psi\in C^1([0,T]\times\mathbb{R}^2\times\mathbb{R}^2)$ compactly supported :

$$-\iint N_s^\eta\partial_t\phi\,dxdt - \iint J^\eta\cdot\nabla_x\phi\,dxdt = \int N_s^\eta(0,x)\phi(0,x)\,dx, \qquad (2.5.35)$$

where

$$N_s^\eta(0,x) = \sum_{k\geq 1}\int f_k^{in}(x,p)\,dp.$$

And

$$\begin{aligned}&\iiint f_k^\eta(-\partial_t\psi - \frac{1}{\eta}(\frac{p}{m}\cdot\nabla_x\psi - \nabla_x\epsilon_k\cdot\nabla_p\psi))\,dtdxdp - \\ &\iiint\frac{Q(f^\eta)_k}{\eta^2}\psi\,dtdxdp = \iint f_k^\eta(0,x,p)\psi(0,x,p)\,dxdp.\end{aligned} \qquad (2.5.36)$$

From Lemma 2.5.5 we can then substitute ψ and ϕ in (2.5.36), by summing over k we obtain (2.5.35). It suffices then to pass to the limit $\eta\to 0$ in the second term of (2.5.35).

Lemma 2.5.6 and 2.5.5 prove that we can choose $\psi = \phi\frac{\Theta}{\mathcal{M}}$ in the weak formulation (2.5.36), for all $\phi\in C^1([0,T]\times\mathbb{R}^2)$ compactly supported. By summing and using (2.5.33), we find :

$$\begin{aligned}&-\eta\sum_k\iiint f_k^\eta\partial_t\left(\phi\frac{\Theta_k}{\mathcal{M}_k}\right)dtdxdp - \sum_k\iiint\frac{f_k^\eta}{\mathcal{M}_k}\frac{p}{m}\nabla_x\phi\cdot\Theta_k\,dtdxdp \\ &-\sum_k\iiint\phi\,\frac{f_k^\eta}{\mathcal{M}_k}(\frac{p}{m}\nabla_x\Theta_k - \nabla_x\epsilon_k\cdot\nabla_p\Theta_k - \frac{p}{m}\Theta_k\nabla_x(-\log\mathcal{Z}))\,dtdxdp \\ &+\iint J^\eta\phi\,dtdx = \sum_k\iint f_k^{in}(x,p)\phi(0,x)\frac{\Theta_k(0,x,p)}{\mathcal{M}_k(0,x,p)}\,dxdp.\end{aligned} \qquad (2.5.37)$$

We have that $f^\eta\in L^2_{\mathcal{M}}$ thus using Lemma 2.5.6, the limit of the first term vanishes.

From Lemma 2.5.4, we have that,

$$\forall\, g\in X, \qquad \sum_{k\geq 1}\iiint f_k^\eta g_k\,dtdxdp \to \sum_{k\geq 1}\iiint N_s\mathcal{M}_k g_k\,dtdxdp.$$

Lemma 2.5.6 proves that $(\frac{p}{m}\cdot\frac{\Theta_k}{\mathcal{M}_k})$ and $(\frac{p}{m}\cdot\frac{\nabla_s\Theta_k}{\mathcal{M}_k})$ for $s=t,x,p$ are in X. Moreover with Assumption 2.2.2, we have that ϵ_k is bounded in $L^\infty([0,T],H^1(\mathbb{R}^2))$. Thus we can pass to the limit in (2.5.37). Taking $\phi(t=0,x)=0$, we obtain

$$\begin{aligned}\iint J^0\phi\,dtdx = &\sum_k\iiint(N_s(\frac{p}{m}\cdot\nabla_x\phi)\Theta_k+N_s\phi\frac{p}{m}\nabla_x\Theta_k)\,dtdxdp\\ &-\sum_k\iiint N_s\phi(\nabla_x\epsilon_k\cdot\nabla_p\Theta_k+\frac{p}{m}\Theta_k\nabla_x(-\log\mathcal{Z}))\,dtdxdp.\end{aligned}$$

After an integration by parts, we recover the expression J^0 in (2.5.34). Thus the proof of Theorem 2.5.1 is over if we prove the two following lemmata. □

Lemma 2.5.5 *For all function $p\mapsto\gamma(p)$ polynomially increasing as well as all its derivatives and for all $\phi\in C^\infty([0,T]\times\mathbb{R}^2)$ compactly supported, the function $\psi=\gamma\phi$ can be taken as test function in the weak formulation of Boltzmann* (2.5.36)*.*

Proof. Let $p\mapsto\xi_R(p)$ such that $\xi_R\in\mathcal{D}([-R,R]^2)$, $0\le\xi_R\le1$, $|\nabla_p\xi_R|\le1$ and $\xi_R\longrightarrow1$ a.e. when $R\to+\infty$. We set $\psi_R=\phi\gamma\xi_R$, function with which we can write the weak formulation (2.5.36). To pass to the limit $R\to+\infty$, it suffices from a Lebesgue theorem that $\gamma f_k^\eta\in L_p^1(\mathbb{R}^2)$ and $p\gamma f_k^\eta\in L_p^1(\mathbb{R}^2)$ as well as for $\nabla_p\gamma$. However with the Cauchy-Schwarz inequality,

$$\int_{\mathbb{R}^2}|\gamma f_k^\eta|(1+|p|)\,dp\le\int_{\mathbb{R}^2}(1+|p|)^2M(p)\gamma^2(p)\,dp\int_{\mathbb{R}^2}\frac{f_k^\eta}{M(p)}\,dp<\infty$$

because γ is polynomially increasing and $M(p)=\dfrac{1}{2\pi}e^{-\frac{p^2}{2m}}$. □

Lemma 2.5.6 *Let Θ be defined in* (2.3.13)*. There exist nonnegative constants C_0, C_1 and C_2 such that: $\forall\,(t,x)\in[0,T]\times\mathbb{R}^2$,*

$$C_1(1+|p|)\le\left|\frac{\Theta_k}{\mathcal{M}_k}\right|\le C_2(1+|p|),$$

$$\left|\frac{\nabla_s\Theta_k}{\mathcal{M}_k}\right|\le C_0(1+|p|^2)\quad\textit{for } s=t,x,p.$$

Proof. By definition of Θ in (2.3.13) we have

$$Q_B(\Theta)_k=-\frac{p}{m}\mathcal{M}_k=Q_B^+(\Theta)_k-\lambda_k\Theta_k,$$

where we denote $Q_B^+(\Theta)_k=\mathcal{M}_k\sum_{k'}\int\alpha_{k,k'}\Theta'_{k'}\,dp'$ and $\lambda_k=\sum_{k'}\int\alpha_{k,k'}\mathcal{M}'_{k'}$. From Assumption 2.2.1, we have $0<\alpha_1\le\lambda_k\le\alpha_2$. Moreover, since $\Theta\in L^2_{\mathcal{M}}$,

$$|Q_B^+(\Theta)_k|\le\alpha_2\mathcal{M}_k\sum_{k'}\int\frac{(\Theta'_{k'})^2}{\mathcal{M}'_{k'}}\,dp'\le c.$$

Then the first inequality follows directly from the identity

$$\lambda_k \Theta_k = Q_B^+(\Theta)_k + \frac{p}{m}\mathcal{M}_k,$$

and we just have to derive it to obtain the second one. □

2.6 Formal derivation for Fermi-Dirac statistics

In this section we will consider the formal diffusive limit of the Boltzmann equation for degenerated semiconductors. We use now Fermi-Dirac statistics and the collision operator reads :

$$Q_{FD}(f)_k = \sum_{k'} \int_{\mathbb{R}^2} \alpha_{k,k'}(p,p')(\mathcal{M}_k(p) f_{k'}(p')(1-f_k(p)) - \mathcal{M}_{k'}(p') f_k(p)(1-f_{k'}(p')))\,dp'. \tag{2.6.38}$$

The diffusive limit is then the limit as η goes to 0 of the Boltzmann equation :

$$\partial_t f_k^\eta + \frac{1}{\eta}(\frac{p}{m}\cdot\nabla_x f_k^\eta - \nabla_x \epsilon_k \cdot \nabla_p f_k^\eta) = \frac{1}{\eta^2} Q_{FD}(f^\eta)_k, \quad (x,p)\in\mathbb{R}^2\times\mathbb{R}^2. \tag{2.6.39}$$

We couple this equation with the initial condition (2.2.9). Physically, f_k represents the occupation rate of the kth subband. Thus f has a physical meaning if and only if $0 \le f \le 1$. If $f = 1$ there is no gain and if $f = 0$, the term of loss vanishes.

Definition 2.6.1 *We define the Fermi-Dirac distribution for a real function $\mu(t,x)$ by*

$$F_k^\mu(t,x,p) = \frac{1}{1+\exp(\frac{p^2}{2m}+\epsilon_k-\mu)}. \tag{2.6.40}$$

2.6.1 Properties of the collision operator

The following proposition states important properties of the collision operator.

Proposition 2.6.2 *Let f be such that $0 \le f(t,x,p) \le 1$ for all $t\in[0,T]$, $x\in\mathbb{R}^2$ and $p\in\mathbb{R}^2$. We suppose that the cross-section α satisfies Assumption 2.2.1. Then the collision operator defined in* (2.6.38) *satisfies the following properties :*

(i) $\displaystyle\sum_k \int_{\mathbb{R}^2} Q_{FD}(f)\,dp = 0.$

(ii) $Q_{FD}(f) = 0$ *if and only if* $\exists\,\mu(t,x)\in\mathbb{R}$ *such that* $f(p) = F^\mu(p)$.

Proof. The first point is obvious thanks to the symmetry of the cross-section α (2.2.8) and corresponds to the conservation of the mass of the particles. For the second, it suffices to write :

$$Q_{FD}(f)_k = \sum_{k'} \int_{\mathbb{R}^2} \alpha_{k,k'}\mathcal{M}_k\mathcal{M}'_{k'}(1-f_k)(1-f'_{k'})\left(\frac{f'_{k'}}{\mathcal{M}'_{k'}(1-f'_{k'})} - \frac{f_k}{\mathcal{M}_k(1-f_k)}\right)dp'.$$

Since we have $0 \leq f \leq 1$, this integral is null if and only if

$$\frac{f'_{k'}}{\mathcal{M}'_{k'}(1-f'_{k'})} - \frac{f_k}{\mathcal{M}_k(1-f_k)} = 0.$$

It means that $f_k/(1-f_k)$ is a Maxwellian. This is equivalent to the existence of $\mu(t,x) \in \mathbb{R}$ such that $f_k(p) = F_k^\mu(p)$. □

Let $\mu(t,x)$ be a given real-valued function. For the rest of this part, we omit to write the dependency in t and x. We define the linearization of the collision operator around equilibrium function by :

$$\mathcal{K}^\mu(f)_k = \sum_{k'} \int \alpha_{k,k'} \left(\frac{\mathcal{M}'_{k'}}{F_{k'}^{\mu'}} F_k^\mu f'_{k'} - \frac{\mathcal{M}_k}{F_k^\mu} F_{k'}^{\mu'} f_k \right) dp'. \tag{2.6.41}$$

Straightforward calculations using the definition (2.6.40) lead to

$$\mathcal{K}^\mu(f)_k = \sum_{k'} \int \alpha_{k,k'} [(\mathcal{M}_k(1-F_k^\mu) + \mathcal{M}'_{k'} F_k^\mu) f'_{k'} - (\mathcal{M}'_{k'}(1-F_{k'}^{\mu'}) + \mathcal{M}_k F_{k'}^{\mu'}) f_k]\, dp'.$$

Thus, if we consider a small perturbation g of the equilibrium defined by $g = F^\mu + \eta f + O(\eta^2)$. We have

$$Q_{FD}(g) = Q_{FD}(F^\mu + \eta f + O(\eta^2)) = \eta \mathcal{K}^\mu(f) + O(\eta^2). \tag{2.6.42}$$

Since $\mathcal{K}$ is linear, we can do the same analysis as in paragraph 2.3.1. We define then

$$\mathcal{N}_k^\mu = \frac{(F_k^\mu)^2}{\mathcal{M}_k} \tag{2.6.43}$$

and the space

$$L^2_{\mathcal{N}} = \{ f = (f_k)_{k \geq 1} \text{ such that } \sum_k \int_{\mathbb{R}^2} \frac{f_k^2}{\mathcal{N}_k^\mu}\, dp < \infty \}, \tag{2.6.44}$$

which is an Hilbert space with the scalar product

$$\langle f, g \rangle_{\mathcal{N}} = \sum_k \int_{\mathbb{R}^2} \frac{f_k g_k}{\mathcal{N}_k^\mu}\, dp.$$

And we denote $\| \cdot \|_{\mathcal{N}}$ the corresponding norm.

Proposition 2.6.3 *Let $\mathcal{K}^\mu$ be defined in (2.6.41) for a given real-valued function $\mu(t,x)$. We assume that the cross-section α satisfies Assumption 2.2.1. Then we have :*

(i) $\mathcal{K}^\mu$ is a linear, selfadjoint and negative bounded operator on $L^2_{\mathcal{N}}$.

(ii) $Ker\, \mathcal{K}^\mu = \{ f \in L^2_{\mathcal{N}}$ such that $\exists\, \lambda \in \mathbb{R},\ f = \lambda N^\mu \}$.

(iii) If $\mathcal{P}^\mu$ is the orthogonal projection on $Ker\, \mathcal{K}^\mu$ with the scalar product $\langle \cdot, \cdot \rangle_{\mathcal{N}}$, then there exists a nonnegative constant C_μ depending on μ such that

$$-\langle \mathcal{K}^\mu(f), f \rangle_{\mathcal{N}} \geq C_\mu \| f - \mathcal{P}^\mu(f) \|^2_{\mathcal{N}}. \tag{2.6.45}$$

(iv) $Im\, \mathcal{K}^\mu = \{ f \in L^2_{\mathcal{N}}$ such that $\sum_k \int f_k\, dp = 0 \}$.

Proof. We have

$$\langle \mathcal{K}^\mu(f), g\rangle_{\mathcal{N}} = \sum_{k,k'} \iint \alpha_{k,k'} F^{\mu'}_{k'} F^\mu_k \left(\frac{\mathcal{M}'_{k'}}{(F^{\mu'}_{k'})^2} f'_{k'} - \frac{\mathcal{M}_k}{(F^\mu_k)^2} f_k \right) \frac{g_k}{\mathcal{N}^\mu_k}\, dpdp'.$$

Thanks to the definition of F^μ_k (2.6.40) and $\mathcal{M}_k$ (2.2.7), we have the estimate

$$\frac{F^\mu_k}{\mathcal{M}_k} = \frac{2\pi\mathcal{Z}}{e^{-p^2/(2m)-\epsilon_k} + e^{-\mu}} \geq \frac{2\pi\mathcal{Z}}{1+e^{-\mu}}.$$

Thus,

$$\sum_k \int F^\mu_k \frac{f_k^2}{(\mathcal{N}^\mu_k)^2}\, dp \leq \sum_k \int \frac{1+e^{-\mu}}{2\pi\mathcal{Z}} \frac{f_k^2}{\mathcal{N}^\mu_k}\, dp = \frac{1+e^{-\mu}}{2\pi\mathcal{Z}} \|f\|^2_{\mathcal{N}}. \tag{2.6.46}$$

Then, we have thanks to Assumption 2.2.1

$$\begin{aligned} |\langle \mathcal{K}^\mu(f), g\rangle_{\mathcal{N}}| &\leq \alpha_2 \sum_{k,k'} \iint F^{\mu'}_{k'} F^\mu_k \left(\frac{|f'_{k'}|}{\mathcal{N}^{\mu'}_{k'}} + \frac{|f_k|}{\mathcal{N}^\mu_k} \right) \frac{|g_k|}{\mathcal{N}^\mu_k}\, dpdp' \\ &\leq \alpha_2 N^\mu \sum_k \int F^\mu_k \frac{|f_k|}{\mathcal{N}^\mu_k} \frac{|g_k|}{\mathcal{N}^\mu_k}\, dp + \\ &\quad + \alpha_2 \left(\sum_{k'} \int F^{\mu'}_{k'} \frac{|f'_{k'}|}{\mathcal{N}^{\mu'}_{k'}}\, dp' \right) \left(\sum_k \int F^\mu_k \frac{|g_k|}{\mathcal{N}^\mu_k}\, dp \right), \end{aligned}$$

where we note $N^\mu = \sum_k \int F^\mu_k\, dp$. From (2.6.46) and a Cauchy-Schwarz inequality, we deduce

$$\sum_k \int F^\mu_k \frac{|f_k|}{\mathcal{N}^\mu_k} \frac{|g_k|}{\mathcal{N}^\mu_k}\, dp \leq \frac{(1+e^{-\mu})^2}{2\pi\mathcal{Z}} \|f\|_{\mathcal{N}} \|g\|_{\mathcal{N}}.$$

Consequently,

$$|\langle \mathcal{K}^\mu(f), g\rangle_{\mathcal{N}}| \leq \alpha_2 \left(N^\mu \frac{(1+e^{-\mu})^2}{2\pi\mathcal{Z}} + 1 \right) \|f\|_{\mathcal{N}} \|g\|_{\mathcal{N}}.$$

It provides the continuity on $L^2_{\mathcal{N}}$ of the operator $\mathcal{K}^\mu$. Moreover, we can rewrite

$$\langle \mathcal{K}^\mu(f), g\rangle_{\mathcal{N}} = -\frac{1}{2} \sum_{k,k'} \iint \alpha_{k,k'} F^{\mu'}_{k'} F^\mu_k \left(\frac{f'_{k'}}{\mathcal{N}^{\mu'}_{k'}} - \frac{f_k}{\mathcal{N}^\mu_k} \right) \left(\frac{g'_{k'}}{\mathcal{N}^{\mu'}_{k'}} - \frac{g_k}{\mathcal{N}^\mu_k} \right) dpdp'. \tag{2.6.47}$$

We deduce easily the symmetry and negativity of $\mathcal{K}^\mu$. Thus (i) holds true.

Moreover, $f \in Ker\, \mathcal{K}^\mu$ iff $\langle \mathcal{K}^\mu(f), g\rangle_{\mathcal{N}} = 0$, for all $g \in L^2_{\mathcal{N}}$. If we chose $g = f$ in (2.6.47) we have,

$$-\langle \mathcal{K}^\mu(f), f\rangle_{\mathcal{N}} = \frac{1}{2} \sum_{k,k'} \iint \alpha_{k,k'} F^{\mu'}_{k'} F^\mu_k \left(\frac{f'_{k'}}{\mathcal{N}^{\mu'}_{k'}} - \frac{f_k}{\mathcal{N}^\mu_k} \right)^2 dpdp'.$$

Thus (ii) holds. Besides, we deduce from the estimate $F^\mu_k \geq \dfrac{e^{-\mu}}{2\pi\mathcal{Z}} \mathcal{N}^\mu_k$ and Assumption 2.2.1 the bound

$$-\langle \mathcal{K}^\mu(f), f\rangle_{\mathcal{N}} \geq \frac{\alpha_1 e^{-\mu}}{4\pi\mathcal{Z}} \sum_{k,k'} \iint \mathcal{N}^{\mu'}_{k'} \mathcal{N}^\mu_k \left(\frac{f'_{k'}}{\mathcal{N}^{\mu'}_{k'}} - \frac{f_k}{\mathcal{N}^\mu_k} \right)^2 dpdp'.$$

Thus if $f \in (Ker\,\mathcal{K}^\mu)^\perp$, we have

$$-\langle \mathcal{K}^\mu(f), f\rangle_{\mathcal{N}} \geq \frac{\alpha_1 e^{-\mu}}{4\pi\mathcal{Z}} \left(\sum_k \int \mathcal{N}_k^\mu \, dp\right) \|f_k\|^2_{\mathcal{N}}.$$

Else, we chose $g = f - \mathcal{P}^\mu(f) \in (Ker\,\mathcal{K}^\mu)^\perp$. Since $\langle \mathcal{K}^\mu(f), f\rangle_{\mathcal{N}} = \langle \mathcal{K}^\mu(g), g\rangle_{\mathcal{N}}$, thanks to the selfadjointness of $\mathcal{K}^\mu$, we deduce easily (iii).

Since $\mathcal{K}^\mu$ is selfadjoint, it suffices to prove that $Im\,\mathcal{K}^\mu$ is closed to have $Im\,\mathcal{K}^\mu = (Ker\,\mathcal{K}^\mu)^\perp = \{f \in L^2_{\mathcal{N}}$ such that $\sum_k \int f_k \, dp = 0\}$. This proof is the same that for Proposition 2.3.2. □

Corollary 2.6.4 *The equation $\mathcal{K}^\mu(f) = h$ admits a solution in $L^2_{\mathcal{N}}$ iff $h \in (Ker\,\mathcal{K}^\mu)^\perp$. Moreover this solution is unique if we impose $f \in (Ker\,\mathcal{K}^\mu)^\perp$.*

We can state of course the same result as in Proposition 2.3.4 :

Proposition 2.6.5 *There exists $\Theta^\mu \in (L^2_{\mathcal{N}})^2$ such that for all $k \geq 1$,*

$$\mathcal{K}^\mu(\Theta)_k = -\frac{p}{m}\mathcal{N}_k^\mu \quad \textit{and} \quad \sum_k \int_{\mathbb{R}^2} \Theta_k \, dp = 0. \tag{2.6.48}$$

As before, we define the diffusion matrix by

$$\mathbb{D}^\mu = \int \sum_k \Theta_k^\mu \otimes \frac{p}{m} \, dp. \tag{2.6.49}$$

Then $\mathbb{D}^\mu$ is a symmetric coercive matrix.

2.6.2 Formal derivation

We give without proof the following existence and uniqueness result for the problem (2.6.39) with the initial condition (2.2.9).

Theorem 2.6.6 *Let $T > 0$. Under assumptions 2.2.1 and 2.2.2, if we suppose moreover that for all $t \in [0, T]$, $x \in \mathbb{R}^2$ and $p \in \mathbb{R}^2$, $0 \leq f^{in}(x,p) \leq 1$, with $f^{in} \in \ell^1(L^1_{x,p})$.*

Then, the problem (2.6.39) *with the initial condition* (2.2.9) *admits an unique weak solution $f \in \ell^1(L^1_{t,x,p})$ satisfying $0 \leq f \leq 1$.*

Proposition 2.6.7 *Under Assumption 2.2.1, if the solution f^η in Theorem 2.6.6 admits a Hilbert expansion with respect to η, $f^\eta = f^0 + \eta f^1 + \ldots$. Then $f^0 = F^\mu(p)$ where μ is the solution of the equation*

$$\partial_t N_\mu + \mathrm{div}_x\, (\mathbb{D}^\mu \cdot \nabla_x \mu \, \frac{e^{-\mu}}{2\pi\mathcal{Z}}) = 0, \tag{2.6.50}$$

where

$$N_\mu := \sum_{k\geq 1} \int_{\mathbb{R}^2} F_k^\mu \, dp = \sum_k \int_{\mathbb{R}^2} \frac{1}{1 + e^{\frac{p^2}{2m} + \epsilon_k - \mu}} \, dp = 2\pi m \sum_{k\geq 1} \log(1 + e^{\mu - \epsilon_k}).$$

Proof. We follow the same idea as before. Formally, we have:

$$Q_{FD}(f^0 + \eta f^1 + O(\eta^2))_k = \eta(\frac{p}{m} \cdot \nabla_x f_k^0 - \nabla_x \epsilon_k \cdot \nabla_p f_k^0) + O(\eta^2). \tag{2.6.51}$$

If we can pass to the limit $\eta \to 0$, then we have $Q_{FD}(f^0) = 0$. Thus, from 2.6.2, there exists μ such that:

$$f_k^0 = F_k^\mu \ , \forall k \geq 1.$$

Therefore, a straightforward calculation leads to

$$\frac{p}{m} \cdot \nabla_x f_k^0 - \nabla_x \epsilon_k \cdot \nabla_p f_k^0 = \exp(\frac{p^2}{2m} + \epsilon_k - \mu)(F_k^\mu)^2 \, \frac{p}{m} \cdot \nabla_x \mu.$$

The choice of the linear operator $\mathcal{K}^\mu$ in (2.6.42) allows us to write

$$Q_{FD}(f^\eta) = \eta \mathcal{K}^\mu(f^1) + O(\eta^2).$$

Thus by identifying the terms at the order 1 in η in (2.6.51), we deduce

$$\mathcal{K}^\mu(f^1) = \exp(\frac{p^2}{2m} + \epsilon_k - \mu)(F_k^\mu)^2 \, \frac{p}{m} \cdot \nabla_x \mu = (\frac{p}{m} \cdot \nabla_x \mu) \, \frac{e^{-\mu}}{2\pi \mathcal{Z}} \, \mathcal{N}_k^\mu.$$

Thus, by definition of Θ^μ in (2.6.48), we have

$$f_k^1 = -(\Theta_k^\mu \cdot \nabla_x \mu) \, \frac{e^{-\mu}}{2\pi \mathcal{Z}}.$$

If we integrate over p and sum the Boltzmann equation (2.6.39), we find

$$\partial_t \left(\sum_k \int f_k^\eta \, dp \right) + \frac{1}{\eta} \sum_k \int \frac{p}{m} \cdot \nabla_x f_k^\eta \, dp = 0. \tag{2.6.52}$$

And with the Hilbert expansion of f^η,

$$\frac{1}{\eta} \sum_k \int \frac{p}{m} \cdot \nabla_x f_k^\eta \, dp = \frac{1}{\eta} \sum_k \int \frac{p}{m} \cdot \nabla_x F_k^\mu \, dp + \sum_k \int \frac{p}{m} \cdot \nabla_x f_k^1 \, dp + O(\eta).$$

Since the function $p \mapsto p \cdot \nabla_x F_k$ is odd, the first term of the right hand side vanishes. Moreover,

$$\sum_k \int \frac{p}{m} \cdot \nabla_x f_k^1 \, dp = -\mathrm{div}_x \, \left(\left(\sum_k \int \frac{p}{m} \otimes \Theta^\mu \, dp \right) \nabla_x \mu \, \frac{e^{-\mu}}{2\pi \mathcal{Z}} \right).$$

We recognize the diffusion matrix $\mathbb{D}^\mu$ defined in (2.6.49). Thus if we take the limit $\eta \to 0$ in (2.6.52), we obtain the equation (2.6.50) for μ.

□

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PARTIE I

Existence, unicité et comportement en temps long

Chapter 3

Le système classique dérive-diffusion-Poisson revisité

Ce chapitre reprend et étend une note [6]
en collaboration avec N. Ben Abdallah [1] et F. Méhats [2].

3.1 Introduction

Le système couplé dérive-diffusion-Poisson est très largement utilisé pour modéliser le transport de charges dans des dispositifs à semiconducteurs ou à plasmas dans un contexte fortement collisionnel [23, 22]. Il convient aussi de rapprocher ce système aux modèles de Keller-Segel [8] et de Fokker-Planck [2]. Soit $\Omega \subset \mathbb{R}^3$ un domaine régulier borné de l'espace. L'équation de dérive-diffusion est une équation de conservation dont l'inconnue est la densité des porteurs de charges $N(t,x)$ pour $t \in \mathbb{R}^+$ et $x \in \Omega$. Cette équation s'écrit :

$$\partial_t N - \text{div}\,(\mathbb{D}(\nabla N + N\nabla V)) = 0, \tag{3.1.1}$$

où $\mathbb{D} = \mathbb{D}(x)$ est la matrice de diffusion symétrique et définie positive que l'on supposera suffisamment régulière.

Hypothèse 3.1.1 *La fonction $\mathbb{D}$ est de classe C^1 de $\overline{\Omega}$ dans l'ensemble des matrices symétriques définies positives et telle que pour tout $x \in \Omega$ on a $\mathbb{D}(x) \geq \alpha I$, avec α donné.*

Le courant, noté J, est la somme d'un courant de dérive proportionnel à la densité de particule et aux forces électrostatiques et d'un courant de diffusion proportionnel au gradient de la densité de particules :

$$J(t,x) = \mathbb{D}(x)(\nabla N(t,x) + N(t,x)\nabla V(t,x)).$$

[1] MIP, UMR 5640, Université Paul Sabatier, Toulouse.
[2] IRMAR, Université Rennes 1, Rennes.

Le potentiel électrostatique $V(t,x)$ est généré par les électrons via l'équation de Poisson :

$$-\Delta V(t,x) = N(t,x). \tag{3.1.2}$$

Le système (3.1.1)–(3.1.2) est complété par la condition initiale : $N(0,x) = N_0(x)$, $x \in \Omega$ et par des conditions aux bords de type Dirichlet :

$$N(t,x) = N_b(x) \quad \text{et} \quad V(t,x) = V_b(x) \qquad \text{pour } x \in \partial\Omega. \tag{3.1.3}$$

On peut prendre d'autres conditions aux bords, l'essentiel pour notre analyse étant qu'elles permettent d'utiliser la régularité elliptique sur l'équation de Poisson et qu'elles garantissent l'unicité des solutions de l'équation de Poisson (3.1.2).

On suppose que les données vérifient l'hypothèse suivante :

Hypothèse 3.1.2 *La donnée de Cauchy N_0 est positive et appartient à $L^{6/5}(\Omega)$. De plus, les données de Dirichlet sont telles que $V_b \in C^2(\partial\Omega)$ et il existe un réel $u_\infty > 0$ tel que $N_b = u_\infty e^{-V_b}$.*

Il est coutume d'introduire le niveau de Fermi ϵ_F et la variable de slotboom u définis par

$$u = e^{\epsilon_F} = Ne^V.$$

On peut donc réécrire le courant sous la forme :

$$J = \mathbb{D}\, N\nabla\epsilon_F = \mathbb{D}\, e^{-V}\nabla u.$$

Les méthodes basées sur l'entropie sont maintenant des outils classiques de l'analyse de l'existence de solutions et du comportement en temps long des modèles de transport diffusif. Gajewski [16] a utilisé l'entropie relative pour construire des solutions et prouver leur convergence vers l'équilibre pour un système de dérive-diffusion-Poisson avec une matrice de diffusion scalaire. En [17], il a été prouvé que la convergence est exponentielle. Plus récemment des résultats sur le comportement en temps long utilisant des techniques d'entropie ont été obtenus dans un domaine non borné avec un potentiel de confinement [2] et pour des systèmes bipolaires [3], et aussi dans un domaine borné avec des conditions de non-flux aux bords [9] et pour des systèmes avec une diffusion non-linéaire [10]. Ces résultats utilisant les inégalités de Sobolev logarithmique s'appuient fortement sur le fait que les systèmes sont isolés (la norme L^1 de la densité N est conservée). On se propose de présenter un résultat d'existence et de comportement en temps long dans le cas où des contacts ohmiques n'assurent plus la conservation de la masse totale. Pour ce faire, on utilise une entropie relative quadratique. Une idée similaire a été utilisée en [2] pour analyser le trou spectral de l'opérateur défini en (3.1.1) et pour l'étude en temps long d'un système couplé quantique-classique en [5].

Pour présenter nos résultats, on introduit maintenant le système stationnaire sur les inconnues (N_∞, V_∞)

$$-\text{div}\,(\mathbb{D}(\nabla N_\infty + N_\infty\nabla V_\infty)) = 0, \qquad -\Delta V_\infty = N_\infty. \tag{3.1.4}$$

On complète ce système par les mêmes conditions aux bords que le problème dépendant du temps :

$$N_\infty = N_b \quad \text{et } V_\infty = V_b \quad \text{sur } \partial\Omega. \tag{3.1.5}$$

Proposition 3.1.3 *Sous l'hypothèse 3.1.2, le système* (3.1.4)–(3.1.5) *admet une solution unique* (N_∞, V_∞) *qui se met sous la forme* $N_\infty = u_\infty e^{-V_\infty}$ *avec* $V_\infty \in C^2(\overline{\Omega})$.

Nous allons dans cette partie énoncer deux résultats portant sur le comportement en temps long des solutions de dérive-diffusion-Poisson d'une part, et d'autre part sur l'existence de telles solutions. Plus précisément,

Théorème 3.1.1 *Sous les hypothèses 3.1.1 et 3.1.2 et si* (N, V) *est une solution de* (3.1.1)–(3.1.3) *telle que* $N \in C(\mathbb{R}^+, L^2(\Omega)) \cap L^2_{loc}(\mathbb{R}^+, H^1(\Omega))$ *et* $V \in C(\mathbb{R}^+, H^1(\Omega))$. *Alors il existe deux constantes* $C > 0$ *et* $\lambda > 0$ *telles que pour tout* $t > 0$,

$$\|N - N_\infty\|_{L^2(\Omega)}(t) + \|V - V_\infty\|_{H^1(\Omega)}(t) \leq Ce^{-\lambda t}. \tag{3.1.6}$$

On remarque que ce théorème suppose de manière implicite que la donnée initiale appartienne à $L^2(\Omega)$, ce qui est plus fort que l'hypothèse 3.1.2. En fait les estimations a priori obtenues grâce à l'entropie relative ne fournissent une borne sur la densité que dans $L \log L$. Cependant, on peut montrer que les hypothèses du théorème précédent sont verifiées à partir d'un certain temps :

Théorème 3.1.2 *Sous les hypothèse 3.1.1 et 3.1.2, il existe une solution faible* (N, V) *de* (3.1.1)–(3.1.3) *satisfaisant*

$$N(1 + |\log N|) \in L^\infty_{loc}(\mathbb{R}^+, L^1(\omega)), \ \sqrt{N} \in L^2(\mathbb{R}^+, H^1(\Omega)) \quad et \quad V \in L^\infty_{loc}(\mathbb{R}^+, H^1(\Omega)). \tag{3.1.7}$$

De plus il existe $T > 0$ *tel que* $N \in C([T, +\infty); L^2(\Omega))$ *et* $V \in C([T, +\infty); H^1(\Omega))$. *Alors on peut trouver deux constantes* $C > 0$ *et* $\lambda > 0$ *telles que cette solution satisfasse* (3.1.6) *pour* $t \geq T$.

Ce chapitre est organisé de la manière suivante. Au paragraphe 3.2, on s'intéresse au comportement en temps long des solutions et on prouve le théorème 3.1.1. Pour cela on montrera dans un premier temps la convergence de l'entropie relative vers 0 quand t tend vers $+\infty$. Puis, on établira l'estimation 3.1.6 en linéarisant cette entropie. Dans une dernière sous-partie, on rappelera, pour être complet, dans un cas simple d'autres techniques utilisant les inégalités de Sobolev logarithmiques. La section 3.3 est consacrée à l'existence des solutions. De manière connue, on obtient l'existence avec des techniques reposant sur l'entropie dans un cadre $L \log L$ pour la densité. Ensuite, en utilisant la linéarisation de cette entropie, on obtient plus de régularité à partir d'un certain temps.

3.2 Comportement en temps long

Dans cette section, nous allons étudier le comportement des solutions en temps grand. Pour cela il convient de s'intéresser au système stationnaire (3.1.4)–(3.1.5). De manière évidente, l'équation de dérive-diffusion implique que la variable de Slotboom définie par $N_\infty e^{V_\infty}$ est constante sur Ω. Elle est alors égale à sa valeur aux frontières du domaine donc $N_\infty = u_\infty e^{-V_\infty}$ grâce à l'hypothèse 3.1.2. Alors V_∞ est la solution du problème :

$$-\Delta V_\infty = u_\infty e^{-V_\infty}.$$

Donc (voir [15]) V_∞ est l'unique minimum de la fonctionnelle convexe

$$J(V) = \int_\Omega |\nabla V|^2\, dx + u_\infty \int_\Omega e^{-V}\, dx.$$

Compte tenu de nos hypothèses aux bords, on a que $V_\infty \in C^2(\overline{\Omega})$. On retrouve ainsi le résultat énoncé dans la Proposition 3.1.3.

Pour prouver le théorème 3.1.1, on va dans un premier temps établir la convergence de l'entropie relative vers 0 puis prouver l'estimation 3.1.6.

3.2.1 Convergence de l'entropie relative

On définit l'entropie relative de (N, V) par rapport (N_∞, V_∞) par

$$E(t) = \int_\Omega (N \log \frac{N}{N_\infty} + N_\infty - N)\, dx + \frac{1}{2}\int_\Omega |\nabla(V - V_\infty)|^2\, dx. \tag{3.2.8}$$

Le lemme suivant établi la décroissance de cette quantité vers 0 quand t tend vers $+\infty$:

Lemma 3.2.1 *Soit (N, V) solution faible de* (3.1.1),(3.1.2) *et soit (N_∞, V_∞) solution du problème stationnaire* (3.1.4). *Alors l'entropie relative definie en* (3.2.8) *decroît vers* 0 *quand t tends vers $+\infty$. Cela implique la convergence de N et V vers N_∞ et V_∞ resp. dans $L^1(\Omega)$ et $H^1(\Omega)$.*

Démonstration. Par un calcul direct utilisant (3.1.1), (3.1.2), (3.1.3), on a

$$\frac{d}{dt}E(t) = -\int_\Omega e^{-V}\frac{\mathbb{D}\nabla u.\nabla u}{u}\, dx \le -\alpha \int_\Omega e^{-V}\frac{|\nabla u|^2}{u}\, dx,$$

où on a utilisé l'hypothèse 3.1.1 dans la dernière inégalité. Donc l'entropie est une fonction décroissante du temps et pour tout $t \ge 0$ on a

$$E(t) + \alpha \int_0^t \int_\Omega e^{-V}\frac{|\nabla u|^2}{u}\, dxd\tau \le E(0). \tag{3.2.9}$$

Cette inégalité suffit à prouver le Lemme en reprenant l'argumentation de Gajewski [16]. Par soucis de complétude et de clairté, on reprend les grandes lignes de la démonstration. Tout d'abord, il existe une suite $t_j \to +\infty$ telle que

$$\lim_{j\to+\infty} \int_\Omega e^{-V(t_j)}\frac{|\nabla u(t_j)|^2}{u(t_j)}\, dx = 0. \tag{3.2.10}$$

De plus, on déduit après un calcul direct que

$$\int_\Omega e^{-V}\frac{|\nabla u|^2}{u}\,dx = \int_\Omega 4|\nabla\sqrt{N}|^2\,dx + \int_\Omega N|\nabla V|^2\,dx + \int_\Omega 2N^2\,dx + \int_{\partial\Omega} N_b\,\partial_\nu V\,ds$$

(où $\nu(x)$ est le vecteur normal sortant en $x\in\partial\Omega$ et ds est la mesure surfacique). Comme, d'après l'équation de Poisson (4.1.4) et la régularité elliptique standard pour celle-ci, on a

$$\left|\int_{\partial\Omega} N_b\partial_\nu V\,ds\right| \le C\|V\|_{H^2(\Omega)} \le C(\|N\|_{L^2(\Omega)} + \|V_b\|_{H^{3/2}(\partial\Omega)}) \le C + \int_\Omega N^2\,dx,$$

on déduit que

$$\int_\Omega e^{-V}\frac{|\nabla u|^2}{u}\,dx \ge \int_\Omega 4|\nabla\sqrt{N}|^2\,dx - C_0. \tag{3.2.11}$$

Alors (3.2.10) et (3.2.11) impliquent que $\|\sqrt{N(t_j)}\|_{H^1(\Omega)} \le C$. A extraction d'une sous-suite près, on peut prouver que $\lim_{j\to+\infty} E(t_j) = 0$. Comme E est decroissant, on a : $\lim_{t\to+\infty} E(t) = 0$. Grâce à l'inégalité de Csiszár-Kullback [1, 12, 20], on déduit que $\|N - N_\infty\|_{L^1(\Omega)}(t) \longrightarrow 0$ et $\|V - V_\infty\|_{H^1(\Omega)}(t) \longrightarrow 0$, quand $t\to+\infty$. □

3.2.2 Convergence exponentielle

Danc cette partie on prouve la convergence exponentielle en temps long des solutions vers les solutions du problème stationnaire. On définit $n = N - N_\infty$ et $v = V - V_\infty$. L'idée est de linéariser l'entropie relative E par rapport à ces quantités. On pose donc :

$$L(t) = \frac{1}{2}\int_\Omega \frac{n^2}{N_\infty}\,dx + \frac{1}{2}\int_\Omega |\nabla v|^2\,dx. \tag{3.2.12}$$

De (3.1.1), (3.1.2), on déduit que les quantités n et v sont solutions de :

$$\begin{cases} \partial_t n - \operatorname{div}_x\left(\mathbb{D}(\nabla_x n + N_\infty\nabla_x v + n\nabla_x V_\infty + n\nabla_x v)\right) = 0, \\ -\Delta_{x,z} v = n. \end{cases} \tag{3.2.13}$$

De (3.2.13), (3.2.12) et après une integration par parties, il vient

$$\frac{d}{dt}L(t) = -\int_\Omega N_\infty\mathbb{D}\nabla(\frac{n}{N_\infty}+v)\cdot\nabla(\frac{n}{N_\infty}+v)\,dx - \int_\Omega n\mathbb{D}\nabla v\cdot\nabla(\frac{n}{N_\infty}+v)\,dx. \tag{3.2.14}$$

Grâce à l'inégalité de Poincaré, le premier terme du membre de droite est contrôlé par $L(t)$. Nous allons montrer que le second terme peut être contrôlé par le premier et par $L(t)$. Avec l'inégalité de Cauchy-Schwarz, on a

$$-\int_\Omega n\mathbb{D}\nabla v\cdot\nabla(\frac{n}{N_\infty}+v)\,dx \le \frac{1}{2}\int_\Omega N_\infty\mathbb{D}\nabla(\frac{n}{N_\infty}+v)\cdot\nabla(\frac{n}{N_\infty}+v)\,dx + \frac{1}{2}\int_\Omega \frac{n^2}{N_\infty}\mathbb{D}\nabla v\cdot\nabla v\,dx.$$

Alors en utilisant l'hypothèse 3.1.1 et le fait que N_∞ est borné inférieurement, on obtient

$$\frac{d}{dt}L(t) \leq -C_1 \int_\Omega (|\nabla(\frac{n}{N_\infty})|^2 + 2\frac{n^2}{N_\infty} + |\nabla v|^2)\, dx + C_2 \int_\Omega n^2 |\nabla v|^2\, dx, \tag{3.2.15}$$

où C_1 et C_2 sont deux constantes positives. Avec une interpolation, on a

$$\|n\|^2_{L^4(\Omega)} \leq \|n\|^{1/2}_{L^2(\Omega)} \|n\|^{3/2}_{L^6(\Omega)}. \tag{3.2.16}$$

Grâce à l'injection de $H^1(\Omega)$ dans $L^6(\Omega)$ et la régularité elliptique de l'équation de Poisson dans (3.2.13), on a

$$\|\nabla v\|^2_{L^4(\Omega)} \leq \|\nabla v\|^{1/2}_{L^2(\Omega)} \|\nabla v\|^{3/2}_{L^6(\Omega)} \leq C \|\nabla v\|^{1/2}_{L^2(\Omega)} \|n\|^{3/2}_{L^2(\Omega)}. \tag{3.2.17}$$

Donc en utilisant de plus le fait que N_∞ est borné inférieurement, on a après une inégalité de Cauchy-Schwarz et en utilisant (3.2.16) et (3.2.17),

$$\int_\Omega n^2 |\nabla v|^2\, dx \leq C \|\nabla v\|^{1/2}_{L^2(\Omega)} \|n\|^2_{L^2(\Omega)} \left\| \frac{n}{N_\infty} \right\|^{3/2}_{H^1(\Omega)} \leq C\varepsilon \left\| \frac{n}{N_\infty} \right\|^2_{H^1(\Omega)} + \frac{C}{\varepsilon^3} \|n\|^8_{L^2(\Omega)},$$

où on a aussi utilisé le fait que ∇v est borné dans $L^\infty(\mathbb{R}_+, L^2(\Omega))$ (voir (3.2.9)). Donc, en se fixant $\varepsilon > 0$ suffisamment petit, on déduit de (3.2.15) et de l'inégalité de Poincaré qu'il existe deux constantes positives C_1 et C_2 telles que

$$\frac{d}{dt}L(t) \leq -C_1 L(t) + C_2 L(t)^4. \tag{3.2.18}$$

On a vu dans la preuve du Lemme 3.2.1 qu'il existe une suite $(t_j)_{j\in\mathbb{N}}$ tendant vers $+\infty$ et telle que $(\sqrt{N(t_j)})_{j\in\mathbb{N}}$ soit bornée dans $H^1(\Omega)$. Grâce à l'injection $H^1(\Omega) \hookrightarrow L^6(\Omega)$, $\|n(t_j)\|_{L^3(\Omega)}$ est bornée pour tout $j \in \mathbb{N}$. De plus, le Lemme 3.2.1 implique $\lim_{j\to+\infty} \|n(t_j)\|_{L^1(\Omega)} = 0$. Donc, par interpolation, on déduit que $\lim_{j\to+\infty} L(t_j) = 0$. Par conséquent, on peut trouver t_* tel que $C_2 L(t_*)^3 \leq C_1/2$. Avec (3.2.18), on a

$$\frac{d}{dt}L(t_*) \leq -\frac{C_1}{2} L(t_*) < 0. \tag{3.2.19}$$

On définit l'ensemble $A := \{t \in [t_*, +\infty)$ tels que $\forall\, s \in [t_*, t), C_2 L(s)^3 \leq \frac{C_1}{2}\}$. Par continuité de L, A est un ensemble fermé contenant t_* par (3.2.19). De plus, si $t_1 \in A$, par (3.2.18), on a

$$\frac{d}{dt}L(t_1) \leq -(C_1 - C_2 L(t_1)^3) L(t_1) \leq -\frac{C_1}{2} L(t_1).$$

Par continuité de L, il existe $\delta > 0$ tel que $\forall\, s \in [t_1, t_1 + \delta), L(s) \leq L(t_1)$. Donc A est ouvert et par connexité, $A = [t_*, +\infty)$ i.e.

$$\forall\, t \in [t_*, +\infty), \qquad L(t) \leq L(t_*) e^{-\frac{C_1}{2}(t - t_*)}.$$

□

3.2.3 Remarque dans le cas $\mathbb{R}^3$

Par soucis de complétude nous allons présenter de manière succinte une analyse plus connue du comportement en temps long, reposant sur les inégalités Sobolev logarithmique, dans le cas où l'espace d'étude n'est plus un borné mais $\mathbb{R}^3$ tout entier (voir [2, 3, 10, 14] pour plus de détail). On suit le développement présenté dans [3].

Tout d'abord, il convient de remarquer que dans ce cas la masse totale du système se conserve :

$$\forall\, t \in \mathbb{R}^+, \qquad \int_{\mathbb{R}^3} N(t,x)\,dx = \int_{\mathbb{R}^3} N_0(x)\,dx = \mathcal{N}_I.$$

On introduit l'entropie relative de (N,V) par rapport à (N_∞, V_∞) :

$$E(t) = \int_\Omega (N \log \frac{N}{N_\infty} + N_\infty - N)\,dx + \frac{1}{2}\int_\Omega |\nabla(V - V_\infty)|^2\,dx. \tag{3.2.20}$$

Dans ce cas, N_∞ et V_∞ sont définis sur Ω par

$$N_\infty(x) = \frac{\mathcal{N}_I}{\int_\Omega e^{-V_\infty(y)}\,dy}\; e^{-V_\infty(x)}$$
$$-\Delta V_\infty = N_\infty.$$

On peut montrer après un calcul direct utilisant (3.1.1), (3.1.2), (3.1.3) et les hypothèses 3.1.1 et 3.1.2 que

$$\frac{d}{dt}E(t) = -\int_{\mathbb{R}^3} N\frac{\mathbb{D}\nabla u.\nabla u}{u^2}\,dx \le -\alpha\int_{\mathbb{R}^3} N|\nabla \log u|^2\,dx.$$

Par conservation de la masse, on a que la constante u_∞ vaut $u_\infty = \mathcal{N}_I/(\int_{\mathbb{R}^3} e^{-V_\infty}\,dx)$, où $\mathcal{N}_I$ est la masse totale. Alors

$$\frac{d}{dt}E(t) \le -\alpha\int_{\mathbb{R}^3} N|\nabla(\log \frac{Ne^V}{u_\infty})|^2\,dx.$$

On rappelle l'inégalité de Sobolev logarithmique [2, 14, 19] : soient deux fonctions f et g positives telles que $\int_{\mathbb{R}^3} f\,dx = \int_{\mathbb{R}^3} g\,dx$ alors il existe un constante positive λ telle que

$$\int_{\mathbb{R}^3} f\log(f/g)\,dx \le \frac{1}{\lambda}\int_{\mathbb{R}^3} f|\nabla \log(f/g)|^2\,dx. \tag{3.2.21}$$

En appliquant (3.2.21) pour $f = N$ et $g = u_\infty e^{-V}$, on a

$$\frac{d}{dt}E(t) \le -\alpha\lambda\int_{\mathbb{R}^3} N\log\frac{N}{u_\infty e^{-V_\infty}}\,dx = -\alpha\lambda(\int_{\mathbb{R}^3} N\log\frac{N}{N_\infty}\,dx + \int_{\mathbb{R}^3} N\log\frac{N_\infty}{u_\infty e^{-V}}\,dx).$$

Par l'inégalité de Jensen sur la fonction convexe $-\log$, on a

$$-\log\frac{N_\infty}{u_\infty e^{-V}} = V_\infty - V - \log\left(\int_{\mathbb{R}^3} e^{V_\infty - V}\frac{N_\infty}{N}\,dx\right) \le V_\infty - V - \int_{\mathbb{R}^3}(V_\infty - V)\frac{N_\infty}{N}\,dx.$$

Donc on aboutit à

$$\begin{aligned}\frac{d}{dt}E(t) &\leq -\alpha\lambda \int_{\mathbb{R}^3} N \log \frac{N}{N_\infty}\, dx - \alpha\lambda \int_{\mathbb{R}^3} (N - N_\infty)(V - V_\infty)\, dx) \\ &\leq -\alpha\lambda \int_{\mathbb{R}^3} N \log \frac{N}{N_\infty}\, dx - \alpha\lambda \int_{\mathbb{R}^3} |\nabla_x (V - V_\infty)|^2\, dx,\end{aligned}$$

où on a utilisé l'équation de Poisson (3.1.2) dans la dernière inégalité. On en déduit donc avec l'expression de l'entropie relative (3.2.20) que $\frac{d}{dt}E(t) \leq -\alpha\lambda E(t)$. Finalement, $E(t) \leq E(0)\, e^{-\alpha\lambda t}$.

3.3 Existence des solutions

3.3.1 Cas d'une matrice de diffusion scalaire

Par soucis de complétude nous rappelons ici une méthode classique de démonstration de l'existence des solutions au problème dérive-diffusion-Poisson dans le cas où la matrice de diffusion vérifie $\mathbb{D} = Id$. Dans ce cas, une estimation L^2 locale de la densité peut être obtenue et l'existence est alors prouvée par une méthode de point fixe.

Tout d'abord, nous introduisons $\underline{N}$ et $\underline{V}$ des prolongements de classe C^2 au domaine Ω des données aux bords N_b et V_b.

Proposition 3.3.1 *Soit $T > 0$ et soit $N_0 \in L^2(\Omega)$. Si (N, V) est une solution faible de dérive-diffusion-Poisson* (3.1.1)-(3.1.2)-(3.1.3) *telle que $0 \leq N \in C([0,T], L^2(\Omega)) \cap L^2(0,T; H^1(\Omega))$ et $V \in C([0,T], H^2(\Omega))$. Alors il existe une constante C_T ne dépendant que de T, N_b, V_b et $\|N_0\|_{L^2(\Omega)}$ telle que $\forall\, t \in [0,T]$*

$$\|N\|_{L^2(\Omega)}(t) + \int_0^t \|N\|^2_{H^1(\Omega}\, dx \leq C_T.$$

Preuve. On multiplie l'équation de dérive-diffusion (3.1.1) par $(N - \underline{N})$ et on intègre. Après des intégrations par parties, on aboutit à

$$\begin{aligned}\frac{1}{2}\frac{d}{dt}\int_\Omega (N - \underline{N})^2\, dx + \int_\Omega \mathbb{D}(\nabla(N - \underline{N}) + (N - \underline{N})\nabla V) \cdot \nabla(N - \underline{N})\, dx = \\ \int_\Omega \text{div}\,(\mathbb{D}\nabla\underline{N})(N - \underline{N})\, dx + \int_\Omega \mathbb{D}(\underline{N}\nabla V) \cdot \nabla(N - \underline{N})\, dx\end{aligned} \tag{3.3.22}$$

Dans le cas où la matrice de diffusion $\mathbb{D} = Id$, on peut utiliser l'équation de Poisson pour traiter le 3$^{\text{ème}}$ terme du membre de gauche, contrairement au cas d'une matrice non scalaire :

$$\begin{aligned}\int_\Omega \mathbb{D}(N - \underline{N})\nabla V \cdot \nabla(N - \underline{N})\, dx &= \frac{1}{2}\int_\Omega \nabla(N - \underline{N})^2 \cdot \nabla V\, dx \\ &= \frac{1}{2}\int_\Omega N(N - \underline{N})^2\, dx.\end{aligned}$$

Grâce à la positivité de la densité, ce terme est positif. L'identité (3.3.22) devient donc

$$\frac{1}{2}\frac{d}{dt}\int_\Omega (N-\underline{N})^2\,dx + \int_\Omega |\nabla(N-\underline{N})|^2\,dx \le \int_\Omega \Delta\underline{N}(N-\underline{N})\,dx + \int_\Omega \underline{N}\nabla V\cdot\nabla(N-\underline{N})\,dx. \tag{3.3.23}$$

Par construction, la fonction $\underline{N}$ est de classe C^2, donc avec une inégalité de Cauchy-Schwarz, on peut facilement borner le permier terme du membre de droite par $C_1\|N-\underline{N}\|_{L^2(\Omega)}$ où C_1 est une constante positive. Pour le second terme du membre de droite, après des inégalités de Cauchy-Schwarz, on obtient

$$\int_\Omega \underline{N}\nabla V\cdot\nabla(N-\underline{N})\,dx. \le \|\nabla(N-\underline{N})\|^2_{L^2(\Omega)}\|\underline{N}\|_{L^4(\Omega)}\|\nabla V\|_{L^4(\Omega)}.$$

On peut maintenant utiliser la régularité elliptique de l'équation de Poisson qui nous donne

$$\|\nabla V\|_{L^4(\Omega)} \le C_2\|N\|_{L^2(\Omega)} + C_3 \le C_2\|N-\underline{N}\|_{L^2(\Omega} + C_4.$$

Donc, on a

$$\int_\Omega \underline{N}\nabla V\cdot\nabla(N-\underline{N})\,dx. \le \frac{1}{2}\int_\Omega |\nabla(N-\underline{N})|^2\,dx + C_5\int_\Omega (N-\underline{N})^2\,dx + C_6. \tag{3.3.24}$$

En injectant (3.3.24) dans (3.3.22), on obtient

$$\frac{1}{2}\frac{d}{dt}\int_\Omega (N-\underline{N})^2\,dx + \int_\Omega |\nabla(N-\underline{N})|^2\,dx \le C_1\|N-\underline{N}\|_{L^2(\Omega)} + C_5\int_\Omega (N-\underline{N})^2\,dx + C_6.$$

Le résultat énoncé dans la proposition s'obtient alors directement par un lemme de Gronwall.
□

Proposition 3.3.2 *Soient $T>0$ et $N_0 \in L^2_+(\Omega)$. Si $\mathbb{D} = Id$, il existe une unique solution faible (N,V) au système* (3.1.1)–(3.1.2)–(3.1.3) *telle que*

$$N \in C([0,T],L^2(\Omega)) \cap L^2(0,T;H^1(\Omega)), \qquad V \in C([0,T],H^2(\Omega)).$$

Preuve. On construit l'application $F : N \mapsto \widehat{N}$ définie par :

1. Pour $N \ge 0$ donné, on résoud l'équation de Poisson (3.1.2) : $-\Delta V = N$ avec les conditions aux bords $V = V_b$ sur $\partial\Omega$. On obtient alors V.

2. On résoud alors l'équation parabolique d'inconnue $\widehat{N}$:

$$\partial_t\widehat{N} - \text{div}\,(\nabla\widehat{N} + \widehat{N}\nabla V) = 0,$$

avec les conditions aux bords

$$\widehat{N}(t,x) = N_b(x) \quad \text{sur } \partial\Omega; \qquad \widehat{N}(0,x) = N_0(x) \quad \text{pour } x \in \Omega.$$

Des résultats classiques sur les équations paraboliques [21] prouvent l'existence et l'unicité de $\widehat{N} \geq 0$ et permettent de donner un sens à l'application F ainsi construite. En s'appuyant sur l'argumentation de [22], nous allons montrer que F réalise une contraction sur l'espace M_T définie par $M_T = \{n : \|n\|_T \leq 1\}$ où la norme est définie par

$$\|n\|_T = \left[\max_{0\leq t\leq T} \|n(t)\|_{L^2(\Omega)}^2 + \int_0^T \|n(t)\|_{H^1(\Omega)}\, dt\right]^{1/2}.$$

La valeur du paramètre T sera fixée durant la démonstration. Soient N et $\widetilde{N}$ deux éléments de M_T. On note $\delta F = F(\widetilde{N}) - F(N)$ qui vérifie :

$$\partial_t \delta F - \operatorname{div}\left(\nabla \delta F + \delta F \nabla V + F(\widetilde{N})\nabla(\delta V)\right) = 0, \tag{3.3.25}$$

avec les conditions aux frontières

$$\delta F(0,x) = 0 \quad x \in \Omega; \quad \delta F(t,x) = 0 \quad x \in \partial\omega.$$

En multipliant l'équation (3.3.25) par δF et en intégrant, on obtient après une intégration par parties

$$\frac{1}{2}\frac{d}{dt}\int_\Omega |\delta F|^2\, dx + \int_\Omega |\nabla(\delta F)|^2\, dx + \frac{1}{2}\int_\Omega \nabla((\delta F)^2)\cdot\nabla V\, dx + \int_\Omega F(\widetilde{N})\nabla(\delta V)\cdot\nabla(\delta F)\, dx = 0.$$

Grâce à l'équation de Poisson, le troisième terme s'écrit après une intégration par parties

$$\int_\Omega \nabla((\delta F)^2)\cdot\nabla V\, dx = \int_\Omega N((\delta F)^2)\, dx \geq 0.$$

Pour le dernier terme, avec des inégalités de Cauchy-Schwarz on a

$$\int_\Omega F(\widetilde{N})\nabla(\delta V)\cdot\nabla(\delta F)\, dx \leq \|\nabla(\delta F)\|_{L^2(\Omega)}\|F(\widetilde{N})\|_{L^4(\Omega)}\|\nabla(\delta V)\|_{L^4(\Omega)}.$$

La régularité elliptique de l'équation de Poisson permet alors d'écrire $\|\nabla(\delta V)\|_{L^4(\Omega)} \leq C_1\|\delta N\|_{L^2(\Omega)}$. On aboutit finalement à

$$\frac{1}{2}\frac{d}{dt}\int_\Omega |\delta F|^2\, dx + \frac{1}{2}\int_\Omega |\nabla(\delta F)|^2\, dx \leq C_2\|F(\widetilde{N})\|_{L^4(\Omega)}^2\|\delta N\|_{L^2(\Omega)}^2. \tag{3.3.26}$$

En prenant $\widetilde{N} = 0$ dans cette identité, on trouve après une intégration

$$\|F(N)\|_T \leq C_3 T,$$

où C_3 est une constante positive qui ne dépend que des données. Bien évidemment on a la même estimation si on remplace N par $\widetilde{N}$ et donc en intégrant (3.3.26) il suit,

$$\begin{aligned}\forall\, t \in [0,T], \quad \int_\Omega |\delta F|^2\, dx + \int_0^t \int_\Omega |\nabla(\delta F)|^2\, dxds \;&\leq C_4 T\int_0^t \|\delta N\|_{L^2(\Omega)}^2\, ds \\ &\leq C_4 T^2\|\delta N\|_T^2.\end{aligned}$$

Donc en prenant T assez petit, F réalise une contraction sur M_T. On construit alors une unique solution sur un intervalle $[0,T_0]$. Ensuite, grâce à l'estimation L^2 uniforme et en changeant l'origine des temps en T_0, on peut prouver de même l'existence et l'unicité d'une solution sur $[T_0, 2T_0]$. En réitérant ce procédé, on construit une solution sur $[0,T]$. □

3.3.2 Régularisation

Dans la cas où la matrice de diffusion $\mathbb{D}$ n'est plus scalaire, l'estimation L^2 sur la densité n'est plus valable. Donc on doit travailler dans le cadre $L \log L$. Une technique classique (voir [4, 25]) consiste à régulariser le système : pour $\varepsilon > 0$ et m assez grand ($m \geq 2$ suffit), on considère le problème modifié :

$$\partial_t N^\varepsilon - \text{div}\,(\mathbb{D}(\nabla N^\varepsilon + N^\varepsilon \nabla V^\varepsilon)) = 0 \tag{3.3.27}$$
$$-(1-\varepsilon\Delta)^{2m}\Delta V^\varepsilon = N^\varepsilon \tag{3.3.28}$$

soumis à la condition initiale régularisée $N(0,x) = N^{0,\varepsilon}(x)$ et aux conditions aux bords :

$$N^\varepsilon(t,x) = N_b \quad ; \quad V^\varepsilon(t,x) = V_b \quad \text{et} \quad \Delta V^\varepsilon = \ldots = \Delta^{2m} V^\varepsilon = 0 \quad \text{pour } x \in \partial\Omega. \tag{3.3.29}$$

Pour ce système, on définit de même les solutions N^ε_∞, V^ε_∞ du système stationnaire correspondant. L'entropie relative de ce nouveau système est :

$$E^\varepsilon(t) = \int_\Omega (N^\varepsilon \log \frac{N^\varepsilon}{N^\varepsilon_\infty} + N^\varepsilon_\infty - N^\varepsilon)\, dx + \frac{1}{2}\int_\Omega |(1-\varepsilon\Delta)^m \nabla(V^\varepsilon - V^\varepsilon_\infty)|^2\, dx. \tag{3.3.30}$$

On définit l'application $F : N \mapsto \widehat{N}$ par :

1. Pour N donné, on résout l'équation de Poisson (3.3.28) et on obtient un potentiel V.

2. Pour ce potentiel V, on résout dérive-diffusion 3.3.27 et on appelle $\widehat{N}$ la solution.

On peut alors montrer de la même manière que dans la preuve de la Proposition 3.3.2 (voir [22]; ce point est aussi détaillé au chapitre suivant avec en plus un couplage quantique) que F réalise une contraction sur $\{n : \max_{0\leq t\leq T} \|n(t)\|^2_{L^2(\Omega)} + \int_0^T \|n(s)\|^2_{H^1(\Omega)}\, ds < \infty\}$ pour $T \leq T_0$ assez petit. Donc on construit une solution sur $[0, T_0]$ qu'on peut étendre sur $[0, T]$ pour T quelconque.

Ainsi, on est capable de construire une solution $(N^\varepsilon, V^\varepsilon)$ du problème modifié (3.3.27)–(3.3.28) telle que $N^\varepsilon \in C(\mathbb{R}_+, L^2(\Omega))$ et $V^\varepsilon \in C(\mathbb{R}_+, H^{4m+2}(\Omega))$.

3.3.3 Passage à la limite $\varepsilon \to 0$

Pour obtenir des solutions au système non régularisé, il convient de passer à la limite $\varepsilon \to 0$. Pour ce faire, nous allons tout d'abord obtenir des estimations indépendantes de ε puis utiliser une méthode de compacité de Aubin-Lions. On rappelle un lemme d'Aubin :

Lemma 3.3.3 (Aubin) *Soient $T > 0$, $q \in (1, +\infty)$ et soit $(f_n)_{n\in\mathbb{N}}$ une suite bornée de fonctions dans $L^q(0,T;H)$ où H est un espace de Banach. Si $(f_n)_{n\in\mathbb{N}}$ est bornée dans $L^q(0,T;V)$ où V s'injecte de manière compacte dans H et $\partial f_n/\partial t$ est bornée dans $L^q(0,T;V')$ uniformément par rapport à $n \in \mathbb{N}$, alors $(f_n)_{n\in\mathbb{N}}$ est relativement compact dans $L^q(0,T;H)$.*

On a pour tout $t > 0$,

$$\frac{d}{dt}E^\varepsilon(t) = -\int_\Omega e^{-V^\varepsilon}\frac{\mathbb{D}\nabla u^\varepsilon.\nabla u^\varepsilon}{u^\varepsilon}\,dx \le -\alpha\int_\Omega e^{-V^\varepsilon}\frac{|\nabla u^\varepsilon|^2}{u^\varepsilon}\,dx.$$

Notre hypothèse sur la donnée initiale $N_0 \in L^{6/5}(\Omega)$ nous permet de borner l'entropie relative initiale $E^\varepsilon(0)$ par une constante C_0 indépendante de ε. Donc en intégrant sur $[0,t]$ pour tout $t > 0$, on a :

$$E^\varepsilon(t) + \alpha\int_0^t\int_\Omega e^{-V^\varepsilon}\frac{|\nabla u^\varepsilon|^2}{u^\varepsilon}\,dxd\tau \le E^\varepsilon(0) \le C_0. \tag{3.3.31}$$

D'après le lemme 3.4 de [4], on a $\|\Delta V^\varepsilon\|_{L^2(\Omega)} \le \|(1-\varepsilon\Delta)^m\Delta V^\varepsilon\|_{L^2(\Omega)}$. Donc on peut montrer comme en (3.2.11) que

$$\int_\Omega e^{-V^\varepsilon}\frac{|\nabla u^\varepsilon|^2}{u^\varepsilon}\,dx \ge \int_\Omega 4|\nabla\sqrt{N^\varepsilon}|^2\,dx - C, \tag{3.3.32}$$

où C est une constante positive indépendante de ε. Grâce aux estimations (3.3.31) et (3.3.32), on obtient directement que $\sqrt{N^\varepsilon}$ est borné dans $L^2_{loc}(\mathbb{R}^+, H^1(\Omega))\cap L^\infty(\mathbb{R}^+, L^2(\Omega))$. En écrivant $\nabla N = 2\sqrt{N}\nabla\sqrt{N}$, on obtient par l'inégalité de Hölder :

$$\int_\Omega |\nabla V|^{6/5}\,dx \le 2^{6/5}\left(\int_\Omega |\nabla\sqrt{N}|^2\,dx\right)^{3/5}\left(\int_\Omega |\sqrt{N}|^3\,dx\right)^{2/5}.$$

Et avec une interpolation, on a

$$\left(\int_\Omega |\sqrt{N}|^3\,dx\right)^{2/5} = \|\sqrt{N}\|^{6/5}_{L^3(\Omega)} \le \|\sqrt{N}\|^{3/5}_{L^2(\Omega)}\|\sqrt{N}\|^{6/5}_{L^6(\Omega)}.$$

Donc avec l'injection $H^1(\Omega) \hookrightarrow L^6(\Omega)$, on a :

$$\int_\Omega |\nabla V|^{6/5}\,dx \le C\|\sqrt{N}\|^{3/5}_{L^2(\Omega)}\|\sqrt{N}\|^{9/5}_{H^1(\Omega)}.$$

Il en résulte que N^ε est borné dans $L^{10/9}_{loc}(\mathbb{R}_+, W^{1,6/5}(\Omega))$ indépendamment de ε. Et par l'inégalité de Cauchy-Schwarz, on a pour tout $t \in \mathbb{R}^+$

$$\int_0^t\left(\int_\Omega |\nabla N^\varepsilon + N^\varepsilon\nabla V^\varepsilon|\,dx\right)^2 dt \le \sup_{s\in[0,t]}\|N^\varepsilon\|_{L^1(\Omega)}(s)\int_0^t\int_\Omega \frac{|\nabla N^\varepsilon + N^\varepsilon\nabla V^\varepsilon|^2}{N^\varepsilon}\,dxdt.$$

En rappelant l'expression de la variable de Slotboom $u^\varepsilon = N^\varepsilon e^{V^\varepsilon}$, on déduit de (3.3.31) et de l'inégalité précédente que le courant $J^\varepsilon = \mathbb{D}(\nabla N^\varepsilon + N^\varepsilon\nabla V^\varepsilon)$ est borné indépendamment de ε dans $L^2_{loc}(\mathbb{R}^+, L^1(\Omega))$. Donc avec l'équation de dérive-diffusion (3.3.27), on a que $\partial_t N^\varepsilon$ est borné dans $L^2_{loc}(\mathbb{R}^+, W^{-1,1}(\Omega))$. On peut donc utiliser le lemme d'Aubin pour en déduire qu'il existe une sous-suite, que nous dénoterons abusivement N^ε, qui converge vers N dans $L^1_{loc}(\mathbb{R}_+, L^1(\Omega))$. Pour ce N, on pose alors V la solution du problème de Poisson

$-\Delta V = N$ avec les conditions aux bords $V = V_b$ sur $\partial\Omega$. On a alors, $V^\varepsilon \to V$ dans $L^2_{loc}(\mathbb{R}^+, H^1(\Omega))$. Par les propriétés de la trace et l'injection compacte de $W^{1/2,6/5}(\Omega) \hookrightarrow L^1(\Omega)$, on retrouve que $N_{|\partial\Omega} = N_b$. De plus, grâce à la semi-continuité, on a pour tout $t > 0$

$$E(t) + \int_0^t \int_\Omega e^{-V} \frac{\mathbb{D}\nabla u.\nabla u}{u}\, dxds \le \liminf_{\varepsilon\to 0} E^\varepsilon(t) + \int_0^t \int_\Omega e^{-V^\varepsilon} \frac{\mathbb{D}\nabla u^\varepsilon.\nabla u^\varepsilon}{u^\varepsilon}\, dx \le C_0.$$

Ceci permet de récupérer la borne de $\sqrt{N}$ dans $L^2_{loc}(\mathbb{R}^+, H^1(\Omega))$ qu'on avait en (3.2.11) et la borne de V dans $L^\infty_{loc}(\mathbb{R}^+, H^1(\Omega))$. De plus, le courant est borné dans $L^2_{loc}(\mathbb{R}^+, L^1(\Omega))$. Donc l'équation (3.3.27) pour $\varepsilon = 0$ a un sens. On peut passer à la limite dans cette équation de dérive-diffusion et montrer que le courant J^ε converge au sens des distributions vers J.

On a alors obtenu des solutions (N, V) de (3.1.1)–(3.1.2)–(3.1.3) satisfaisant (3.1.7).

Remarque 3.3.4 *Dans le cas où on considère que le domaine n'est plus borné, il faut de plus avoir une estimation sur $|x|^2 N^\varepsilon(t,x)$ dans $L^\infty_{loc}(\mathbb{R}^+, L^1(\Omega))$ indépendante de ε. En effet, on n'a qu'une majoration sur la quantité $\int_{\mathbb{R}^3} N^\varepsilon \log N^\varepsilon\, dx$ et il faut pouvoir s'assurer qu'elle n'explose pas vers $-\infty$ (voir [8]).*

3.3.4 Régularité en temps long

Comme dans la partie 3.2.1, on peut montrer grâce à (3.3.30) et (3.3.32) que l'entropie E^ε décroît vers 0 quand t tends vers $+\infty$. Considérons maintenant l'entropie linéarisée (avec les notations $n^\varepsilon = N^\varepsilon - N^\varepsilon_\infty$, $v^\varepsilon = V^\varepsilon - V^\varepsilon_\infty$):

$$L^\varepsilon(t) = \frac{1}{2}\int_\Omega \frac{(n^\varepsilon)^2}{N^\varepsilon_\infty}\, dx + \frac{1}{2}\int_\Omega |\nabla v^\varepsilon|^2\, dx. \tag{3.3.33}$$

Des calculs similaires à la partie 3.2.2 amènent à l'inegalité :

$$\frac{d}{dt} L^\varepsilon(t) \le -C_1 L^\varepsilon(t) + C_2 L^\varepsilon(t)^4, \tag{3.3.34}$$

où C_1 et C_2 sont indépendantes de ε. Dans la partie 3.2.2 on a démontré l'existence de $t^\varepsilon_* > 0$ tel que $L^\varepsilon(t^\varepsilon_*)^3 \le C_1/(2C_2)$. Alors il existe deux constantes positives C et λ indépendantes de ε telle que pour tout $t \ge t^\varepsilon_*$, $L^\varepsilon(t) \le Ce^{-\lambda t}$. Le point crucial est de trouver un tel t^ε_* borné uniformément par rapport à ε.

Tout d'abord, on peut prouver facilement par une argumentation par l'absurde que pour tout $\eta > 0$ il existe $\alpha(\eta) > 0$ tel que,

$$\left(\forall\, \varepsilon > 0, \quad \forall\, t \ge 0, \quad \int_\Omega e^{-V^\varepsilon(t)} \frac{|\nabla u^\varepsilon(t)|^2}{u^\varepsilon(t)}\, dx \le \alpha(\eta)\right) \implies L^\varepsilon(t) \le \eta. \tag{3.3.35}$$

Ensuite, l'inégalité (3.3.31) implique qu'il existe une constant positive C_0 telle que

$$\forall\, T > 0, \quad \exists\, t^\varepsilon(T) \in [0, T] \quad \text{tel que} \quad \int_\Omega e^{-V^\varepsilon(t^\varepsilon(T))} \frac{|\nabla u^\varepsilon(t^\varepsilon(T))|^2}{u^\varepsilon(t^\varepsilon(T))}\, dx \le \frac{C_0}{T} \tag{3.3.36}$$

Donc , en choisissant $\eta = (C_1/(2C_2))^{1/3}$ dans (3.3.35) et $T \geq C_0/\alpha(\eta)$ dans (3.3.36), on déduit que le $t^\varepsilon(T)$ correspondant peut être pris comme notre t_*^ε.

Finalement, sur $[T, \infty)$ on a l'estimation $L^\varepsilon(t) \leq Ce^{-\lambda t}$. Comme pour tout $t \geq T$ on a $L(t) \leq \liminf_{\varepsilon \to 0} L^\varepsilon(t) \leq Ce^{-\lambda t}$ (L défini en (4.3.11)), on déduit que N appartient à $C([T, \infty), L^2(\Omega))$. □

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Chapter 4

Théorie L^2 pour le système DDSP (dérive-diffusion-Schrödinger-Poisson)

Joint work with N. Ben Abdallah [1] and F. Méhats [2].

4.1 Introduction and main result

In this chapter, we present the analysis of the DDSP system introduced in the beginning of this PhD in the case where the diffusion matrix is assumed to be the identity. We recall that this system models the transport of a particle system which is partially quantized in one direction (denoted by z) and which, in the transport direction denoted by x, has a diffusive motion. The system is at equilibrium in the confined direction with a local Fermi level ϵ_F which depends on the transport variable x. The variable x is assumed to lie in a bounded regular domain $\omega \in \mathbb{R}^2$ while z belongs to the interval $(0,1)$. The spatial domain is then $\Omega = \omega \times (0,1)$. At a time t and a position (x,z), we recall that the particle density $N(t,x,z)$ is given by :

$$N(t,x,z) = N_s(t,x) \sum_{k=1}^{+\infty} \frac{e^{-\epsilon_k(t,x)}}{\mathcal{Z}(t,x)} |\chi_k(t,x,z)|^2, \tag{4.1.1}$$

where the repartition function $\mathcal{Z}$ is defined by

$$\mathcal{Z}(t,x) = \sum_{k=1}^{+\infty} e^{-\epsilon_k(t,x)}, \tag{4.1.2}$$

[1] MIP, UMR 5640, Université Paul Sabatier, Toulouse.
[2] IRMAR, Université Rennes 1, Rennes.

and (χ_k, ϵ_k) is the complete set of eigenfunctions and eigenvalues of the Schrödinger operator in the z variable

$$\begin{cases} -\frac{1}{2}\,\partial_z^2\chi_k + V\chi_k = \epsilon_k\chi_k & (k \geq 1), \\ \chi_k(t,x,\cdot) \in H_0^1(0,1), & \int_0^1 \chi_k\,\chi_\ell\,dz = \delta_{k\ell}\,. \end{cases} \tag{4.1.3}$$

The electrostatic potential V is a solution of the Poisson equation

$$-\Delta_{x,z}V = N. \tag{4.1.4}$$

The surface density N_s satisfies the drift-diffusion equation

$$\partial_t N_s - \mathrm{div}_x\,(\nabla_x N_s + N_s\,\nabla_x V_s) = 0, \tag{4.1.5}$$

where the effective potential V_s is given by

$$V_s = -\log\sum_k e^{-\epsilon_k}. \tag{4.1.6}$$

The unknowns of the overall system are the surface density $N_s(t,x)$, the eigenenergies $\epsilon_k(t,x)$, the eigenfunctions $\chi_k(t,x,z)$ and the electrostatic potential $V(t,x,z)$. The Fermi level ϵ_F is determined by :

$$\epsilon_F(t,x) = \log\frac{N_s(t,x)}{\mathcal{Z}(t,x)}. \tag{4.1.7}$$

This will be useful for the study of global equilibria. The system (4.1.3)–(4.1.2) is completed with the initial condition

$$N_s(0,x) = N_s^0(x) \tag{4.1.8}$$

and with the following boundary conditions :

$$\begin{cases} N_s(t,x) = N_b(x), \quad V(t,x,z) = V_b(x,z), & \text{for } x \in \partial\omega, \quad z \in (0,1), \\ \partial_z V(t,x,0) = \partial_z V(t,x,1) = 0, & \text{for } x \in \omega. \end{cases} \tag{4.1.9}$$

In application like the Double-Gate transistor [4], the frontier $\partial\omega\times[0,1]$ includes the source and the drain contacts as well as insulating or artificial boundary. On the other hand $\omega\times\{0\}$ and $\omega\times\{1\}$ represent the gate contacts (in addition to possible insulating boundaries). Mixed type boundary conditions are then to be prescribed. The boundary conditions (4.1.9) do not take into account this complexity and are chosen for the mathematical convenience : elliptic regularity properties of the Poisson equation (4.1.4) are needed in our proofs.

4.1.1 Main Results

Assumption 4.1.1

- *The initial condition satisfies* $N_s^0 \in L^2(\omega)$ *and* $N_s^0 \geq 0$, *a.e.*
- *The boundary data for the surface density satisfy* $0 < N_1 \leq N_b \leq N_2$ *a.e., where* N_1 *and* N_2 *are positive constants,* $N_b \in C^2(\partial\omega)$.
- *The Dirichlet datum for the potential satisfies* $V_b \in C^2(\partial\omega \times [0,1])$ *and the compatibility condition*
$$\frac{\partial V_b}{\partial z}(x,0) = \frac{\partial V_b}{\partial z}(x,1) = 0, \quad \forall\, x \in \partial\omega.$$

The first result of this paper is the following existence and uniqueness theorem:

Theorem 4.1.2 *Let* $T > 0$ *be fixed. Under Assumption* 4.1.1*, the system* (4.1.3)–(4.1.9) *admits a unique weak solution such that*

$$N_s \in C([0,T], L^2(\omega)) \cap L^2((0,T), H^1(\omega)), \qquad V \in C([0,T], H^2(\Omega)).$$

The second result concerns the asymptotic behaviour of the solution as times tends to $+\infty$. To this aim, we shall first define the notion of global equilibrium for boundary data, under which we show that there exists a unique stationary solution, and finally prove that the time dependent solution converges exponentially fast to this stationary solution.

Assumption 4.1.3 *The boundary is said to be at global equilibrium if there exists a real number* $u^\infty > 0$ *such that* $\forall\, x \in \partial\omega$, $N_b(x) = u^\infty e^{-V_s^\infty(x)}$*, where* V_s^∞ *is defined by*

$$V_s^\infty(x) = -\log\Big(\sum_k e^{-\epsilon_k[V_b](x)}\Big).$$

In view of (4.1.7)*, it means that the Fermi level at the boundary is constant.*

In this assumption, as well as in the sequel of the paper, for each potential V, the notation $\epsilon_k[V]$ stands for the kth eigenvalue of the Hamiltonian $-\frac{1}{2}\partial_z^2 + V$ and $\chi_k[V]$ denotes the corresponding eigenfunction (solving (4.1.3)).

The stationary problem reads

$$\begin{cases} -\mathrm{div}_x \left(\nabla_x N_s^\infty + N_s^\infty \nabla_x V_s^\infty\right) = 0, \\ -\dfrac{1}{2}\partial_z^2 \chi_k^\infty + V^\infty \chi_k^\infty = \epsilon_k^\infty\, \chi_k^\infty, \\ -\Delta_{x,z} V^\infty = N^\infty = \dfrac{N_s^\infty}{\mathcal{Z}^\infty} \displaystyle\sum_{k=1}^{+\infty} |\chi_k^\infty|^2 e^{-\epsilon_k^\infty}, \\ \mathcal{Z}^\infty = \displaystyle\sum_{\ell=1}^{+\infty} e^{-\epsilon_\ell^\infty}, \end{cases} \tag{4.1.10}$$

with the boundary conditions

$$\begin{cases} N_s^\infty(x) = N_b(x), \quad V^\infty(x,z) = V_b(x,z) & \text{for } x \in \partial\omega, \quad z \in (0,1), \\ \partial_z V^\infty(x,0) = \partial_z V^\infty(x,1) = 0 & \text{for } x \in \omega, \end{cases} \tag{4.1.11}$$

where we have used the short notation ϵ_k^∞ for $\epsilon_k[V^\infty]$ and χ_k^∞ for $\chi_k[V^\infty]$.

Proposition 4.1.4 *Under Assumptions* 4.1.1 *and* 4.1.3*, the stationary problem* (4.1.10)–(4.1.11) *admits a unique solution such that* $N_s^\infty \in C^2(\overline{\omega})$ *and* $V^\infty \in C^2(\overline{\Omega})$.

The following theorem proves the exponential convergence of the time dependent solution towards the stationary one.

Theorem 4.1.5 *Let Assumptions* 4.1.1 *and* 4.1.3 *hold. Let* N_s, V *and* N_s^∞, V^∞ *be respectively the time dependent and the stationary solutions defined respectively in Theorem* 4.1.2 *and Proposition* 4.1.4. *There exist two constants* $\lambda > 0$ *and* $C > 0$ *such that for all* $t \geq 0$,

$$\|N_s - N_s^\infty\|_{L^2(\omega)}(t) + \|V - V^\infty\|_{H^1(\omega)}(t) \leq C e^{-\lambda t}.$$

The outline of the chapter is as follows. In Section 4.2, we prove Theorem 4.1.2. The strategy of the proof as well as various notations are detailed in Subsection 4.2.1. Let us just mention that two essential ingredients are used : the first is a relative entropy inequality which provides preliminary estimates on the solution, which are then completed with an L^2 estimate on the surface density. The second ingredient is the analysis of the Schrödinger-Poisson system (4.1.3)-(4.1.4) which is shown to be uniquely solvable by convex minimization techniques in the spirit of [28, 29, 30]. Section 4.3 is devoted to the proof of Theorem 4.1.5 which uses a quadratic approximation of the relative entropy given in section 4.2, and which is a Lyapunov functional for the linearized system around the stationary solution. We will usually refer to the Appendix (at the end of this PhD) for some technical lemmata and classical results for Sturm-Liouville operators.

4.2 Existence and uniqueness (Proof of Theorem 4.1.2)

4.2.1 Notations and strategy of the proof

As done in [7], we view the system as a two dimensional drift-diffusion equation (4.1.5) for the surface density coupled to the quasistatic Schrödinger-Poisson system (4.1.3), (4.1.4). The drift-diffusion equation determines the value of the surface density in terms of the electrostatic potential, while the Schrödinger-Poisson systems allows to compute the potential as a function of the surface density.

The overall problem is then solved by a fixed-point procedure for the unknown N_s, as for the standard drift-diffusion-Poisson problem [18, 26, 27]. The global in time existence heavily relies on an entropy estimate.

The first block now in the proof is to consider the quasistatic Schrodinger-Poisson system which consists, for any given nonnegative function $N_s(x)$ defined on ω, in finding a potential $V(x,z)$ defined on Ω and satisfying

$$
\left\{
\begin{array}{l}
-\Delta_{x,z} V = N(x,z); \quad (x,z) \in \Omega \\
N(x,z) = N_s(x) \displaystyle\sum_{k=1}^{+\infty} \frac{e^{-\epsilon_k(x)}}{\mathcal{Z}(x)} \, |\chi_k(x,z)|^2 \,; \quad \mathcal{Z}(x) = \sum_{\ell=1}^{+\infty} e^{-\epsilon_\ell(x)} \\
\left\{
\begin{array}{ll}
-\dfrac{1}{2}\, \partial_z^2 \chi_k + V \chi_k = \epsilon_k \chi_k & (k \geq 1), \\
\chi_k(t,x,\cdot) \in H_0^1(0,1), & \displaystyle\int_0^1 \chi_k \, \chi_\ell \, dz = \delta_{k\ell} \,,
\end{array}
\right. \\
V = V_b \text{ on } \partial\omega \times (0,1), \quad \partial_z V(x,0) = \partial_z V(x,1) = 0 \quad \text{for } x \in \omega.
\end{array}
\right.
\tag{4.2.12}
$$

For this problem, we have the following result whose proof (which relies on technical properties of the spectrum of the Hamiltonian stated in the Appendix) is postponed.

Proposition 4.2.1 *Let $N_s \in L^2(\omega)$ such that $N_s \geq 0$. Then the system* (4.2.12) *admits a unique solution $(V, (\epsilon_k, \chi_k)_{k\geq 1})$, which satisfies the estimates $\|V\|_{H^2(\Omega)} \leq C(N_s)$, the constant $C(N_s)$ depending only on the $L^2(\omega)$ norm of N_s. Moreover, for two arbitrary data N_s and $\widetilde{N_s}$, the corresponding solutions satisfy :*

$$
\|V - \widetilde{V}\|_{H^2(\Omega)} \leq C(N_s, \widetilde{N_s}) \, \|N_s - \widetilde{N_s}\|_{L^2(\omega)}.
$$

In order to prove existence of solutions of the overall problem, we need to show some *a priori* estimates for the solution. We shall begin with a relative entropy inequality (see e.g. [2, 3, 16] for classical counterparts), then show a uniform L^p estimate for the surface density. In order to do so, we proceed like in the standard drift-diffusion case [18] and define the slotboom variable

$$
u = e^{\epsilon_F} = \frac{N_s}{\mathcal{Z}}. \tag{4.2.13}
$$

We also define the surface current density

$$
J_s = -\nabla_x N_s - N_s \nabla_x V_s = -\sum_k e^{-\epsilon_k} \nabla_x u, \tag{4.2.14}
$$

in such a way that the drift-diffusion equation is written

$$
\partial_t N_s + \operatorname{div}_x \, J_s = 0.
$$

We denote by ρ_k the occupation factor of the kth subband

$$
\rho_k = u \, e^{-\epsilon_k} \tag{4.2.15}
$$

so that

$$
N = \sum_k \rho_k \, |\chi_k|^2 \quad ; \quad N_s = \sum_k \rho_k.
$$

Now we introduce two extensions $\underline{N_s}$ and $\underline{V}$ of the boundary data. These extensions are respectively defined on ω and Ω and chosen in such a way that

- $\underline{N_s} \in C^2(\overline{\omega})$, $0 < \underline{N_1} \leq \underline{N_s} \leq \underline{N_2}$ with two nonnegative constants N_1 and N_2, and $\underline{N_s}|_{\partial\omega} = N_b$.
- $\underline{V} \in C^2(\overline{\Omega})$ and satisfies the boundary conditions: $\underline{V}|_{\partial\omega\times(0,1)} = V_b$ and for all $x \in \omega$, $\partial_z \underline{V}(x,0) = \partial_z \underline{V}(x,1) = 0$.

It is clear that for regular enough domains such functions exist. Solving (4.1.3) with $\underline{V}$ instead of V, we find two sequences $\epsilon_k[\underline{V}](x)$ and $\chi_k[\underline{V}](x,z)$, that we shall shortly denote by $\underline{\epsilon_k}$ and $\underline{\chi_k}$. We then define $\underline{u}$, $\underline{\epsilon_F}$, $\underline{\mathcal{Z}}$ and $\underline{\rho_k}$ by

$$\underline{u} = \frac{\underline{N_s}}{\underline{\mathcal{Z}}} \quad ; \quad \underline{\mathcal{Z}} = \sum_k e^{-\underline{\epsilon_k}} \quad ; \quad \underline{\epsilon_F} = \log \underline{u} \quad ; \quad \underline{\rho_k} = \underline{u} e^{-\underline{\epsilon_k}} = e^{\underline{\epsilon_F} - \underline{\epsilon_k}},$$

as well as the density

$$\underline{N}(x,z) = \sum_k \underline{\rho_k}(x) |\underline{\chi_k}(x,z)|^2.$$

It is readily seen that

$$\|\nabla_x \underline{u}/\underline{u}\|_{L^\infty(\omega)} < \infty. \tag{4.2.16}$$

The relative entropy of (ρ_k, V) with respect to $(\underline{\rho_k}, \underline{V})$ is defined by:

$$\begin{aligned} W = & \sum_k \int_\omega (\rho_k \log(\rho_k/\underline{\rho_k}) - \rho_k + \underline{\rho_k})\, dx + \frac{1}{2} \iint_\Omega |\nabla_{x,z}(V - \underline{V})|^2 \, dxdz \\ & + \int_\omega \sum_k u\, e^{-\epsilon_k} \left(\epsilon_k[V] - \epsilon_k[\underline{V}] - \langle |\chi_k|^2 (V - \underline{V}) \rangle \right) \, dx, \end{aligned} \tag{4.2.17}$$

where we use the notation $\langle f \rangle = \int_0^1 f\, dz$. As will be shown later on, the three terms of right hand side of the above identity are nonnegative. Besides, W has the following compact form

$$W = \iint_\Omega \left(N(\epsilon_F - V - (\underline{\epsilon_F} - \underline{V})) - N + \underline{N} \right) \, dxdz + \frac{1}{2} \iint_\Omega |\nabla_{x,z}(V - \underline{V})|^2 \, dxdz.$$

Let us comment on this formula. One can note that the familiar form of the relative entropy for classical drift-diffusion systems is recovered here. The main difference is that, in the classical case, the relation between the Fermi level, the electrostatic potential and the density is local: $\epsilon_F - V = \log N$ (see e.g. [2, 10, 18]), while here this relation is non local in space. This form is also similar to the one recently obtained in [20] for a fully quantum drift-diffusion model (QDD). This model was derived in [13] by following the strategy of quantum moments developed in [15] (see also the review paper [14]). It consists of a 3D drift-diffusion equation involving a quantum chemical potential which depends on the density in a non local way, *via* the resolution of a quasistatic auxiliary quantum problem. In the QDD model, the quantum chemical potential is the generalization of the term $\epsilon_F - V$ of the present model.

The following two propositions provide some *a priori* estimates needed for the resolution of the coupled system:

Proposition 4.2.2 *Let $T>0$. Let (N_s, V) be a weak solution of* (4.1.5), (4.1.3), (4.1.4), (4.1.9) *such that $N_s \in C([0,T], L^2(\omega)) \cap L^2([0,T], H^1(\omega))$ and $V \in C([0,T], H^2(\Omega))$. Then we have*

$$\forall t \in [0,T], \qquad 0 \leq W(t) < C_T,$$

where C_T is a constant only depending on T, $W(0)$ and $\underline{u}$.

Proposition 4.2.3 *Let $T > 0$ and assume that $N_s^0 \in L^p(\omega)$ for some $p \in [2, +\infty]$ and let (N_s, V) be weak solution of* (4.1.5), (4.1.3), (4.1.4), (4.1.9) *such that $N_s \in C([0,T], L^2(\omega)) \cap L^2([0,T], H^1(\omega))$ and $V \in C([0,T], H^2(\Omega))$. Then*

$$N_s \in C([0,T], L^p(\omega)),$$

for any $T > 0$, with a bound depending only on T, N_b, V_b and $\|N_s^0\|_{L^p(\omega)}$.

4.2.2 Proof of the entropy inequality

The aim of this subsection is the proof of Proposition 4.2.2. Let (N_s, V) be a weak solution of (4.1.5), (4.1.3), (4.1.4). Since $V \in C([0,T], H^2(\Omega))$, by Lemma B.0.9, we deduce that $V_s \in C([0,T], H^2(\Omega))$. This is enough to ensure that $N_s \geq 0$, thanks to the maximum principle for parabolic equations (see for instance [25]).

The relative entropy is the sum of three positive terms.
Let us now show that the relative entropy W defined by (4.2.17) is nonnegative. This is obviously the case for the two first terms. In order to deal with the third one, let us denote $\epsilon_k^s := \epsilon_k[sV + (1-s)\underline{V}]$, and $\chi_k^s = \chi_k[sV + (1-s)\underline{V}]$. Straightforward computations using Lemma B.0.3 of the Appendix lead to

$$\sum_k u\, e^{-\epsilon_k} \left(\epsilon_k[V] - \epsilon_k[\underline{V}] - \langle |\chi_k|^2 (V - \underline{V})\rangle\right) =$$
$$= \int_0^1 \int_1^s \sum_{k,\ell \neq k} u \, \frac{e^{-\epsilon_k} - e^{-\epsilon_\ell}}{\epsilon_k^\sigma - \epsilon_\ell^\sigma} \langle \chi_k^\sigma (V - \underline{V}) \chi_\ell^\sigma \rangle^2 \, d\sigma ds \;\geq 0,$$

since the sequence $(\epsilon_k = \epsilon_k[V])_{k \geq 1}$ is increasing. This is enough to conclude that $W \geq 0$, as the sum of three nonnegative terms.

The initial relative entropy is finite.
Since $N_s^0 \in L^2(\omega)$, then by Proposition 4.2.1 we have $V \in H^2(\Omega) \subset L^\infty(\Omega)$. From Lemma B.0.1 we deduce that

$$\|\epsilon_k - \frac{1}{2}\pi^2 k^2\|_{L^\infty(\omega)} \leq \|V\|_{L^\infty(\Omega)}.$$

This is enough to deduce that $W(0) < +\infty$.

Relative entropy dissipation.
Let us now compute dW/dt. We first remark that

$$\frac{d}{dt} \sum_k \int_\omega (\rho_k \log(\rho_k/\underline{\rho_k}) - \rho_k + \underline{\rho_k}) \, dx = \sum_k \int_\omega \partial_t \rho_k \, \log(\rho_k/\underline{\rho_k}) \, dx.$$

Taking advantage from the identity $N_s = \sum \rho_k$ and from $\log \rho_k = \log u - \epsilon_k$, the right hand side is equal to

$$\int_\omega \partial_t N_s \log(u/\underline{u})\, dx - \sum_k \int_\omega \partial_t \rho_k\, (\epsilon_k - \underline{\epsilon_k})\, dx.$$

With the identity $\partial_t \epsilon_k = \langle |\chi_k|^2\, \partial_t V \rangle$ (see Lemma (B.0.3)) and (4.1.5) we obtain

$$\begin{aligned}\frac{d}{dt}\sum_k \int_\omega (\rho_k \log(\rho_k/\underline{\rho_k}) - \rho_k + \underline{\rho_k})\, dx = & \int_\omega \mathrm{div}_x \left(\sum_k e^{-\epsilon_k} \nabla_x u \right) \log \frac{u}{\underline{u}}\, dx \\ & -\frac{d}{dt}\int_\omega \sum_k \rho_k (\epsilon_k - \underline{\epsilon_k})\, dx \\ & + \iint_\Omega \sum_k \rho_k |\chi_k|^2 \partial_t V\, dxdz.\end{aligned}$$

The Poisson equation and the fact that $V = \underline{V}$ on $\partial\omega \times (0,1)$ give

$$\begin{aligned}\frac{d}{dt}\frac{1}{2}\iint_\Omega |\nabla_{x,z}(V - \underline{V})|^2\, dxdz &= \iint_\Omega \partial_t N (V - \underline{V})\, dxdz \\ &= \frac{d}{dt}\iint_\Omega N(V - \underline{V})\, dxdz - \iint_\Omega N \partial_t V\, dxdz.\end{aligned}$$

By using (4.1.6) and the expression of ρ_k, we obtain

$$\frac{d}{dt}W = \int_\omega \mathrm{div}_x \left(\sum_k e^{-\epsilon_k} \nabla_x u \right) \log(u/\underline{u})\, dx.$$

After an integration by parts, we deduce thanks to $u = \underline{u}$ on $\partial\omega$ that

$$\frac{d}{dt}W = -\int_\omega \sum_k e^{-\epsilon_k} \frac{|\nabla_x u|^2}{u}\, dx + \int_\omega \sum_k e^{-\epsilon_k} \frac{\nabla_x u . \nabla_x \underline{u}}{\underline{u}}\, dx. \tag{4.2.18}$$

In the sequel, we shall use the notation

$$D(t) = \int_\omega \sum_k e^{-\epsilon_k} \frac{|\nabla_x u|^2}{u}\, dx \tag{4.2.19}$$

and we shall refer to this term as the entropy dissipation rate. Let now define $\beta = \|\nabla_x \underline{u}/\underline{u}\|_{L^\infty(\omega)} < +\infty$ (from (4.2.16)). A straightforward Cauchy-Schwarz inequality leads to :

$$\frac{d}{dt}W + D \le \beta\sqrt{D}\sqrt{\|N_s\|_{L^1(\omega)}}.$$

Using the inequality $2ab \le \varepsilon^2 a^2 + 1/\varepsilon^2 b^2$ for $\varepsilon > 0$ small enough, we get

$$\frac{d}{dt}W \le C\|N_s\|_{L^1(\omega)}$$

Since the function $F(t) = t\log(t) - t + 1$, satisfies $F(t) \geq t + (1-e)$, we obtain

$$\begin{aligned} W &\geq \sum_k \int_\omega \underline{\rho_k}\, F(\rho_k/\underline{\rho_k})\, dx \geq \sum_k \int_\omega \underline{\rho_k}\left(\rho_k/\underline{\rho_k} + 1 - e\right)\, dx \\ &\geq \int_\omega N_s\, dx - (e-1)\int_\omega \underline{N_s}\, dx, \end{aligned}$$

which leads to the differential inequality

$$\frac{d}{dt}W \leq C\int_\omega N_s\, dx \leq C(W + C_0),$$

where C_0 only depends on the data of the problem (and not on the considered solution). The Gronwall lemma implies $W(t) \leq C_T$ for all $t \in [0,T]$, where C_T only depends on T, $W(0)$ and data ($W(0) < +\infty$ if $N_s^0 \in L^2(\omega)$).

Remark 4.2.4 The above manipulations are formal for weak solutions (defined such that $N_s \in C([0,T], L^2(\omega))$). To make the argument rigorous, it is enough to regularize the data, obtain a regular solution for which the result holds, then pass to the limit in the regularization parameter and use the uniqueness of the weak solution (proved in Section 4.2.5).

4.2.3 Proof of the L^p estimate

The aim of this subsection is the proof of Proposition 4.2.3. We have seen in Section 4.2.2 that $W(0) < C(\|N_s^0\|_{L^2(\omega)})$. Hence Proposition 4.2.2 implies

$$\forall\, t \leq T, \qquad \|V(t)\|_{H^1(\Omega)} + \|N_s(t)\|_{L^1(\omega)} \leq C_T. \tag{4.2.20}$$

Thanks to the Trudinger inequality (B.0.18) and to (B.0.16), as well as Lemma B.0.8 the functions

$$S_1(t,x) = \sup_{k\geq 1} \|\chi_k(t,x,\cdot)\|^2_{L^\infty_z} \quad ; \quad S_2(t,x) = \sum_{k\geq 1} \frac{e^{-\epsilon_k(t,x)}}{\mathcal{Z}(t,x)}\,(\epsilon_k(t,x))^2 \tag{4.2.21}$$

are in $L^\infty((0,T), L^p(\omega))$ for any finite p and satisfy the bound

$$\forall p < +\infty, \quad \|S_1(t,.)\|_{L^p(\omega)} + \|S_2(t,.)\|_{L^p(\omega)} \leq C_p\,, \tag{4.2.22}$$

where C_p is a constant only depending on $\|V(t)\|_{H^1(\Omega)}$. From now on, we denote

$$n_s = N_s - \underline{N_s} \quad ; \quad n = N - \underline{N} \quad ; \quad v_s = V_s - \underline{V_s} \quad ; \quad v = V - \underline{V}\,. \tag{4.2.23}$$

Proof of Proposition 4.2.3 for $p \in [2, +\infty)$***.***
Multiply (4.1.5) by $n_s|n_s|^{p-2}$ and integrate on ω. After an integration by parts, we get

$$\begin{aligned} \frac{1}{p}\frac{d}{dt}\int_\omega |n_s|^p\, dx + (p-1)\int_\omega |\nabla_x n_s|^2 |n_s|^{p-2}\, dx + \frac{p-1}{p}\int_\omega \nabla_x |n_s|^p \cdot \nabla_x V_s\, dx = \\ = \int_\omega \Delta_x \underline{N_s}\, n_s|n_s|^{p-2}\, dx + \int_\omega \mathrm{div}_x\, (\underline{N_s}\nabla_x V_s) n_s|n_s|^{p-2}\, dx. \end{aligned}$$

The last term of the left hand side can be written after an integration by parts

$$-\frac{p-1}{p}\int_\omega |n_s|^p \Delta_x V_s\,dx.$$

The above computations follow closely the standard drift-diffusion Poisson system for which the above term is nonnegative. In our case however, $-\Delta_x V_s \neq N_s$ which induces additional difficulties. Indeed, with the Poisson equation (4.1.4), we have: $-\Delta_x V = \partial_z^2 V + N$. And, after some integrations by parts,

$$\langle \partial_z^2 V|\chi_k|^2\rangle = 2\langle V\chi_k\partial_z^2\chi_k\rangle + 2\langle V|\partial_z\chi_k|^2\rangle.$$

Thanks to the Schrödinger equation (4.1.3), we have:

$$\partial_z^2\chi_k = 2(V-\epsilon_k)\chi_k \quad \text{and} \quad 2\langle V|\chi_k|^2\rangle + |\partial_z\chi_k|^2 = 2\epsilon_k.$$

Thus,

$$\langle \partial_z^2 V|\chi_k|^2\rangle = 4\langle V^2|\chi_k|^2\rangle + 2\langle (V+\epsilon_k)|\partial_z\chi_k|^2\rangle - 4\epsilon_k^2.$$

These remarks lead to the following identity:

$$\begin{aligned}
-\Delta_x V_s \;=\; & -4S_2(t,x) + \frac{\langle N^2 + 4V^2\,N\rangle}{N_s} + 2\sum_k \frac{e^{-\epsilon_k}}{\mathcal{Z}}\left\langle (V+\epsilon_k)|\partial_z\chi_k|^2\right\rangle \\
& -\frac{1}{\mathcal{Z}}\sum_k\sum_{\ell\neq k}\left(\frac{e^{-\epsilon_k}-e^{-\epsilon_\ell}}{\epsilon_k-\epsilon_\ell}\right)\langle \chi_k\chi_\ell\,\nabla_x V\rangle^2 \\
& +\sum_k \frac{e^{-\epsilon_k}}{\mathcal{Z}}\left\langle |\chi_k|^2\,\nabla_x V\right\rangle^2 - \left(\sum_k \frac{e^{-\epsilon_k}}{\mathcal{Z}}\left\langle |\chi_k|^2\,\nabla_x V\right\rangle\right)^2,
\end{aligned} \tag{4.2.24}$$

where S_2 is defined in (4.2.21). By the Cauchy-Schwarz inequality, the sum of the last two terms of the right hand side is nonnegative. Moreover, except for the first one, the other terms are obviously nonnegative. By an integration by parts, we deduce

$$\frac{1}{p}\frac{d}{dt}\int_\omega |n_s|^p\,dx + (p-1)\int_\omega |\nabla_x n_s|^2|n_s|^{p-2}\,dx \leq I + II + III \tag{4.2.25}$$

where

$$\begin{aligned}
I &= 4\frac{p-1}{p}\int_\omega |n_s|^p S_2\,dx, \\
II &= \int_\omega \Delta_x \underline{N_s} n_s|n_s|^{p-2}\,dx, \\
III &= \int_\omega \mathrm{div}_x\,(\underline{N_s}\nabla_x V_s) n_s|n_s|^{p-2}\,dx.
\end{aligned}$$

Let us now analyze each term separately.

Estimating I.

Thanks to the Hölder inequality, for all $r>1$ and $r' = r/(r-1)$ we have:

$$I = 4\frac{p-1}{p}\int_\omega |n_s|^p S_2\,dx \leq C\||n_s|^{\frac{p}{2}}\|_{L^{2r}}^2\|S_2\|_{L^{r'}}.$$

By applying Gagliardo-Nirenberg and Young inequalities we have for $r > 1$

$$\left\| |n_s|^{\frac{p}{2}} \right\|^2_{L^{2r}(\omega)} \le C \left\| |n_s|^{\frac{p}{2}} \right\|^{2/r}_{L^2(\omega)} \left\| |n_s|^{\frac{p}{2}} \right\|^{2(1-1/r)}_{H^1(\omega)} \le C \left(\frac{1}{\varepsilon^r} \|n_s\|^p_{L^p} + \varepsilon^{\frac{r}{r-1}} \left\| |n_s|^{\frac{p}{2}} \right\|^2_{H^1(\omega)} \right).$$

By using the estimate (4.2.22) and Poincaré inequality we obtain

$$I \le C_\varepsilon \|n_s\|^p_{L^p} + C\varepsilon \int_\omega |\nabla_x |n_s|^{p/2}|^2 \, dx. \tag{4.2.26}$$

Estimating II.
This is an easy task. By a straightforward Hölder inequality, we have

$$|II| = \left| \int_\omega \Delta_x \underline{N_s} n_s |n_s|^{p-2} \, dx \right| \le \|n_s\|^{p-1}_{L^p(\omega)} \|\Delta_x \underline{N_s}\|_{L^p(\omega)}. \tag{4.2.27}$$

Estimating III.
This term needs more work. We first begin by an integration by parts and obtain

$$III = -(p-1) \iint_\Omega \underline{N_s} \sum_k \frac{e^{-\epsilon_k}}{\mathcal{Z}} |\chi_k|^2 \, \nabla_x V \cdot \nabla_x n_s |n_s|^{p-2} \, dx dz.$$

This leads to the inequality

$$|III| \le (p-1) \|\underline{N_s}\|_{L^\infty} \iint_\Omega |S_1(t,x)| \, |\nabla_x V| \, |\nabla_x n_s| \, |n_s|^{p-2} \, dx dz,$$

where S_1 is defined in (4.2.21). Taking advantage of (4.2.22), we find after a Hölder inequality

$$|III| \le C_{q,r} \|\underline{N_s}\|_{L^\infty} \|\nabla_x V\|_{L^q} \|\nabla_x n_s |n_s|^{p-2}\|_{L^r} \tag{4.2.28}$$

for any (q,r) such that $q < +\infty$ and $r > q'$, where $q' = q/(q-1)$. By choosing $r = \frac{p}{p-1}$, we have by a Hölder inequality

$$\|\nabla_x n_s |n_s|^{p-2}\|_{L^r} \le \|\nabla_x n_s |n_s|^{\frac{p-2}{2}}\|_{L^2} \|n_s\|^{\frac{p-2}{2}}_{L^p}.$$

Now one can apply (4.2.28) with any $q > p$. By choosing q close enough to p, the following Sobolev inequality holds

$$\|\nabla_x V\|_{L^q} \le C_1 \|V\|_{W^{2,s}} \le C_2 \|N\|_{L^s} + C_3$$

for some $s < p$. Using again the inequality

$$N \le N_s S_1, \tag{4.2.29}$$

where S_1 is defined by (4.2.21) and satisfies the uniform bound (4.2.22), we immediately obtain $\|N\|_{L^s} \le C \|N_s\|_{L^p} \le C(\|\underline{N_s}\|_{L^p} + \|n_s\|_{L^p})$. Besides, we have

$$\int_\omega |\nabla_x n_s|^2 |n_s|^{p-2} \, dx = \frac{4}{p^2} \int_\omega |\nabla_x (|n_s|^{p/2})|^2 \, dx. \tag{4.2.30}$$

All in all, (4.2.28) becomes

$$|III| \le C\|\nabla_x(|n_s|^{p/2})\|_{L^2(\omega)}\|n_s\|_{L^p(\omega)}^{(p-2)/2}(\|n_s\|_{L^p(\omega)} + \|\underline{N_s}\|_{L^p(\omega)} + 1),$$

which leads, after a Young inequality to

$$|III| \le C_1\varepsilon^2\int_\omega |\nabla_x(|n_s|^{p/2})|^2\,dx + \frac{C_2}{\varepsilon^2}\|n_s\|_{L^p(\omega)}^p + \frac{C_3}{\varepsilon^2}\|n_s\|_{L^p(\omega)}^{p-2}, \tag{4.2.31}$$

where ε is an arbitrarily small constant and C_1, C_2, C_3 are independent from ε.

Consider now the inequality (4.2.25). Inserting the inequalities (4.2.30), (4.2.27), (4.2.26) and (4.2.31) in (4.2.25) and fixing ε small enough, there exists $A > 0$ and non-negative constants still denoted by C_1, C_2 and C_3 such that

$$\begin{aligned}\frac{1}{p}\frac{d}{dt}\int_\omega |n_s|^p\,dx + A\int_\omega |\nabla_x(|n_s|^{p/2})|^2\,dx \\ \le C_1\int_\omega |n_s|^p\,dx + C_2\|n_s\|_{L^p(\omega)}^{p-1} + C_3\|n_s\|_{L^p(\omega)}^{p-2}.\end{aligned}$$

A Gronwall argument leads to the boundedness on $[0,T]$ of $\|n_s(t)\|_{L^p(\omega)}$.

Proof of Proposition 4.2.3 for $p = +\infty$.

Since $N_s \in L^p(\omega)$ for all $1 \le p < +\infty$, then by (4.2.29) and (4.2.22), $n \in L^r(\Omega)$ for all $1 \le r < +\infty$. Therefore the Poisson equation (4.1.4) leads to $V \in W^{2,r}(\Omega)$. By Sobolev embeddings, the potential V lies in $L^\infty([0,T]\times\Omega)$. Hence from (4.2.24) and (B.0.2) we deduce that there exists a nonnegative constant a such that $\Delta_x V_s \le a$. We use the standard notation f_+ for the positive part of f:

$$f_+ = \begin{cases} f & \text{if } f \ge 0, \\ 0 & \text{else.}\end{cases}$$

Let us define

$$A(t) = \lambda e^{at}, \quad \text{where} \quad \lambda \ge \max(\|N_s^0\|_{L^\infty(\omega)}, \|N_b\|_{L^\infty(\partial\omega)}). \tag{4.2.32}$$

Then, from (4.1.5) and the choice of a,

$$\partial_t(N_s - A(t)) - \mathrm{div}_x\,(\nabla_x(N_s - A(t)) + (N_s - A(t))\nabla_x V_s) \le 0.$$

Multiplying this equation by $(N_s - A(t))_+$ and integrating over ω, we get after an integration by part

$$\frac{1}{2}\frac{d}{dt}\int_\omega (N_s - A(t))_+^2\,dx + \int_\omega |\nabla_x(N_s - A(t))_+|^2\,dx + \frac{1}{2}\int_\omega \nabla_x(N_s - A(t))_+^2\nabla_x V_s\,dx \le 0.$$

After another integration by parts and since $\Delta_x V_s \le a$,

$$\frac{d}{dt}\int_\omega (N_s - A(t))_+^2\,dx - a\int_\omega (N_s - A(t))_+^2\,dx \le 0.$$

We deduce from this inequality and the choice of λ in (4.2.32) that for all $t \in [0,T]$, $N_s \le A(t)$ thus $N_s \le \lambda e^{aT}$.

4.2.4 Analysis of the Schrödinger-Poisson system

In this subsection, we prove Proposition 4.2.1. We use the functional spaces

$$H^1_\omega = \left\{ V \in H^1(\Omega) \ : \forall x \in \partial\omega,\ z \in [0,1],\ V(x,z) = 0 \right\}$$

and

$$L^p_x L^q_z(\Omega) = \{u \in L^1_{loc}(\Omega) \text{ such that } \|u\|_{L^p_x L^q_z(\Omega)} = \left(\int_\omega \|u(x,\cdot)\|^p_{L^q(0,1)}\, dx \right)^{1/p} < +\infty\}.$$

Thanks to Gagliardo-Nirenberg inequalities and interpolation estimates, one can prove the

Lemma 4.2.5 *We have the Sobolev imbedding of $H^1(\Omega)$ into $L^2_x L^\infty_z(\Omega)$.*

Let $V_0 \in H^2(\Omega)$ be such that $V_0 = V_b$ on $\partial\omega \times (0,1)$ and $\partial_z V_0(x,0) = \partial_z V_0(x,1) = 0$ for all $x \in \omega$ (for instance we can take $V_0 = \underline{V}$). Proceeding as in [7] and in the spirit of [28] we can show that a weak solution of (4.2.12) in the affine space $V_0 + H^1_\omega$ is a critical point with respect to V of the functional

$$\begin{aligned} J(V, N_s) &= J_0(V) + J_1(V, N_s) \\ &= \frac{1}{2} \iint_\Omega |\nabla_{x,z} V|^2 + \int_\omega N_s \log \sum_k e^{-\epsilon_k[V]}\, dx, \end{aligned}$$

where we recall that $(\epsilon_k[V])_{k\geq 1}$ denote the eigenvalues of the Hamiltonian $-\frac{1}{2}\frac{d^2}{dz^2} + V$, *i.e.* satisfy (4.1.3).

The functional J_0 is clearly continuous and strongly convex on $H^1(\Omega)$. The analysis of the functional $V \mapsto J_1(V, N_s)$ relies on the properties of $\epsilon_k[V]$. From the inequality (see Lemma B.0.1)

$$|\epsilon_k[V] - \epsilon_k[\widetilde{V}]|(x) \leq \|V(x,\cdot) - \widetilde{V}(x,\cdot)\|_{L^\infty_z(0,1)}$$

and

$$\log \frac{\sum_k e^{-\epsilon_k[V]}}{\sum_k e^{-\epsilon_k[\widetilde{V}]}} \leq \log \frac{\sum_k e^{-\epsilon_k[\widetilde{V}] + \sup_\ell(|\epsilon_\ell[V] - \epsilon_\ell[\widetilde{V}]|)}}{\sum_k e^{-\epsilon_k[\widetilde{V}]}},$$

we deduce

$$\begin{aligned} |J_1(V, N_s) - J_1(\widetilde{V}, N_s)| &\leq \int_\omega |N_s(x)| \sup_k \Big(|\epsilon_k[V] - \epsilon_k[\widetilde{V}]|(x) \Big)\, dx \\ &\leq \|N_s\|_{L^2(\omega)} \|V - \widetilde{V}\|_{L^2_x L^\infty_z(\Omega)}. \end{aligned} \tag{4.2.33}$$

The functional $J_1(\cdot, N_s)$ is globally Lipschitz continuous on $L^2_x L^\infty_z(\Omega)$, thus on $H^1(\Omega)$, thanks to Lemma 4.2.5.

Next, $J_1(\cdot, N_s)$ is twice Gâteaux differentiable on $L^\infty(\Omega)$ and

$$\begin{aligned} d^2_V J_1(V, N_s) W \cdot W &= -\int_\omega \frac{N_s}{\mathcal{Z}} \sum_k \sum_{\ell \neq k} \frac{e^{-\epsilon_k} - e^{-\epsilon_\ell}}{\epsilon_k - \epsilon_\ell} \langle \chi_k \chi_\ell W \rangle^2\, dx \\ &\quad + \int_\omega N_s \left\{ \sum_k \frac{e^{-\epsilon_k}}{\mathcal{Z}} \langle |\chi_k|^2 W \rangle^2 - \left(\frac{\sum_k e^{-\epsilon_k} \langle |\chi_k|^2 W \rangle}{\mathcal{Z}} \right)^2 \right\} dx. \end{aligned}$$

When N_s is nonnegative, this quantity is nonnegative thanks to the Cauchy-Schwarz inequality. Thus $J_1(\cdot, N_s)$ is convex. As a consequence, the functional $J(\cdot, N_s) = J_0 + J_1(\cdot, N_s)$ is continuous and strongly convex on $V_0 + H^1_\omega$. Moreover, using the Poincaré inequality on H^1_ω and (4.2.33) with $\widetilde{V} = 0$, we have

$$J(V, N_s) \geq C\|V\|^2_{H^1(\Omega)} - C\|N_s\|_{L^2(\Omega)}\|V\|_{H^1(\Omega)} + J(0, N_s),$$

thus $J(\cdot, N_s)$ is coercive and bounded from below on H^1_ω : it admits a unique minimizer, denoted by V, which is then solution of our problem with the boundary conditions (4.1.9).

Now we prove the H^2 estimate of V. Since V is a minimizer of $J(\cdot, N_s)$ we have $J(V, N_s) \leq J(0, N_s)$. Thus,

$$\frac{1}{2}\iint_\Omega |\nabla_{x,z}V|^2\, dxdz \leq J_1(0, N_s) - J_1(V, N_s).$$

Applying (4.2.33), we deduce that V is bounded in $H^1(\Omega)$, with a bound only depending on the L^2 norm of N_s. Therefore the function S_1 defined in (4.2.21) satisfies the bound (4.2.22). Since $N \leq N_s S_1$, we deduce that the density N lies in $L^r(\Omega)$ for any $r < 2$, which implies by elliptic regularity that $V \in W^{2,r}(\Omega)$. This implies that V actually lies in L^∞ which leads, in view of (B.0.16), to $S_1 \in L^\infty$. Therefore, N is bounded in $L^2(\Omega)$, which gives $V \in H^2(\Omega)$ thanks to the elliptic regularity.

Let us now prove the Lipschitz dependence of V with respect to N_s in $H^2(\Omega)$. Let V and $\widetilde{V}$ denote the minimizers of $J(\cdot, N_s)$ and $J(\cdot, \widetilde{N_s})$. Using the linearity of J_1 with respect to N_s, its Lipschitz dependence with respect to V from (4.2.33), the strong convexity of J and the fact that $\widetilde{V}$ minimizes $J(\cdot, \widetilde{N_s})$, we get

$$\begin{aligned}\frac{1}{C}\|V - \widetilde{V}\|^2_{H^1(\Omega)} \leq\ & J(\widetilde{V}, N_s) - J(V, N_s)\\ &= J_1(\widetilde{V}, N_s - \widetilde{N_s}) - J_1(V, N_s - \widetilde{N_s}) + J(\widetilde{V}, \widetilde{N_s}) - J(V, \widetilde{N_s})\\ &\leq C'\|V - \widetilde{V}\|_{H^1(\Omega)}\, \|N_s - \widetilde{N_s}\|_{L^2(\omega)}.\end{aligned}$$

Thus, we have first the Lipschitz dependence of V in $H^1(\Omega)$. The Poisson equation gives $-\Delta(V - \widetilde{V}) = N - \widetilde{N}$, and

$$\begin{aligned}N - \widetilde{N} =\ & (N_s - \widetilde{N_s})\sum_k \frac{e^{-\epsilon_k}|\chi_k|^2}{\mathcal{Z}} + \widetilde{N_s}\sum_k \left(\frac{e^{-\epsilon_k}}{\mathcal{Z}} - \frac{e^{-\widetilde{\epsilon_k}}}{\widetilde{\mathcal{Z}}}\right)|\chi_k|^2\\ &+\widetilde{N_s}\sum_k \frac{e^{-\widetilde{\epsilon_k}}}{\widetilde{\mathcal{Z}}}(|\chi_k|^2 - |\widetilde{\chi_k}^2|)\end{aligned}$$

(we denote $\widetilde{\epsilon_k}$ instead of $\epsilon_k[\widetilde{V}]$ and $\widetilde{\chi_k}$ instead of $\chi_k[\widetilde{V}]$). With Lemma B.0.4,

$$\|\chi_k - \widetilde{\chi_k}\|_{L^\infty_z} \leq C_1 e^{C_2(\|V\|_{L^2_z} + \|\widetilde{V}\|_{L^2_z})}\|V - \widetilde{V}\|_{L^1_z}. \tag{4.2.34}$$

Denoting $\chi_k^s = \chi_k[\widetilde{V} + s(V - \widetilde{V})]$ and $\epsilon_k^s = \epsilon_k[\widetilde{V} + s(V - \widetilde{V})]$, we have with Lemma B.0.3,

$$\sum_k \left(\frac{e^{-\epsilon_k}}{\mathcal{Z}} - \frac{e^{-\widetilde{\epsilon_k}}}{\widetilde{\mathcal{Z}}} \right) |\chi_k|^2 = \int_0^1 \frac{\sum_k \langle |\chi_k^s|^2 (V - \widetilde{V}) \rangle e^{-\epsilon_k^s}}{\sum_\ell e^{-\epsilon_\ell^s}} \frac{\sum_k |\chi_k|^2 e^{-\epsilon_k^s}}{\sum_\ell e^{-\epsilon_\ell^s}} \, ds - \int_0^1 \sum_k \frac{\langle |\chi_k^s|^2 (V - \widetilde{V}) \rangle e^{-\epsilon_k^s}}{\sum_\ell e^{-\epsilon_\ell^s}} |\chi_k|^2 \, ds.$$

Thus, since we have proved that $\chi_k^s \in L^\infty(\Omega)$, $\forall s \in [0,1]$, we deduce

$$\left| \sum_k \left(\frac{e^{-\epsilon_k}}{\mathcal{Z}} - \frac{e^{-\widetilde{\epsilon_k}}}{\widetilde{\mathcal{Z}}} \right) |\chi_k|^2 \right| \leq C \|V - \widetilde{V}\|_{L^1_z}. \tag{4.2.35}$$

Hence, from (4.2.34) and (4.2.35), it yields,

$$\|N - \widetilde{N}\|_{L^2(\Omega)} \leq C \|N_s - \widetilde{N_s}\|_{L^2(\omega)} + C \|V - \widetilde{V}\|_{L^2(\Omega)}.$$

Finally, from the Lipschitz dependence of V with respect to N_s in $H^1(\Omega)$, we have locally $\|V - \widetilde{V}\|_{L^2(\Omega)} \leq C \|N_s - \widetilde{N_s}\|_{L^2(\omega)}$. Thus, $\|N - \widetilde{N}\|_{L^2(\Omega)} \leq C \|N_s - \widetilde{N_s}\|_{L^2(\omega)}$ with a constant C depending on $\|N_s\|_{L^2(\omega)}$ and $\|\widetilde{N_s}\|_{L^2(\omega)}$. Applying the elliptic regularity, we conclude $\|V - \widetilde{V}\|_{H^2(\Omega)} \leq C(\|N_s\|_{L^2(\omega)}, \|\widetilde{N_s}\|_{L^2(\omega)}) \|N_s - \widetilde{N_s}\|_{L^2(\Omega)}$. □

Remark 4.2.6 We can also solve this problem by assuming that $u \in L^2(\omega)$ is given such that $u \geq 0$. More precisely, the system (4.1.3), (4.1.4) is now written

$$\begin{cases} \dfrac{1}{2} \partial_z^2 \chi_k + V \chi_k = \epsilon_k \\ -\Delta_{x,z} V = u \displaystyle\sum_k |\chi_k|^2 e^{-\epsilon_k}. \end{cases}$$

Following the same idea as above, a weak solution of this system in the affine space $V_0 + H^1(\Omega)$ is the unique minimizer with respect to V of the convex functional :

$$J(V) = \frac{1}{2} \iint_\Omega |\nabla_x V|^2 \, dx dz + \int_\omega u \sum_k e^{-\epsilon_k[V]} \, dx,$$

(in fact, for H^1 potentials, it is not guaranteed that this functional takes finite values; to circumvent this difficulty, one can instead solve an auxiliary problem where the exponential is truncated for negative arguments, then estimate its solution and show that it is nonnegative). As before, we have $V \in H^2(\Omega)$ for $u \in L^2(\omega)$.

Proof of Proposition 4.1.4. We consider the stationary problem (4.1.10)–(4.1.11). First, we remark that the stationary drift-diffusion equation and the boundary conditions gives

$$\begin{cases} -\text{div} \, (\displaystyle\sum_k e^{-\epsilon_k^\infty} \nabla_x u) = 0 & \text{for } x \in \omega, \\ u = u^\infty & \text{for } x \in \partial\omega, \end{cases}$$

Thus $u = u^\infty$. Then (4.1.10) can be written

$$\begin{cases} -\frac{1}{2}\partial_z^2 \chi_k^\infty + V^\infty \chi_k^\infty = \epsilon_k^\infty \, \chi_k^\infty \,, \\ -\Delta_{x,z} V^\infty = u^\infty \sum_k |\chi_k^\infty|^2 e^{-\epsilon_k^\infty} \,. \end{cases}$$

And the solution of this Schrödinger-Poisson system is the minimum of the convex functional (see Remark 4.2.6):

$$J(V) = \frac{1}{2} \iint_\Omega |\nabla_{x,z} V|^2 \, dxdz + \int_\omega u^\infty \sum_k e^{-\epsilon_k[V]} \, dx,$$

where $(\epsilon_k[V])_{p\geq 1}$ are the eigenvalues of the Hamiltonian, i.e. satisfy (4.1.3). □

4.2.5 Proof of Theorem 4.1.2

The proof of existence and uniqueness relies on a contraction argument in the spirit of [26]. We first define the map $F : N_s \mapsto \widehat{N_s}$ as follows :

Step 1. For a given $N_s \geq 0$, solve the Schrödinger-Poisson system (4.2.12) as in Section 4.2.4. From the obtained $V \in C([0,T], H^2(\Omega))$ (see Proposition 4.2.1), define V_s by (4.1.6). Thanks to Lemma B.0.9, V_s belongs to $C([0,T], H^2(\omega))$.

Step 2. The surface potential V_s being known, solve the following parabolic equation for the unknown $\widehat{N_s}$:

$$\partial_t \widehat{N_s} - \text{div}\,_x(\nabla_x \widehat{N_s} + \widehat{N_s} \nabla_x V_s) = 0, \tag{4.2.36}$$

with the boundary condition:

$$\widehat{N_s}(t,x) = N_b(x) \qquad \text{for } x \in \partial\omega, \tag{4.2.37}$$

and the initial value:

$$\widehat{N_s}(0,x) = N_s^0(x) \qquad \text{for } x \in \omega.$$

Standard results on parabolic equations ([25]) leads to the existence and uniqueness of the solution $\widehat{N_s}$ of (4.2.36), (4.2.37). Of course, $\widehat{N_s} \geq 0$. The map F is then defined after these two steps by $F(N_s) := \widehat{N_s}$.

Let us now show that F is a contraction on the space $M_{a,T}$ defined by $M_{a,T} = \{n : \|n\|_T \leq a\}$, where the norm is:

$$\|n\|_T = \left[\max_{0\leq t\leq T} \|n(t)\|^2_{L^2(\omega)} + \int_0^T \|n(t)\|^2_{H^1(\omega)} \, dt \right]^{1/2}. \tag{4.2.38}$$

These two parameters T and a will be specified later on. Let N_s and $\widetilde{N_s}$ be two elements of $M_{a,T}$. The difference $\delta F = F(\widetilde{N_s}) - F(N_s)$ verify

$$\partial_t \delta F - \text{div}\,_x(\nabla_x \delta F + \delta F \nabla_x V_s + F(\widetilde{N_s}) \nabla_x \delta V_s) = 0\,, \tag{4.2.39}$$

with the notation $\delta V_s = V_s - \widetilde{V}_s$. The boundary conditions become:

$$\delta F(0,x) = 0, \quad \forall x \in \omega \ ; \qquad \delta F(t,x) = 0, \quad \forall x \in \partial\omega, \ \forall t \in [0,T].$$

Multiplying (4.2.39) by δF and integrating on ω, we get after an integration by parts

$$\frac{1}{2}\frac{d}{dt}\int_\omega |\delta F|^2\,dx + \int_\omega |\nabla_x(\delta F)|^2\,dx + \int_\omega \nabla_x(\delta F)(\delta F \nabla_x V_s + F(\widetilde{N_s})\nabla_x(\delta V_s))\,dx = 0.$$

The Cauchy-Schwarz inequality applied to the third term leads to:

$$\frac{1}{2}\frac{d}{dt}\|\delta F\|_{L^2}^2 + \|\nabla_x(\delta F)\|_{L^2}^2 \ \le \ \|\nabla_x(\delta F)\|_{L^2}\left(\|\delta F\nabla_x V_s\|_{L^2} + \|F(\widetilde{N_s})\nabla_x(\delta V_s)\|_{L^2}\right).$$

Thus,

$$\begin{aligned}\frac{d}{dt}\|\delta F\|_{L^2}^2 + \|\nabla_x(\delta F)\|_{L^2}^2 \ &\le \ 2\|\delta F\nabla_x V_s\|_{L^2}^2 + 2\|F(\widetilde{N_s})\nabla_x(\delta V_s)\|_{L^2}^2 \\ &\le \ 2\|\delta F\|_{L^4}^2\|\nabla_x V_s\|_{L^4}^2 + 2\|F(\widetilde{N_s})\|_{L^4}^2\|\nabla_x(\delta V_s)\|_{L^4}^2 .\end{aligned} \tag{4.2.40}$$

Besides, we have

$$|\nabla_x V_s| = \frac{|\sum_k \int_0^1 |\chi_k|^2 \nabla_x V e^{-\epsilon_k}\,dz|}{\sum_k e^{-\epsilon_k}} \le |S_2(t,x)| \int_0^1 |\nabla_x V|\,dz,$$

where S_2 is defined by (4.2.21). From Proposition 4.2.1 and the fact that $N_s \in M_{a,T}$, we deduce that

$$\max_{0\le t\le T}\|V(t)\|_{H^2(\Omega)} \le C_1(a)\,,$$

where $C_1(a)$ is a constant only depending on a. From Lemma B.0.9 and the imbedding $H^2(\Omega) \hookrightarrow L^\infty(\Omega)$, we deduce the pointwise in time inequalities

$$\max_{0\le t\le T}\left(\|S_2(t)\|_{L^\infty} + \|V_s(t)\|_{H^2(\omega)}\right) \le C_2(a).$$

From Lemma B.0.9 and Proposition 4.2.1, we know that there exists a constant $C_2(a)$ such that,

$$\|\nabla_x(\delta V_s)\|_{L^4} \le C\|\delta V_s\|_{H^2(\omega)} \le C_2(a)\|\delta N_s\|_{L^2(\omega)}.$$

Inserting the above inequalities in (4.2.40), we obtain the inequality

$$\frac{d}{dt}\|\delta F\|_{L^2}^2 + \|\nabla_x(\delta F)\|_{L^2}^2 \ \le \ C_3(a)\left(\|\delta F\|_{L^4}^2 + \|F(\widetilde{N_s})\|_{L^4}^2\|\delta N_s\|_{L^2}^2\right).$$

The Gagliardo Nirenberg inequality leads to

$$\frac{d}{dt}\|\delta F\|_{L^2}^2 + \frac{1}{2}\|\nabla_x(\delta F)\|_{L^2}^2 \ \le \ C_4(a)\left(\|\delta F\|_{L^2}^2 + \|F(\widetilde{N_s})\|_{L^4}^2\|\delta N_s\|_{L^2}^2\right). \tag{4.2.41}$$

Taking $\widetilde{N_s} = 0$ in the above inequality leads to

$$\begin{aligned}\frac{d}{dt}\|F(N_s) - F(0)\|_{L^2}^2 + \frac{1}{2}\|\nabla_x(F(N_s) - F(0))\|_{L^2}^2 \ &\le \\ C_4(a)\left(\|F(N_s) - F(0)\|_{L^2}^2 + \|F(0)\|_{L^4}^2\|N_s\|_{L^2}^2\right),&\end{aligned}$$

which implies

$$\|F(N_s)(t) - F(0)(t)\|_{L^2}^2 \leq \|F(N_s)(0) - F(0)(0)\|_{L^2}^2 \, e^{C_4(a)t} + C_4(a)\|F(0)\|_{L^4}^2 \int_0^t \|N_s(\tau)\|_{L^2}^2 \, e^{C_4(a)(t-\tau)} \, d\tau \,.$$

We then obtain

$$\|F(N_s)\|_T \leq C_5(a) e^{C_5(a)T},$$

where $\| \cdot \|_T$ is defined in (4.2.38) and C_5 only depends on a. Of course, since N_s and $\widetilde{N_s}$ play the same role, we obviously have

$$\|F(\widetilde{N_s})\|_T \leq C_5(a) e^{C_5(a)T}. \tag{4.2.42}$$

Let us now go back to (4.2.41), which after a Gronwall inequality yields

$$\begin{aligned}
\|\delta F(t)\|_{L^2}^2 &\leq C_4(a) \|\delta N_s\|_T^2 \int_0^t e^{C_4(a)(t-\tau)} \, \|F(\widetilde{N_s})(\tau)\|_{L^4}^2 \, d\tau \\
&\leq C_4(a) \, e^{C_4(a)t} \, \|\delta N_s\|_T^2 \int_0^t \|F(\widetilde{N_s})(\tau)\|_{L^2} \, \|\nabla_x F(\widetilde{N_s})(\tau)\|_{L^2} \, d\tau \\
&\leq C_4(a) \, e^{C_4(a)t} \, \|\delta N_s\|_T^2 \, \sqrt{T} \, \|F(\widetilde{N_s})\|_T^2 \,.
\end{aligned}$$

We then deduce from (4.2.42) that

$$\|\delta F(t)\|_T \leq C_6(a) \, T^{1/4} \, e^{C_6(a)T} \, \|\delta N_s\|_T \,.$$

Let us now take $a = 2\|F(0)\|_1$ and choose the parameter $T \leq 1$ small enough so that $C_6(a) \, T^{1/4} \, e^{C_6(a)T} \leq 1/2$. Since $\| \cdot \|_T$ is increasing with respect to T, it is readily seen that F leaves $M_{a,T}$ invariant and is a contraction on this set. We have then constructed a unique solution on a time interval T_0 which only depends on the L^2 norm of the initial datum and on the $H^{1/2}(\partial\omega)$ norm of the boundary values for N_s and V_s. In order to construct a global solution, we take T_0 as the origin and prove as above the existence and uniqueness of the solution on $[T_0, 2T_0]$. This is made possible thanks to the locally uniform in time L^2 *a priori* estimate on the self-consistent solution, given in Proposition 4.2.3. Proceeding analogously we construct the solution $[2T_0, 3T_0]$ until covering completely the interval $[0, T]$.

4.3 Long time behaviour

The study of the exponential convergence to the equilibrium is established in two steps. First we prove the convergence towards 0 as t goes to $+\infty$ and the decreasing of the relative entropy defined by

$$\begin{aligned}
W(t) = \; & \sum_k \int_\omega (\rho_k \log(\rho_k/\rho_k^\infty) - \rho_k + \rho_k^\infty) \, dx + \frac{1}{2} \iint_\Omega |\nabla_{x,z}(V - V^\infty)|^2 \, dxdz \\
& + \int_\omega \sum_k u \, e^{-\epsilon_k} \left(\epsilon_k[V] - \epsilon_k[V^\infty] - \int_0^1 |\chi_k|^2 (V - V^\infty) \, dz \right) \, dx,
\end{aligned} \tag{4.3.1}$$

where we define $\rho_k^\infty = u^\infty e^{-\epsilon_k^\infty}$. We denote

$$n = N - N^\infty, \quad v = V - V^\infty, \quad v_s = V_s - V_s^\infty, \quad n_s = N_s - N_s^\infty. \tag{4.3.2}$$

We deduce:

$$\begin{cases} \partial_t n_s - \mathrm{div}_x \left(\nabla_x n_s + N_s^\infty \nabla_x v_s + n_s \nabla_x V_s^\infty + n_s \nabla_x v_s\right) = 0, \\ -\Delta_{x,z} v = n. \end{cases} \tag{4.3.3}$$

Next we consider a quadratic approximation of the relative entropy and prove its exponential convergence to 0 as t goes to $+\infty$.

In the sequel, the letter C stands for a positive constant depending only on the data and ε stands for an arbitrarily small positive constant.

4.3.1 Convergence of the relative entropy

This section is devoted to the following preliminary result:

Proposition 4.3.1 *Under Assumption* 4.1.1 *and* 4.1.3*, the solution of the drift-diffusion-Schrödinger-Poisson system* (4.1.1)–(4.1.9) *is such that:*

(i) The relative entropy W defined by (4.3.1) *is decreasing and*

$$\lim_{t \to +\infty} W(t) = 0.$$

(ii) We have $n_s \longrightarrow 0$ in $L^1(\omega)$ and $v \longrightarrow 0$ in $H^1(\omega)$ as t goes to $+\infty$.

Proof. This proof is based on an idea developed in [18]. Let (N_s^∞, V^∞) solve the stationary problem (4.1.10). We deduce from (4.2.18) that the relative entropy satisfies:

$$\frac{d}{dt} W(t) = -D(t),$$

where D is given by (4.2.19). Then, for all $t \geq 0$, we have

$$W(t) + \int_0^t D(\tau)\, d\tau = W(0), \tag{4.3.4}$$

which implies that there exists a sequence $t_j \longrightarrow +\infty$ such that

$$D(t_j) \longrightarrow 0 \qquad \text{as} \qquad j \longrightarrow +\infty. \tag{4.3.5}$$

Now, straightforward calculations using $N_s = u e^{-V_s}$ give

$$D = \int_\omega \left(4 |\nabla_x \sqrt{N_s}|^2 + 2 \nabla_x N_s \cdot \nabla_x V_s + N_s |\nabla_x V_s|^2\right) dx. \tag{4.3.6}$$

After an integration by parts, we get

$$\int_\omega \nabla_x N_s \cdot \nabla_x V_s \, dx = -\int_\omega N_s \, \Delta_x V_s \, dx + \int_{\partial\omega} N_s \, \partial_\nu V_s \, d\sigma,$$

where $\nu(x)$ denotes the outward unitary normal vector at $x \in \partial\omega$ and $d\sigma$ the surface measure on $\partial\omega$ induced by the Lebesgue measure. Therefore we deduce from (4.3.6) that

$$\begin{aligned} 4\|\nabla_x\sqrt{N_s}\|_{L^2}^2 &\le D + 2\int N_s\Delta_x V_s\,dx - 2\int_{\partial\omega} N_s\partial_\nu V_s\,d\sigma \\ &\le D + 8\int_\omega N_s S_2\,dx - 2\int_{\partial\omega\times(0,1)} N\partial_\nu V\,d\sigma dz \\ &\le D + 8\|N_s\|_{L^4}\|S_2\|_{L^{4/3}} + 2\|N_b\|_{L^\infty}\|V\|_{H^2} \\ &\le D + C\|N_s\|_{L^4} + C\|N\|_{L^2} + C, \end{aligned}$$

where we recall that S_2 is given by (4.2.21) and satisfies (4.2.22). Besides, it is readily seen that $N \le N_s S_1$ where S_1 is given in (4.2.21) and satisfies (4.2.22). Therefore $\|N\|_{L^2} \le C\|N_s\|_{L^4}$. We conclude from the above inequality that

$$4\|\nabla_x\sqrt{N_s}\|_{L^2}^2 \le D + C\|N_s\|_{L^4} + C.$$

Applying a Gagliardo-Nirenberg inequality to the function $\sqrt{N_s}$ in the right-hand side, we obtain (for any $\varepsilon > 0$)

$$4\|\nabla_x\sqrt{N_s}\|_{L^2}^2 \le D + C\|N_s\|_{L^1}^{1/2}\|\sqrt{N_s}\|_{H^1} + C \le D + C_\varepsilon\|N_s\|_{L^1} + \varepsilon\|\nabla_x\sqrt{N_s}\|_{L^2}^2 + C,$$

which leads, in view of (4.2.20), to the inequality

$$\|\nabla_x\sqrt{N_s}\|_{L^2}^2(t) \le C(D(t)+1). \tag{4.3.7}$$

By evaluating (4.3.5) and (4.3.7) at $t = t_j$, we deduce the boundedness in $H^1(\omega)$ of the sequence $(\sqrt{N_s(t_j)})_j$. Because of the compactness embedding of $H^1(\omega)$ into $L^4(\omega)$, we can assume without loss of generality that there exists $\overline{N_s}$ belonging to $L^2(\omega)$ such that $\sqrt{\overline{N_s}} \in H^1(\omega)$ and

$$N_s(t_j) \longrightarrow \overline{N_s} \text{ in } L^2(\omega). \tag{4.3.8}$$

Thanks to the properties of the trace of $H^1(\omega)$ functions and the compact embedding $H^{1/2}(\partial\omega) \hookrightarrow L^4(\partial\omega)$, we have $\overline{N_s}|_{\partial\omega} = N_b$. From Proposition 4.2.1, we know that the mapping $N_s \mapsto V$ defined by

$$\begin{cases} -\dfrac{1}{2}\partial_z^2\chi_k + V\chi_k = \epsilon_k\chi_k \qquad (k \ge 1), \\ -\Delta_{x,z}V = N = N_s\displaystyle\sum_k \frac{|\chi_k|^2 e^{-\epsilon_k}}{\mathcal{Z}}, \end{cases}$$

(with the boundary conditions of V in (4.1.9)) is well-posed for $N_s \in L^2(\omega)$ such that $N_s \ge 0$ a.e. and is continuous from $L^2(\omega)$ into $H^2(\Omega)$. Moreover, by Lemma B.0.9 we also know that the mapping $V \mapsto V_s$ defined by

$$\begin{cases} V_s = -\log(\displaystyle\sum_k e^{-\epsilon_k}) \\ -\dfrac{1}{2}\partial_z^2\chi_k + V\chi_k = \epsilon_k\chi_k \end{cases}$$

is continuous from $H^2(\Omega)$ to $H^2(\omega)$. It follows that

$$\exists\, \overline{V_s} \in H^2(\omega) \text{ such that } V_s(t_j) \longrightarrow \overline{V_s} \text{ in } H^2(\omega) \subset C(\overline{\omega}).$$

Hence,

$$u(t_j) = N_s(t_j)e^{V_s(t_j)} \longrightarrow \overline{N_s}e^{\overline{V_s}} \text{ in } L^2(\omega). \tag{4.3.9}$$

Now (4.3.5) and (4.3.8) imply that, for any $h \in (L^4(\omega))^2$, we have

$$\begin{aligned}\left|\int_\omega \nabla_x(N_s(t_j)e^{V_s(t_j)})h\,dx\right| &= \left|\int_\omega \nabla_x u(t_j)\,h\,dx\right|\\ &\leq \left(\int_\omega e^{-V_s(t_j)}\frac{|\nabla_x u(t_j)|^2}{u(t_j)}\,dx\right)\|N_s(t_j)e^{2V_s(t_j)}\|^{1/2}_{L^2(\omega)}\|h\|_{L^4(\omega)}\\ &\longrightarrow 0 \text{ as } j\to+\infty.\end{aligned}$$

Taking into account (4.3.9), we deduce that $\overline{N_s}e^{\overline{V_s}}$ is constant in ω. Since $\overline{N_s}|_{\partial\omega} = N_b$ and $\overline{V_s}|_{\partial\omega} = V_s^\infty$, Assumption 4.1.3 implies $\overline{N_s}e^{\overline{V_s}} = u^\infty$. Thus, $(\overline{N_s},\overline{V_s})$ can be identified as the unique solution of the stationary Schrödinger-Poisson system (see Remark 4.2.6):

$$\overline{N_s} = N_s^\infty,\ \overline{V_s} = V_s^\infty \text{ and analogously } V(t_j) \longrightarrow V^\infty \text{ as } j\to+\infty.$$

Since the function W is decreasing, we have

$$\lim_{t\to+\infty} W(t) = \lim_{j\to+\infty} W(t_j) = 0.$$

Consequently, $\|v(t)\|_{H^1(\Omega)} \to 0$ and $\|n_s\|_{L^1(\omega)} \to 0$ as $t\to+\infty$ by a Poincaré inequality and the Csiszár-Kullback inequality presented in the appendix (A.3.4) (cf [3, 11, 24]). □

4.3.2 Exponential convergence

This section is devoted to the proof of the main result of this paper, i.e. the exponential convergence of the surface density N_s and the electrostatic potential V to the equilibrium functions. We will consider the differences n, n_s, v, v_s defined in (4.3.2) and introduce the quadratic approximation of the relative entropy:

$$L(t) = \frac{1}{2}\int_\omega \frac{(n_s)^2}{N_s^\infty}\,dx + \int_\omega n_s v_s\,dx - \frac{1}{2}\iint_\Omega |\nabla v|^2\,dxdz + \int_\omega N_s^\infty v_s\,dx - \iint_\Omega N^\infty v\,dxdz. \tag{4.3.10}$$

Since the Poisson equation gives $\iint_\Omega nv\,dxdz = \iint_\Omega |\nabla v|^2\,dxdz$, we can rewrite

$$L(t) = \frac{1}{2}\int_\omega \frac{(n_s)^2}{N_s^\infty}\,dx + \frac{1}{2}\iint_\Omega |\nabla v|^2\,dxdz + \int_\omega N_s v_s\,dx - \iint_\Omega Nv\,dxdz. \tag{4.3.11}$$

In order to prove Theorem 4.1.5, we need three technical lemmata that we prove further in subsection 4.3.2.2:

Lemma 4.3.2 *Consider a weak solution of* (4.1.3)–(4.1.9). *Then for all* $t \geq 0$, *we have*

$$\frac{1}{2}\int_\omega \frac{(n_s)^2}{N_s^\infty}\,dx + \frac{1}{2}\iint_\Omega |\nabla v|^2\,dxdz \leq L(t) \leq \frac{1}{2}\int_\omega \frac{(n_s)^2}{N_s^\infty}\,dx + \int_\omega n_s v_s\,dx.$$

Lemma 4.3.3 *Let V and $\underline{V}$ belong to $L^2(0,1)$ and V_s, $\underline{V_s}$ be defined by*

$$V_s = -\log\sum_k \exp(-\epsilon_k[V]) \quad ; \quad \underline{V_s} = -\log\sum_k \exp(-\epsilon_k[\underline{V}]).$$

Then, by setting $v = V - \underline{V}$ and $v_s = V_s - \underline{V_s}$, we have

$$|\nabla_x v_s|^2 \leq C_1 e^{C_2(\|\underline{V}\|_{L^2_z(0,1)}+\|v\|_{L^2_z(0,1)})}(\langle|\nabla_x v|\rangle^2 + \langle|v|\rangle^2\langle|\nabla_x \underline{V}|\rangle^2), \tag{4.3.12}$$

where C_1 and C_2 are two positive constants.

Lemma 4.3.4 *Consider a weak solution of* (4.1.3)–(4.1.9). *Then there exist two nonnegative constants C_1 and C_2 such that for all $t \geq 0$,*

$$\int_\omega \frac{(n_s)^2}{N_s^\infty}|\nabla_x v_s|^2\,dx \leq \frac{1}{2}\int_\omega N_s^\infty \left|\nabla_x\left(\frac{n_s}{N_s^\infty} + v_s\right)\right|^2 dx + C_1 L(t)^4 + C_2 L(t)\|v\|_{H^1(\Omega)},$$

where L is defined in (4.3.11). *Moreover, we have*

$$\|v_s\|_{L^6(\Omega)} \leq C\|v\|_{H^1(\Omega)}, \tag{4.3.13}$$

for a nonnegative constant C.

4.3.2.1 Proof of Theorem 4.1.5

From (4.3.10) and the Poisson equation, we deduce that

$$\frac{d}{dt}L(t) = \int_\omega \partial_t n_s\left(\frac{n_s}{N_s^\infty} + v_s\right)\,dx + \int_\omega N_s\partial_t v_s\,dx - \iint_\Omega N\partial_t v\,dxdz.$$

Furthermore, $e^{-V_s} = \sum_k e^{-\epsilon_k} = \mathcal{Z}$ and $\partial_t\epsilon_k = \langle|\chi_k|^2\partial_t v\rangle$ imply

$$\partial_t v_s = \frac{1}{\mathcal{Z}}\sum_k \langle|\chi_k|^2\partial_t v\rangle\, e^{-\epsilon_k}.$$

Hence $\int_\omega N_s\partial_t v_s\,dx = \iint_\Omega N\partial_t v\,dxdz$. With (4.3.3) and after an integration by parts, we get

$$\frac{d}{dt}L(t) = -\int_\omega (\nabla_x n_s + N_s^\infty\nabla_x v_s + n_s\nabla_x V_s^\infty + n_s\nabla_x v_s)\cdot\nabla_x\left(\frac{n_s}{N_s^\infty} + v_s\right)\,dx.$$

Since $\nabla_x N_s^\infty + N_s^\infty\nabla_x V_s^\infty = 0$, we deduce that

$$\frac{d}{dt}L(t) = -\int_\omega N_s^\infty\left|\nabla_x\left(\frac{n_s}{N_s^\infty} + v_s\right)\right|^2 dx - \int_\omega n_s\nabla_x v_s\cdot\nabla_x\left(\frac{n_s}{N_s^\infty} + v_s\right)\,dx. \tag{4.3.14}$$

Now we will show that the second term of the right-hand side of can be controlled by the first one for long time. From Lemma 4.3.4, we deduce

$$\begin{aligned}
-\int_\omega n_s \nabla_x v_s \cdot \nabla_x \left(\frac{n_s}{N_s^\infty} + v_s\right) dx \\
&\le \frac{1}{2}\int_\omega \frac{(n_s)^2}{N_s^\infty} |\nabla_x v_s|^2 \, dx + \frac{1}{2}\int_\omega N_s^\infty \left|\nabla_x \left(\frac{n_s}{N_s^\infty} + v_s\right)\right|^2 dx \\
&\le \frac{3}{4}\int_\omega N_s^\infty \left|\nabla_x \left(\frac{n_s}{N_s^\infty} + v_s\right)\right|^2 dx + C_1 L(t)^4 + C_2 \|v\|_{H^1(\Omega)} L(t).
\end{aligned}$$

Thanks to the Poincaré inequality and Lemma 4.3.2, we have

$$\begin{aligned}
-\frac{1}{4}\int_\omega N_s^\infty \left|\nabla_x (\frac{n_s}{N_s^\infty} + v_s)\right|^2 dx &\le -\frac{C}{4}\int_\omega N_s^\infty \left(\frac{n_s}{N_s^\infty} + v_s\right)^2 dx \\
&\le -\frac{C}{2}\int_\omega \left(\frac{1}{2}\frac{(n_s)^2}{N_s^\infty} + n_s v_s\right) dx \le -\frac{C}{2} L(t).
\end{aligned}$$

Hence, we have obtained from (4.3.14)

$$\frac{d}{dt} L(t) \le -C_0 L(t) + C_1 L(t)^4 + C_2 \|v\|_{H^1(\Omega)} L(t). \tag{4.3.15}$$

By Proposition 4.3.1 (ii), there exists $T > 0$ such that, for all $t \ge T$, $C_2 \|v\|_{H^1(\omega)}(t) \le C_0/2$. Thus, for all $t \ge T$,

$$\frac{d}{dt} L(t) \le -\frac{C_0}{2} L(t) + C_1 L(t)^4. \tag{4.3.16}$$

From (4.3.5) and (4.3.7), there exists a sequence $t_j \to +\infty$ as $j \to +\infty$ such that the sequence $(\sqrt{N_s(t_j)})_{j\in\mathbb{N}}$ is bounded in $H^1(\omega)$. Up to a renumbering, we can suppose that for all $j \in \mathbb{N}$, $t_j \ge T$. Moreover, by interpolation, we have

$$\left\|\frac{n_s}{\sqrt{N_s^\infty}}\right\|_{L^2(\omega)} \le C \|n_s\|_{L^1(\omega)}^{1/4} \|n_s\|_{L^3(\omega)}^{3/4}.$$

By the Sobolev embedding of $H^1(\omega)$ into $L^6(\omega)$, we deduce that $\|n_s\|_{L^3(\omega)}(t_j)$ is bounded. Since we have proved in Proposition 4.3.1 (ii) that $n_s \to 0$ in $L^1(\omega)$ as t goes to $+\infty$, this insures the convergence towards 0 of $\|n_s/\sqrt{N_s^\infty}\|_{L^2(\omega)}(t_j)$ as j goes to $+\infty$. Moreover, with the bound of L in Lemma 4.3.2 we deduce

$$L(t) \le \frac{1}{2}\left\|\frac{n_s}{\sqrt{N_s^\infty}}\right\|_{L^2(\omega)}^2 + C\|n_s\|_{L^2(\omega)} \|v_s\|_{L^6(\omega)}.$$

And (4.3.13) provides a bound of $\|v_s\|_{L^6(\omega)}$ by $\|v\|_{H^1(\Omega)}$ which converges towards 0 as t goes to $+\infty$ thanks to Proposition 4.3.1. We can conclude now that $\lim_{j\to+\infty} L(t_j) = 0$. Hence,

$$\exists\, t_* > 0 \text{ such that } C_1 L(t_*)^3 \le \frac{C_0}{4}. \tag{4.3.17}$$

Now we define the set

$$\mathcal{A} := \left\{ t \in [t_*, +\infty) \text{ such that } \forall\, s \in [t_*, t], C_1 L(s)^3 \leq \frac{C_0}{4} \right\}.$$

By continuity of L, $\mathcal{A}$ is a closed set which contains t_* from (4.3.17). Moreover, if $t_0 \in \mathcal{A}$, from (4.3.16) we deduce that L is decreasing near t_0. By continuity of L, it yields that $\mathcal{A}$ is open. Thus, $\mathcal{A} = [t_*, +\infty)$, i.e.

$$\forall\, t \in [t_*, +\infty),\ \frac{d}{dt} L(t) \leq -\frac{C_0}{4} L(t).$$

We obtain the announced result by integrating this last inequality.

4.3.2.2 Proofs of the technical lemmata

Proof of Lemma 4.3.2. The concavity of the function $x \mapsto \log x$ leads to the inequality

$$v_s = \log\left(\frac{\sum_k e^{-\epsilon_k^\infty}}{\sum_k e^{-\epsilon_k}}\right) = \log\left(\sum_k \frac{e^{-\epsilon_k}}{\sum_\ell e^{-\epsilon_\ell}} e^{\epsilon_k - \epsilon_k^\infty}\right) \geq \sum_k \frac{e^{-\epsilon_k}}{\sum_\ell e^{-\epsilon_\ell}} (\epsilon_k - \epsilon_k^\infty). \qquad (4.3.18)$$

Therefore

$$\begin{aligned} N_s v_s - \langle N v \rangle &= N_s \left(v_s - \sum_k \frac{e^{-\epsilon_k}}{\sum_\ell e^{-\epsilon_\ell}} \langle |\chi_k|^2 v \rangle \right) \\ &\geq \frac{N_s}{\sum_\ell e^{-\epsilon_\ell}} \sum_k e^{-\epsilon_k} (\epsilon_k - \epsilon_k^\infty - \langle |\chi_k[V]|^2) v \rangle). \end{aligned}$$

The right hand side of this inequality is exactly the third term of (4.2.17) which is positive. Therefore

$$\int_\omega N_s v_s \, dx - \iint_\Omega N v \, dx dz \geq 0. \qquad (4.3.19)$$

By exchanging the roles of (N, N^∞) and (V, V^∞), we find

$$\iint_\Omega N^\infty v \, dx dz - \int_\omega N_s^\infty v_s \, dx \geq 0 \qquad (4.3.20)$$

which leads, by (4.3.11) and for all $t \geq 0$, to

$$0 \leq \frac{1}{2} \int_\omega \frac{(n_s)^2}{N_s^\infty} \, dx + \frac{1}{2} \iint_\Omega |\nabla v|^2 \, dx dz \leq L(t).$$

This ends the proof of Lemma 4.3.2. Remark that the sum of (4.3.19) and (4.3.20) leads to the inequality

$$\int_\omega n_s v_s \, dx \geq \iint_\Omega n v \, dx dz = \iint_\Omega |\nabla v|^2 \geq 0.$$

□

Proof of Lemma 4.3.3. We have

$$\nabla_x v_s = \sum_k \frac{e^{-\epsilon_k}}{\mathcal{Z}}(\partial_x \epsilon_k - \partial_x \underline{\epsilon_k}) + \sum_k \left(\frac{e^{-\epsilon_k}}{\mathcal{Z}} - \frac{e^{-\underline{\epsilon_k}}}{\underline{\mathcal{Z}}} \right) \partial_x \underline{\epsilon_k}\,, \tag{4.3.21}$$

with the notation $\underline{\mathcal{Z}} = \sum_\ell e^{-\underline{\epsilon_\ell}}$. Thus, by a Jensen inequality,

$$|\nabla_x v_s|^2 \leq 2 \sum_k \frac{e^{-\epsilon_k}}{\mathcal{Z}} |\partial_x \epsilon_k - \partial_x \underline{\epsilon_k}|^2 + 2 \left| \sum_k \left(\frac{e^{-\epsilon_k}}{\mathcal{Z}} - \frac{e^{-\underline{\epsilon_k}}}{\underline{\mathcal{Z}}} \right) \partial_x \underline{\epsilon_k} \right|^2 . \tag{4.3.22}$$

For the first term of the right hand side, we use the results stated in Lemma B.0.2 and B.0.4:

$$\begin{aligned}
&\sum_k \frac{e^{-\epsilon_k}}{\mathcal{Z}} |\partial_x \epsilon_k - \partial_x \underline{\epsilon_k}|^2 \\
&\quad \leq 2 \sum_k \frac{e^{-\epsilon_k}}{\mathcal{Z}} \langle |\chi_k|^2 \nabla_x v \rangle^2 + 2 \sum_k \frac{e^{-\epsilon_k}}{\mathcal{Z}} \langle (|\chi_k|^2 - |\underline{\chi_k}|^2) \nabla_x \underline{V} \rangle^2 \\
&\quad \leq C_1 e^{C_2 \|V(x,.)\|_{L^2(0,1)}} \langle |\nabla_x v| \rangle^2 + \int_0^1 C_1 e^{C_2 \|\underline{V}(x,.)+sv(x,.)\|_{L^2(0,1)}} \langle |v| \rangle^2 \langle |\nabla_x \underline{V}| \rangle^2 \, ds.
\end{aligned}$$

Consequently, we have

$$\sum_k \frac{e^{-\epsilon_k}}{\mathcal{Z}} |\partial_x \epsilon_k - \partial_x \underline{\epsilon_k}|^2 \leq C_1 e^{C_2 (\|\underline{V}\|_{L^2(0,1)} + \|v\|_{L^2(0,1)})} (\langle |\nabla_x v| \rangle^2 + \langle |v| \rangle^2 \langle |\nabla_x \underline{V}| \rangle^2). \tag{4.3.23}$$

We can write the second term of the right hand side of (4.3.22) as follows:

$$\begin{aligned}
\sum_k \left(\frac{e^{-\epsilon_k}}{\mathcal{Z}} - \frac{e^{\underline{\epsilon_k}}}{\underline{\mathcal{Z}}} \right) \partial_x \underline{\epsilon_k} = \; & \int_0^1 \frac{\sum_k \langle |\chi_k^s|^2 v \rangle e^{-\epsilon_k^s}}{\sum_\ell e^{-\epsilon_\ell^s}} \; \frac{\sum_k \langle |\underline{\chi_k}|^2 \nabla_x \underline{V} \rangle e^{-\epsilon_k^s}}{\sum_\ell e^{-\epsilon_\ell^s}} \, ds \\
& - \int_0^1 \sum_k \frac{\langle |\chi_k^s|^2 v \rangle e^{-\epsilon_k^s}}{\sum_\ell e^{-\epsilon_\ell^s}} \langle |\underline{\chi_k}|^2 \nabla_x \underline{V} \rangle \, ds,
\end{aligned}$$

where we use the notation $\epsilon_k^s = \epsilon_k[\underline{V} + sv]$ and $\chi_k^s = \chi_k[\underline{V} + sv]$. Thus, by applying the L^∞ bound in the z direction for χ_k^s and $\underline{\chi_k}$ stated in Lemma B.0.2, we obtain

$$\left| \sum_k \left(\frac{e^{-\epsilon_k}}{\mathcal{Z}} - \frac{e^{-\underline{\epsilon_k}}}{\underline{\mathcal{Z}}} \right) \partial_x \underline{\epsilon_k} \right|^2 \leq C_1 e^{C_2 (\|\underline{V}\|_{L^2(0,1)} + \|v\|_{L^2(0,1)})} \langle |v| \rangle^2 \langle |\nabla_x \underline{V}| \rangle^2. \tag{4.3.24}$$

By combining (4.3.23) and (4.3.24) in (4.3.22), we obtain (4.3.12). □

Proof of Lemma 4.3.4. From (4.3.12), we deduce

$$\begin{aligned}
&\int_\omega \frac{(n_s)^2}{N_s^\infty} |\nabla_x v_s|^2 \, dx \\
&\qquad \leq C_1 \int_\omega \frac{(n_s)^2}{N_s^\infty} e^{C_2 (\|V^\infty\|_{L_z^2(0,1)} + \|v\|_{L_z^2(0,1)})} (\langle |\nabla_x v| \rangle^2 + \langle |v| \rangle^2 \langle |\nabla_x V^\infty| \rangle^2) \, dx.
\end{aligned} \tag{4.3.25}$$

Throughout the proof, C, C_1 and C_2 stand for universal constants. Since V is bounded in $H^1(\Omega)$ uniformly in time, the Trudinger inequality implies

$$\exp(C_2(\|V^\infty\|_{L^2_z(0,1)} + \|v\|_{L^2_z(0,1)})) \in L^p(\omega), \quad \forall p \in [1,\infty). \tag{4.3.26}$$

Thus a Hölder inequality gives

$$\int_\omega \frac{(n_s)^2}{N_s^\infty} e^{C_2(\|V^\infty\|_{L^2_z(0,1)}+\|v\|_{L^2_z(0,1)})} \langle |\nabla_x v|\rangle^2 \, dx \leq C \left\| \frac{n_s}{\sqrt{N_s^\infty}} \right\|^2_{L^3(\omega)} \|\langle |\nabla_x v|\rangle\|^2_{L^8(\omega)}. \tag{4.3.27}$$

Using the expression given in (4.1.1) for $n = N - N^\infty$, we deduce

$$n = n_s \sum_k \frac{|\chi_k|^2 e^{-\epsilon_k}}{\mathcal{Z}} + N_s^\infty \sum_k \left[(|\chi_k|^2 - |\chi_k^\infty|^2) \frac{e^{-\epsilon_k}}{\mathcal{Z}} + |\chi_k^\infty|^2 \left(\frac{e^{-\epsilon_k}}{\mathcal{Z}} - \frac{e^{-\epsilon_k^\infty}}{\mathcal{Z}^\infty} \right) \right].$$

As we saw before, denoting $\epsilon_k^s = \epsilon_k[V + sv]$, and $\chi_k^s = \chi_k[V + sv]$ we can rewrite with Lemma B.0.3 the third term as follow :

$$\begin{aligned} \sum_k |\chi_k^\infty|^2 \left(\frac{e^{-\epsilon_k}}{\mathcal{Z}} - \frac{e^{-\epsilon_k^\infty}}{\mathcal{Z}^\infty} \right) = \; & \int_0^1 \frac{\sum_k \langle |\chi_k^s|^2 v\rangle e^{-\epsilon_k^s}}{\sum_\ell e^{-\epsilon_\ell^s}} \frac{\sum_k |\chi_k^\infty|^2 e^{-\epsilon_k^s}}{\sum_\ell e^{-\epsilon_\ell^s}} \, ds - \\ & \int_0^1 \sum_k \frac{\langle |\chi_k^s|^2 v\rangle e^{-\epsilon_k^s}}{\sum_\ell e^{-\epsilon_\ell^s}} |\chi_k^\infty|^2 \, ds. \end{aligned}$$

Since Lemma B.0.2 provides a bound of the eigenvectors of the Hamiltonian χ_k uniformly in k, we deduce, thanks to Lemma B.0.2 and Lemma B.0.4,

$$|n|(x,z) \leq C_1 e^{C_2(\|V^\infty\|_{L^2_z(0,1)}+\|v\|_{L^2_z(0,1)})} (|n_s|(x) + N_s^\infty \|v\|_{L^1_z(0,1)}(x)).$$

Therefore, using interpolation inequalities, (4.3.26) and $N_s^\infty \in L^\infty(\omega)$, ones deduces from elliptic regularity for the Poisson equation (4.1.4) that :

$$\|v\|_{H^2(\Omega)} \leq C\|n\|_{L^2(\Omega)} \leq C(\|n_s\|_{L^{18/7}(\omega)} + \|v\|_{H^1(\Omega)}). \tag{4.3.28}$$

With a Gagliardo-Nirenberg inequality and (4.3.28), we have

$$\begin{aligned} \|\langle |\nabla_x v|\rangle\|_{L^8(\omega)} & \leq C \|\langle |\nabla_x v|\rangle\|^{1/4}_{L^2(\omega)} \|\langle |\nabla_x v|\rangle\|^{3/4}_{H^1(\omega)} \\ & \leq C \|v\|^{1/4}_{H^1(\Omega)} (\|n_s\|^{3/4}_{L^{18/7}(\omega)} + \|v\|^{3/4}_{H^1(\Omega)}). \end{aligned} \tag{4.3.29}$$

By interpolation inequalities, we get

$$\left\| \frac{n_s}{\sqrt{N_s^\infty}} \right\|^2_{L^3(\omega)} \leq \left\| \frac{n_s}{\sqrt{N_s^\infty}} \right\|_{L^2(\omega)} \left\| \frac{n_s}{\sqrt{N_s^\infty}} \right\|_{L^6(\omega)} \tag{4.3.30}$$

and

$$\|n_s\|_{L^{18/7}(\omega)} \leq \|n_s\|^{2/3}_{L^2(\omega)} \|n_s\|^{1/3}_{L^6(\omega)}. \tag{4.3.31}$$

Thus by (4.3.27), (4.3.29), (4.3.30) and (4.3.31), we obtain

$$\int_\omega \frac{(n_s)^2}{N_s^\infty} e^{C_2(\|V^\infty\|_{L^2_z(0,1)}+\|v\|_{L^2_z(0,1)})} \langle |\nabla_x v|\rangle^2\, dx \\ \leq C \left\| \frac{n_s}{\sqrt{N_s^\infty}} \right\|_{L^2(\omega)} \left\| \frac{n_s}{\sqrt{N_s^\infty}} \right\|_{L^6(\omega)} \|v\|^{1/2}_{H^1(\Omega)} (\|n_s\|_{L^2(\omega)} \|n_s\|^{1/2}_{L^6(\omega)} + \|v\|^{3/2}_{H^1(\Omega)}).$$

Finally, using $N_s^\infty \geq C > 0$ and Lemma 4.3.2, we have

$$\int_\omega \frac{(n_s)^2}{N_s^\infty} e^{C_2(\|V^\infty\|_{L^2_z(0,1)}+\|v\|_{L^2_z(0,1)})} \langle |\nabla_x v|\rangle^2\, dx \\ \leq C_1 L(t) \|n_s\|^{3/2}_{L^6(\omega)} \|v\|^{1/2}_{H^1(\Omega)} + C_2 L(t)^{1/2} \|n_s\|_{L^6(\omega)} \|v\|^2_{H^1(\Omega)}. \tag{4.3.32}$$

Now, to handle the term $\|n_s\|_{L^6(\omega)}$, we decompose $\|n_s\|_{L^6(\omega)} \leq C(\|n_s/N_s^\infty + v_s\|_{L^6(\omega)} + \|v_s\|_{L^6(\omega)})$. By (4.3.18) we have:

$$|v_s| \leq \max\left\{ \sum_k \frac{e^{-\epsilon_k}}{\sum_\ell e^{-\epsilon_\ell}} |\epsilon_k - \epsilon_k^\infty|, \sum_k \frac{e^{-\epsilon_k^\infty}}{\sum_\ell e^{-\epsilon_\ell^\infty}} |\epsilon_k^\infty - \epsilon_k| \right\}.$$

Hence, with Lemma B.0.4 and (4.3.26), we deduce

$$\|v_s\|_{L^6(\omega)} \leq C \|v\|_{L^8_x L^1_z(\Omega)} \leq C \|v\|_{H^1(\Omega)},$$

thanks to the Sobolev embedding of $H^1(\Omega)$ into $L^8_x L^1_z(\Omega)$, which proves the inequality (4.3.13) in Lemma 4.3.4. Moreover Proposition 4.3.1 provides a uniform bound on $\|v\|_{H^1(\Omega)}$ which, with the inequality (4.3.32) and Lemma 4.3.2, leads to

$$\int_\omega \frac{(n_s)^2}{N_s^\infty} e^{C_2(\|V^\infty\|_{L^2_z(0,1)}+\|v\|_{L^2_z(0,1)})} \langle |\nabla_x v|\rangle^2\, dx \\ \leq C_1 L(t) \left\| \frac{n_s}{N_s^\infty} + v_s \right\|^{3/2}_{L^6(\omega)} + C_2 L(t)^{1/2} \left\| \frac{n_s}{N_s^\infty} + v_s \right\|_{L^6(\omega)} \|v\|_{H^1(\Omega)} + C_3 L(t) \|v\|_{H^1(\Omega)}. \tag{4.3.33}$$

Finally, using $x^{1/4} y^{3/4} \leq \frac{1}{4\varepsilon^3} x + \frac{3}{4}\varepsilon y$, we have

$$L(t) \left\| \frac{n_s}{N_s^\infty} + v_s \right\|^{3/2}_{L^6(\omega)} \leq \frac{1}{4\varepsilon^3} L(t)^4 + \frac{3}{4}\varepsilon \left\| \frac{n_s}{N_s^\infty} + v_s \right\|^2_{L^6(\omega)} \\ \leq \frac{1}{4\varepsilon^3} L(t)^4 + C\varepsilon \left\| \nabla_x \left(\frac{n_s}{N_s^\infty} + v_s \right) \right\|^2_{L^2(\omega)},$$

where the Sobolev embedding $H^1 \hookrightarrow L^6(\omega)$ and the Poincaré inequality are used. Proceeding analogously for the second term in (4.3.33), we obtain the desired inequality for ε fixed small enough.

In order to estimate the second term in (4.3.25), we first use the Sobolev embedding $H^1(\Omega) \hookrightarrow L^8_x L^1_z(\Omega)$ and (4.3.26), we have

$$\int_\omega \frac{(n_s)^2}{N_s^\infty} e^{C_2(\|V^\infty\|_{L^2_z(0,1)}+\|v\|_{L^2_z(0,1)})} \langle |v|\rangle^2 \langle |\nabla_x V^\infty|\rangle^2\, dx \leq C \|v\|^2_{H^1(\Omega)} \left\| \frac{n_s}{\sqrt{N_s^\infty}} \right\|^2_{L^3(\omega)}.$$

With (4.3.30) and Lemma 4.3.2, it yields

$$\begin{aligned}\int_\omega \frac{(n_s)^2}{N_s^\infty} e^{C_2(\|V^\infty\|_{L_z^2(0,1)}+\|v\|_{L_z^2(0,1)})}\langle|v|\rangle^2\langle|\nabla_x V^\infty|\rangle^2\,dx \\ \leq CL(t)^{1/2}\|v\|_{H^1(\Omega)}^2\left(\left\|\frac{n_s}{N_s^\infty}+v_s\right\|_{L^6(\omega)}+\|v_s\|_{L^6(\omega)}\right).\end{aligned} \tag{4.3.34}$$

By proceeding as above, we obtain the desired inequality for the second term, which concludes the proof. □

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Chapter 5

Théorie $L \log L$ pour DDSP pour un système isolé

5.1 Introduction and main results

5.1.1 Presentation of the model

In this work we will analyzed the DDSP system when the diffusion matrix is not assumed to be scalar. Thus, we have to work in a $L \log L$ framework given by the entropy estimate.

We assume that the transport variable x lies in a bounded regular domain $\omega \subset \mathbb{R}^2$, the drift-diffusion equation is given in ω by

$$\partial_t N_s - \text{div}_x(\mathbb{D}(\nabla_x N_s + N_s \nabla_x V_s)) = 0, \tag{5.1.1}$$

where $\mathbb{D}$ is the diffusion matrix and V_s is the effective potential defined in (1.0.5). At a time t and a position $(x, z) \in \Omega = \omega \times (0, 1)$, we denote the particle density by $N(t, x, z)$, for Boltzmann statistics it is given by

$$N(t, x, z) = N_s(t, x) \sum_k \frac{e^{-\epsilon_k(t,x)}}{\mathcal{Z}(t, x)} |\chi_k(t, x, z)|^2 , \tag{5.1.2}$$

where the repartition function $\mathcal{Z}$ is defined in (4.1.2) and $(\epsilon_k, \chi_k)_{k\geq 1}$ is the complete set of eigenvalues and eigenfunctions of the 1D Schrödinger operator in the z variable

$$\begin{cases} -\dfrac{1}{2}\,\partial_z^2 \chi_k + V\chi_k = \epsilon_k \chi_k & (k \geq 1), \\ \chi_k(t, x, \cdot) \in H_0^1(0, 1), & \displaystyle\int_0^1 \chi_k\, \chi_\ell\, dz = \delta_{k\ell}\,. \end{cases} \tag{5.1.3}$$

The electrostatic potential V is obtained thanks to the resolution of the Poisson equation

$$-\Delta_{x,z} V = N = N_s \sum_k \frac{e^{\epsilon_k}}{\mathcal{Z}} |\chi_k|^2 \,. \tag{5.1.4}$$

We usually define the slotboom variable u and the Fermi level ϵ_F by

$$u(t,x) = e^{\epsilon_F(t,x)} = \frac{N_s(t,x)}{\mathcal{Z}(t,x)}. \tag{5.1.5}$$

We have then $\rho_k(t,x) = u(t,x)e^{-\epsilon_k(t,x)}$. The unknowns of the overall system are the surface density $N_s(t,x)$, the electrostatic potential $V(t,x,z)$, the eigenenergies $\epsilon_k(t,x)$ and the eigenvectors $\chi_k(t,x,z)$.

The system is completed with the initial condition

$$N_s(0,x) = N_s^0(x), \tag{5.1.6}$$

and by the following boundary conditions :

$$\partial_\nu V(t,x,z) = 0 \text{ on } \partial\omega \times (0,1), \qquad V(t,x,0) = V(t,x,1) = 0 \text{ for } x \in \omega, \tag{5.1.7}$$

for the potential and

$$\partial_\nu N_s(t,x) = 0 \text{ on } \partial\omega \times (0,1), \tag{5.1.8}$$

where $\partial\omega$ is the boundary of ω and $\nu(x)$ denotes the outward unit normal vector at $x \in \partial\omega$.

5.1.2 Main results

In the previous chapter we have analyzed the DDSP system and proved an existence and uniqueness result and studied the long time behaviour. But we prove this result only in the case of a scalar and constant diffusion matrix. If we want to consider a non-scalar and non-constant but regular enough diffusion matrix we can not apply these results here. Indeed we lose some regularity such that the only estimate that we have on the density is the entropy estimate : we have to work with a surface density in $L \log L$.

In this work we propose to extend the previous results on the existence and long time behaviour in the case of a general but smooth diffusion matrix :

Assumption 5.1.1 *The function $\mathbb{D}$ is assumed to be a C^1 function on $\overline{\Omega}$ into the set of 2×2 symmetric positive definite matrix such that for all $x \in \Omega$ we have $\mathbb{D}(x) \geq \alpha I$, where $\alpha > 0$ is given.*

Moreover we make the following assumption on the initial conditions

Assumption 5.1.2 *The initial condition satisfies $N_s^0 \in L^2(\omega)$ and $N_s^0 \geq 0$ a.e. And we denote*

$$\mathcal{N}_I = \int_\omega N_s^0 \, dx.$$

The first result of this work concerns the existence of solutions for the drift-diffusion-Schrödinger-Poisson system presented above.

Theorem 5.1.3 *Let $T > 0$. Under Assumptions 5.1.1 and 5.1.2 the system* (5.1.1)-(5.1.3)–(5.1.8) *admits a weak solution such that*

$$N_s \log N_s \in L^\infty([0,T], L^1(\omega)) \text{ and } \sqrt{N_s} \in L^2([0,T], H^1(\omega)),$$
$$V \in L^\infty([0,T], H^1(\omega)).$$

In order to present our second result, we introduce the steady state (N_s^∞, V^∞) of our system. The stationary drift-diffusion equation implies directly that the Slotboom variable u is constant and with the conservation of the mass we have

$$u = \frac{\mathcal{N}_I}{\sum_k \int_\Omega e^{-\epsilon_k[V^\infty](x)}\,dx}\,,$$

where V^∞ is defined by

$$\begin{cases} N_s^\infty(x) = \dfrac{\mathcal{N}_I}{\sum_k \int_\Omega e^{-\epsilon_k[V^\infty](x)}\,dx} \displaystyle\sum_k e^{-\epsilon_k[V^\infty](x)} \\ -\dfrac{1}{2}\,\partial_z^2 \chi_k + V^\infty \chi_k = \epsilon_k \chi_k \qquad (k \geq 1), \\ \chi_k(t,x,\cdot) \in H_0^1(0,1), \qquad \displaystyle\int_0^1 \chi_k\,\chi_\ell\,dz = \delta_{k\ell}\,, \\ -\Delta V^\infty = N_s^\infty \displaystyle\sum_k \frac{e^{-\epsilon_k[V^\infty]}}{\sum_k e^{-\epsilon_k[V^\infty]}} |\chi_k[V^\infty]|^2, \end{cases} \tag{5.1.9}$$

with the boundary conditions

$$\partial_\nu V^\infty(x,z) = 0 \text{ on } \partial\omega \times (0,1), \qquad V^\infty(x,0) = V^\infty(x,1) = 0 \text{ for } x \in \omega.$$

We can prove that this system admits a unique solution $V^\infty \in C^2(\overline{\Omega})$ (see [10, 18]).

Theorem 5.1.4 *Under assumptions 5.1.1 and 5.1.2, if N_s, V is a solution defined in Theorem 5.1.3 and if N^∞, V^∞ is defined in* (5.1.9)*. Then there exists two constants $\kappa > 0$ and $C > 0$ such that for all $t \geq 0$*

$$\|N_s - N_s^\infty\|_{L^1(\omega)}(t) + \|V - V^\infty\|_{H^1(\Omega)}(t) \leq C e^{-\kappa t}.$$

Compared to chapter 4, the main difference is the general framework of our study. In the previous work, we worked with a density in L^2. But with a non-scalar diffusion matrix we are not able to prove that the solutions of the drift-diffusion equation stay in L^2 for a regular initial data. Thus we have to work in a $L \log L$ framework. It can be done thanks to precise estimates on the spectrum of the Hamiltonian which is given in the Appendix.

We present our results only in the case of conservative boundary conditions (5.1.7)-(5.1.8) for the sake of simplicity and to present a different way based on the logarithmic Sobolev inequalities to study the long time behaviour. But we can easily extend them to Dirichlet boundary conditions.

5.1.3 Strategy of the proofs

Regarding the whole system, we shall take advantage of its structure : an evolution drift-diffusion equation (5.1.1) coupled to a quasistatic Schrödinger-Poisson problem (5.1.3)-(5.1.4). Therefore following [4], we will use a fixed point procedure to construct solutions. The main ingredients for the existence will be some a priori estimates and the wellposedness of the Schrödinger-Poisson system in our framework.

In order to insure sufficient regularity we have to consider a regularized system. For a parameter $\varepsilon \in [0,1]$, we define the linear regularization operator by

$$\begin{array}{rcl} R^\varepsilon : L^1(\Omega) & \to & C^\infty(\overline{\Omega}) \\ V & \to & R^\varepsilon[V](x,z) = (\overline{V} *_x \xi_{\varepsilon,x} *_z \xi_{\varepsilon,z})|_{\overline{\Omega}} \end{array} \tag{5.1.10}$$

where $\overline{V}$ is the extension of V by zero outside Ω and $\xi_{\varepsilon,x}$ and $\xi_{\varepsilon,z}$ are C^∞ nonnegative compactly supported even approximations of the unity, respectively on $\mathbb{R}^2$ and $\mathbb{R}$. We write then the regularized system:

$$\partial_t N_s^\varepsilon - \operatorname{div}_x(\mathbb{D}(\nabla_x N_s^\varepsilon + N_s^\varepsilon \nabla_x V_s^\varepsilon)) = 0, \tag{5.1.11}$$

$$\begin{cases} -\dfrac{1}{2}\,\partial_z^2 \chi_k^\varepsilon + R^\varepsilon[V^\varepsilon]\chi_k^\varepsilon = \epsilon_k^\varepsilon \chi_k^\varepsilon \qquad (k \geq 1), \\ \chi_k^\varepsilon(t,x,\cdot) \in H_0^1(0,1), \qquad \displaystyle\int_0^1 \chi_k^\varepsilon\, \chi_\ell^\varepsilon\, dz = \delta_{k\ell}\,, \end{cases} \tag{5.1.12}$$

$$-\Delta_{x,z} V^\varepsilon = R^\varepsilon\left[\sum_k \int_{\mathbb{R}^2} N_s^\varepsilon \frac{e^{-\epsilon_k^\varepsilon}}{\mathcal{Z}^\varepsilon} |\chi_k^\varepsilon|^2\, dv\right]. \tag{5.1.13}$$

Remark 5.1.5 *When $\varepsilon = 0$, we have $R^0 = Id$ and the regularized problem reduces to the unregularized system.*

Therefore the solutions of the overall problem are obtained thanks to the passage to the limit $\varepsilon \to 0$ on solutions of the regularized problem (5.1.11)–(5.1.13). The key points for the passage at the limit is then to establish uniform estimates independent of ε. Section 5.2 is devoted to these estimates. In section 5.3 we analyze the Schrödinger-Poisson system in the general framework given by our estimates. And in section 5.4 we detail the proof of Theorem 5.1.3 which is decomposed into several steps : existence of solutions for the regularized system, using the uniform estimates to pass to the limit $\varepsilon \to 0$ in the solutions of the regularized system to obtain solutions of the unregularized system. In the last section, we present the proof of Theorem 5.1.4. We use a general method based on the logarithmic Sobolev inequalities (see [1, 2, 7, 9, 14]). This method consists in proving the exponential decay as t grows to $+\infty$ of the relative entropy.

5.2 Free energy and a priori estimates

In this section, we will establish some uniform estimates on the solution of the regularized system (5.1.11)–(5.1.13). For the sake of clarity we skip all the exponent ε. We define the total free energy of the system by

$$W = \sum_{k\geq 1} \int_\omega \rho_k \log \rho_k\, dx + \frac{1}{2} \iint_\Omega |\nabla_{x,z} V|^2\, dxdz + \frac{1}{2} \sum_k \int_\omega \rho_k \langle |\partial_z \chi_k|^2 \rangle\, dx. \tag{5.2.14}$$

Lemma 5.2.1 *Let $\varepsilon \in [0,1]$. Consider any weak solution (N_s, V) of the regularized system (5.1.11)–(5.1.13) such that $N_s \log N_s \in L^\infty_{loc}(\mathbb{R}^+, L^1(\omega))$, $V \in L^\infty_{loc}(\mathbb{R}^+, H^1(\Omega))$ and $\sqrt{N_s} \in L^2_{loc}(\mathbb{R}^+, H^1(\omega))$. Then we have*

$$\frac{d}{dt}W(t) = -D(t) := -\int_\omega \mathcal{Z}\,\mathbb{D}\,\frac{\nabla_x u \cdot \nabla_x u}{u}\,dx.$$

Proof. First, we notice that our boundary conditions (5.1.7)-(5.1.8) implies $\partial_\nu u = 0$ on $\partial\omega$. Hence $J \cdot \nu = 0$ on $\partial\omega$ and the total mass of the system is conserved :

$$\frac{d}{dt}\int_\omega N_s\,dx = 0.$$

We have

$$\frac{d}{dt}\sum_k \int_\omega \rho_k \log \rho_k\,dx = \frac{d}{dt}\sum_{k\geq 1}\int_\omega (\rho_k \log\rho_k - \rho_k)\,dx = \sum_{k\geq 1}\int_\omega \partial_t\rho_k \log\rho_k\,dx.$$

Taking advantage of the identity $\log\rho_k = \log u - \epsilon_k$ and from $N_s = \sum_k \rho_k$, we find

$$\frac{d}{dt}\sum_{k\geq 1}\int_\omega (\rho_k\log\rho_k - \rho_k)\,dx = \int_\omega \partial_t N_s \log u\,dx - \sum_{k\geq 1}\int_\omega \partial_t\rho_k \epsilon_k\,dx.$$

With the notation $\langle f\rangle = \int_0^1 f(z)\,dz$, the linearity of the regularization R^ε and Lemma B.0.3 imply that

$$\partial_t\epsilon_k = \langle |\chi_k|^2 \partial_t R^\varepsilon[V]\rangle = \langle |\chi_k|^2 R^\varepsilon[\partial_t V]\rangle.$$

This identity and the drift-diffusion equation (5.1.11) lead to

$$\begin{aligned}\frac{d}{dt}\sum_{k\geq 1}\int_\omega (\rho_k\log\rho_k - \rho_k)\,dx \quad &= \int_\omega \operatorname{div}_x\left(\mathbb{D}\left(\sum_k e^{-\epsilon_k}\nabla_x u\right)\right)\log u\,dx \\ &+\sum_k \iint_\Omega \rho_k |\chi_k|^2 R^\varepsilon[\partial_t V]\,dxdz - \frac{d}{dt}\sum_k\int_\omega \rho_k\epsilon_k\,dx.\end{aligned} \tag{5.2.15}$$

The selfadjointness of the operator R^ε on $L^2(\Omega)$ and the Poisson equation (5.1.13) imply

$$\sum_k \iint_\Omega \rho_k|\chi_k|^2 R^\varepsilon[\partial_t V]\,dxdz = \frac{d}{dt}\sum_k\int_\omega \rho_k\langle|\chi_k|^2 R^\varepsilon[V]\rangle\,dx - \frac{1}{2}\frac{d}{dt}\iint_\Omega |\nabla_{x,z}V|^2\,dxdz.$$

Hence, after an integration by parts on the first term of the right hand side of (5.2.15), we obtain

$$\begin{aligned}&\frac{d}{dt}\sum_k\int_\omega(\rho_k\log\rho_k - \rho_k)\,dx + \frac{1}{2}\frac{d}{dt}\iint_\Omega |\nabla_{x,z}V|^2\,dxdz \\ &+\frac{d}{dt}\sum_k\int_\omega \rho_k(\epsilon_k - \langle|\chi_k|^2R^\varepsilon[V]\rangle)\,dx = -\int_\omega\left(\sum_k e^{-\epsilon_k}\right)\frac{\mathbb{D}\nabla_x u\cdot\nabla_x u}{u}\,dx.\end{aligned}$$

To conclude the proof it suffices to notice that, from the Schrödinger equation 5.1.12, we have

$$\epsilon_k - \langle |\chi_k|^2 R^\varepsilon[V] \rangle = \frac{1}{2} \langle |\partial_z \chi_k|^2 \rangle.$$

□

This allows us to prove some a priori estimates :

Corollary 5.2.2 *Let $\varepsilon \in [0,1]$ and (N_s, V) such as in Lemma 5.2.1 and satisfying Assumptions 5.1.1 and 5.1.2. Then the following estimates holds :*

(i) mass :

$$\forall t \in \mathbb{R}^+, \int_\omega N_s \, dx = \mathcal{N}_I$$

(ii) entropy : there exist nonnegative constants C_1, C_2 and C_3 independent of ε, such that

$$\forall t \in \mathbb{R}^+, \quad \sum_{k \geq 1} \int_\omega \rho_k (1 + k^2 + |\log \rho_k|) \, dx \leq C_1, \tag{5.2.16}$$

$$\forall t \in \mathbb{R}^+, \quad \int_\omega N_s |\log N_s| \, dx \leq C_2, \tag{5.2.17}$$

$$\forall t \in \mathbb{R}^+, \quad \iint_\Omega |\nabla_{x,z} V|^2 \, dxdz \leq C_3. \tag{5.2.18}$$

(iii) dissipation : there exist nonnegative constants C_4 and C_5 independent of ε such that

$$\forall t \in \mathbb{R}^+, \quad \int_0^t \int_\omega |\nabla_x \sqrt{N_s}|^2 \, dxds \leq C_4, \tag{5.2.19}$$

$$\forall t \in \mathbb{R}^+, \ \forall p \in [1, +\infty) \quad \int_0^t \int_\omega \|N_s\|_{L^p(\omega)}(s) \, ds \leq C_5. \tag{5.2.20}$$

Proof. The first point in an easy consequence of our choice of boundary conditions. From Lemma 5.2.1 we deduce after an integration in time that

$$\forall t \in \mathbb{R}^+, \quad W(t) = W(0) - \int_0^t D(s) \, ds \leq W(0). \tag{5.2.21}$$

Assumption 5.1.2 on initial data insures that $W(0)$ is bounded independently on ε. In fact, solving the Schrödinger-Poisson system for a given N_s^0 in $L^2(\omega)$ furnishes $V(t=0,\cdot,\cdot) \in H^2(\Omega) \subset L^\infty(\Omega)$ and then $\epsilon_k(t=0,\cdot) \in L^\infty(\omega)$ and $\partial_z \chi_k(t=0,\cdot) \in L^\infty(\Omega)$ (see [5] and the Appendix).

If we denote $\epsilon_k^\sigma = \epsilon_k[\sigma R^\varepsilon[V]]$ and $\chi_k^\sigma = \chi_k[\sigma R^\varepsilon[V]]$. Straightforward computations using Lemma B.0.3 lead to

$$\sum_k u e^{-\epsilon_k} (\epsilon_k - \epsilon_k[0] - \langle |\chi_k|^2 R^\varepsilon[V] \rangle) =$$

$$= \int_0^1 \int_1^s \sum_{k, \ell \neq k} u \frac{e^{-\epsilon_k} - e^{-\epsilon_\ell}}{\epsilon_k^\sigma - \epsilon_\ell^\sigma} \langle \chi_k^\sigma R^\varepsilon[V] \chi_\ell^\sigma \rangle^2 \, d\sigma ds \geq 0,$$

since the sequence $(\epsilon_k)_{k\geq 1}$ is increasing. And we have $\epsilon_k[0] = \pi^2 k^2/2$. Thus (5.2.21) implies that

$$\sum_k \int_\omega \rho_k\left(\frac{\pi^2 k^2}{2} + \log \rho_k\right) dx + \frac{1}{2} \iint_\Omega |\nabla_{x,z} V|^2 \, dxdz \leq W(0). \tag{5.2.22}$$

If we denote $K = \sum e^{-k^2}$, by a Jensen inequality we have,

$$\begin{aligned} W(0) \geq \sum_k \int_\omega \rho_k(k^2 + \log \rho_k)\, dx \quad &= K \sum_k \int_\omega \frac{\rho_k}{e^{-k^2}} (\log \frac{\rho_k}{e^{-k^2}}) \frac{e^{-k^2}}{K} \, dx \\ &\geq \int_\omega N_s \log(N_s/K) \, dx. \end{aligned}$$

Thus from (5.2.22),

$$\forall\, t \in \mathbb{R}^+, \qquad \int_\omega N_s \log N_s \, dx \leq W(0) + \mathcal{N}_I \log K.$$

Then estimate (5.2.17) is a direct consequence of the remark that $\forall\, a > 0$, $a|\log a| \leq a \log a + 2/e$. Moreover it leads to

$$\begin{aligned} \sum_k \int_\omega \rho_k |\log \rho_k| \, dx \quad &\leq \sum_k \int_\omega \rho_k(|\log(\rho_k/e^{-k^2})| + k^2)\, dx \\ &\leq \sum_k \int_\omega \rho_k(\log(\rho_k/e^{-k^2}))\, dx + \frac{2}{e} \sum_k \int_\omega e^{-k^2} \, dx \\ &\qquad + \sum_k \int_\omega \rho_k k^2 \, dx \\ &\leq \sum_k \int_\omega \rho_k(\log \rho_k + 2k^2)\, dx + \frac{2}{e} |\omega| K, \end{aligned}$$

where $|\omega|$ denotes the Lebesgue measure of ω. Thus, we deduce from (5.2.22) that we have

$$\forall\, t \in \mathbb{R}^+, \quad \sum_k \int_\omega \rho_k |\log \rho_k| \, dx \leq W(0) + \frac{2}{e}|\omega| K. \tag{5.2.23}$$

Hence from (5.2.22), we obtain

$$\frac{1}{2} \iint_\Omega |\nabla_{x,z} V|^2 \, dxdz \leq 2W(0) + \frac{2}{e}|\omega| K,$$

and

$$\sum_k \int_\omega \rho_k k^2 \, dx \leq 2W(0) + \frac{2}{e}|\omega| K.$$

For the point (iii), we remark that thanks to Assumption 5.1.1 and the expression of the Slotboom variable u (5.1.5), we have

$$\begin{aligned} D &\geq \alpha \int_\omega \frac{|\nabla_x N_s + N_s \nabla_x V_s|^2}{N_s} \, dx \\ &= \alpha \int_\omega (4|\nabla_x \sqrt{N_s}|^2 + 2\nabla_x N_s \cdot \nabla_x V_s + N_s |\nabla_x V_s|^2)\, dx. \end{aligned} \tag{5.2.24}$$

An integration by parts proves that

$$\int_\omega \nabla_x N_s \cdot \nabla_x V_s \, dx = -\int_\omega N_s \Delta_x V_s \, dx + \int_{\partial\omega} N_s \partial_\nu V_s \, d\sigma, \tag{5.2.25}$$

where $d\sigma$ is the surface measure on $\partial\omega$. From the expression of V_s in (1.0.5), we deduce that

$$\int_{\partial\omega} N_s \partial_\nu V_s \, d\sigma = \int_{\partial\omega\times(0,1)} N \partial_\nu V \, d\sigma dz = 0,$$

with our boundary conditions (5.1.7). Moreover, straightforward computations lead to the following identity

$$\begin{aligned} -\Delta_x V_s &= -4S_2(t,x) + \frac{\langle N^2 + 4V^2\, N\rangle}{N_s} + 2\sum_k \frac{e^{-\epsilon_k}}{\mathcal{Z}} \left\langle (V+\epsilon_k)|\partial_z \chi_k|^2 \right\rangle \\ &\quad -\frac{1}{\mathcal{Z}} \sum_k \sum_{\ell\neq k} \left(\frac{e^{-\epsilon_k} - e^{-\epsilon_\ell}}{\epsilon_k - \epsilon_\ell} \right) \langle \chi_k \chi_\ell \, \nabla_x V \,\rangle^2 \\ &\quad + \sum_k \frac{e^{-\epsilon_k}}{\mathcal{Z}} \left\langle |\chi_k|^2 \, \nabla_x V \right\rangle^2 - \left(\sum_k \frac{e^{-\epsilon_k}}{\mathcal{Z}} \left\langle |\chi_k|^2 \, \nabla_x V \right\rangle \right)^2, \end{aligned}$$

where S_2 is given by

$$S_2(t,x) = \sum_k \frac{e^{-\epsilon_k(t,x)}}{\mathcal{Z}(t,x)} (\epsilon_k(t,x))^2.$$

By the Cauchy-Schwarz inequality, the sum of the last two terms of the right hand side is nonnegative. Moreover, except for the first one, the other terms are obviously nonnegative. From (5.2.25), we have

$$\int_\omega \nabla_x N_s \cdot \nabla_x V_s \, dx \geq -4 \int_\omega S_2 N_s \, dx \geq -4 \|N_s\|_{L^4(\omega)} \|S_2\|_{L^{4/3}(\omega)}.$$

It is proved in Lemma B.0.8 that S_2 is bounded in $L^p(\omega)$ for all $p \in [1, +\infty)$. Thus we deduce from (5.2.24) that

$$4\alpha \int_\omega |\nabla_x \sqrt{N_s}|^2 \, dx \leq D + 8 \|S_2\|_{L^{4/3}(\omega)} \|N_s\|_{L^4(\omega)}. \tag{5.2.26}$$

We recall the Gagliardo-Nirenberg inequality for all $p \in [2, +\infty]$:

$$\|u\|_{L^p(\omega)} \leq C \|u\|_{L^2(\omega)}^{2/p} \|\nabla u\|_{L^2(\omega)}^{1-2/p}. \tag{5.2.27}$$

If we apply it for $p = 8$ and $u = \sqrt{N_s}$, we have

$$\|N_s\|_{L^4(\omega)} \leq C \|N_s\|_{L^1(\omega)}^{1/4} \|\nabla_x \sqrt{N_s}\|_{L^2(\omega)}^{3/2} = C \mathcal{N}_I^{1/4} \|\nabla_x \sqrt{N_s}\|_{L^2(\omega)}^{3/2}. \tag{5.2.28}$$

Thus if we inject (5.2.28) in (5.2.26), we deduce that there exists a nonnegative constant C such that

$$\forall\, t \in \mathbb{R}^+, \qquad \int_\omega |\nabla_x \sqrt{N_s}|^2 \, dx \leq C(1 + D(t)).$$

Since we have from Lemma 5.2.1 that $\int_0^t D(s)\,ds \le W(0)$, for all $t \in \mathbb{R}^+$, we obtain (5.2.19) and from (5.2.27) with $u = \sqrt{N_s}$, we have (5.2.20).

$\square$

5.3 The regularized Schrödinger-Poisson system

In this section the surface density N_s is assumed to be given and we only consider the resolution of the "quasistatic" regularized Schrödinger-Poisson system. By analogy with section 4.2.4, it is important to analyze the Schrödinger-Poisson block. However in this case the lack of regularity forces us to regularized the system with a small parameter ε. It is then necessary to clarify the evolution of this system as $\varepsilon \to 0$ and to be able to analyze it for a density only in $L \log L$. This regularized system is defined for $\varepsilon \in [0,1]$ by:

$$\begin{cases} -\dfrac{1}{2}\,\partial_z^2 \chi_k^\varepsilon + R^\varepsilon[V^\varepsilon]\chi_k^\varepsilon = \epsilon_k^\varepsilon \chi_k^\varepsilon \qquad (k \ge 1), \\ \chi_k^\varepsilon(t,x,\cdot) \in H_0^1(0,1), \qquad \displaystyle\int_0^1 \chi_k^\varepsilon\,\chi_\ell^\varepsilon\,dz = \delta_{k\ell}\,, \end{cases} \tag{5.3.29}$$

$$-\Delta_{x,z} V^\varepsilon = R^\varepsilon\left[N_s \sum_k \frac{e^{\epsilon_k^\varepsilon}}{\mathcal{Z}^\varepsilon} |\chi_k^\varepsilon|^2 \right]. \tag{5.3.30}$$

The system is completed by the following boundary conditions:

$$\partial_\nu V^\varepsilon(t,x,z) = 0 \text{ on } \partial\omega \times (0,1), \qquad V^\varepsilon(t,x,0) = V^\varepsilon(t,x,1) = 0 \text{ for } x \in \omega.$$

We remark that in the case $\varepsilon = 0$, we have $R^0 = Id$ and we recover the unregularized Schrödinger-Poisson system (5.1.3)–(5.1.4).

We assume that N_s satisfies the following assumption:

H1 : $N_s \ge 0$ and there exists a nonnegative constant C_T such that:

$$\forall\, t \in [0,T], \qquad \int_\omega (N_s |\log N_s| + 1)\,dx \le C_T, \tag{5.3.31}$$

In the sequel we will use the functional space $H_{01}^1 = \{V \in L^\infty((0,T), H^1(\Omega)) : V(t,x,0) = V(t,x,1) = 0\}$.

We can prove straightforwardly from convolution results that the regularization operator R^ε defined in (5.1.10) satisfies the following properties :

Lemma 5.3.1 *(i) R^ε is a bounded operator on $L_x^p L_z^q(\Omega)$ for $1 \le p,q \le +\infty$ and satisfies*

$$\forall\, V \in L_x^p L_z^q(\Omega), \quad \|R^\varepsilon[V]\|_{L_x^p L_z^q(\Omega)} \le \|V\|_{L_x^p L_z^q(\Omega)}.$$

$$\textit{if } 1 \le p,q < +\infty \textit{ and } V \in L_x^p L_z^q(\Omega), \textit{ then } \lim_{\varepsilon \to 0} \|R^\varepsilon[V] - V\|_{L_x^p L_z^q(\Omega)} = 0.$$

(ii) R^ε is selfadjoint on $L^2(\Omega)$.

(iii) Let $r \ge 1$ be given and $V \in W^{1,r}(\Omega)$. Then

$$\nabla_x R^\varepsilon[V] = R^\varepsilon[\nabla_x V]\,; \qquad \lim_{\varepsilon \to 0} \|\nabla_x R^\varepsilon[V] - \nabla_x V\|_{L^r(\Omega)} = 0.$$

By analogy with section 4.2.4 and [4, 18, 19, 20], we can establish an existence and uniqueness result for the regularized Schrödinger-Poisson system by using a method based on a functional. The difficulty here is that we have to establish estimates for a density only in $L\log L$ which should be independent of ε. The tools to allow this analysis are a precise analysis of the spectral properties of the Hamiltonian (see Appendix B) and the Trudinger inequality combined with the Young inequality (see Appendix A).

Proposition 5.3.2 (Existence and uniqueness) *Let $\varepsilon \in [0,1]$ and $T>0$ and assume $N_s \in L^\infty(0,T;L^1(\omega))$ satisfies* **H1***.*

Then the regularized Schrödinger-Poisson system (5.3.29)–(5.3.30) *admits a unique solution $(V^\varepsilon, (\epsilon_k[V^\varepsilon], \chi_k[V^\varepsilon]))$ such that $V^\varepsilon \in H^1_{01}$ with a bound independent of ε.*

Proof. We consider the functional defined on H^1_{01} by

$$J(V) = \frac{1}{2}\iint_\Omega |\nabla V|^2\,dxdz + \int_\omega N_s \log\sum_k e^{-\epsilon_k[R^\varepsilon[V]]}\,dx = J_0(V) + J_1(V,N_s). \quad (5.3.32)$$

We will prove that this functional is continuous, coercive and strongly convex on H^1_{01}. Thus it admits a unique minimizer which defines a solution of (5.3.29)–(5.3.30).

The functional J_0 is clearly continuous and strongly convex on H^1_{01}. For the functional J_1, we use the properties of $\epsilon_k[V]$ stated in (B.0.14) to prove

$$\begin{aligned}|J_1(V,N_s) - J_1(\widetilde{V},N_s)| &\le \int_\omega N_s(x)\sup_k(|\epsilon_k[R^\varepsilon[V]] - \epsilon_k[R^\varepsilon[\widetilde{V}]]|(x))\,dx \\ &\le C\int_\omega N_s(1 + \|R^\varepsilon[V]\|^{1/2}_{L^2_z(0,1)} + \|R^\varepsilon[\widetilde{V}]\|^{1/2}_{L^2_z(0,1)})\|R^\varepsilon[V-\widetilde{V}]\|_{L^2_z(0,1)}\,dx.\end{aligned} \quad (5.3.33)$$

In the following C and C_T will stand for nonnegative constants depending only on the data and not on ε. Using the Young inequality given in the appendix (A.1.1), we have

$$\begin{aligned}\int_\omega N_s\|R^\varepsilon[V-\widetilde{V}]\|_{L^2_z(0,1)}\,dx &= \int_\omega N_s\frac{\|R^\varepsilon[V-\widetilde{V}]\|_{L^2_z(0,1)}}{\|R^\varepsilon[V-\widetilde{V}]\|_{H^1(\Omega)}}\,dx\|R^\varepsilon[V-\widetilde{V}]\|_{H^1(\Omega)} \\ &\le \int_\omega\left(N_s\log N_s - N_s + \exp\frac{\|R^\varepsilon[V-\widetilde{V}]\|_{L^2_z(0,1)}}{\|R^\varepsilon[V-\widetilde{V}]\|_{H^1(\Omega)}}\right)dx\ \|R^\varepsilon[V-\widetilde{V}]\|_{H^1(\Omega)}.\end{aligned}$$

Therefore, the Trudinger inequality (A.2.3) and **H1** lead to

$$\int_\omega N_s\|R^\varepsilon[V-\widetilde{V}]\|_{L^2_z(0,1)}\,dx \le C_T\|R^\varepsilon[V-\widetilde{V}]\|_{H^1(\Omega)}.$$

Besides the properties of the regularization R^ε (Proposition 5.3.1) implies

$$\|R^\varepsilon[V-\widetilde{V}]\|_{H^1(\Omega)} \le \|V-\widetilde{V}\|_{H^1(\Omega)}.$$

Thus we have

$$\int_\omega N_s\|R^\varepsilon[V-\widetilde{V}]\|_{L^2_z(0,1)}\,dx \le C_T\|V-\widetilde{V}\|_{H^1(\Omega)}. \quad (5.3.34)$$

Doing the same for the others term, we have

$$\int_\omega N_s \|R^\varepsilon[V]\|^{1/2}_{L^2_z(0,1)} \|R^\varepsilon[V-\widetilde{V}]\|_{L^2_z(0,1)}\,dx \le C\|V\|^{1/2}_{H^1(\Omega)}\|V-\widetilde{V}\|_{H^1(\Omega)} \times \int_\omega \left(N_s \log N_s - N_s + \exp \frac{\gamma \|R^\varepsilon[V]\|^{1/2}_{L^2_z(0,1)} \|R^\varepsilon[V-\widetilde{V}]\|_{L^2_z(0,1)}}{\|R^\varepsilon[V]\|^{1/2}_{H^1(\Omega)} \|R^\varepsilon[V-\widetilde{V}]\|_{H^1(\Omega)}} \right) dx,$$

where γ is the constant defined in the Trudinger inequality (A.2.3). An interpolation gives

$$\int_\omega \exp \frac{\gamma \|R^\varepsilon[V]\|^{1/2}_{L^2_z(0,1)} \|R^\varepsilon[V-\widetilde{V}]\|_{L^2_z(0,1)}}{\|R^\varepsilon[V]\|^{1/2}_{H^1(\Omega)} \|R^\varepsilon[V-\widetilde{V}]\|_{H^1(\Omega)}}\,dx \le$$

$$\le \left(\int_\omega \exp \frac{\gamma \|R^\varepsilon[V]\|_{L^2_z(0,1)}}{\|R^\varepsilon[V]\|_{H^1(\Omega)}}\,dx \right)^{1/2} \left(\int_\omega \exp \frac{\gamma \|R^\varepsilon[V-\widetilde{V}]\|^2_{L^2_z(0,1)}}{\|R^\varepsilon[V-\widetilde{V}]\|^2_{H^1(\Omega)}}\,dx \right)^{1/2} \le C,$$

thanks to the Trudinger inequality (A.2.3) and **H1**. Thus,

$$\int_\omega N_s \|R^\varepsilon[V]\|^{1/2}_{L^2_z(0,1)} \|R^\varepsilon[V-\widetilde{V}]\|_{L^2_z(0,1)}\,dx \le C_T \|V\|^{1/2}_{H^1(\Omega)} \|V-\widetilde{V}\|_{H^1(\Omega)}. \tag{5.3.35}$$

Obviously we have the same estimate (5.3.35) if we change V to $\widetilde{V}$ and $\widetilde{V}$ to V. Thus (5.3.34) and (5.3.35) injected in (5.3.33) prove

$$|J_1(V,N_s) - J_1(\widetilde{V},N_s)| \le C_T(1 + \|V\|^{1/2}_{H^1(\Omega)} + \|\widetilde{V}\|^{1/2}_{H^1(\Omega)}) \|V-\widetilde{V}\|_{H^1(\Omega)}. \tag{5.3.36}$$

Hence $J_1(\cdot,N_s)$ is Lipschitz continuous on H^1_{01}. Now if we take $\widetilde{V}=0$ in (5.3.36), from **H1** we have that $0 \ge J_1(0,N_s) \ge -C_T$. Thus, there exist two nonnegative constants C_1 and C_2 such that

$$J(V) \ge \frac{1}{2}\|\nabla V\|^2_{L^2(\Omega)} - C_1(1 + \|V\|^{1/2}_{H^1(\Omega)})\|V\|_{H^1(\Omega)} - C_2.$$

If we apply the Poincaré inequality in H^1_{01}, we find

$$J(V) \ge C_3\|V\|^2_{H^1(\Omega)} - C_4\|V\|^{3/2}_{H^1(\Omega)} - C_5.$$

Hence the functional J_ρ is coercive and admits a minimizer in H^1_{01}. Moreover, from Lemma B.0.3, it is clear that J_ρ is twice Gâteaux differentiable on H^1_{01} and for any $W \in H^1(\Omega)$,

$$d_V J(V)\cdot W = \iint_\Omega \nabla V \cdot \nabla W\,dxdz - \sum_k \int_\omega N_s \frac{e^{-\epsilon_k[R^\varepsilon[V]]}}{\sum_\ell e^{-\epsilon_\ell[R^\varepsilon[V]]}} \langle |\chi_k[R^\varepsilon[V]]|^2 R^\varepsilon[W]\rangle\,dx.$$

From the selfadjointness of R^ε on $L^2(\Omega)$, one deduces that each minimizer of the functional J is a weak solution of the Schrödinger-Poisson system (5.3.29)–(5.3.30). And

$$d^2_V J_1(V,N_s)W\cdot W = -\int_\omega \frac{N_s}{\mathcal{Z}^\varepsilon} \sum_k \sum_{\ell\ne k} \frac{e^{-\epsilon^\varepsilon_k} - e^{-\epsilon^\varepsilon_\ell}}{\epsilon^\varepsilon_k - \epsilon^\varepsilon_\ell} \langle \chi^\varepsilon_k \chi^\varepsilon_\ell R^\varepsilon[W]\rangle^2\,dx + \int_\omega N_s \left\{ \sum_k \frac{e^{-\epsilon^\varepsilon_k}}{\mathcal{Z}^\varepsilon} \langle |\chi^\varepsilon_k|^2 R^\varepsilon[W]\rangle^2 - \left(\frac{\sum_k e^{\epsilon^\varepsilon_k} \langle |\chi^\varepsilon_k|^2 R^\varepsilon[W]\rangle}{\mathcal{Z}^\varepsilon} \right)^2 \right\} dx.$$

When N_s is nonnegative, this quantity is nonnegative thanks to the Cauchy-Schwarz inequality. Thus $J_1(\cdot, N_s)$ is convex. As a consequence, the functional J is convex and admits a unique minimum which is the weak solution of the Schrödinger-Poisson system (5.3.29)–(5.3.30). □

Proposition 5.3.3 (Continuity) *Let $\varepsilon \in [0,1]$ and $T > 0$. Assume N_s and $\widetilde{N_s}$ are given in $L^\infty(0,T;L^1(\omega))$ and satisfy* **H1**.

Then the corresponding solutions V^ε and respectively $\widetilde{V}^\varepsilon$ of the Schrödinger-Poisson system (5.3.29)–(5.3.30) *verify*

$$\forall\, t \in [0,T], \quad \|V^\varepsilon - \widetilde{V}^\varepsilon\|_{H^1(\Omega)} \le C_T \|N_s - \widetilde{N_s}\|^{1/8}_{L^1(\omega)}, \tag{5.3.37}$$

for a nonnegative constant C_T depending only on the data and not on ε.

Moreover, as $\varepsilon \to 0$, the solution V^ε of the regularized problem (5.3.29)–(5.3.30) *converges to the solution V of the unregularized problem* (5.1.3)–(5.1.4) *in $L^\infty(0,T;H^1(\Omega))$ and uniformly with respect to $N_s \in L^\infty(0,T;L^1(\omega))$ satisfying* **H1**.

Proof. In the proof all the constants are nonnegative and depend only on the data and not on ε. If we multiply the Poisson equation (5.3.30) by $(V^\varepsilon - \widetilde{V}^\varepsilon)$ and integrate :

$$\begin{aligned}\iint_\Omega |\nabla(V^\varepsilon - \widetilde{V}^\varepsilon)|^2\,dxdz &= \sum_k \iint_\Omega (N_s - \widetilde{N_s})\frac{e^{-\epsilon_k^\varepsilon}}{\mathcal{Z}^\varepsilon}|\chi_k^\varepsilon|^2 R^\varepsilon[V^\varepsilon - \widetilde{V}^\varepsilon]\,dxdz \\ &+ \sum_k \iint_\Omega \widetilde{N_s}\left(\frac{e^{-\epsilon_k^\varepsilon}}{\mathcal{Z}^\varepsilon}|\chi_k^\varepsilon|^2 - \frac{e^{-\widetilde{\epsilon_k}^\varepsilon}}{\mathcal{Z}[\widetilde{V}^\varepsilon]}|\widetilde{\chi_k}^\varepsilon|^2\right) R^\varepsilon[V^\varepsilon - \widetilde{V}^\varepsilon]\,dxdz,\end{aligned} \tag{5.3.38}$$

where we use the selfadjointness of the linear operator R^ε on $L^2(\Omega)$.

We use the notation of the Appendix : $\epsilon_k^s = \epsilon_k[sR^\varepsilon[V^\varepsilon] + (1-s)R^\varepsilon[\widetilde{V}^\varepsilon]]$ and $\chi_k^s = \chi_k[sR^\varepsilon[V^\varepsilon] + (1-s)R^\varepsilon[\widetilde{V}^\varepsilon]]$. Then we have, (we recall that the regularization is a linear operator)

$$\frac{e^{-\epsilon_k[V]}}{\mathcal{Z}[V]}|\chi_k[V]|^2 - \frac{e^{-\epsilon_k^\varepsilon}}{\mathcal{Z}^\varepsilon}|\widetilde{\chi_k}^\varepsilon|^2 = \int_0^1 \frac{d}{ds}\left(\frac{e^{-\epsilon_k^s}}{\mathcal{Z}^s}|\chi_k^s|^2\right)\,ds.$$

From Lemma B.0.3, we deduce

$$\begin{aligned}\sum_k \int_0^1 \frac{d}{ds}\left(\frac{e^{-\epsilon_k^s}}{\mathcal{Z}^s}|\chi_k^s|^2\right) R^\varepsilon[V^\varepsilon - \widetilde{V}^\varepsilon]\,dz = -\sum_k \frac{e^{-\epsilon_k^s}}{\mathcal{Z}^s}\langle |\chi_k^s|^2\, R^\varepsilon[V^\varepsilon - \widetilde{V}^\varepsilon]\rangle^2 + \\ \left(\frac{\sum_k e^{-\epsilon_k^s}\langle |\chi_k^s|^2\, R^\varepsilon[V^\varepsilon - \widetilde{V}^\varepsilon]\rangle}{\mathcal{Z}^s}\right)^2 + \frac{1}{\mathcal{Z}^s}\sum_k\sum_{\ell\neq k}\frac{e^{-\epsilon_k^s} - e^{-\epsilon_\ell^s}}{\epsilon_k^s - \epsilon_\ell^s}\left\langle \chi_k^s\chi_\ell^s\, R^\varepsilon[V^\varepsilon - \widetilde{V}^\varepsilon]\right\rangle^2.\end{aligned}$$

Thanks to the Cauchy-Schwarz inequality, this last term is nonpositive. Thus the second term of the right hand side of (5.3.38) is nonpositive.

For the first term of the right hand side of (5.3.38), we use the bound of $\|\chi_k\|_{L^\infty_z}$ given in Lemma B.0.5. We deduce

$$\begin{aligned}\sum_k \iint_\Omega (N_s - \widetilde{N_s})\frac{e^{-\epsilon_k^\varepsilon}}{\mathcal{Z}^\varepsilon}|\chi_k^\varepsilon|^2 R^\varepsilon[V^\varepsilon - \widetilde{V}^\varepsilon]\,dxdz \le \\ \le C_1\int_\omega |N_s - \widetilde{N_s}|(1 + \|R^\varepsilon[V^\varepsilon]\|^{1/2}_{L^2_z})\|R^\varepsilon[V^\varepsilon - \widetilde{V}^\varepsilon]\|_{L^2_z}\,dx.\end{aligned} \tag{5.3.39}$$

By a Hölder inequality,

$$\int_\omega |N_s - \widetilde{N_s}|(1 + \|R^\varepsilon[V^\varepsilon]\|_{L^2_z}^{1/2})\|R^\varepsilon[V^\varepsilon - \widetilde{V}^\varepsilon]\|_{L^2_z}\,dxdz \le$$
$$\le \|N_s - \widetilde{N_s}\|_{L^1(\omega)}^{1/4}\left(\int_\omega (N_s + \widetilde{N_s})(1 + \|R^\varepsilon[V^\varepsilon]\|_{L^2_z}^{2/3})\|R^\varepsilon[V^\varepsilon - \widetilde{V}^\varepsilon]\|_{L^2_z}^{4/3}\,dx\right)^{3/4}. \tag{5.3.40}$$

The assumption **H1** implies a bound in $L\log L$ of the densities N_s and $\widetilde{N_s}$. Thus we can follow the idea of the proof of Proposition 5.3.2 and prove after straightforward calculations using the Young inequality (A.1.1) and the Trudinger inequality (A.2.3), that

$$\int_\omega (N_s + \widetilde{N_s})(1 + \|R^\varepsilon[V^\varepsilon]\|_{L^2_z}^{2/3})\|R^\varepsilon[V^\varepsilon - \widetilde{V}^\varepsilon]\|_{L^2_z}^{4/3}\,dx \le C_2(1 + \|V^\varepsilon\|_{H^1(\Omega)}^{2/3})\|V^\varepsilon - \widetilde{V}^\varepsilon\|_{H^1(\Omega)}^{4/3},$$

which is bounded since V^ε and $\widetilde{V}^\varepsilon$ are bounded in $H^1(\Omega)$ with Proposition 5.3.2. Thus if we look at (5.3.39), we have proved that there exists a nonnegative constant C_3 such that

$$\|V^\varepsilon - \widetilde{V}^\varepsilon\|_{H^1(\Omega)}^2 \le C_3\|N_s - \widetilde{N_s}\|_{L^1(\omega)}^{1/4}.$$

This leads to (5.3.37).

For the convergence when $\varepsilon \to 0$, we consider V^ε and V the solutions of the unregularized and respectively regularized problem for $N_s \in L^\infty(0,T;L^1(\omega))$ satisfying **H1**. We have

$$-\Delta(V^\varepsilon - V) = (R^\varepsilon - Id)\left[N_s \frac{e^{-\epsilon_k^\varepsilon}}{\mathcal{Z}^\varepsilon}|\chi_k^\varepsilon|^2\right] + N_s\sum_k\left(\frac{e^{-\epsilon_k^\varepsilon}}{\mathcal{Z}^\varepsilon}|\chi_k^\varepsilon|^2 - \frac{e^{-\epsilon_k}}{\mathcal{Z}}|\chi_k|^2\right).$$

Multiplying by $(V^\varepsilon - V)$ and integrate, we obtain after a integration by parts and thanks to the selfadjointness of R^ε in $L^2(\Omega)$

$$\iint_\Omega |\nabla(V^\varepsilon - V)|^2\,dxdz = I + II + III, \tag{5.3.41}$$

where

$$I = \iint_\Omega N_s\sum_k \frac{e^{-\epsilon_k^\varepsilon}}{\mathcal{Z}^\varepsilon}|\chi_k^\varepsilon|^2(R^\varepsilon - Id)[V^\varepsilon - V]\,dxdz,$$
$$II = \iint_\Omega N_s\sum_k\left(\frac{e^{-\epsilon_k^\varepsilon}}{\mathcal{Z}^\varepsilon}|\chi_k^\varepsilon|^2 - \frac{e^{-\epsilon_k}}{\mathcal{Z}}|\chi_k|^2\right)(V^\varepsilon - R^\varepsilon[V^\varepsilon])\,dxdz,$$
$$III = \iint_\Omega N_s\sum_k\left(\frac{e^{-\epsilon_k^\varepsilon}}{\mathcal{Z}^\varepsilon}|\chi_k^\varepsilon|^2 - \frac{e^{-\epsilon_k}}{\mathcal{Z}}|\chi_k|^2\right)(R^\varepsilon[V^\varepsilon] - V)\,dxdz.$$

For the first term, we have with Lemma B.0.5

$$|I| \le C\int_\omega N_s(1 + \|R^\varepsilon[V^\varepsilon]\|_{L^2_z})\|(R^\varepsilon - Id)[V^\varepsilon - V]\|_{L^2_z}\,dx.$$

As above, with assumption **H1** and the Young and Trudinger inequalities, we can prove

$$|I| \leq C_1 \|(R^\varepsilon - Id)[V^\varepsilon - V]\|_{H^1(\Omega)}.$$

From the properties of the regularization R^ε (see Proposition 5.3.1), we deduce easily that, since V^ε is bounded in $H^1(\Omega)$ independently of ε as proved in Proposition 5.3.2, we have $\lim_{\varepsilon\to 0} |I| = 0$. For the second term, we use the same idea and obtain

$$|II| \leq C \int_\omega N_s(1 + \|R^\varepsilon[V^\varepsilon]\|_{L^2_z} + \|V\|_{L^2_z})\|(R^\varepsilon - Id)[V^\varepsilon]\|_{L^2_z}\, dx.$$

And the Young and Trudinger inequalities with **H1** lead to

$$|II| \leq C_2(1 + \|V^\varepsilon\|_{H^1(\Omega)} + \|V\|_{H^1(\Omega)})\|(R^\varepsilon - Id)[V^\varepsilon]\|_{H^1(\Omega)},$$

which converges towards 0 as ε goes to 0. Finally, as we have shown for the second term of the right hand side of (5.3.38), the term III is nonpositive. Thus a Poincaré inequality in (5.3.41) implies that

$$\lim_{\varepsilon\to 0} \|V^\varepsilon - V\|_{L^\infty(0,T;H^1(\Omega))} = 0.$$

□

5.4 Existence of solutions

This section is devoted to the proof of Theorem 5.1.3

5.4.1 Existence of solutions for the regularized system

Proposition 5.4.1 *Let $T > 0$ and $\varepsilon \in (0,1)$ be fixed. Then the regularized problem* (5.1.11)–(5.1.13) *with the initial condition* (5.1.6) *and the boundary condition* (5.1.7)–(5.1.8) *admits a unique solution $(N_s^\varepsilon, V^\varepsilon)$ with $N_s^\varepsilon \in C(0,T;L^2(\mathbb{R}^2)) \cap L^2(0,T;H^1(\omega))$.*

Proof. We do not give in detail the proof which can be straightforwardly adapted from the proof of the existence result in [5]. The proof relies on a fixed point argument on the map $F : N_s \mapsto \widehat{N_s}$ defined on the set

$$\mathcal{S}_T = \{n : \left(\max_{0\leq t\leq T} \|n(t)\|^2_{L^2(\omega)} + \int_0^T \|n(t)\|^2_{H^1(\omega)}\, dt\right) < +\infty\}$$

by

1. For a given $N_s \geq 0$, we solve the regularized Schrödinger-Poisson system (5.3.29)–(5.3.30) and obtained $V \in L^\infty(0,T;C^\infty(\overline{\Omega}))$.

2. We construct $V_s = -\log \sum_k e^{-\epsilon_k[V]}$. From the spectral properties of the Hamiltonian, we have $V_s \in L^\infty(0,T;C^\infty(\overline{\omega}))$.

3. For this effective potential V_s, we solve the following parabolic equation for the unknown $\widehat{N_s}$:
$$\partial_t \widehat{N_s} - \text{div}_x(\mathbb{D}(\nabla_x \widehat{N_s} + \widehat{N_s}\nabla_x V_s)) = 0,$$
with the initial condition N_s^0 and the boundary condition $\partial_\nu N_s = 0$ for $x \in \partial\omega$.

We can prove as in section 4.2.5 that F is a contraction on the set $\mathcal{S}_{T_0}$ for T_0 small enough. Thus we have a solution on $[0, T_0]$ that we can extend to $[0, T]$. □

5.4.2 Passing to the limit $\varepsilon \to 0$

We have now all matters to construct solutions of the unregularized problem and to prove Theorem 5.1.3. We will use the Aubin-Lions compactness method to show that the solution of the regularized system converges when the parameter of regularization goes to 0 towards solutions of the unregularized system, up to an extraction of a subsequence. However this method does not give any uniqueness result. We first recall a simple statement of a Aubin-Lions lemma [2, 15]:

Lemma 5.4.2 (Aubin Lemma) *Take $T > 0$, $q \in (1, +\infty)$ and let $(f_n)_{n\in\mathbb{N}}$ be a bounded sequence of functions in $L^q(0, T; H)$ where H is a Banach space. If $(f_n)_{n\in\mathbb{N}}$ is bounded in $L^q(0, T; V)$ where V is compactly imbedded in H and $\partial f_n/\partial t$ is bounded in $L^q(0, T; V')$ uniformly with respect to $n \in \mathbb{N}$, then $(f_n)_{n\in\mathbb{N}}$ is relatively compact in $L^q(0, T; H)$.*

Proof of Theorem 5.1.3. We fix T>0. From Proposition 5.4.1, there exist N_s^ε and V^ε solution of the regularized problem (5.1.11)–(5.1.13) with the initial data N_s^0. Assertion (iii) of Corollary 5.2.2 proves that we have $\sqrt{N_s^\varepsilon} \in L^2(0, T; H^1(\omega))$ and with (i), $\sqrt{N_s^\varepsilon} \in L^\infty(0, T; L^2(\omega))$. Thus since we have $\nabla_x N_s^\varepsilon = 2\sqrt{N_s^\varepsilon}\nabla_x\sqrt{N_s^\varepsilon}$, we deduce that $N_s^\varepsilon \in L^2(0, T; W^{1,1}(\omega))$ with a uniform bound with respect to ε. Moreover, with (5.2.24), we have after a Cauchy-Schwarz inequality :

$$\begin{aligned}\int_0^T \left(\int_\omega |\nabla_x N_s^\varepsilon + N_s^\varepsilon \nabla_x V_s^\varepsilon|\, dx\right)^2 dt \quad &\le \mathcal{N}_I \int_0^T \int_\omega \frac{|\nabla_x N_s^\varepsilon + N_s^\varepsilon \nabla_x V_s^\varepsilon|^2}{N_s^\varepsilon}\, dxdt \\ &\le \frac{\mathcal{N}_I}{\alpha} \int_0^T D^\varepsilon(t)\, dt,\end{aligned}$$

where D^ε is defined in Lemma 5.2.1 and is bounded in $L^1(0, T)$ uniformly with respect to ε. Therefore we conclude with (5.1.11) that $\partial_t N_s^\varepsilon$ is bounded in $L^2(0, T; W^{-1,1}(\omega))$ uniformly with respect to ε.

Hence we can apply Lemma 5.4.2 for $q = 2$, $H = L^1(\omega)$ and $V = W^{1,1}(\omega)$. There exists a subsequence (still denoted abusively N_s^ε) such that $N_s^\varepsilon \to N_s$ strongly in $L^2(0, T; L^1(\omega))$. From the weak continuity we have that for a.e. $t \in [0, T]$,

$$\int_\omega N_s(1 + |\log N_s|)\, dx \le C_T,$$

for a nonnegative constant C_T. For this function N_s, we can solve the unregularized Schrödinger-Poisson system (5.1.3)–(5.1.4) and construct the set $(V, (\epsilon_k, \chi_k)_{k\geq 1})$ with $V \in L^\infty(0,T; H^1(\Omega))$ as proved in Proposition 5.3.2. Thanks to Proposition 5.3.3, we have that

$$\|V^\varepsilon - V\|_{L^2(0,T;H^1(\Omega))} \to 0 \quad \text{ as } \varepsilon \to 0.$$

We want now to pass to the limit $\varepsilon \to 0$ in the drift-diffusion equation. Thanks to Lemma B.0.5, we have

$$\begin{aligned}\iint_{[0,T]\times\omega} N_s^\varepsilon \nabla_x V_s^\varepsilon \, dxdt &= \iint_{[0,T]\times\omega} N_s^\varepsilon \sum_k \frac{e^{-\epsilon_k^\varepsilon}}{\mathcal{Z}^\varepsilon} \langle |\chi_k^\varepsilon|^2 \nabla_x V^\varepsilon \rangle \, dxdt \\ &\leq \iint_{[0,T]\times\omega} N_s^\varepsilon (1 + \|R^\varepsilon[V^\varepsilon]\|_{L_z^2}^{1/2}) \|\nabla_x V^\varepsilon\|_{L_z^2} \, dxdt.\end{aligned}$$

By the Cauchy-Schwarz inequality and the Sobolev imbedding $H^1(\Omega) \hookrightarrow L_x^p L_z^2(\Omega)$ for all $p \in [1, +\infty)$, we deduce :

$$\iint_{[0,T]\times\omega} N_s^\varepsilon \nabla_x V_s^\varepsilon \, dxdt \leq C_T \|V^\varepsilon\|_{L^\infty(0,T;H^1(\Omega))} (1 + \|V^\varepsilon\|_{L^\infty(0,T;H^1(\Omega))}) \|N_s^\varepsilon\|_{L^1(0,T;L^4(\omega))}.$$

But assertion (iii) of Corollary 5.2.2 shows that $\|N_s^\varepsilon\|_{L^1(0,T;L^4(\omega))}$ is bounded independently of ε. Thus there exists a nonnegative constant C_T independent of ε such that :

$$\iint_{[0,T]\times\omega} N_s^\varepsilon \nabla_x V_s^\varepsilon \, dxdt \leq C_T.$$

Hence we can give a sense to the drift-diffusion equation as $\varepsilon \to 0$. From Lemma B.0.3, we have

$$\nabla_x \epsilon_k^\varepsilon [V^\varepsilon] = \langle |\chi_k^\varepsilon|^2 \nabla_x V^\varepsilon \rangle.$$

The convergence of V^ε in $L^2(0,T; H^1(\Omega))$ and the local Lipschitz dependency of the eigenvectors of the Hamiltonian with respect to the potential (see Appendix B) allow us to conclude that $\nabla_x \epsilon_k^\varepsilon [V^\varepsilon] \to \nabla_x \epsilon_k[V]$ in $L^p((0,T)\times\omega)$ for all $p \in [1,2)$. Thus,

$$\nabla_x V_s^\varepsilon = \frac{\sum_k \nabla_x \epsilon_k^\varepsilon e^{-\epsilon_k^\varepsilon}}{\mathcal{Z}^\varepsilon}$$

converges for a.e. $(t,x) \in [0,T]\times\omega$. This is enough to prove

$$N_s^\varepsilon \nabla_x V_s^\varepsilon \rightharpoonup N_s \nabla_x V_s \quad \text{ in } \mathcal{D}'([0,T]\times\omega).$$

By the weak semi-continuity we get moreover

$$\iint_{[0,T]\times\omega} N_s \nabla_x V_s \, dxdt \leq \liminf_{\varepsilon\to 0} \iint_{[0,T]\times\omega} N_s^\varepsilon \nabla_x V_s^\varepsilon \, dxdt.$$

The convexity of the functional $N_s \mapsto \int_\omega |\nabla_x \sqrt{N_s}|^2 \, dx$ gives

$$\iint_{[0,T]\times\omega} |\nabla_x \sqrt{N_s}|^2 \, dxdt \leq \liminf_{\varepsilon\to 0} \iint_{[0,T]\times\omega} |\nabla_x \sqrt{N_s^\varepsilon}|^2 \, dxdt.$$

And for a.e. $t \in [0,T]$,

$$W(t) + \int_0^t D(s)\, ds \leq \liminf_{\varepsilon\to 0} \ (W^\varepsilon(t) + \int_0^t D^\varepsilon(s)\, ds).$$

5.5 Long time behaviour

This section is devoted to the proof of Theorem 5.1.4. We use an entropy method relying on the logarithmic Sobolev inequalities and on the Csiszàr-Kullback inequalities. This method has been widely used by several authors (see for instance [1, 2, 7, 8, 9]). We introduce the relative entropy of (ρ_k, V) with respect to the stationary solutions $(\rho_k^\infty, V^\infty)$:

$$\begin{aligned} W^\infty(t) = \; & \sum_k \int_\omega (\rho_k \log(\rho_k/\rho_k^\infty) - \rho_k + \rho_k^\infty)\, dx + \frac{1}{2}\iint_\Omega |\nabla_{x,z}(V - V^\infty)|^2\, dxdz \\ & + \sum_k \int_\omega \rho_k \left(\epsilon_k[V] - \epsilon_k[V^\infty] - \int_0^1 |\chi_k|^2 (V - V^\infty)\, dz \right) dx. \end{aligned} \tag{5.5.42}$$

We recall that the decay of ρ_k with respect to k insures that the last term is nonnegative. We can prove with the same calculations as in Lemma 5.2.1 that

$$\frac{d}{dt} W^\infty(t) = -\int_\omega N_s \mathbb{D} \frac{\nabla_x u \cdot \nabla_x u}{u^2}\, dx \le -\alpha \int_\omega N_s |\nabla_x (\log u)|^2\, dx,$$

where we use Assumption 5.1.1 for the last inequality. We denote $\overline{u} = \mathcal{N}_I / \int_\omega \mathcal{Z}(x)\, dx$. Therefore we have

$$\frac{d}{dt} W^\infty(t) \le -\alpha \int_\omega N_s |\nabla_x \log \frac{u}{\overline{u}}|^2\, dx. \tag{5.5.43}$$

We recall the Gross logarithmic Sobolev inequality [1, 9, 14] : for two nonnegative functions f and g such that $\int_\omega f\, dx = \int_\omega g\, dx$ then there exists a nonnegative constant λ such that

$$\int_\omega f \log \frac{f}{g} \le \frac{1}{\lambda} \int_\omega f |\nabla \log(f/g)|^2\, dx.$$

Hence if we apply it in (5.5.42) with $f = N_s$ and $g = \overline{u}\mathcal{Z}$, we obtain

$$\frac{d}{dt} W^\infty(t) \le -\alpha\lambda \int_\omega N_s \log \frac{u}{\overline{u}}\, dx.$$

We can then decompose

$$\log \frac{u}{\overline{u}} = \log \frac{\rho_k}{\rho_k^\infty} + \epsilon_k - \epsilon_k^\infty + \log \frac{\rho_k^\infty}{\overline{u} e^{-\epsilon_k^\infty}} = \log \frac{\rho_k}{\rho_k^\infty} + \epsilon_k - \epsilon_k^\infty + \log \frac{u^\infty}{\overline{u}}.$$

Moreover, we have seen that u^∞ is a constant. Thus

$$\frac{u^\infty}{\overline{u}} = \left(\frac{u^\infty}{\mathcal{N}_I} \int_\omega \mathcal{Z}(x)\, dx \right) = \sum_k \int_\omega u^\infty e^{-\epsilon_k} \frac{dx}{\mathcal{N}_I}$$

Therefore with the identity $u^\infty = \rho_k^\infty e^{-\epsilon_k^\infty}$ and a Jensen inequality, we have

$$\log \frac{u^\infty}{\overline{u}} = \log \sum_k \int_\omega \rho_k^\infty e^{\epsilon_k^\infty - \epsilon_k} \frac{dx}{\mathcal{N}_I} \ge \sum_k \int_\omega (\epsilon_k^\infty - \epsilon_k) \frac{\rho_k^\infty}{\mathcal{N}_I}\, dx.$$

(We recall that we have $\sum_k \int_\omega \rho_k^\infty = \mathcal{N}_I$). Finally we have obtained

$$\begin{aligned}
\frac{d}{dt}W^\infty(t) &\leq -\alpha\lambda\Big(\sum_k \int_\omega \rho_k \log\frac{\rho_k}{\rho_k^\infty}\,dx + \sum_k \int_\omega (\rho_k - \rho_k^\infty)(\epsilon_k - \epsilon_k^\infty)\,dx\Big) \\
&\leq -\alpha\lambda\Big(\sum_k \int_\omega \rho_k \log\frac{\rho_k}{\rho_k^\infty}\,dx + \iint_\Omega (N - N^\infty)(V - V^\infty)\,dxdz \\
&\quad + \sum_k \int_\omega \rho_k(\epsilon_k - \epsilon_k^\infty - \langle|\chi_k|^2(V - V^\infty)\rangle)\,dx \\
&\quad + \sum_k \int_\omega \rho_k^\infty(\epsilon_k^\infty - \epsilon_k - \langle|\chi_k^\infty|^2(V^\infty - V)\rangle\,dx\Big).
\end{aligned}$$

As we have seen before, properties of the spectrum of the Hamiltonian insure that the last term of the right hand side is nonnegative. According to the Poisson equation, the second term of the right hand side is equal to

$$\iint |\nabla_{x,z}(V - V^\infty)|^2\,dxdz.$$

Thus, we have shown

$$\frac{d}{dt}W^\infty(t) \leq -\alpha\lambda W^\infty(t),$$

and a Gronwall argument yields the exponential convergence of the relative entropy : $W^\infty(t) \leq W^\infty(0)\,e^{-\alpha\lambda t}$. Next we shall use the Csiszàr-Kullback inequality presented in the Appendix (A.3.4). We deduce that

$$\|\rho_k - \rho_k^\infty\|_{\ell^1(L^1(\omega))} \leq \sqrt{2\mathcal{N}_I W^\infty(0)}\,e^{-\frac{\alpha\lambda}{2}t}.$$

□

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PARTIE II

De Boltzmann vers DDSP

Chapter 6

Le cas de la dimension 2

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6.1 Introduction and main results

In the first part of this PhD, we have presented and analyzed a drift-diffusion-Schrödinger-Poisson system which models the transport of electrons confined in a nanostructure. In this subband model, electrons are assumed to behave like wave in the confinement directions (z) and to have a classical behaviour in the transport direction parallel to the electron gas (x). This system was obtained formally thanks to a diffusive limit of a kinetic system for partially quantized particles, when the mean free path becomes small with respect to the macroscopic lengthscale. This chapter is devoted to the rigorous study of this limit for a transport in one dimension ($x \in [a, b]$).

6.1.1 Presentation of the system of equations

In the transversal direction (referred by z), the electrons are confined in the nanostructure. The description of the system needs the diagonalization of the 1D stationary Schrödinger equation. We define then on $\Omega = (a, b)\times(0, 1)$, the set $(\chi_k[V], \epsilon_k[V])_{k\geq 1}$ as the complete set of eigenfunctions and eigenvalues of the Schrödinger operator in the z variable, $z \in (0, 1)$:

$$\begin{cases} -\dfrac{1}{2}\,\partial_z^2\chi_k[V] + V\chi_k[V] = \epsilon_k[V]\chi_k[V] \qquad (k \geq 1), \\ \chi_k[V] \in H_0^1(0, 1), \qquad \displaystyle\int_0^1 \chi_k[V]\,\chi_\ell[V]\,dz = \delta_{k\ell}\,. \end{cases} \tag{6.1.1}$$

If we denote ρ_k the occupation number of the kth subband, the particle density for a partially quantized system can be written

$$N(t, x, z) = \sum_{k=1}^{+\infty} \rho_k(t, x)|\chi_k[V(t, x, \cdot)](z)|^2.$$

The electrostatic potential V generates by the charge carriers is then the solution of the Poisson equation :

$$-\Delta_{x,z}V(t,x,z) = \sum_k \rho_k(t,x)|\chi_k[V(t,x,\cdot)](z)|^2, \tag{6.1.2}$$

with the boundary conditions :

$$\begin{cases} \dfrac{dV}{dx}(t,a,z) = \dfrac{dV}{dx}(t,b,z) = 0, & \text{for } z \in (0,1), \\ V(t,x,0) = V(t,x,1) = 0, & \text{for } x \in (a,b). \end{cases} \tag{6.1.3}$$

In the transport direction, the motion of particles is described by a 1D Boltzmann equation. Let $\eta > 0$ be the scaled mean free path assumed to be small. We consider here the scaled Boltzmann equation in one dimension for the subband model defined on the phase space $(a,b)\times\mathbb{R}$. The position x belongs to (a,b), the velocity v belongs to $\mathbb{R}$ and the time variable t is nonnegative. Then the occupation number ρ_k^η is defined by $\rho_k^\eta = \int_{\mathbb{R}} f_k^\eta\, dv$ where the distribution function $f_k^\eta(t,x,v)$ satisfies ([26, 29])

$$\partial_t f_k^\eta + \frac{1}{\eta}\{\mathcal{H}_k^\eta, f_k^\eta\} = \frac{1}{\eta^2}Q^\eta(f^\eta)_k\,, \tag{6.1.4}$$

where $\{\cdot,\cdot\}$ is the Poisson bracket : $\{g,h\} = \nabla_x h\cdot\nabla_v g - \nabla_v h\cdot\nabla_x g$. And $\mathcal{H}_k$ denotes the energy of the system in the kth subband which is the sum of the kinetic energy and the potential energy :

$$\mathcal{H}_k^\eta(t,x,v) = \frac{1}{2}v^2 + \epsilon_k[V^\eta(t,x,\cdot)].$$

The collision operator Q^η in the linear BGK approximation reads in the following form :

$$Q^\eta(f)_k = \sum_{k'}\int_{\mathbb{R}} \alpha_{k,k'}(v,v')(\mathcal{M}_k^\eta(v)f_{k'}(v') - \mathcal{M}_{k'}^\eta(v')f_k(v))\,dv', \tag{6.1.5}$$

where the function $\mathcal{M}_k^\eta$ is the normalized Maxwellian

$$\mathcal{M}_k^\eta(t,x,v) = \frac{1}{2\pi\mathcal{Z}^\eta}e^{-\mathcal{H}_k^\eta(t,x,v)} \tag{6.1.6}$$

and where the repartition function $\mathcal{Z}^\eta$ is given by

$$\mathcal{Z}^\eta(t,x) = \sum_{k=1}^{+\infty} e^{-\epsilon_k[V^\eta(t,x,\cdot)]}. \tag{6.1.7}$$

We refer the reader to [8, 28, 29] for a physical background of the equation (6.1.4).

We consider the specular reflexion boundary conditions :

$$f_k^\eta(t,a,v) = f_k^\eta(t,a,-v)\,,\ f_k^\eta(t,b,v) = f_k^\eta(t,b,-v), \quad v>0, t\in\mathbb{R}^+. \tag{6.1.8}$$

The surface density of particles is defined by

$$N_s^\eta(t,x) = \sum_k \int_{\mathbb{R}} f_k^\eta(t,x,v)\,dv = \sum_k \rho_k^\eta(t,x).$$

The cross section α is assumed to be symmetric and bounded from above and below :

(**A-1**) $\alpha_{k,k'}(v,v') = \alpha_{k,k'}(v',v)$ and $0 < \alpha_1 \le \alpha_{k,k'}(v,v') \le \alpha_2$, for all $(v,v') \in \mathbb{R}^2, k,k' \ge 1$.

We considered the well-prepared initial condition that we assume to be at the *thermal equilibrium*:

$$f_k^\eta(0,x,v) = f_k^{in}(x,v) := \frac{N_s^{in}(x)}{2\pi \sum_k e^{-\epsilon_k[V^{in}]}}\, e^{-v^2/2-\epsilon_k[V^{in}]}, \quad (x,v) \in [a,b]\times\mathbb{R}, \tag{6.1.9}$$

where $(V^{in}, (\epsilon_k[V^{in}], \chi_k[V^{in}])_{k\ge1})$ is the set of solutions of the Schrödinger-Poisson system at the thermal equilibrium :

$$\begin{cases} -\dfrac{1}{2}\,\partial_z^2\chi_k[V^{in}] + V^{in}\chi_k[V^{in}] = \epsilon_k[V^{in}]\chi_k[V^{in}] & (k\ge1), \\ \chi_k[V^{in}](x,\cdot) \in H_0^1(0,1), \qquad \displaystyle\int_0^1 \chi_k[V^{in}]\,\chi_\ell[V^{in}]\,dz = \delta_{k\ell}\,. \end{cases}$$

$$-\Delta_{x,z}V^{in} = \sum_k \frac{N_s^{in}(x)}{\sum_k e^{-\epsilon_k[V^{in}]}}|\chi_k[V^{in}]|^2 e^{-\epsilon_k[V^{in}]},$$

We assume that we have

(**A-2**) $N_s^{in} \ge 0$, $N_s^{in} \in C^0[a,b]$.

Under this assumption, we know that the Schrödinger-Poisson system at the thermal equilibrium admits a unique solution $(V^{in}, (\epsilon_k[V^{in}], \chi_k[V^{in}])_{k\ge1})$ with $0 \le V^{in} \in C^1(\Omega)$ (see Proposition 4.2.1).

Moreover, we can verify that we have,

$$f_k^{in} \ge 0, \qquad \exists\,\delta > 2 \text{ such that } ((1+v^\delta+k^2)f_k^{in}) \in \ell^1(L^1([a,b]\times\mathbb{R})),$$

When η goes to 0, we tends to a fluid description and are in a diffusive regime. It is well-known that in a diffusion approximation the surface density N_s satisfies at the limit a drift-diffusion equation [26, 16]. But there is no result of diffusion limit in a coupled quantum-classical case.

6.1.2 Main results

We write here the full Boltzmann-Schrödinger-Poisson system with the dependence in η :

$$\partial_t f_k^\eta + \frac{1}{\eta}(v.\nabla_x f_k^\eta - \nabla_x\epsilon_k^\eta.\nabla_v f_k^\eta) = \frac{1}{\eta^2}Q^\eta(f^\eta)_k, \quad (x,v) \in (a,b)\times\mathbb{R}. \tag{6.1.10}$$

$$\begin{cases} -\dfrac{1}{2}\,\partial_z^2\chi_k^\eta + V^\eta\chi_k^\eta = \epsilon_k^\eta\chi_k^\eta & (k\ge1), \\ \chi_k^\eta(t,x,\cdot) \in H_0^1(0,1), \qquad \displaystyle\int_0^1 \chi_k^\eta\,\chi_\ell^\eta\,dz = \delta_{k\ell}\,, \end{cases} \tag{6.1.11}$$

$$-\Delta_{x,z}V^\eta = \sum_k \int_{\mathbb{R}} f_k^\eta |\chi_k^\eta|^2\, dv, \tag{6.1.12}$$

which is coupled with the boundary condition (6.1.8)-(6.1.3) and the initial boundary condition (6.1.9). We point out the fact that in this Boltzmann equation the energy levels $(\epsilon_k)_{k\geq 1}$ depend on η (contrary to chapter 2). Moreover in the Schrödinger-Poisson system, the given is no more N_s like in DDSP but the occupation number ρ_k. The aim of this paper is to prove rigorously the limit of this system to DDSP.

Hydrodynamics limits for the Boltzmann equation have been widely studied by several authors ([1, 2, 10, 15, 14, 17, 19, 27] and see C. Villani [30] for a good review on the subject). Others diffusion limits are presented for instance in the context of parabolic hydrodynamical limit we refer to [11] which considers linear kinetic equations arising in models of plasma, semi-conductor, rarefied gases and for a diffusive limit of generalized two-velocity models we refer to [18]. If we want to work in a framework which is physically acceptable, we have to deal with solutions defined in the renormalized sense [12, 13, 21]. Namely, the entropy of this kind of system only gives a $L\log L$ bound on the distribution function . With the elliptic regularity on the Poisson equation and properties of the Hamiltonian (see Appendix), we can not hope to have a stronger estimate than $\nabla_x \epsilon_k$ in $L^\infty([0,T], L^2(\Omega))$. Thus the product $f_k \nabla_x \epsilon_k$ has no signification even in a weak sense. Thus we can only prove existence of renormalized solutions. The result established here is the following

Theorem 6.1.1 *Let $T>0$ and assume that Assumptions* **(A-1)** *and* **(A-2)** *hold. If we denote :*

$$\mathcal{N}_{in} = \int_a^b N_s^{in}\, dx.$$

Then, there exists $\mathcal{N}_0 > 0$ such that if $\mathcal{N}_{in} \leq \mathcal{N}_0$, the system (6.1.10)-(6.1.1)-(6.1.2) - (6.1.8)-(6.1.9)-(6.1.3) *admits a renormalized solution $(V^\eta, (\epsilon_k^\eta, \chi_k^\eta, f_k^\eta)_{k\geq 1})$ on $[0,T]$ which satisfies*

(i) $\forall\, \beta \in C^1(\mathbb{R}^+)$, $\beta(f^\eta)$ is a weak solution of:

$$\begin{cases} \eta\partial_t \beta(f^\eta)_k + v\cdot\nabla_x \beta(f^\eta)_k - \nabla_x \epsilon_k^\eta \cdot \nabla_v \beta(f^\eta)_k = \dfrac{Q^\eta(f^\eta)_k}{\eta}\beta'(f^\eta)_k, \\ \beta(f^\eta)_k(t=0) = \beta(f^{in})_k. \end{cases}$$

(ii) $\forall\, \lambda>0$, $\Theta_{k,\lambda}^\eta := (f_k^\eta + \lambda \exp(-\frac{1}{2}(v^2+k^2)))^{1/2}$ satisfies

$$\eta\partial_t \Theta_{k,\lambda}^\eta + v\cdot\nabla_x \Theta_{k,\lambda}^\eta - \nabla_v(\nabla_x \epsilon_k^\eta\ \Theta_{k,\lambda}^\eta) = \frac{Q^\eta(f^\eta)_k}{2\eta\Theta_{k,\lambda}^\eta} + \lambda \nabla_x \epsilon_k^\eta\ \frac{ve^{-\frac{1}{2}(v^2+k^2)}}{2\Theta_{k,\lambda}^\eta}.$$

(iii) We have the local mass conservation

$$\partial_t N_s^\eta + \nabla_x \cdot J^\eta = 0, \qquad \text{where} \qquad J^\eta = \frac{1}{\eta}\sum_{k\geq 1}\int_{\mathbb{R}} v f_k^\eta\, dv.$$

(iv) The entropy inequality (6.2.22) *holds :*

$$\forall\, t \in [0,T], \quad 0 \le W^\eta(t) + \frac{\alpha_1}{2\eta^2}\int_0^t \mathcal{R}^\eta(s)\,ds \le C_T, \tag{6.1.13}$$

where the entropy of the system is defined as in (4.2.17) *by*

$$W^\eta(t) = \sum_k \iint_{(a,b)\times\mathbb{R}} \left(f_k^\eta \log\frac{f_k^\eta}{M_k} - f_k^\eta + M_k \right) dxdv + \frac{1}{2}\iint_\Omega |\nabla_{x,z}V^\eta|^2\,dxdz$$

and the dissipation rate by

$$\mathcal{R}^\eta(t) = \frac{1}{2}\sum_k \iint_{(a,b)\times\mathbb{R}} \left(\sqrt{f_k^\eta} - \sqrt{N_s^\eta \mathcal{M}_k^\eta}\right)^2 dxdv.$$

The diffusion approximation can be approached by an asymptotic expansion of the solution with respect to the power of the mean free path η. Using such technics, Poupaud [26] has proved the convergence of the rescaled Boltzmann equation when the potential is given and Ben Abdallah and Tayed [7] have extended this result for the Boltzmann-Poisson system in one dimension. In a general case we do not have enough regularity to pass to the limit on weak solutions. Masmoudi and Tayeb [20] have established the diffusive limit of the Boltzmann-Poisson system towards the drift-diffusion-Poisson system, using renormalized solutions and compactness technics. Here we extend these technics to prove the following theorem :

Theorem 6.1.2 *Let, for $\eta > 0$, $(V^\eta, (f_k^\eta, \epsilon_k^\eta, \chi_k^\eta)_{k\ge1})$ be a renormalized solution of the Boltzmann-Schrödinger-Poisson system as defined in Theorem 6.1.1. Then as $\eta \to 0$, this solution converges to a solution $(V, N_s, (\epsilon_k, \chi_k)_{k\ge1})$ of the drift-diffusion-Schrödinger-Poisson system defined by*

$$\partial_t N_s + \mathrm{div}_x\, J = 0, \qquad J = -\mathbb{D}(\nabla_x N_s + N_s \nabla_x V_s), \tag{6.1.14}$$

$$\begin{cases} -\dfrac{1}{2}\,\partial_{zz}\chi_k + V\chi_k = \epsilon_k\chi_k & (k \ge 1), \\ \chi_k(t,x,\cdot) \in H_0^1(0,1), & \displaystyle\int_0^1 \chi_k\,\chi_\ell\,dz = \delta_{k\ell}\,, \end{cases} \tag{6.1.15}$$

$$-\Delta_{x,z} V = N, \tag{6.1.16}$$

where the density N and the effective potential V_s are defined by

$$N = N_s \sum_k \frac{e^{-\epsilon_k}}{\sum_\ell e^{-\epsilon_\ell}}\,|\chi_k|^2\,, \qquad V_s = -\log\sum_k e^{-\epsilon_k}. \tag{6.1.17}$$

And this system is completed with an initial condition $N_s(0,x) = N_s^{in}(x)$ and with the following conservative boundary conditions :

$$\begin{cases} J(t,a) = J(t,b) = 0, \quad \dfrac{dV}{dx}(t,a,z) = \dfrac{dV}{dx}(t,b,z) = 0 & \text{for } z \in (0,1), \\ V(t,x,0) = V(t,x,1) = 0 & \text{for } x \in (a,b). \end{cases} \tag{6.1.18}$$

We have up to an extraction of a subsequence, as $\eta \to 0$,

$$\|f_k^\eta - N_s \mathcal{M}_k\|_{\ell^1(L^1([0,T]\times[a,b]\times\mathbb{R}))} \to 0 \qquad \textit{and} \qquad \|V^\eta - V\|_{L^2([0,T],H^1(\Omega))} \to 0.$$

The existence of solutions of the drift-diffusion-Schrödinger-Poisson system has been established with the long time behaviour in chapter 4 when the diffusion matrix $\mathbb{D}$ is assumed to be the identity. In this case we have enough regularity to establish the uniqueness of solutions. But for a non constant diffusion matrix, we do not insure the uniqueness of these solutions (cf chapter 5). Moreover with our construction of solutions of Theorem 6.1.1 we can not have uniqueness.

The main difficulties of this result is the fact that the collision operator Q^η is not independent of the mean free path η and that the Schrödinger-Poisson system does not give regularity in time. To overcome these problems we use widely spectral properties of the Hamiltonian (given in Appendix B). The main estimate which gives us the regularity to pass to the limit is the entropy estimate. An other key point is the study of the Schrödinger-Poisson system. Ben Abdallah and Méhats [4] have established existence and uniqueness of the solution of this system for an occupation number ρ_k in L^p for $p > 1$. The proof is based on a idea of Nier [22, 23, 24]. It is important to conserve this existence and uniqueness result if we want to obtain the existence of the whole system Boltzmann-Schrödinger-Poisson. Nevertheless with the technic used here we need the assumption of small data to establish the uniqueness of the solution of the Schrödinger-Poisson system. Thus Theorem 6.1.1 is proved only under the assumption of small initial data. We are not able to insure this uniqueness result in the 3D case when the transport direction is assumed to lie in a bounded domain of $\mathbb{R}^2$. We will try to explain here and in the following chapter the main difficulties to pass from the 2D case to the 3D case.

The outline of the paper is as follows.

In the second section, after briefly recalling basic properties of the collision operator, we establish the a priori estimate, which is the natural estimate for our system.

In the third part, we analyze the Schrödinger-Poisson system under physical assumptions obtain on the whole system.

In section 6.4, we prove Theorem 6.1.2 if we assume that we have constructed a solution of the Boltzmann-Schrödinger-Poisson system as defined in Theorem 6.1.1.

In section 6.5 and 6.6, we investigate the existence problem under the assumption of small data. We first recall useful results on the Vlasov equation and finally detail the different steps of the regularization and passing to the limit in the regularized system to prove Theorem 6.1.1.

The Appendix recall useful inequalities and is devoted to spectral properties of the Schrödinger operator.

We denote for any Banach space E by $\ell^1(E)$ the space of sequences $(h_k)_{k\geq 1}$ such that for all $k \geq 1$ we have $h_k \in E$ and $\sum_{k\geq 1} \|h_k\|_E < +\infty$, this last quantity being the norm of $(h_k)_{k\geq 1}$ in $\ell^1(E)$. We will usually shortly denote by $\|h_k\|_{L^p_{t,x,v}}$ the $L^p((0,T)\times[a,b]\times\mathbb{R})$ norm of h_k. Moreover when there is no confusion possible, we will denote $\epsilon_k(t,x)$ (resp. $\chi_k(t,x,z)$) instead of $\epsilon_k[V(t,x,\cdot)]$ (resp. $\chi_k[V(t,x,\cdot)](z)$).

6.2 A priori estimate

6.2.1 Properties of the collision operator

In this section, we just enumerate some properties of the collision operator which will be useful for the rest of the paper. These properties are proved in section 2.3.1. We assume that η is fixed and we omit to write the dependency of the quantities in this parameter.

Proposition 6.2.1 *Let Q be defined by (6.1.5) with a cross section α symmetric and bounded from above and below i.e. satisfying (**A-1**). Then we get :*
(i) $\sum_k \int Q(f)_k(v)\,dv = 0$.
(ii) Q is a linear, bounded, selfadjoint and negative operator on $L^2_{\mathcal{M}}$.
(iii) The nullspace : $Ker\, Q = \{f \in L^2_{\mathcal{M}} \text{ s.t. } \exists\, N_s \in \mathbb{R} \text{ with } f_k = N_s \mathcal{M}_k, \forall k \geq 1\}$.
(iv) The equation $Q(f) = g$ admits a solution $f \in L^2_{\mathcal{M}}$ iff

$$\sum_k \int_{\mathbb{R}} g_k(v)\,dv = 0,$$

and this solution is unique if we impose the same relation on f.

An easy consequence of this result is the following proposition which allows us to define the diffusion matrix.

Proposition 6.2.2 *There exists $\Theta \in (L^2_{\mathcal{M}})^2$ such that for all $k \geq 1$,*

$$Q(\Theta)_k = -v\mathcal{M}_k \quad \text{and} \quad \sum_k \int_{\mathbb{R}} \Theta_k\,dv = 0.$$

We define the diffusion matrix by

$$\mathbb{D} = \sum_k \int_{\mathbb{R}} \Theta_k \otimes v\,dv. \tag{6.2.19}$$

Then $\mathbb{D}$ is a symmetric coercive matrix.

6.2.2 A priori estimate

Let $T > 0$. We set $M_k = K \exp(-\frac{1}{2}(v^2 + k^2))$ with a constant K chosen such that $\sum_k \int M_k\,dv = 1$. We define the entropy of the whole system (6.1.10)–(6.1.1)–(6.1.2) by :

$$W^\eta(t) = \sum_k \iint_{[a,b]\times\mathbb{R}} \left(f_k^\eta \log \frac{f_k^\eta}{M_k} - f_k^\eta + M_k \right) dxdv + \frac{1}{2} \iint_{\Omega} |\nabla_{x,z} V^\eta|^2\,dxdz. \tag{6.2.20}$$

The *distance* to equilibrium is defined by :

$$\mathcal{R}^\eta(t) = \frac{1}{2} \sum_k \iint_{[a,b]\times\mathbb{R}} \left(\sqrt{f_k^\eta} - \sqrt{N_s^\eta \mathcal{M}_k^\eta} \right)^2 dxdv. \tag{6.2.21}$$

All along the paper, we will use the following functional space :

$$L^p_x L^q_z(\Omega) = \{u \in L^1_{loc}(\Omega) \text{ such that } \|u\|_{L^p_x L^q_z(\Omega)} = \left(\int_a^b \|u\|^p_{L^q(0,1)}\right)^{1/p} < +\infty\}.$$

Thanks to Gagliardo-Nirenberg inequalities and interpolation estimates, one can prove that

Lemma 6.2.3 *We have the Sobolev imbedding of $H^1(\Omega)$ into $L^\infty_x L^2_z(\Omega)$.*

We notice that we do not have this imbedding if the transport is assumed to take place in a bounded domain of $\mathbb{R}^2$ but holds only in a 1D transport.

Proposition 6.2.4 *Let $T > 0$ and let $(V^\eta, (f^\eta_k, \epsilon^\eta_k, \chi^\eta_k)_{k\geq 1})$ be a global weak solution on the interval $[0,T]$ of the Boltzmann-Schrödinger-Poisson system* (6.1.10)–(6.1.1)–(6.1.2) *with the boundary condition* (6.1.9)–(6.1.8). *We assume that* **(A-1)** *holds and the initial data satisfy* **(A-2)**.

Then, there exists a nonnegative constant C_T such that,

$$\forall\, t \in [0,T], \quad 0 \leq W^\eta(t) + \frac{\alpha_1}{2\eta^2}\int_0^t \mathcal{R}^\eta(s)\, ds \leq C_T. \tag{6.2.22}$$

Moreover,

$$\forall\, t \in [0,T], \quad \int_a^b N^\eta_s(t,x) = \mathcal{N}_{in} = \int_a^b N^{in}_s(x)\, dx. \tag{6.2.23}$$

We point out the fact that this entropy only gives a bound on the distance between the distribution function f^η_k and the equilibrium state. Contrary to works of Bardos, Golse, Levermore, Lions, Masmoudi, Saint-Raymond, we can not find initial conditions and a maxwellian M such that the relative entropy of f^η_k with respect to this Maxwellian M converges toward 0 as η goes to 0.

Proof. We will prove this result in the case of smooth solutions for which all calculations are justified. In a general case, we regularize the system to have smooth solutions and pass to the limit in the estimate obtained for these smooth solutions. These steps are explain in section 6.6.

It is readily seen that with our assumption on the initial condition, the initial entropy is bounded. Indeed, we recall that we have $N^{in}_s \in C^0[a,b]$ then $V^{in} \in C^1(\Omega)$. Let us prove the a priori bound.

We first remark that with our boundary conditions, the system conserves the mass:

$$\frac{d}{dt}\sum_k \iint f^\eta_k\, dxdv = 0. \tag{6.2.24}$$

Thus we have (6.2.23)

We multiply (6.1.10) by $\left(1+\log f_k^\eta+\frac{|v|^2}{2}+\epsilon_k^\eta\right)$ and then integrate on $(a,b)\times\mathbb{R}$ and sum over k. We have,

$$\sum_k\iint \partial_t f_k^\eta\left(\log f_k^\eta+\frac{|v|^2}{2}+\epsilon_k^\eta+1\right)\,dxdv = \frac{d}{dt}\sum_k\iint f_k^\eta\left(\log f_k^\eta+\frac{|v|^2}{2}+\epsilon_k^\eta\right)\,dxdv-\sum_k\iint f_k^\eta\partial_t\epsilon_k^\eta\,dxdv.$$

Moreover, using the standard notation $\langle f\rangle=\int_0^1 f(z)\,dz$, we have $\partial_t\epsilon_k^\eta=\langle|\chi_k^\eta|^2\partial_t V^\eta\rangle$. Thus we obtain:

$$\begin{aligned}\sum_k\iint f_k^\eta\partial_t\epsilon_k^\eta\,dxdv &=\sum_k\iiint f_k^\eta|\chi_k^\eta|^2\partial_t V^\eta\,dxdvdz\\ &=\frac{d}{dt}\sum_k\iint f_k^\eta\langle|\chi_k^\eta|^2V^\eta\rangle\,dxdv-\frac{1}{2}\frac{d}{dt}\iint|\nabla_{x,z}V^\eta|^2\,dxdz,\end{aligned}$$

where we use (6.1.2). Therefore,

$$\begin{aligned}\sum_k\iint \partial_t f_k^\eta\left(\log f_k^\eta+\frac{|v|^2}{2}+\epsilon_k^\eta+1\right)\,dxdv &=\frac{1}{2}\frac{d}{dt}\iint|\nabla_{x,z}V^\eta|^2\,dxdz\\ &+\frac{d}{dt}\sum_k\iint f_k^\eta\left(\log f_k^\eta+\frac{|v|^2}{2}+\epsilon_k^\eta-\langle|\chi_k^\eta|^2V^\eta\rangle\right)\,dxdv.\end{aligned}\tag{6.2.25}$$

And we obtain easily from the Schrödinger equation (6.1.1):

$$\frac{1}{2}\langle|\partial_z\chi_k^\eta|^2\rangle+\langle|\chi_k^\eta|^2V^\eta\rangle=\epsilon_k^\eta.$$

For the second term, we have after an integration by parts

$$\begin{aligned}\sum_k\iint(v\cdot\nabla_x f_k^\eta+\nabla_x\epsilon_k^\eta\cdot\nabla_v f_k^\eta)\left(\log f_k^\eta+\frac{|v|^2}{2}+\epsilon_k^\eta+1\right)\,dxdv &=\\ \left[\sum_k\int_{\mathbb{R}} vf_k^\eta\left(\log f_k^\eta+\frac{|v|^2}{2}+\epsilon_k^\eta\right)\,dv\right]_a^b &=0,\end{aligned}\tag{6.2.26}$$

where we take into account the boundary conditions (6.1.8). Finally, with (6.1.5) and since $\sum_k\int Q^\eta(f^\eta)_k\,dv=0$,

$$\begin{aligned}&\sum_k\int Q^\eta(f^\eta)_k\left(\log f_k^\eta+\frac{|v|^2}{2}+\epsilon_k^\eta+1\right)\,dv=\\ &\frac{1}{2}\sum_{k,k'}\iint\alpha_{k,k'}(\mathcal{M}_k^\eta(v)f_{k'}^\eta(v')-\mathcal{M}_{k'}^\eta(v')f_k^\eta(v))\log\left[\left(\frac{f_k^\eta(v)}{\mathcal{M}_k^\eta(v)}\right)\left(\frac{\mathcal{M}_{k'}^\eta(v')}{f_{k'}^\eta(v')}\right)\right]\,dvdv'.\end{aligned}$$

Using the relation $(a-b)\log(a/b) \geq (\sqrt{a}-\sqrt{b})^2$, for all positive a and b, and the Jensen inequality, we obtain:

$$\sum_k \iint Q^\eta(f^\eta)_k \left(\log f_k^\eta + \frac{|v|^2}{2} + \epsilon_k^\eta + 1\right) dvdx \leq -\alpha_1 \mathcal{R}^\eta(t). \tag{6.2.27}$$

Finally, (6.2.25), (6.2.26) and (6.2.27) lead to:

$$\begin{aligned}\frac{d}{dt}\sum_k \iint f_k^\eta \left(\log f_k^\eta + \frac{|v|^2}{2} + \frac{1}{2}\langle|\partial_z \chi_k^\eta|^2\rangle\right) dxdv + \frac{1}{2}\frac{d}{dt}\iint |\nabla_{x,z} V^\eta|^2\, dxdz \\ + \frac{\alpha_1}{2\eta^2}\mathcal{R}^\eta(t) \leq 0.\end{aligned} \tag{6.2.28}$$

From (6.2.28) we have after an integration on $[0,T]$,

$$\begin{aligned}\sum_k \iint f_k^\eta \left(\log f_k^\eta + \frac{|v|^2}{2} + \frac{k^2}{2} - 1\right) dxdv + \frac{1}{2}\iint |\nabla_{x,z} V^\eta|^2\, dxdz \\ + \frac{\alpha_1}{2\eta^2}\int_0^T \mathcal{R}^\eta(t)\, dt \leq C_1 + \sum_k \int_a^b \rho_k^\eta \left(\frac{k^2}{2} - \frac{1}{2}\langle|\partial_z \chi_k^\eta|^2\rangle\right) dx.\end{aligned} \tag{6.2.29}$$

Moreover, since the potential V^η is nonnegative, we have with a Hölder inequality

$$\frac{1}{2}\langle|\partial_z \chi_k^\eta|^2\rangle = \epsilon_k^\eta - \langle|\chi_k^\eta|^2 V^\eta\rangle \geq \epsilon_k[0] - \|\chi_k^\eta\|^2_{L^4_z(0,1)} \|V^\eta\|_{L^2_z(0,1)}.$$

Using an interpolation and Lemma B.0.5 imply the existence of a nonnegative constant C_2 such that

$$\|\chi_k^\eta\|^2_{L^4_z(0,1)} \leq C\|\chi_k^\eta\|_{L^2_z(0,1)}\|\chi_k^\eta\|_{L^\infty_z(0,1)} \leq C_2(1 + \|V^\eta\|^{1/2}_{L^2_z(0,1)})$$

Thus

$$\frac{k^2}{2} - \frac{1}{2}\langle|\partial_z \chi_k^\eta|^2\rangle \leq \frac{1}{2}k^2 - \frac{1}{2}\pi^2 k^2 + C_2(1 + \|V^\eta\|^{1/2}_{L^2_z(0,1)}) \leq C_2(1 + \|V^\eta\|^{1/2}_{L^2_z(0,1)}). \tag{6.2.30}$$

By the Sobolev imbedding $H^1(\Omega) \hookrightarrow L^\infty_x L^2_z(\Omega)$, we have

$$\begin{aligned}\sum_k \int_a^b \rho_k^\eta \left(\frac{k^2}{2} - \frac{1}{2}\langle|\partial_z \chi_k^\eta|^2\rangle\right) dx &\leq C_3 \|\rho_k^\eta\|_{\ell^1(L^1(a,b))}(1 + \|V^\eta\|^{1/2}_{H^1(\Omega)}) \\ &= C_3 \mathcal{N}_{in}(1 + \|V^\eta\|^{1/2}_{H^1(\Omega)}).\end{aligned} \tag{6.2.31}$$

This last inequality in (6.2.29) provides

$$\iint |\nabla_{x,z} V^\eta|^2\, dxdz \leq C_4 + C_5 \|V^\eta\|^{1/2}_{H^1(\Omega)}.$$

Thus after a Poincaré inequality, we deduce that $\|V^\eta\|_{H^1(\Omega)}$ is bounded. Then (6.2.29) and (6.2.31) provides the desired estimate. □

Corollary 6.2.5 *Let $T>0$, there exists a constant $C_T>0$ such that :*

$$\forall\, t \in [0,T], \quad \sum_k \iint_{\omega\times\mathbb{R}^2} f_k^\eta(|\log f_k^\eta| + |v|^2 + k^2 + 1)\, dxdv \le C_T,$$

$$\int_0^T \int_\omega (N_s^\eta \log N_s^\eta - N_s^\eta + 1)\, dxdt \le C_T.$$

Proof. The second estimate is a direct application of the Jensen inequality. The first follows from the remark $a|\log a| \le a\log a + 2/e$. Indeed,

$$\begin{aligned}\sum_k \iint f_k^\eta |\log f_k^\eta|\, dxdv &\le \sum_k \iint f_k^\eta(|\log(f_k^\eta e^{v^2+k^2})| + v^2 + k^2)\, dxdv \\ &\le \sum_k \iint f_k^\eta \log(f_k^\eta e^{v^2+k^2})\, dxdv + \frac{2}{e}\sum_k \iint e^{-v^2-k^2}\, dxdv \\ &\quad + \sum_k \iint (v^2+k^2) f_k^\eta\, dxdv \le C_T.\end{aligned}$$

□

6.3 Analysis of the quasistatic part

This section is devoted to the study of the “quasi-static” Schrödinger-Poisson system defined by :

$$\begin{cases} -\dfrac{1}{2}\,\partial_z^2 \chi_k + V\chi_k = \epsilon_k \chi_k & (k \ge 1), \\ \chi_k(t,x,\cdot) \in H_0^1(0,1), & \displaystyle\int_0^1 \chi_k\, \chi_\ell\, dz = \delta_{k\ell}\,, \end{cases} \tag{6.3.32}$$

$$-\Delta_{x,z} V = \sum_k \rho_k |\chi_k|^2\,, \tag{6.3.33}$$

where we consider now that $\rho = (\rho_k)_{k\ge1}$ is given in $L^\infty((0,T), \ell^1(L^1(a,b)))$. We define $N_s = \sum_k \rho_k$. The system is completed by the following boundary conditions :

$$\begin{cases} \dfrac{dV}{dx}(t,a,z) = \dfrac{dV}{dx}(t,b,z) = 0 & \text{for } z \in (0,1), \\ V(t,x,0) = V(t,x,1) = 0 & \text{for } x \in (a,b). \end{cases}$$

We assume that ρ satisfies the following assumptions :

H1 : $\forall\, k \ge 1$, $\rho_k \ge 0$ and there exists a nonnegative constant C_T such that :

$$\forall\, t \in [0,T], \qquad \sum_k \int_\omega \rho_k (1+k^2)\, dx \le C_T. \tag{6.3.34}$$

In the sequel we will use the functional space $H_{01}^1 = \{V \in H^1(\Omega) \,:\, V(x,0) = V(x,1) = 0\}$.

Proposition 6.3.1 (Existence and uniqueness) *Let us suppose that $\rho = (\rho_k)_{k\geq 1}$ is given in $L^\infty((0,T),\ell^1(L^1(a,b)))$ and satisfy* **H1**. *Then the Schrödinger-Poisson system* (6.3.32)–(6.3.33) *admits a solution in H^1_{01}.*

Moreover, denoting $\mathcal{N} = \|N_s\|_{L^\infty((0,T),L^1(a,b))}$, if $\mathcal{N}$ is small enough, then this solution $(V,(\epsilon_k,\chi_k)_{k\geq 1})$ is unique.

This result is obtained thanks to an idea of Nier [22] which has been developed in [4] and chapter 4 and 5. The main difference here with the first part of the PhD is the fact that the quantity which is assumed to be known is not the surface density N_s but ρ_k. In the DDSP model, the occupation factor is equal to $N_s e^{-\epsilon_k}$ and then decreases with respect to k. It allows to insure the convexity of the functional used in the variational method (see section 4.2.4). Here we have to consider an other functional which is no more convex. This functional is defined on H^1_{01} by

$$J_\rho(V) = \frac{1}{2}\iint_\Omega |\nabla V|^2\,dxdz - \sum_{k\geq 1}\int_\omega \rho_k\epsilon_k[V]\,dx = J_0(V) + J_1(V,\rho). \tag{6.3.35}$$

We first prove that this functional has a minimizer and that this minimizer defines a solution of (6.3.32)–(6.3.33).

Lemma 6.3.2 *Assume that $(\rho_k)_{k\geq 1} \in L^\infty((0,T),\ell^1(L^1(a,b)))$ and satisfy* **H1**. *Then the functional J_ρ defined in* (6.3.35) *is continuous, locally Lipschitz and weakly lower semi-continuous on H^1_{01}. It is coercive : there exist nonnegative constants C_1, C_2 and C_3 such that*

$$J_\rho(V) \geq C_1\|V\|^2_{H^1(\Omega)} - C_2\|V\|^{3/2}_{H^1(\Omega)} - C_3. \tag{6.3.36}$$

Thus the system (6.3.32)–(6.3.33) *admits a solution $(V,(\epsilon_k,\chi_k)_{k\geq 1})$ such that $V \in H^1_{01}$.*

Proof. The functional J_0 is clearly continuous and strongly convex on H^1_{01}. For the functional J_1, we use the properties of $\epsilon_k[V]$ summarized in (B.0.14) to prove

$$\begin{aligned} |J_1(V,\rho) - J_1(\widetilde{V},\rho)| &\leq \sum_{k\geq 1}\int_a^b \rho_k|\epsilon_k[V] - \epsilon_k[\widetilde{V}]|\,dx \\ &\leq C_1\sum_{k\geq 1}\int_a^b \rho_k(1 + \|V\|^{1/2}_{L^2_z(0,1)} + \|\widetilde{V}\|^{1/2}_{L^2_z(0,1)})\|V - \widetilde{V}\|_{L^2_z(0,1)}\,dx. \end{aligned} \tag{6.3.37}$$

If we use the Sobolev imbedding stated in Lemma 6.2.3, we obtain

$$|J_1(V,\rho) - J_1(\widetilde{V},\rho)| \leq C_2(1 + \|V\|^{1/2}_{H^1(\Omega)} + \|\widetilde{V}\|^{1/2}_{H^1(\Omega)})\|N_s\|_{L^1(a,b)}\|V - \widetilde{V}\|_{H^1(\Omega)}. \tag{6.3.38}$$

Hence $J_1(\cdot,\rho)$ is Lipschitz and weakly continuous on H^1_{01}. Now if we take $\widetilde{V} = 0$ in (6.3.38), from **H1**, we have that $0 \geq J_1(0,\rho) \geq -C_T$. Thus,

$$J_\rho(V) \geq \frac{1}{2}\|\nabla V\|^2_{L^2(\Omega)} - C_3(1 + \|V\|^{1/2}_{H^1(\Omega)})\|V\|_{H^1(\Omega)} - C_4.$$

We apply the Poincaré inequality in H^1_{01} to find (6.3.36). Hence the functional J_ρ admits a minimizer in H^1_{01}. Moreover, from Lemma (B.0.3), it is clear that J_ρ is Gâteaux differentiable on H^1_{01} and for any $W \in H^1(\Omega)$,

$$d_V J_\rho(V) \cdot W = \iint_\Omega \nabla V \cdot \nabla W \, dxdz - \sum_k \int_\omega \rho_k \langle |\chi_k[V]|^2 W \rangle \, dx.$$

Thus each minimizer of the functional J_ρ is a weak solution of the Schrödinger-Poisson system (6.3.32)–(6.3.33). □

Lemma 6.3.3 *Let* $(\rho_k)_{k\geq 1}$ *in* $L^\infty((0,T), \ell^1(L^1(a,b)))$ *satisfying* **H1**. *Then, for* $\mathcal{N} = \|N_s\|_{L^\infty((0,T),L^1(a,b))}$ *small enough, the corresponding solution* $(V, (\epsilon_k[V], \chi_k[V]_{k\geq 1})$ *of the Schödinger-Poisson system* (6.1.1)–(6.1.2) *is unique.*

Proof. Let $(\rho_k)_{k\geq 1}$ be in $L^\infty((0,T), \ell^1(L^1(a,b)))$ satisfying **H1**. We assume that we can find two solutions of the Schödinger–Poisson system denoted V and $\widetilde{V}$. Multiplying the Poisson equation (6.3.33) by $(\widetilde{V} - V)$ and integrating provides:

$$\iint_\Omega |\nabla(\widetilde{V} - V)|^2 \, dxdz = \sum_k \int_a^b \rho_k \langle (|\chi_k[\widetilde{V}]|^2 - |\chi_k[V]|^2)(\widetilde{V} - V) \rangle \, dx. \tag{6.3.39}$$

From (B.0.4), we deduce that we have

$$\iint_a^b |\nabla(\widetilde{V} - V)|^2 \, dxdz \leq C_1 \int_\omega N_s \, e^{C_2(\|V\|_{L^2_z(0,1)} + \|\widetilde{V}\|_{L^2_z(0,1)})} \|V - \widetilde{V}\|^2_{L^2_z(0,1)} \, dx.$$

Then the Sobolev imbedding $H^1(\Omega) \hookrightarrow L^\infty_x L^2_z(\Omega)$ and a Poincaré inequality lead to

$$\|V - \widetilde{V}\|^2_{H^1(\Omega)} \leq C_3 e^{C_4(\|V\|_{H^1(\Omega)} + \|\widetilde{V}\|_{H^1(\Omega)})} \|N_s\|_{L^1(a,b)} \|V - \widetilde{V}\|^2_{H^1(\Omega)}. \tag{6.3.40}$$

Thanks to Lemma 6.3.2 we deduce that V and $\widetilde{V}$ are bounded in $H^1(\Omega)$. Thus, there exists a nonnegative constant C_5 such that

$$\|V - \widetilde{V}\|^2_{H^1(\Omega)} \leq C_5 \mathcal{N} \|V - \widetilde{V}\|^2_{H^1(\Omega)}. \tag{6.3.41}$$

Thus it suffices to chose $\mathcal{N}$ small enough to have $C_5\mathcal{N} \leq 1/2$ to prove that $V = \widetilde{V}$ on $[0,T] \times \Omega$. □

Proposition 6.3.4 (Continuity) *Let* $(\rho_k)_{k\geq 1}$ *and* $(\widetilde{\rho_k})_{k\geq 1}$ *in* $L^\infty((0,T), \ell^1(L^1(a,b)))$ *and satisfy* **H1**. *We denote by* $\mathcal{N} = \|N_s\|_{L^\infty((0,T),L^1(a,b))}$, $\widetilde{\mathcal{N}} = \|\widetilde{N_s}\|_{L^\infty((0,T),L^1(a,b))}$ *and* V *and* $\widetilde{V}$ *the corresponding solutions of the Schrödinger-Poisson system* (6.3.32)–(6.3.33). *Then there exists* $\mathcal{N}_0$ *such that if* $\max(\mathcal{N}, \widetilde{\mathcal{N}}) \leq \mathcal{N}_0$, *then*

$$\|V - \widetilde{V}\|_{L^2([0,T],H^1(\Omega))} \leq C_T \|\rho_k - \widetilde{\rho_k}\|_{L^\infty((0,T),\ell^1(L^1(a,b)))},$$

where C_T *is a nonnegative constant depending only on* T.

Proof. Let $(\rho_k)_{k\geq 1}$ and $(\widetilde{\rho_k})_{k\geq 1}$ be two sequences in $L^\infty((0,T),\ell^1(L^1(\omega)))$ satisfying **H1**. Multiplying the Poisson equation (6.3.33) by $(V-\widetilde{V})$ and integrating provides:

$$\begin{aligned}\iint_\Omega |\nabla(V-\widetilde{V})|^2\,dxdz = \sum_k \iint_\Omega (\rho_k-\widetilde{\rho_k})|\chi_k[V]|^2(V-\widetilde{V})\,dxdz \\ +\sum_k \int_a^b \widetilde{\rho_k}\langle(|\chi_k[V]|^2-|\chi_k[\widetilde{V}]|^2)(V-\widetilde{V})\rangle\,dx.\end{aligned} \tag{6.3.42}$$

We treat the second term as in the proof of Lemma 6.3.3 and obtain :

$$\sum_k \int_a^b \widetilde{\rho_k}\langle(|\chi_k[V]|^2-|\chi_k[\widetilde{V}]|^2)(V-\widetilde{V})\rangle\,dx \leq C_1\widetilde{\mathcal{N}}\|V-\widetilde{V}\|^2_{H^1(\Omega)}\,, \tag{6.3.43}$$

where C_1 is a nonnegative constant.

For the first one, we have with Lemma B.0.2

$$\begin{aligned}\sum_k \iint_\Omega (\rho_k-\widetilde{\rho_k})|\chi_k[V]|^2(V-\widetilde{V})\,dxdz \leq \\ \leq C_2\int_a^b \sum_{k\geq 1}|\rho_k-\widetilde{\rho_k}|e^{C_3\|V\|_{L^2_z}}\|V-\widetilde{V}\|_{L^2_z}\,dx.\end{aligned}$$

And by Lemma 6.2.3 and the bound of V and $\widetilde{V}$ in $H^1(\Omega)$, we have

$$\sum_{k\geq 1}\int_\omega (\rho_k-\widetilde{\rho_k})|\chi_k[V]|^2(V-\widetilde{V})\,dxdz \leq C_4\|\rho_k-\widetilde{\rho_k}\|_{\ell^1(L^1(a,b))}. \tag{6.3.44}$$

Therefore if we inject (6.3.43) and (6.3.44) in (6.3.42), we obtain after a Poincaré inequality:

$$\|V-\widetilde{V}\|^2_{H^1(\Omega)} \leq C_5\mathcal{N}\|V-\widetilde{V}\|^2_{H^1(\Omega)} + C_6\|\rho_k-\widetilde{\rho_k}\|_{\ell^1(L^1(a,b))}.$$

Thus it is readily seen after a integration in time that we can find $\mathcal{N}^0$ small enough such that for all $\mathcal{N}\leq\mathcal{N}^0$, we have

$$\|V-\widetilde{V}\|^2_{L^2([0,T],H^1(\Omega))} \leq C_6\|\rho_k-\widetilde{\rho_k}\|_{\ell^1(L^1(a,b))}.$$

□

Remark 6.3.5 *Since the Sobolev imbedding of Lemma 6.2.3 does not hold true for a two dimensional transport, we are not able to insure the uniqueness in Lemma 6.3.3 in this case. Nevertheless we can establish that we have the existence of solutions of the Schrödinger-Poisson system as we will see in chapter 7.*

6.4 Diffusive limit

In this section we assume to have the existence of a solution of the Boltzmann-Schrödinger-Poisson system for η fixed. Thus we suppose that we have constructed a renormalized solution of this system (6.1.10)–(6.1.12) considered with the conditions (6.1.8)-(6.1.9)-(6.1.3), which satisfies Theorem 6.1.1. The proof of this theorem will be discussed in section 6.6.

Here we will establish the diffusive limit when $\eta \to 0$ of this system. Namely, we prove Theorem 6.1.2. The rigorous proof of this convergence result is based on several steps. First the entropy inequality gives a first bound which allows us to obtain a weak convergence of the distribution function. An averaging lemma improves it to a strong convergence of the occupation factor which thanks to the continuity of the Schrödinger-Poisson system provides the strong convergences of the potential. With this kind of convergence we can pass to the limit in the equation in the last step and recover the drift-diffusion system. In the following we will abusively use the same notation $(f_k^\eta)_{k\geq 1}$ for subsequences. All results are proved up to an extraction.

6.4.1 Convergence of the density

We consider a renormalized solution of the Boltzmann equation. That is, $\forall\, \beta \in C^1(\mathbb{R}^+)$, $\beta(f^\eta)$ is a weak solution of :

$$\begin{cases} \eta\partial_t\beta(f^\eta)_k + v\cdot\nabla_x\beta(f^\eta)_k - \nabla_x\epsilon_k^\eta\cdot\nabla_v\beta(f^\eta)_k = \dfrac{Q^\eta(f^\eta)_k}{\eta}\beta'(f^\eta)_k, \\ \beta(f^\eta)_k(t=0) = \beta(f^{in})_k. \end{cases} \tag{6.4.45}$$

We fix $\delta > 0$. Let β_δ be an approximation of the identity, namely $\beta_\delta(s)_k = \frac{1}{\delta}\beta_k(\delta s)$. We choose β_k a C^∞ function satisfying $\beta_k(s) = s_k$ for $s_k \leq 1$, $0 \leq \beta'(s) \leq 1$ for all s and $\beta_k(s) = 2$ for $s \geq 3$.

Lemma 6.4.1 *Let f^η be a renormalized solution of the Boltzmann equation defined in Theorem 6.1.1, we have*

(i) f^η is weakly relatively compact in $\ell^1(L^1((0,T)\times(a,b)\times\mathbb{R}))$.

(ii) $\frac{Q^\eta(f^\eta)}{\eta}$ is weakly relatively compact in $\ell^1(L^1((0,T)\times(a,b)\times\mathbb{R}))$.

Proof. The first point is a consequence of the Dunford-Pettis theorem and the energy estimate.

Let us define

$$r_k^\eta = \frac{\sqrt{f_k^\eta} - \sqrt{N_s^\eta\mathcal{M}_k^\eta}}{\eta\sqrt{\mathcal{M}_k^\eta}}. \tag{6.4.46}$$

Thanks to the dissipation rate control (6.1.13), we have

$$\sum_k \int_0^T \iint |r_k^\eta|^2\mathcal{M}_k^\eta\, dxdvdt \leq C. \tag{6.4.47}$$

Using r^η we can rewrite

$$f_k^\eta = N_s^\eta \mathcal{M}_k^\eta + 2\eta\sqrt{N_s^\eta}\mathcal{M}_k^\eta r_k^\eta + \eta^2 (r_k^\eta)^2 \mathcal{M}_k^\eta.$$

Thanks to the linearity of Q^η and since with (6.4.47), $\sum_k \int_0^T \iint Q^\eta((r^\eta)^2\mathcal{M}^\eta)_k \, dxdvdt \le C$, then we have

$$\frac{Q^\eta(f^\eta)_k}{\eta} = 2\sqrt{N_s^\eta} Q^\eta(\mathcal{M}^\eta r^\eta)_k + \mathbf{O}(\eta)_{\ell^1(L^1_{t,x,v})}.$$

We deduce $\frac{Q^\eta(f^\eta)}{\eta} \in \ell^1(L^1_{t,x,v})$.

Moreover, let $\varepsilon > 0$, we have thanks to a Cauchy-Schwarz inequality,

$$\begin{aligned}\sum_k \int_A |\sqrt{N_s^\eta} Q^\eta(\mathcal{M}^\eta r^\eta)_k| \, dxdvdt \le \quad & C\sum_k \int_A N_s^\eta \mathcal{M}_k^\eta \, dxdvdt + \\ & \frac{1}{4C}\sum_k \int_A \frac{(Q^\eta(\mathcal{M}^\eta r^\eta)_k)^2}{\mathcal{M}_k^\eta} \, dxdvdt.\end{aligned}$$

We choose $C > 0$ such that the second term of the right hand side is bounded by $\varepsilon/2$. For such C, the equi-integrability of N_s^η imply

$$\exists\, \alpha > 0, \forall\, A \subset (0,T)\times(a,b)\times\mathbb{R}, \quad |A| < \alpha \Rightarrow C\sum_k \int_A N_s^\eta \mathcal{M}_k^\eta \, dxdvdt \le \frac{\varepsilon}{2}.$$

Thus $\sqrt{N_s^\eta} Q^\eta(\mathcal{M}^\eta r^\eta)$ is equi-integrable. Besides, for $R > 0$,

$$\sum_k \int_{|v|\ge R} |\sqrt{N_s^\eta} Q^\eta(\mathcal{M}^\eta r^\eta)_k| \, dxdvdt \le \frac{1}{R}\|N_s^\eta\|_{L^1_{t,x}} \left\| \frac{(Q^\eta(r^\eta\mathcal{M}^\eta))^2}{\mathcal{M}^\eta}\right\|^{1/2}_{\ell^1(L^1_{t,x,v})}.$$

And the right hand side goes to 0 uniformly in η as R tends to $+\infty$. This proves the weak compactness of $\frac{Q^\eta(f^\eta)}{\eta}$ thanks to the Dunford-Pettis theorem. □

Lemma 6.4.2 *Let $\rho^\eta = \int f^\eta \, dv$ where f^η is defined in Theorem 6.1.1. Then ρ^η is relatively compact in $\ell^1(L^1((0,T)\times(a,b)))$.*

Proof. We have

$$\eta\partial_t \beta_\delta(f^\eta)_k + v\cdot\nabla_x \beta_\delta(f^\eta)_k = h_k^\eta + \nabla_v g_k^\eta,$$

where $h_k^\eta = \frac{1}{\eta} Q^\eta(f^\eta)_k \beta'_\delta(f^\eta)_k$ and $g_k^\eta = \nabla_x \epsilon_k^\eta \beta_\delta(f^\eta)_k$. Since we have $0 \le \beta'_\delta(f^\eta)_k \le 1$ and $\frac{1}{\eta}Q^\eta(f^\eta)$ is weakly relatively compact in $\ell^1(L^1(dtdxdv))$, we deduce that h_k^η is weakly relatively compact in $\ell^1(L^1(dtdxdv))$. As the choice of β_δ implies $\beta_\delta(f^\eta)_k \le 2/\delta$ then $\beta_\delta(f^\eta)_k \in L^\infty_{t,x,v}$. The spectral properties of the Hamiltonian imply $\nabla_x \epsilon_k = \langle |\chi_k|^2 \nabla_x V\rangle$. The bound of V in $H^1(\Omega)$ implies a bound of $\nabla_x \epsilon_k$ in $L^2(a,b)$. Thus, $g_k^\eta \in \ell^1_{loc}(L_t^\infty L_x^2 L_v^\infty)$. Thanks to an averaging lemma [15, 9], we deduce that $\forall\, \psi_k \in \mathcal{D}(\mathbb{R})$

$$\int_{\mathbb{R}} \beta_\delta(f^\eta)_k \psi_k \, dv \qquad \text{is relatively compact in } L^1_{t,x}.$$

Using the fact that $|v|^2 f_k^\eta$ is uniformly bounded in $L^1_{t,x,v}$, we obtain thanks to standard arguments that $\int_{\mathbb{R}} \beta_\delta(f^\eta)_k\, dv$ is relatively compact in $L^1_{t,x}$. Moreover the definition of β_δ gives

$$\sum_k \int_0^T \iint |\beta_\delta(f^\eta)_k - f_k^\eta|\, dxdvdt \leq 3 \sum_{\{f_k^\eta \geq 1/\delta\}} \int_0^T \iint_{\{f_k^\eta \geq 1/\delta\}} f_k^\eta\, dxdvdt.$$

Thus, the equi-integrability of f_k^η implies

$$\sup_{\eta \leq 1} \|\beta_\delta(f^\eta) - f^\eta\|_{\ell^1(L^1_{t,x,v})} \to 0 \quad \text{as } \delta \to 0. \tag{6.4.48}$$

Let $\varepsilon > 0$, up to an extraction, we have

$$\begin{aligned} \int |f_k^\eta - f_k^{\eta'}|\, dtdxdv \leq & \int |f_k^\eta - \beta_\delta(f^\eta)_k|\, dtdxdv + \int |\beta_\delta(f^\eta)_k - \beta_\delta(f^{\eta'})_k|\, dtdxdv \\ & + \int |\beta_\delta(f^{\eta'})_k - f_k^{\eta'}|\, dtdxdv. \end{aligned}$$

We fix δ such that the first and the third term of the right hand side is $< \varepsilon/3$. For such a $\delta > 0$, $\int_{\mathbb{R}} \beta_\delta(f^\eta)_k\, dv$ is relatively compact. Thus with η and η' small enough the second term is bounded by $\varepsilon/3$. Then the Cauchy criterion proves, up to an extraction,

$$\rho_k^\eta \to \rho_k \text{ strongly in } L^1([0,T] \times (a,b)) \text{ and a.e.}$$

By the Dunford-Pettis theorem, we have that N_s^η converges weakly in $L^1_{t,x}$ towards N_s. By a Lebesgue theorem, the convergence almost everywhere of ρ_k^η implies that for all $\psi \in \mathcal{D}((0,T) \times (a,b))$,

$$\sum_k \iint_{(0,T)\times(a,b)} \rho_k^\eta \psi\, dxdt \longrightarrow \sum_k \iint_{(0,T)\times(a,b)} \rho_k \psi\, dxdt \quad \text{as } \eta \to 0.$$

By uniqueness of the weak limit, we have $N_s = \sum_k \rho_k$. Since N_s and N_s^η are bounded in $L^1_{t,x}$,

$$\exists\, K \in \mathbb{N}, \forall\, k \geq N, \quad \sum_{k \geq N} \int_{(0,T)\times(a,b)} \rho_k\, dtdx < \frac{\varepsilon}{3} \text{ and } \sum_{k \geq N} \int_{(0,T)\times(a,b)} \rho_k^\eta\, dtdx < \frac{\varepsilon}{3}.$$

Thus

$$\sum_k \int_{(0,T)\times(a,b)} |\rho_k^\eta - \rho_k|\, dxdt \leq \frac{2\varepsilon}{3} + \sum_{k \leq N} \int_{(0,T)\times(a,b)} |\rho_k^\eta - \rho_k|\, dxdt.$$

It means that, up to an extraction,

$$\rho^\eta \to \rho \text{ strongly in } \ell^1(L^1((0,T) \times (a,b))) \text{ and a.e.} \tag{6.4.49}$$

□

Proposition 6.4.3 *Let (f^η, V^η) be a solution of the renormalized system defined in Theorem 6.1.1, then there exist V in $L^\infty((0,T),H^1(\Omega))$ and N_s in $L^\infty((0,T),L^1(a,b))$ such that, up to an extraction,*

$$V^\eta \to V \text{ in } L^2((0,T),H^1(\Omega)) \text{ and } f^\eta \to N_s\mathcal{M} \text{ in } \ell^1(L^1((0,T)\times(a,b)\times\mathbb{R})) \text{ and a.e.}$$

Proof. Since with (6.4.49) we have proved the strong and a.e. convergence of ρ^η towards ρ, the Fatou Lemma and estimate (6.1.13) imply that for a.e. $t \in [0,T]$,

$$\sum_k \int_a^b (\rho_k \log \rho_k - \rho_k)\, dx \le C_T \qquad \text{and} \qquad \sum_k \int_a^b \rho_k(1+k^2)\, dx \le C_T.$$

Thus from Lemma 6.3.2, we deduce that there exists $V \in L^\infty([0,T],H^1(\Omega))$ weak solution of the Schrödinger-Poisson system (6.3.32)–(6.3.33). But in the framework of Theorem 6.1.2 we do not impose to have small data. We can not apply the uniqueness result of the Schrödinger-Poisson system in Lemma 6.3.3. Nevertheless, we can prove that

$$\|V - V^\eta\|_{L^2([0,T],H^1(\Omega))} \to 0 \quad \text{ as } \eta \to 0.$$

In fact, we multiply the Poisson equation by $(V - V^\eta)$ and integrate, we have

$$\int_0^T \iint_\Omega |\nabla(V^\eta - V)|^2\, dxdzdt = I + II + III,$$

where

$$I = \sum_k \int_0^T \int_a^b (\rho_k - \rho_k^\eta)\langle|\chi_k[V]|^2(V - V^\eta)\rangle\, dxdt,$$

$$II = \sum_k \int_0^T \iint_{(a,b)\times\mathbb{R}} (f_k^\eta - N_s^\eta\mathcal{M}_k^\eta)\langle(|\chi_k[V]|^2 - |\chi_k[V^\eta]|^2)(V - V^\eta)\rangle\, dxdvdt,$$

$$III = \sum_k \int_0^T \iint_{(a,b)\times\mathbb{R}} N_s^\eta\mathcal{M}_k^\eta\langle(|\chi_k[V]|^2 - |\chi_k[V^\eta]|^2)(V - V^\eta)\rangle\, dxdvdt,$$

We will used the same idea to treat the first and second term as in the proof of Proposition 6.3.4. For the third term we remark that as η goes to 0 we are closer from the equilibrium. And the occupation factors at the equilibrium decrease with respect to k. The distance to the equilibrium is measured thanks to $\mathcal{R}^\eta$ (6.2.21). Therefore, for the third term, we have using Lemma (B.0.3),

$$III = \int_0^T \iint_{(a,b)\times\mathbb{R}} \frac{N_s^\eta}{2} \int_0^1 \sum_{k,\ell\neq k} \frac{\mathcal{M}_k^\eta - \mathcal{M}_\ell^\eta}{\epsilon_k^\sigma - \epsilon_\ell^\sigma}\langle\chi_k^\sigma(V - V^\eta)\chi_\ell^\sigma\rangle^2\, d\sigma\, dxdvdt \le 0, \tag{6.4.50}$$

where we denote $\epsilon_k^\sigma := \epsilon_k[\sigma V + (1-\sigma)\widetilde{V}]$ and $\chi_k^\sigma := \chi_k[\sigma V + (1-\sigma)\widetilde{V}]$.

For the first term, as in the proof of Proposition 6.3.4, we can show that

$$|I| \le C_1\|\rho_k - \rho_k^\eta\|_{\ell^1(L^1_{t,x})}. \tag{6.4.51}$$

For the second term, we use Lemma (B.0.5) to write

$$|II| \leq C_2 \sum_k \int_0^T \iint_{(a,b)\times\mathbb{R}} |f_k^\eta - N_s^\eta \mathcal{M}_k^\eta| \, e^{C_3(\|V\|_{L_z^2} + \|V^\eta\|_{L_z^2})} \|V - V^\eta\|_{L_z^2} \, dxdvdt.$$

Thus Lemma 6.2.3 implies

$$|II| \leq C_4 \sum_k \int_0^T \iint_{(a,b)\times\mathbb{R}} |f_k^\eta - N_s^\eta \mathcal{M}_k^\eta| \, dxdvdt. \tag{6.4.52}$$

We show that the a priori estimate in Proposition 6.2.4 implies to convergence towards 0 of this term. Indeed, by a Cauchy-Schwarz inequality

$$\sum_k \int_0^T \iint_{(a,b)\times\mathbb{R}} |f_k^\eta - N_s^\eta \mathcal{M}_k^\eta| \, dxdvdt \leq 2\sqrt{2} \|N_s^\eta\|_{L_{t,x}^1}^{1/2} \left(\int_0^T \mathcal{R}^\eta(t) \, dt \right)^{1/2}.$$

Then to the properties of the eigenvalues of the Hamiltonian (B.0.3) and the injection of $H^1(\Omega)$ into $L_x^\infty L_z^2(\Omega)$ implies that

$$\|\epsilon_k[V^\eta] - \epsilon_k[V]\|_{L^2([0,T],L^\infty(\omega))} \to 0 \quad \text{as } \eta \to 0.$$

Moreover, using Lemma B.0.3, we have

$$\mathcal{M}_k^\eta - \mathcal{M}_k = \int_0^1 M(v) \frac{e^{-\epsilon_k^s}}{\mathcal{Z}^s} \left(\frac{\sum_\ell \langle |\chi_\ell^s|^2 (V^\eta - V) \rangle e^{-\epsilon_k^s}}{\mathcal{Z}^s} - \langle |\chi_k^s|^2 (V^\eta - V) \rangle \right) ds,$$

where we use the notation $f^s := f[V + s(V^\eta - V)]$. Then by Lemma B.0.2 we have

$$|\mathcal{M}_k^\eta - \mathcal{M}_k| \leq C \, e^{\|V^\eta\|_{L_z^2} + \|V\|_{L_z^2}} \|V - V^\eta\|_{L_z^2} \int_0^1 M(v) \frac{e^{-\epsilon_k^s}}{\mathcal{Z}^s} \, ds \tag{6.4.53}$$

Thus the injection $H^1(\Omega) \hookrightarrow L_x^\infty L_z^2(\Omega)$ provides the convergence $\mathcal{M}^\eta \to \mathcal{M}$ as $\eta \to 0$ in $L^2([0,T], \ell^1(L^\infty((a,b)\times\mathbb{R})))$ and in $L^2([0,T], \ell^\infty(L^\infty((a,b)\times\mathbb{R})))$ Furthermore,

$$\|N_s \mathcal{M} - N_s^\eta \mathcal{M}^\eta\|_{\ell^1(L_{t,x,v}^1)} \leq \|N_s - N_s^\eta\|_{L_{t,x}^1} + \|N_s^\eta (\mathcal{M} - \mathcal{M}^\eta)\|_{\ell^1(L_{t,x,v}^1)}. \tag{6.4.54}$$

The bound (6.4.53) provides

$$\|N_s^\eta (\mathcal{M} - \mathcal{M}^\eta)\|_{\ell^1(L_{t,x,v}^1)} \leq C \int_0^T \int_a^b N_s^\eta \, e^{\|V^\eta\|_{L_z^2} + \|V\|_{L_z^2}} \|V - V^\eta\|_{L_z^2} \, dxdt.$$

Thus the a priori bound in Proposition 6.2.4 and Lemma 6.2.3 imply that there exists a nonnegative constant C such that

$$\|N_s^\eta (\mathcal{M} - \mathcal{M}^\eta)\|_{\ell^1(L_{t,x,v}^1)} \leq C \|V - V^\eta\|_{L^2([0,T],H^1(\Omega))}^{1/2}.$$

This last estimate combines with the strong convergence of N_s^η in $L^1_{t,x}$ imply thanks to (6.4.54) that

$$\|N_s\mathcal{M} - N_s^\eta \mathcal{M}^\eta\|_{\ell^1(L^1_{t,x,v})} \to 0 \quad \text{as } \eta \to 0.$$

Moreover, the entropy estimate (6.1.13) implies a control of the dissipation rate :

$$\int_0^T \mathcal{R}^\eta(t)\,dt = \frac{1}{2}\sum_{k\geq 1}\int_0^T \iint_{(a,b)\times\mathbb{R}} \left(\sqrt{f_k^\eta} - \sqrt{N_s^\eta \mathcal{M}_k^\eta}\right)^2 dxdvdt \leq C_T\eta^2.$$

Thus, by a Cauchy-Schwarz inequality,

$$\begin{aligned}\|f^\eta - N_s\mathcal{M}\|_{\ell^1(L^1_{t,x,v})} &\leq \|f^\eta - N_s^\eta\mathcal{M}^\eta\|_{\ell^1(L^1_{t,x,v})} + \|N_s^\eta\mathcal{M}^\eta - N_s\mathcal{M}\|_{\ell^1(L^1_{t,x,v})} \\ &\leq 4\|N_s^\eta\|^{1/2}_{L^1_{t,x}}\left(\int_0^T \mathcal{R}^\eta(t)\,dt\right)^{1/2} + \|N_s^\eta\mathcal{M}^\eta - N_s\mathcal{M}\|_{\ell^1(L^1_{t,x,v})}.\end{aligned}$$

Thus $f^\eta \to N_s\mathcal{M}$ strongly in $\ell^1(L^1_{t,x,v})$ and one can extract a subsequence converging a.e.

□

6.4.2 The limit equation

Proposition 6.4.4 *Let (f^η, V^η) be a solution of the renormalized system defined in Theorem 6.1.1, then the current J^η, defined by*

$$J^\eta := \frac{1}{\eta}\sum_k \int_{\mathbb{R}^2} v f_k^\eta\,dv, \tag{6.4.55}$$

satisfies

$$\begin{cases} J^\eta \rightharpoonup J = -\mathbb{D}(\nabla_x N_s + N_s\nabla_x V_s) & \text{in weak} - L^1_{t,x}, \\ J(t,a) = J(t,b) = 0, \end{cases}$$

where the diffusion matrix $\mathbb{D}$ is defined in (6.2.19) *and the autoconsistant potential is* $V_s = -\log(\sum_{k\geq 1} e^{-\epsilon_k[V]})$.

Proof. Thanks to Proposition 6.4.3 and the inequality $|\sqrt{a}-\sqrt{b}|^2 \leq |a-b|$ for two nonnegative reals a and b, we have

$$(\sqrt{f_k^\eta})_{k\geq 1} \to (\sqrt{N_s\mathcal{M}_k})_{k\geq 1} \text{ in } \ell^2(L^2_{t,x,v}).$$

Thanks to the definition of r_k^η (6.4.46), we have

$$J^\eta = \frac{1}{\eta}\sum_k \int_{\mathbb{R}^2} v f_k^\eta\,dv = 2\sqrt{N_s^\eta}\sum_k \int_{\mathbb{R}^2} v r_k^\eta \mathcal{M}_k^\eta\,dv + \mathbf{O}(\eta)_{\ell^1(L^1_{t,x,v})}.$$

Besides, $\mathcal{M}_k^\eta \le 1$ and the bound (6.4.47) imply that $(r^\eta \mathcal{M}^\eta)$ is bounded in $\ell^2(L^2_{t,x,v})$. Thus up to an extraction, there exists $r \in \ell^2(L^2(\mathcal{M} dt dx dv))$ such that $(r^\eta \mathcal{M}^\eta)$ weakly converges towards $(r\mathcal{M})$ in $\ell^2(L^2_{t,x,v})$. We deduce

$$\sum_k \int_{\mathbb{R}^2} v r_k^\eta \mathcal{M}_k^\eta \, dv = \sum_k \int_{\mathbb{R}^2} v \mathcal{M}_k \frac{r_k^\eta \mathcal{M}_k^\eta}{\mathcal{M}_k} \, dv \rightharpoonup \sum_k \int_{\mathbb{R}^2} v r_k \mathcal{M}_k \, dv \quad \text{in } weak - L^2_{t,x}.$$

Proposition 6.4.2 proves that $\sqrt{N_s^\eta} \to \sqrt{N_s}$ in $L^2_{t,x}$ strongly. Thus

$$J^\eta \rightharpoonup J := 2\sqrt{N_s} \sum_k \int_{\mathbb{R}^2} v r_k \mathcal{M}_k \, dv \quad \text{in } weak - L^1_{t,x}. \tag{6.4.56}$$

Since we have $\sum_k \int v \mathcal{M}_k \, dv = 0$, Proposition 6.2.1 shows that we can define $Q^{-1}(v\mathcal{M})$ and the selfadjointness of the operator Q leads to

$$J = 2\sqrt{N_s} \sum_k \int_{\mathbb{R}^2} Q^{-1}(v\mathcal{M})_k Q(r\mathcal{M})_k \frac{dv}{\mathcal{M}_k}. \tag{6.4.57}$$

Now, we will find an expression of J. Considering again the definition of r_k^η, we have

$$\frac{Q^\eta(f^\eta)_k}{\eta} = 2\sqrt{N_s^\eta} Q^\eta(r^\eta \mathcal{M}^\eta)_k + \eta Q^\eta((r^\eta)^2 \mathcal{M}^\eta)_k.$$

With (6.4.47), the second term in the right hand side is of order $\mathbf{O}(\eta)_{\ell^1(L^1_{t,x,v})}$. For the first one, one can prove easily, thanks to a Lebesgue theorem, that $\forall f \in \ell^2(L^2_{t,x,v})$, we have $\|Q^\eta(f) - Q(f)\|_{\ell^2(L^2_{t,x,v})} \to 0$. The weak convergence of $(r^\eta \mathcal{M}^\eta)$ in $\ell^2(L^2_{t,x,v})$ implies then

$$Q^\eta(r^\eta \mathcal{M}^\eta) \rightharpoonup Q(r\mathcal{M}) \quad \text{in } \ell^2(L^2_{t,x,v}).$$

With the strong convergence in $L^2_{t,x}$ of $\sqrt{N_s^\eta}$, we deduce

$$\frac{Q^\eta(f^\eta)_k}{\eta} = 2\sqrt{N_s^\eta \mathcal{M}_k} \frac{Q^\eta(r^\eta \mathcal{M}^\eta)_k}{\sqrt{\mathcal{M}_k}} + \mathbf{O}(\eta)_{\ell^1(L^1_{t,x,v})} \rightharpoonup 2\sqrt{N_s} Q(r\mathcal{M})_k \quad \text{in } \ell^1(L^1_{t,x,v}). \tag{6.4.58}$$

We recall that for every $\lambda > 0$, we have defined $\Theta_{k,\lambda}^\eta = (f_k^\eta + \lambda \exp(-\frac{1}{2}(v^2 + k^2)))^{1/2}$. Thus we have

$$\Theta_{k,\lambda}^\eta \to \Theta_{k,\lambda} = (f_k + \lambda e^{-\frac{1}{2}(v^2+k^2)})^{1/2} \quad \text{strongly in } \ell^2(L^2_{t,x,v}).$$

Moreover we have,

$$\eta \partial_t \Theta_{k,\lambda}^\eta + v \cdot \nabla_x \Theta_{k,\lambda}^\eta - \nabla_v (\nabla_x \epsilon_k^\eta \, \Theta_{k,\lambda}^\eta) = \frac{Q^\eta(f^\eta)_k}{2\eta \Theta_{k,\lambda}^\eta} + \lambda \nabla_x \epsilon_k^\eta \, \frac{v e^{-\frac{1}{2}(v^2+k^2)}}{2\Theta_{k,\lambda}^\eta}. \tag{6.4.59}$$

We can pass to the limit in the previous equation (6.4.59). In fact we have the strong convergence of $\Theta_{k,\lambda}^\eta$ in L^2 and the strong convergence of V^η in H^1. Moreover, with Lemma B.0.3, we have

$$\nabla_x \epsilon_k^\eta - \nabla_x \epsilon_k = \langle (|\chi_k^\eta|^2 - |\chi_k|^2) \nabla_x V^\eta \rangle + \langle |\chi_k|^2 \nabla_x (V^\eta - V) \rangle.$$

Thus with Lemma B.0.2 and (B.0.4),

$$|\nabla_x \epsilon_k^\eta - \nabla_x \epsilon_k| \leq C_1 e^{C_2 \|V\|_{L_z^2}} \left(\|\nabla_x V^\eta\|_{L_z^2} e^{C_2 \|V^\eta\|_{L_z^2}} \|V - V^\eta\|_{L_z^2} + \|\nabla_x (V - V^\eta)\|_{L_z^2} \right).$$

The strong convergence of V^η in $L^2((0,T), H^1(\Omega))$ and the Sobolev imbedding in Proposition 6.2.3, $H^1(\Omega) \hookrightarrow L_x^\infty L_z^2(\Omega)$, imply that

$$\nabla_x \epsilon_k^\eta \to \nabla_x \epsilon_k \quad \text{strongly in } \ell^2(L^2_{t,x}).$$

Therefore,

$$\nabla_x \epsilon_k^\eta \Theta_{k,\lambda}^\eta \rightharpoonup \nabla_x \epsilon_k \Theta_{k,\lambda} \quad \text{weakly in } L^1_{t,x,v}.$$

Thus we can take the weak limit as $\eta \to 0$ in (6.4.59). For all $k \geq 1$, we find

$$v \cdot \nabla_x \Theta_{k,\lambda} - \nabla_v (\nabla_x \epsilon_k \ \Theta_{k,\lambda}) = \frac{\sqrt{N_s} Q(r\mathcal{M})_k}{\Theta_{k,\lambda}} + \lambda \nabla_x \epsilon_k \ \frac{v e^{-\frac{1}{2}(v^2+k^2)}}{2\Theta_{k,\lambda}}.$$

And if we make $\lambda \to 0$ in the resulting equation, we find

$$\left(\nabla_x \sqrt{N_s} + \frac{1}{2} \sqrt{N_s} \nabla_x V_s \right) \cdot v\mathcal{M}_k = Q(r\mathcal{M})_k, \tag{6.4.60}$$

where we take $V_s = -\log \sum_k e^{-\epsilon_k}$. And we verify that the product $\sqrt{N_s}\nabla_x V_s$ has a meaning in $L^1_{t,x}$. Now, with (6.4.56) and (6.4.60), we can conclude

$$J = -\mathbb{D}\sqrt{N_s} \left(\nabla_x \sqrt{N_s} + \frac{1}{2} \sqrt{N_s} \nabla_x V_s \right), \tag{6.4.61}$$

where the symmetric positive diffusion matrix, defined in (6.2.19), is given by

$$\mathbb{D} = -\sum_k \int_{\mathbb{R}} v \otimes Q^{-1}(v\mathcal{M})_k \, dv.$$

Besides, with our choice of boundary conditions (6.1.8) we have that

$$\sum_{k \geq 1} \int_{\mathbb{R}} v f_k^\eta(t,a,v) \, dv = \sum_{k \geq 1} \int_{\mathbb{R}} v f_k^\eta(t,b,v) \, dv = 0$$

Thus as η goes to 0, it provides that $J(t,a) = 0$ and $J(t,b) = 0$. Now, if we use Lemma 6.4.5, we can rewrite the current J and the proof of the Proposition 6.4.4 is complete. □

Lemma 6.4.5 *Let N_s and V be defined in Proposition 6.4.3. If we suppose that*

$$\nabla_x \sqrt{N_s} + \frac{1}{2} \sqrt{N_s} \nabla_x V_s = G \in L^2((0,T) \times (a,b)), \tag{6.4.62}$$

where $V_s = -\log(\sum_{k \geq 1} e^{-\epsilon_k[V]})$. Then we have

$$\sqrt{N_s} \in L^2([0,T], H^1(\omega)) \quad \textit{and} \quad \sqrt{N_s}\nabla_x V_s \in L^2((0,T) \times (a,b)).$$

Proof. From (6.4.60) we have that (6.4.62) holds. Moreover, we have $\sqrt{N_s}$ bounded in $L^2_{t,x}$ and V in $L^2_t H^1_x$, then from Lemma B.0.2, we deduce that $\sqrt{N_s}\nabla_x V_s \in L^1_{t,x}$. It follows that $\nabla_x \sqrt{N_s} \in L^1_{t,x}$. We consider the approximation of the identity β_δ as before. Namely $\beta_\delta(s) = \frac{1}{\delta}\beta(\delta s)$ where β is a $C^\infty(\mathbb{R}^+)$ function satisfying $\beta(s) = s$ for $0 \leq s \leq 1$, $\beta(s) = 2$ for $s \geq 3$ and $0 \leq \beta'(s) \leq 1$. If we denote $\psi = \sqrt{N_s}$, we have

$$\nabla_x \beta_\delta(\psi) = \nabla_x \psi \beta'_\delta(\psi).$$

Hence we can renormalize the equation (6.4.62) :

$$\nabla_x \beta_\delta(\psi) + \frac{1}{2}\nabla_x V_s\, \beta'_\delta(\psi)\psi = \tilde{G}$$

where $\tilde{G} = G\, \beta'_\delta(\psi) \leq G$. Multiplying (6.4.63) by $\nabla_x \beta_\delta(\psi)$ and integrating provides

$$\iint |\nabla_x \beta_\delta(\psi)|^2\, dxdt + \frac{1}{2}\iint \nabla_x V_s \cdot \nabla_x \beta_\delta(\psi)\, \psi \beta'_\delta(\psi)\, dxdt = \iint \tilde{G}\nabla_x \beta_\delta(\psi)\, dxdt. \quad (6.4.63)$$

By a Cauchy-Schwarz inequality we deduce

$$\iint \tilde{G}\nabla_x \beta_\delta(\psi)\, dxdt \leq \frac{1}{2}\iint \tilde{G}^2\, dxdt + \frac{1}{2}\iint |\nabla_x \beta_\delta(\psi)|^2\, dxdt.$$

If we define $\tilde{\beta}$ by $\tilde{\beta}(s) = \int_0^s \tau \beta'(s)^2\, d\tau$ and $\tilde{\beta}_\delta(s) = \frac{1}{\delta^2}\tilde{\beta}(\delta s)$. Then, $\tilde{\beta}_\delta(s)$ goes to $\frac{s^2}{2}$ when δ goes to 0 and we have

$$\int_\omega \nabla_x V_s \cdot \nabla_x \beta_\delta(\psi)\, \psi \beta'_\delta(\psi)\, dx = \int_\omega \nabla_x V_s \cdot \nabla_x \tilde{\beta}_\delta(\psi)\, dx = -\int_\omega \Delta_x V_s \tilde{\beta}_\delta(\psi)\, dx. \quad (6.4.64)$$

With the Poisson equation (6.3.33) for $f_k = N_s \mathcal{M}_k$, we have :

$$-\Delta_x V = \partial_z^2 V + N_s \sum_{k\geq 1} \frac{e^{-\epsilon_k}|\chi_k|^2}{\mathcal{Z}}.$$

And, after some integrations by parts,

$$\langle \partial_z^2 V |\chi_k|^2\rangle = 2\langle V \chi_k \partial_z^2 \chi_k\rangle + 2\langle V|\partial_z \chi_k|^2\rangle.$$

Thanks to the Schrödinger equation (6.3.32), we have :

$$\partial_z^2 \chi_k = 2(V - \epsilon_k)\chi_k \quad \text{ and } \quad 2\langle V|\chi_k|^2\rangle + |\partial_z \chi_k|^2 = 2\epsilon_k.$$

Thus,

$$\langle \partial_z^2 V |\chi_k|^2\rangle = 4\langle V^2 |\chi_k|^2\rangle + 2\langle (V + \epsilon_k)|\partial_z \chi_k|^2\rangle - 4\epsilon_k^2.$$

These remarks lead to the following identity :

$$\begin{aligned} -\Delta_x V_s \quad = \quad & -4\sum_k \frac{e^{-\epsilon_k}(\epsilon_k)^2}{\mathcal{Z}} + \frac{\langle N^2 + 4V^2\, N\rangle}{N_s} + 2\sum_k \frac{e^{-\epsilon_k}}{\mathcal{Z}}\left\langle (V+\epsilon_k)|\partial_z \chi_k|^2\right\rangle \\ & -\frac{1}{\mathcal{Z}}\sum_k \sum_{\ell\neq k}\left(\frac{e^{-\epsilon_k} - e^{-\epsilon_\ell}}{\epsilon_k - \epsilon_\ell}\right)\langle \chi_k \chi_\ell\, \nabla_x V\,\rangle^2 \\ & + \sum_k \frac{e^{-\epsilon_k}}{\mathcal{Z}}\left\langle |\chi_k|^2\, \nabla_x V\right\rangle^2 - \left(\sum_k \frac{e^{-\epsilon_k}}{\mathcal{Z}}\left\langle |\chi_k|^2\, \nabla_x V\right\rangle\right)^2. \end{aligned} \quad (6.4.65)$$

By the Cauchy-Schwarz inequality, the sum of the last two terms of the right hand side is nonnegative. Moreover, except for the first one, the other terms are obviously nonnegative. Thus we have with (6.4.64),

$$\int_a^b \nabla_x V_s \cdot \nabla_x \beta_\delta(\psi)\, \psi \beta'_\delta(\psi)\, dx \geq -4 \int_a^b \sum_k \frac{e^{-\epsilon_k}(\epsilon_k)^2}{\mathcal{Z}} \tilde{\beta}_\delta(\psi)\, dx.$$

Moreover, Lemma B.0.2 and the Sobolev imbedding $H^1(\Omega) \hookrightarrow L^\infty_x L^2_z(\Omega)$ imply that the quantity $\sum_k \frac{e^{-\epsilon_k}(\epsilon_k)^2}{\mathcal{Z}}$ is bounded in $L^\infty(\omega)$. Thus (6.4.63) leads to

$$\iint |\nabla_x \beta_\delta(\psi)|^2\, dtdx \leq \iint G^2\, dtdx + 4 \int_a^b \sum_k \frac{e^{-\epsilon_k}(\epsilon_k)^2}{\mathcal{Z}} \tilde{\beta}_\delta(\psi)\, dx.$$

Passing to the limit $\delta \to 0$, we have

$$\iint |\nabla_x \sqrt{N_s}|^2\, dtdx \leq \iint G^2\, dtdx + 4 \int_a^b \sum_k \frac{e^{-\epsilon_k}(\epsilon_k)^2}{\mathcal{Z}} N_s\, dx.$$

Thus we deduce that $\sqrt{N_s} \in L^2((0,T), H^1(a,b))$ and with (6.4.62) we conclude easily that $\sqrt{N_s}\nabla_x V_s \in L^2((0,T) \times (a,b))$. □

6.5 The truncated Boltzmann equation

This part deals with well-known existence results and properties for the Boltzmann equation. Most results will be stated for the matter of completeness without proof, we can find these standard results in [3, 4, 10, 13, 21]. We shall assume that $\eta > 0$ is fixed, for the clarity of the notation we choose $\eta = 1$, and that the force fields $F_k := -\nabla_x \epsilon_k$ is given. We consider the equations indexed in k :

$$\begin{cases} \partial_t f_k + v \cdot \nabla_x f_k + F_k \cdot \nabla_v f_k = Q_R(f)_k, & (x,v) \in (a,b) \times \mathbb{R},\ t \in [0,T], \\ f_k(t,a,v) = f_k(t,a,-v), \quad f_k(t,b,v) = f_k(t,b,-v) & \text{for } t \in [0,T], v > 0, \\ f_k(0,x,v) = f_k^{in}(x,v), \end{cases} \tag{6.5.66}$$

where we use the truncated collision operator :

$$Q_R(f)_k = \sum_{k'} \int_{\mathbb{R}} \alpha^R_{k,k'}(v,v')(\mathcal{M}_k(v) f_{k'}(v') - \mathcal{M}_{k'}(v') f_k(v))\, dv', \tag{6.5.67}$$

where the truncated cross-section is defined for a $R > 0$ by

$$\alpha^R_{k,k'}(v,v') = \alpha_{k,k'}(v,v') 1_{k \leq R, |v| \leq R}(k,v) 1_{k' \leq R, |v'| \leq R}(k',v').$$

A simple calculation shows that the regularized collision operator (6.5.67) is bounded in $\ell^1(L^1_{t,x})$ and in $\ell^\infty(L^\infty_{t,x})$ and satisfies $\sum_k \int_{\mathbb{R}} Q_R(f)_k\, dv = 0$.

The following lemma states the existence and uniqueness of the weak solution for each equation of (6.5.66).

Lemma 6.5.1 *Let $T > 0$ and assume that the initial data satisfy for all $k \geq 1$,*

$$f_k^{in} \geq 0, \quad (1+v^2) f_k^{in} \in L^1((a,b)\times\mathbb{R}), \quad f_k^{in} \in L^\infty((a,b)\times\mathbb{R}).$$

Assume that $F_k \in L^1((0,T), W^{1,1}(a,b)\cap L^\infty(a,b))$ and that $\epsilon_k \geq \frac{1}{2}\pi^2 k^2$. Then (6.5.66) *admits an unique weak solution $f_k \in L^\infty((0,T), L^1 \cap L^\infty((a,b)\times\mathbb{R}))$, $f_k \geq 0$ and*

$$\forall\, t \in [0,T], \qquad \sum_{k\geq 1} \int_{\mathbb{R}} f_k(t,x,v)\, dv = \sum_{k\geq 1} \int_{\mathbb{R}} f_k^{in}(x,v)\, dv \tag{6.5.68}$$

Moreover if there exists $\delta > 2$ such that $(v^\delta + k^2) f_k^{in} \in \ell^\infty(L^\infty_{x,v})$, then

$$\forall\, t \in [0,T], \qquad \sum_{k\geq 1} \|f_k(t,\cdot,\cdot)\|_{L^\infty((a,b)\times\mathbb{R})} \leq C(1+(A(t))^2), \tag{6.5.69}$$

where C is a constant depending only on T and the data and A is defined by: $A(t) := \int_0^t \sup_{k\geq 1} \|F_k(s,\cdot)\|_{L^\infty_x}\, ds$.

Proof. All the results are standard for the Vlasov equation and can be find in [10] for instance. The key point is that with our choice of truncated collision operator, we can apply the results of Vlasov on our problem. We define

$$Q_R^+(f)_k = \mathcal{M}_k \left(\sum_{k'} \int_{\mathbb{R}} \alpha^R_{k,k'} f'_{k'}\, dv' \right)$$

and

$$\lambda_k^R = \sum_{k'} \int_{\mathbb{R}^2} \alpha^R_{k,k'} \mathcal{M}'_{k'}\, dv'.$$

Operator Q_R^+ is continuous on $L^1 \cap L^\infty$ and preserve positivity. Thanks to the weak maximum principle of the Vlasov equation, one can construct, (for $R > 0$) from a fixed point with the characteristic formula, a positive solution of

$$\begin{cases} \partial_t f_k + v\cdot\nabla_x f_k + F_k \cdot \nabla_v f_k + \lambda_k^R f_k = Q_R^+(f)_k, & (x,v)\in(a,b)\times\mathbb{R},\ t\in[0,T], \\ f_k(t,a,v) = f_k(t,a,-v), \quad f_k(t,b,v) = f_k(t,b,-v) & \text{for } t\in[0,T], v>0, \\ f_k(0,x,v) = f_k^{in}(x,v). \end{cases} \tag{6.5.70}$$

Let us prove that the L^∞ bound (6.5.69) is independent of R. We first define the charge density N_R by

$$N_R = \sum_{k\leq R} \int_{|v|\leq R} f_k\, dv.$$

We consider the characteristic $Z = (X,Y)$:

$$\begin{cases} \dfrac{dZ}{ds}(s;x,v,t) = (Y(s;x,v,t), F_k(X(s;x,v,t),s)), \\ Z(t;x,v,t) = (x,v). \end{cases}$$

By integrating the Boltzmann equation (6.5.70) over the characteristic Z, we find

$$\begin{aligned} f_k(t,x,v) \le \quad & f_k(\tau_e, Z(\tau_e;x,v,t)) \exp\left(-\int_{\tau_e}^t \lambda_k^R(s)\,ds\right) \\ & + \int_{\tau_e}^t Q_R^+(f)_k(s) \exp\left(-\int_s^t \lambda_k^R(\sigma)\,d\sigma\right) ds, \end{aligned}$$

where τ_e is the incoming instant to $[a,b]\times\mathbb{R}$ of the characteristic curves passing by (x,v) at the time t. Moreover, we have

$$|Q_R^+(f)(t,x,v)| \le \alpha_2 \mathcal{M}_k(t,x,v) N_R(t,x).$$

Thus after a summation over $k \ge 1$, we find

$$\sum_{k\ge 1} f_k(t,x,v) \le \sum_{k\ge 1} \|f_k^{in}\|_{L^\infty_{x,v}} + \frac{\alpha_2}{2\pi}\int_0^t \exp(-\frac{1}{2}(Y(s))^2) N_R(s,X(s))\,ds.$$

And the characteristics satisfy : $v = Y(s) + \int_s^t F_k(X(\sigma),\sigma)\,d\sigma$. Therefore, by definition of A, we have that if $|v| \ge 2A$ then $|Y(s)|^2 \ge (v/2)^2$. With our assumption on the initial condition (f^{in}), we deduce that there exists a nonnegative constant C such that :

$$\sum_{k\ge 1} f_k(t,x,v) \le \begin{cases} \displaystyle\sum_{k\ge 1} \frac{C}{k^2} + \frac{\alpha_2}{2\pi}\int_0^t \|N_R(s,\cdot)\|_{L^\infty_x}\,ds & \text{if } |v| \le 2A, \\ \displaystyle\sum_{k\ge 1} \frac{C}{k^2+(v/2)^\delta} + \frac{\alpha_2}{2\pi} e^{-v^2/8}\int_0^t \|N_R(s,\cdot)\|_{L^\infty_x}\,ds & \text{if } |v| \ge 2A. \end{cases}$$

Integrating this last inequality for $|v| \le 2A$ and for $|v| \ge 2A$, we get

$$\|N_R\|_{L^\infty_x}(t) \le C\left(A^2 + \int_0^t \|N_R\|_{L^\infty_x}(s)\,ds\right)$$

which provides the bound (6.5.69) by a Gronwall argument. □

The following lemma, whose proof can be find in [4], establishes some continuity and compactness result for the solution of (6.5.66)

Lemma 6.5.2 *Let $\epsilon_k^n \in L^1((0,T), W^{1,1}(a,b))$ for any k and n, such that for any fixed k, $\|F_k^n\|_{L^1} = \|\nabla_x \epsilon_k^n\|_{L^1}$ is bounded independently of n. Let (f_k^n) be a corresponding sequence of weak solutions of* (6.5.66).

(i) If for all $k \ge 1$ we have as $n \to \infty$,

$$\epsilon_k^n \to \epsilon_k \text{ in } W^{1,1}_{t,x}, \quad f_k^n \rightharpoonup f_k \text{ in } L^\infty_{t,x,v} - weak*,$$

then the limit f_k is a weak solution of (6.5.66) *with ϵ_k.*

(ii) If additionally we have for all $n \in \mathbb{N}$,

$$\sum_{k\ge 1} (\|f_k^n\|_{L^\infty_{t,x,v}} + \|(v^2+k^2) f_k^n\|_{L^1_{t,x,v}}) \le C,$$

where C is a constant independent of n. Then the sequence of charge densities $(\rho_k^n)_{k\ge 1} = (\int f_k^n\,dv)_{k\ge 1}$ is compact (with respect to n) in the $\ell^1(L^q((0,T)\times(a,b)))$ topology for any $q < 2$.

6.6 Existence for the overall problem

In this section we are interested in the existence of a solution for a fixed $\eta > 0$. The existence result is stated in Theorem 6.1.1. The problem considered is a Boltzmann equation coupled with a Schödinger–Poisson system. The structure of this coupling invite us to use a fixed-point argument for the proof. But to define this fixed-point, we need to have the uniqueness of a solution of the Schödinger–Poisson system. Thus, with our result we are not able to prove the existence for every kind of initial condition.

We do not give in detail the proof of Theorem 6.1.1, because most results are standard. We only give the main steps which follows the idea of [3, 4, 20] : we regularize the system thanks to a parameters, we construct solution for the regularized system and we left go the parameter to 0 to recover solutions of the unregularized system.

First, we introduce a regularization of the overall problem. Let us define the linear regularization operator by

$$\begin{array}{rcl} R^\varepsilon : L^1(\Omega) & \to & C^\infty(\overline{\Omega}) \\ V & \to & R^\varepsilon[V](x,z) = (\overline{V} *_x \xi_{\varepsilon,x} *_z \xi_{\varepsilon,z})|_{\overline{\Omega}} \end{array} \tag{6.6.71}$$

where $\overline{V}$ is the extension of V by zero outside Ω and $\xi_{\varepsilon,x}$ and $\xi_{\varepsilon,z}$ are C^∞ nonnegative compactly supported even approximations of the unity on $\mathbb{R}$. We write then the regularized system :

$$\begin{cases} \partial_t f^\varepsilon_{k,R} + \dfrac{1}{\eta}(v.\nabla_x f^\varepsilon_{k,R} - \nabla_x \epsilon^\varepsilon_{k,R}.\nabla_v f^\varepsilon_{k,R}) = \dfrac{1}{\eta^2} Q^\varepsilon_R(f^\varepsilon_R)_k, \quad (x,v) \in (a,b)\times\mathbb{R}, \\ f^\varepsilon_{k,R}(t,a,v) = f^\varepsilon_{k,R}(t,a,-v),\ f^\varepsilon_{k,R}(t,b,v) = f^\varepsilon_{k,R}(t,b,-v),\ \ v>0, t\in[0,T], \\ f^\varepsilon_{k,R}(0,x,v) = f^{in}_k(x,v), \end{cases} \tag{6.6.72}$$

$$\begin{cases} -\dfrac{1}{2}\,\partial_z^2 \chi^\varepsilon_{k,R} + R^\varepsilon[V^\varepsilon_R]\chi^\varepsilon_{k,R} = \epsilon^\varepsilon_{k,R}\chi^\varepsilon_{k,R} \qquad (k \geq 1), \\ \chi^\varepsilon_{k,R}(t,x,\cdot) \in H^1_0(0,1), \qquad \displaystyle\int_0^1 \chi^\varepsilon_{k,R}\,\chi^\varepsilon_{\ell,R}\,dz = \delta_{k\ell}\,, \end{cases} \tag{6.6.73}$$

$$\begin{cases} -\Delta_{x,z} V^\varepsilon_R = R^\varepsilon\left[\displaystyle\sum_k \int_{\mathbb{R}} f^\varepsilon_{k,R}|\chi^\varepsilon_{k,R}|^2\,dv\right], \\ \dfrac{dV^\varepsilon_R}{dx}(t,a,z) = \dfrac{dV^\varepsilon_R}{dx}(t,b,z) = 0, \qquad \text{for } z\in(0,1), \\ V^\varepsilon_R(t,x,0) = V^\varepsilon_R(t,x,1) = 0, \qquad \text{for } x \in (a,b). \end{cases} \tag{6.6.74}$$

We use the regularization of the collision operator :

$$Q^\varepsilon_R(f)_k = \sum_{k'} \int_{\mathbb{R}} \alpha^R_{k,k'}(v,v')(\mathcal{M}^\varepsilon_k(v) f_{k'}(v') - \mathcal{M}^\varepsilon_{k'}(v') f_k(v))\,dv', \tag{6.6.75}$$

where the truncated cross-section is defined by

$$\alpha^R_{k,k'}(v,v') = \alpha_{k,k'}(v,v') 1_{k\leq R,|v|\leq R}(k,v) 1_{k'\leq R,|v'|\leq R}(k',v').$$

We still use the notations defined in section 6.1 : $N_s^\varepsilon = \sum_{k\geq 1} \int f_k^\varepsilon \, dv$ and the Maxwellian $\mathcal{M}_k^\varepsilon = \frac{1}{2\pi \mathcal{Z}^\varepsilon} \exp(-\frac{1}{2}v^2 - \epsilon_k^\varepsilon)$ for $\mathcal{Z}^\varepsilon = \sum_{k\geq 1} e^{-\epsilon_k^\varepsilon}$.

Since for $\varepsilon = 0$ we have $R^0 = Id$, we will obtain a solution of the unregularized problem by passing to the limits $\varepsilon \to 0$ and $R \to +\infty$ in the regularized one (6.6.72)–(6.6.74), which are done in the followings steps.

Step 1 : Existence for the regularized problem

In the first step we prove that the regularized problem admit a solution. We verify easily that that the regularized collision operator (6.5.67) is bounded in $\ell^1(L^1_{t,x})$ and in $\ell^\infty(L^\infty_{t,x})$ and satisfies $\sum_k \int_{\mathbb{R}} Q_R^\varepsilon(f)_k \, dv = 0$ and

$$\sum_{k\geq 1} \int_{\mathbb{R}} Q_R^\varepsilon(f)_k \log \frac{f_k}{\mathcal{M}_k} \, dv \leq -\frac{\alpha_1}{2} \sum_{k\geq 1} \int_{\mathbb{R}} (\sqrt{f_k} - \sqrt{N_s \mathcal{M}_k})^2 \, dv.$$

Moreover, we can prove straightforwardly from convolution results that the regularization operator R^ε satisfies the following properties :

Lemma 6.6.1 *(i) R^ε is a bounded operator on $L^p_x L^q_z(\Omega)$ for $1 \leq p, q \leq +\infty$ and satisfies*

$$\forall V \in L^p_x L^q_z(\Omega), \quad \|R^\varepsilon[V]\|_{L^p_x L^q_z(\Omega)} \leq \|V\|_{L^p_x L^q_z(\Omega)}.$$

$$\text{if } 1 \leq p, q < +\infty \text{ and } V \in L^p_x L^q_z(\Omega), \text{ then } \lim_{\varepsilon\to 0} \|R^\varepsilon[V] - V\|_{L^p_x L^q_z(\Omega)} = 0.$$

(ii) R^ε is selfadjoint on $L^2(\Omega)$.
(iii) Let $r \geq 1$ be given and $V \in W^{1,r}(\Omega)$. Then

$$\nabla_x R^\varepsilon[V] = R^\varepsilon[\nabla_x V]\,; \qquad \lim_{\varepsilon\to 0} \|\nabla_x R^\varepsilon[V] - \nabla_x V\|_{L^r(\Omega)} = 0.$$

Following the ideas of the proof of Proposition 4.8 of [4] we establish:

Proposition 6.6.2 *Let $T > 0$ and let assume that Assumption* **(A-1)** *holds and that the initial condition is at the thermal equilibrium, i.e. verify* **(A-2)** *and is given by* (6.1.9)*. Then, there exists $\varepsilon_0 > 0$ and $\delta > 0$ such that, if*

$$\sum_{k\geq 1} \|f_k^{in}\|_{L^1_{x,v}} < \delta, \tag{6.6.76}$$

then for all $\varepsilon \in (0, \varepsilon_0)$ the regularized problem (6.6.72)–(6.6.74) *admits a global weak solution $(V_R^\varepsilon, (\epsilon_{k,R}^\varepsilon, \chi_{k,R}^\varepsilon, f_{k,R}^\varepsilon)_{k\geq 1})$ on the interval $[0,T]$ which satisfies the entropy estimate:*

$$\forall t \in [0,T], \quad 0 \leq W_R^\varepsilon(t) + \frac{\alpha_1}{2\eta^2} \int_0^T \mathcal{R}_R^\varepsilon(t)\, dt \leq C_T, \tag{6.6.77}$$

with

$$W_R^\varepsilon(t) = \sum_{k\geq 1} \left(f_{k,R}^\varepsilon \log \frac{f_{k,R}^\varepsilon}{M_k} - f_{k,R}^\varepsilon + M_k \right) dxdv + \frac{1}{2} \iint |\nabla_{x,z} V_R^\varepsilon|^2 \, dxdz$$

and

$$\mathcal{R}^\varepsilon_R(t) = \frac{1}{2}\sum_{k\geq 1}\iint \left(\sqrt{f^\varepsilon_{k,R}} - \sqrt{N^\varepsilon_{s,R}\mathcal{M}^\varepsilon_{k,R}}\right)^2 dxdv.$$

Step 2 : Passing to the limit $R \to +\infty$

For $\varepsilon > 0$ fixed, one can pass to the limit as $R \to +\infty$. We obtain

Proposition 6.6.3 *Let $T > 0$ and let assume that* **(A-1)** *and* **(A-2)** *are satisfied. Let $\varepsilon > 0$ be fixed ($\varepsilon < \varepsilon_0$) and $(V^\varepsilon_R, (f^\varepsilon_{k,R}, \chi^\varepsilon_{k,R}, \epsilon^\varepsilon_{k,R})_{k\geq 1})$ be a weak solution of the regularized Boltzmann-Schrödinger-Poisson system* (6.6.72)–(6.6.74)*. Then as $R \to +\infty$ this solution converges to a weak solution $(V^\varepsilon, (f^\varepsilon_k, \chi^\varepsilon_k, \epsilon^\varepsilon_k)_{k\geq 1})$ of*

$$\begin{cases} \partial_t f^\varepsilon_k + \dfrac{1}{\eta}(v.\nabla_x f^\varepsilon_k - \nabla_x \epsilon^\varepsilon_k . \nabla_v f^\varepsilon_k) = \dfrac{1}{\eta^2} Q^\varepsilon(f^\varepsilon)_k, \quad (x,v) \in (a,b)\times\mathbb{R}, \\ f^\varepsilon_{k,R}(t,a,v) = f^\varepsilon_{k,R}(t,a,-v),\ f^\varepsilon_{k,R}(t,b,v) = f^\varepsilon_{k,R}(t,b,-v),\ v>0, t\in[0,T[\\ f^\varepsilon_k(0,x,v) = f^{in}_k(x,v), \end{cases} \tag{6.6.78}$$

$$\begin{cases} -\dfrac{1}{2}\,\partial^2_z \chi^\varepsilon_k + R^\varepsilon[V^\varepsilon]\chi^\varepsilon_k = \epsilon^\varepsilon_k \chi^\varepsilon_k \qquad (k\geq 1), \\ \chi^\varepsilon_k(t,x,\cdot) \in H^1_0(0,1), \qquad \displaystyle\int_0^1 \chi^\varepsilon_k\,\chi^\varepsilon_\ell\,dz = \delta_{k\ell}\,, \end{cases} \tag{6.6.79}$$

$$\begin{cases} -\Delta_{x,z} V^\varepsilon = R^\varepsilon \left[\displaystyle\sum_k \int_{\mathbb{R}^2} f^\varepsilon_k |\chi^\varepsilon_k|^2\,dv\right], \\ \dfrac{dV^\varepsilon_R}{dx}(t,a,z) = \dfrac{dV^\varepsilon_R}{dx}(t,b,z) = 0, \qquad \textit{for } z\in(0,1), \\ V^\varepsilon(t,x,0) = V^\varepsilon(t,x,1) = 0, \qquad \textit{for } x \in (a,b). \end{cases} \tag{6.6.80}$$

Moreover it satisfies the estimate

$$\forall\, t\in[0,T], \quad 0 \leq W^\varepsilon(t) + \frac{\alpha_1}{2\eta^2}\int_0^T \mathcal{R}^\varepsilon(t)\,dt \leq C_T, \tag{6.6.81}$$

with

$$W^\varepsilon(t) = \sum_{k\geq 1}\left(f^\varepsilon_k \log\frac{f^\varepsilon_k}{M_k} - f^\varepsilon_k + M_k\right) dxdv + \frac{1}{2}\iint |\nabla_{x,z}V^\varepsilon|^2\,dxdz$$

and

$$\mathcal{R}^\varepsilon(t) = \frac{1}{2}\sum_{k\geq 1}\iint\left(\sqrt{f^\varepsilon_k} - \sqrt{N^\varepsilon_s \mathcal{M}^\varepsilon_k}\right)^2 dxdv.$$

Proof. We skip all the index ε in the notation. With our regularization (6.6.71) we have a bound of V in $L^\infty_t(W^{1,\infty}_{x,z})$ depending only on ε and not on R which provides thanks to (6.5.69) a bound of $(f_{k,R})_{k\geq 1}$ in $\ell^\infty(L^\infty_{t,x,v})$ depending only on ε and on the data. And with (6.5.68), we have a bound of $(f_{k,R})_{k\geq 1}$ in $\ell^1(L^1_{t,x,v})$ depending only on the data. Thus we can extract a subsequence converging as $R \to +\infty$ towards a function f in

$\ell^2(L^2_{t,x,v}) - weak$. Arguing as in Proposition 6.4.2, one can prove thanks to an averaging Lemma that $\rho_R := (\int f_{k,R}\,dv)_{k\geq 1} \to \rho := (\int f_k\,dv)_{k\geq 1}$ in $\ell^2(L^2_{x,v}) - strong$.

The conservation of the mass implies that for all $t \in [0,T]$ we have $\|f\|_{\ell^1(L^1_{t,x,v})} = \|f^{in}\|_{\ell^1(L^1_{t,x,v})} = \mathcal{N}_{in}$. Then we can solve the regularized Schrödinger-Poisson system (6.6.79)-(6.6.80) with the given ρ and construct an unique solution $V \in L^\infty_t(H^1_{x,z})$. The continuity of the solution of the Schödinger-Poisson system (cf Proposition 6.3.4) provides $V_R \to V$ in $L^2_t(H^1_{x,z})$ and properties of the eigenvalues of the Hamiltonian shows $\epsilon_k[R^\varepsilon[V_R]] \to \epsilon_k[R^\varepsilon[V]]$ in $L^2_t(W^{2,\infty}_{x,z})$.

Furthermore, we have for all $k \geq 1$

$$\|Q_R(f_R)_k\|_{L^\infty_{x,v}} \leq \alpha_2(\|f_R\|_{\ell^1(L^1_{x,v})} + \|f_R\|_{L^\infty_{x,v}}) \leq C_{T,\varepsilon},$$

where $C_{T,\varepsilon}$ is a nonnegative constant depending only on T and ε and on the data. We deduce that we can extract a subsequence $(Q_R(f_R)_k)_R$ converging as $R \to +\infty$ in $L^\infty - weak^*$. From the previous remarks and the definition of Q_R (6.5.67), we deduce after using some Lebesgue theorems that

$$\forall\,\phi \in L^1((a,b)\times\mathbb{R}), \qquad \iint (Q(f)_k - Q_R(f_R)_k)\phi\,dxdv \to 0 \qquad \text{as } R \to +\infty$$

Thus one can pass to the limit in the weak equation of the Boltzmann-Schrödinger-Poisson system (6.6.72)–(6.6.74) and prove straightforwardly that $(V,(f_k,\epsilon_k,\chi_k)_{k\geq 1})$ is a solution of (6.6.78)–(6.6.80). Finally we recover the estimate (6.6.81) by passing to the limit $R \to +\infty$ in (6.6.77). □

Step 3 : Passing to the limit $\varepsilon \to 0$

In the last step we prove Theorem 6.1.1 by taking the limit $\varepsilon \to 0$ in the system (6.6.78)–(6.6.80).

Since the solution satisfies the estimate (6.6.81), we deduce that

$$\sum_{k\geq 1}\iiint_{(0,T)\times(a,b)\times\mathbb{R}} f_k^\varepsilon(1+v^2+k^2+|\log f_k^\varepsilon|)\,dxdvdt \leq C_T$$

and with a Jensen inequality, one can deduce

$$\iint_{(0,T)\times(a,b)} N_s^\varepsilon(1+|\log N_s^\varepsilon|)\,dxdt \leq C_T,$$

where we recall that we use the notation $N_s^\varepsilon := \sum_{k\geq 1}\int_{\mathbb{R}^2} f_k^\varepsilon\,dv$. Thus the Dunford-Pettis theorem implies that $(f_k^\varepsilon)_{k\geq 1}$ and N_s^ε are weakly relatively compact respectively in $\ell^1(L^1((0,T)\times(a,b)\times\mathbb{R}))$ and in $L^1((0,T)\times(a,b))$. Moreover

$$Q^\varepsilon(f^\varepsilon)_k = \left(\sum_{k'\geq 1}\int_{\mathbb{R}} \alpha_{k,k'} f_{k'}^{\varepsilon'}\right)\mathcal{M}_k^\varepsilon - \left(\sum_{k'\geq 1}\int_{\mathbb{R}} \alpha_{k,k'}\mathcal{M}_{k'}^{\varepsilon'}\right) f_k^\varepsilon.$$

Thus $Q^\varepsilon(f^\varepsilon)$ is bounded in $\ell^1(L^1_{t,x,v})$ and for all $I \subset [0,T]$, $A \subset [a,b]$ and $B \subset \mathbb{R}$, we have

$$\sum_k \int_I \int_A \int_B |Q^\varepsilon(f^\varepsilon)_k| \, dxdvdt \le \alpha_2 \int_{I\times A} N_s^\varepsilon \, dxdt + \alpha_2 \int_{I\times A\times B} f_k^\varepsilon \, dxdvdt.$$

Since N_s^ε and $(f_k^\varepsilon)_{k\ge1}$ are equi-integrable and tight, we deduce that $Q^\varepsilon(f^\varepsilon)$ have the same properties. The Dunford-Pettis theorem implies then that $Q^\varepsilon(f^\varepsilon)$ is weakly relatively compact in $\ell^1(L^1((0,T)\times(a,b)\times\mathbb{R}))$. Then,

$$\eta \partial_t f_k^\varepsilon + v\cdot\nabla_x f_k^\varepsilon = \frac{1}{\eta} Q^\varepsilon(f^\varepsilon)_k + \nabla_v \cdot (\nabla_x \epsilon_k^\varepsilon \, f_k^\varepsilon).$$

Proceeding as in the proof of Proposition 6.4.2, by an averaging lemma, we can prove that

$$\rho^\varepsilon \to \rho \text{ strongly in } \ell^1(L^1((0,T)\times(a,b))). \tag{6.6.82}$$

Moreover ρ satisfies the estimate

$$\sum_{k\ge1} \iint \rho_k (1 + k^2 + |\log \rho_k|) \, dxdt \le C_T. \tag{6.6.83}$$

and the conservation of the mass implies

$$\forall\, t \in [0,T], \forall\, \varepsilon > 0, \quad \int_a^b N_s \, dx = \int_a^b N_s^\varepsilon \, dx = \mathcal{N}_{in}.$$

We can then apply Lemma 6.3.2 to solve the *unregularized* Schrödinger-Poisson system (6.3.32)–(6.3.33) with the density ρ. Thus there exists $V \in L^\infty([0,T], H^1(\Omega))$ weak solution of (6.3.32)–(6.3.33). The conservation of the mass implies with Lemma 6.3.3 that we have the uniqueness of this solution. Moreover multiplying the two Poisson equations by $(V^\varepsilon - V)$ and integrating lead to

$$\begin{aligned} \iint_\Omega |\nabla(V^\varepsilon - V)|^2 \, dxdz = \; & \iint_\Omega R^\varepsilon \left[\sum_k (\rho_k^\varepsilon |\chi_k^\varepsilon|^2 - \rho_k |\chi_k|^2) \right] (V^\varepsilon - V)\, dxdz + \\ & \iint (R^\varepsilon - Id) \left[\sum_k \rho_k |\chi_k|^2 \right] (V^\varepsilon - V)\, dxdz. \end{aligned} \tag{6.6.84}$$

For the second term of the right hand side of (6.6.84), we use the selfadjointness of the operator R^ε (Lemma 6.6.1 (ii)) to write

$$\begin{aligned} & \iint_\Omega (R^\varepsilon - Id) \left[\sum_k \rho_k |\chi_k|^2 \right] (V^\varepsilon - V)\, dxdz \\ & \qquad \le C \sum_{k\ge1} \int_a^b \rho_k (1 + \|V\|_{L_z^2}^{1/2}) \|(R^\varepsilon - Id)[V^\varepsilon - V]\|_{L_z^2} \, dx, \end{aligned}$$

where we use the bound on the eigenvectors of the Hamiltonian established in Lemma B.0.5. Proceeding as in Lemma 6.3.2, we can obtain, thanks to the imbedding $H^1(\Omega) \hookrightarrow L^\infty_x L^2_z(\Omega)$.

$$\iint_\Omega (R^\varepsilon - Id)\left[\sum_k \rho_k|\chi_k|^2\right](V^\varepsilon - V)\,dxdz \le C(1+\|V\|^{1/2}_{H^1(\Omega)})\|(R^\varepsilon - Id)[V^\varepsilon - V]\|_{H^1(\Omega)}.$$

And with Lemma 6.6.1, if we define for the bounded operator R^ε

$$\|R^\varepsilon - Id\|_2 := \sup_{\{V\in L^2(\Omega), V\neq 0\}} \frac{\|(R^\varepsilon - Id)V\|_{L^2(\Omega)}}{\|V\|_{L^2(\Omega)}},$$

then we have thanks to Lemma 6.6.1 (i),

$$\|R^\varepsilon - Id\|_2 \to 0 \quad \text{as } \varepsilon \to 0. \tag{6.6.85}$$

Thus, there exists a nonnegative constant depending only on T such that

$$\iint_\Omega (R^\varepsilon - Id)\left[\sum_k \rho_k|\chi_k|^2\right](V^\varepsilon - V)\,dxdz \le C_1\|R^\varepsilon - Id\|_2\,\|V^\varepsilon - V\|_{H^1(\Omega)}. \tag{6.6.86}$$

For the first term of the right hand side of (6.6.84), we decompose, using the selfadjointness of R^ε

$$\begin{aligned}&\iint_\Omega R^\varepsilon\left[\sum_k(\rho_k^\varepsilon|\chi_k^\varepsilon|^2 - \rho_k|\chi_k|^2)\right](V^\varepsilon - V)\,dxdz = \\ &\sum_{k\ge1}\int_a^b(\rho_k^\varepsilon - \rho_k)\langle|\chi_k|^2 R^\varepsilon[V^\varepsilon - V]\rangle\,dx + \sum_{k\ge1}\int_a^b \rho_k^\varepsilon\langle(|\chi_k^\varepsilon|^2 - |\chi_k|^2)R^\varepsilon[V^\varepsilon - V]\rangle\,dx.\end{aligned} \tag{6.6.87}$$

From the properties of the regularization operator R^ε resumed in Lemma 6.6.1 we have,

$$\|R^\varepsilon[V^\varepsilon - V]\|_{H^1(\Omega)} \le \|V^\varepsilon - V\|_{H^1(\Omega)}.$$

We treat the first term of the right hand side of (6.6.87) exactly as the first term of the right hand side of (6.3.42). Thus there exist two nonnegative constants C_2 and C_3 such that,

$$\sum_{k\ge1}\int_a^b(\rho_k^\varepsilon - \rho_k)\langle|\chi_k|^2 R^\varepsilon[V^\varepsilon - V]\rangle\,dx \le C_2\mathcal{N}_{in}\|V^\varepsilon - V\|^2_{H^1(\Omega)} + C_3\|\rho_k^\varepsilon - \rho_k\|_{\ell^1(L^1_x)}. \tag{6.6.88}$$

For the second term of the right hand side of (6.6.87), we refer to the treatment of the second term of (6.3.42). Therefore, there exists a nonnegative constant C_4 such that

$$\sum_{k\ge1}\int_a^b \rho_k^\varepsilon\langle(|\chi_k^\varepsilon|^2 - |\chi_k|^2)R^\varepsilon[V^\varepsilon - V]\rangle\,dx \le C_4\mathcal{N}_{in}\|V^\varepsilon - V\|^2_{H^1(\Omega)}. \tag{6.6.89}$$

Thus from (6.6.88) and (6.6.89), equation (6.6.87) becomes

$$\iint_\Omega R^\varepsilon \left[\sum_k (\rho_k^\varepsilon |\chi_k^\varepsilon|^2 - \rho_k |\chi_k|^2) \right] (V^\varepsilon - V)\, dxdz \leq \\ \leq C_3 \|\rho_k^\varepsilon - \rho_k\|_{\ell^1(L^1_x)} + C_5 \mathcal{N}_{in} \|V^\varepsilon - V\|^2_{H^1(\Omega)}. \tag{6.6.90}$$

If we inject this last inequality (6.6.90) and (6.6.86) in the expression (6.6.84), we find

$$\iint_\Omega |\nabla(V^\varepsilon - V)|^2\, dxdz \leq \; C_1 \|R^\varepsilon - Id\|_2 \, \|V^\varepsilon - V\|_{H^1(\Omega)} + \\ + C_3 \|\rho_k^\varepsilon - \rho_k\|_{\ell^1(L^1_x)} + C_5 \mathcal{N}_{in} \|V^\varepsilon - V\|^2_{H^1(\Omega)}.$$

Finally after a Poincaré inequality, we deduce that if we take $\mathcal{N}_{in}$ small enough, we have

$$\|V^\varepsilon - V\|^2_{H^1(\Omega)} \leq C_6 \|R^\varepsilon - Id\|_2^2 + C_7 \|\rho_k^\varepsilon - \rho_k\|_{\ell^1(L^1_x)}.$$

It is now easy with (6.6.85) to conclude that

$$\lim_{\varepsilon \to 0} \|V^\varepsilon - V\|^2_{H^1(\Omega)} = 0.$$

Thus there exists $\mathcal{N}_0 > 0$ such that, for all $0 < \mathcal{N}_{in} \leq \mathcal{N}_0$, there exists $V \in L^\infty([0,T], H^1(\Omega))$ weak solution of the *unregularized* Schrödinger-Poisson system (6.3.32)–(6.3.33) and such that the potential V^ε, weak solution of the regularized system, converges towards V in $L^2([0,T], H^1(\Omega))$. The properties of the eigenvectors imply as in Proposition (6.4.3) that we have $\epsilon_k^\varepsilon \to \epsilon_k$ in $L^2_t(L^\infty_x)$. Thus V is a weak solution of the Schrödinger-Poisson system (6.1.11)–(6.1.12).

With standard arguments on Boltzmann equation we can prove then that a renormalized solution of the Boltzmann equation (6.6.78) converges strongly in $\ell^1(L^1_{t,x,v})$ to a renormalized solution f_k of the Boltzmann equation with a force field $\nabla_x \epsilon_k$. Then we pass to the limit $\varepsilon \to 0$ in a renormalized Boltzmann equation and prove (i) (ii) and (iii) of Theorem 6.1.1. Using convexity arguments, we prove (iv) of Theorem 6.1.1. We do not give in detail the end of the existence proof but refer the reader to [21, 12, 10].

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Chapter 7

Le cas de la dimension 3

7.1 Introduction

We will consider the Boltzmann-Schrödinger-Poisson system presented in the previous chapter. We recall that this system models the transport of charged carriers confined in a nanostructure. The confining direction is denoted by $z \in (0,1)$. In the transport direction at a kinetic level, particles are described by their time-dependent distribution function denoted by $f_k(t,x,v)$ for the kth subband, defined on the phase space $(x,v) \in \omega \times \mathbb{R}^2$ and $t \in \mathbb{R}^+$. The evolution of the distribution function is governed by the Boltzmann transport equation, which in a rescaled form is :

$$\partial_t f_k^\eta + \frac{1}{\eta}(v.\nabla_x f_k^\eta - \nabla_x \epsilon_k^\eta . \nabla_v f_k^\eta) = \frac{1}{\eta^2} Q^\eta(f^\eta)_k, \quad (x,v) \in \omega \times \mathbb{R}^2, \tag{7.1.1}$$

where η is a parameter related to the mean free path. The collision operator Q^η is given by :

$$Q^\eta(f)_k = \sum_{k'} \int_{\mathbb{R}^2} \alpha_{k,k'}(v,v')(\mathcal{M}_k^\eta(v) f_{k'}(v') - \mathcal{M}_{k'}^\eta(v') f_k(v))\, dv', \tag{7.1.2}$$

where the function $\mathcal{M}_k^\eta$ is the normalized Maxwellian defined in (6.1.6). We define the occupation factor $\rho_k^\eta(t,x) = \int_{\mathbb{R}^2} f_k^\eta \, dv$ and the surface density $N_s^\eta = \sum_k \rho_k^\eta$.

In the subband decomposition approach [6, 7], this equation is coupled to a Schrödinger-Poisson system :

$$\begin{cases} -\frac{1}{2}\,\partial_z^2 \chi_k^\eta + V^\eta \chi_k^\eta = \epsilon_k^\eta \chi_k^\eta & (k \geq 1), \\ \chi_k^\eta(t,x,\cdot) \in H_0^1(0,1), & \int_0^1 \chi_k^\eta\, \chi_\ell^\eta \, dz = \delta_{k\ell}\,, \end{cases} \tag{7.1.3}$$

$$-\Delta_{x,z} V^\eta = \sum_k \rho_k^\eta |\chi_k^\eta|^2, \tag{7.1.4}$$

with the boundary condition :

$$\begin{cases} \partial_\nu V^\eta(t,x,z) = 0, & \text{for } x \in \partial\omega, \quad z \in (0,1), \\ V^\eta(t,x,0) = V^\eta(t,x,1) = 0, & \text{for } x \in \omega, \end{cases} \tag{7.1.5}$$

where $\nu(x)$ is the unit outward normal vector at x on the boundary $\partial\omega$ of ω.

This system is completed by the specular reflexion boundary conditions :

$$f_k^\eta(t,x,v) = f_k^\eta(t,x,-v+2(\nu(x)\cdot v)\nu(x)), \quad v.\nu(x)<0, x\in\partial\omega, t\in\mathbb{R}^+. \tag{7.1.6}$$

We denote $\Gamma^\pm = \{(x,v)\in\partial\omega\times\mathbb{R}^2/\pm(v.\nu(x))>0\}$ and $\Gamma=\Gamma^+\cup\Gamma^-$. And we consider the well-prepared initial conditions :

$$f_k^\eta(0,x,v) = f_k^{in}(x,v) := \frac{N_s^{in}(x)}{2\pi\sum_k e^{-\epsilon_k[V^{in}]}} e^{-v^2/2-\epsilon_k[V^{in}]}, \quad (x,v)\in\omega\times\mathbb{R}^2, \tag{7.1.7}$$

where N_s^{in} is given and $(V^{in},(\epsilon_k[V^{in}],\chi_k[V^{in}])_{k\geq 1})$ is the set of solutions of the Schrödinger-Poisson system at the thermal equilibrium :

$$\begin{cases} -\dfrac{1}{2}\,\partial_z^2\chi_k[V^{in}] + V^{in}\chi_k[V^{in}] = \epsilon_k[V^{in}]\chi_k[V^{in}] & (k\geq 1), \\ \chi_k[V^{in}](x,\cdot)\in H_0^1(0,1), \qquad \displaystyle\int_0^1 \chi_k[V^{in}]\,\chi_\ell[V^{in}]\,dz = \delta_{k\ell}\,, \end{cases}$$

$$-\Delta_{x,z}V^{in} = \sum_k \frac{N_s^{in}(x)}{\sum_k e^{-\epsilon_k[V^{in}]}}|\chi_k[V^{in}]|^2 e^{-\epsilon_k[V^{in}]},$$

In this chapter, we will only present the diffusive limit of solutions of this system. We are not able to establish an existence result for a 2D transport. However if we assume that we have solutions, we can prove their convergence. More precisely, we make the following assumptions :

Assumption 7.1.1 *The cross section α is symmetric and bounded from above and below : there exists α_1, α_2 such that $0<\alpha_1\leq\alpha_{k,k'}(v,v')=\alpha_{k,k'}(v',v)\leq\alpha_2$ for all $(v,v')\in\mathbb{R}^2\times\mathbb{R}^2$, $k,k'\geq 1$.*

Assumption 7.1.2 *The initial condition is regular : $N_s^{in}\in C^0(\overline{\omega})$ and $N_s^{in}\geq 0$. We can prove then (see [2]) that there exists a unique V which satisfy moreover $V^{in}\in C^2(\overline{\omega})$.*

We assume that the existence Theorem proved for a 1D transport still holds for $x\in\omega\subset\mathbb{R}^2$:

Assumption 7.1.3 *Let $T>0$ and assume that Assumptions 7.1.1 and 7.1.2 are satisfied. Then we assume that the system (7.1.1)-(7.1.3)–(7.1.7) admits a renormalized solution in the following sense :*

(i) $\forall\,\beta\in C^1(\mathbb{R}^+)$, $\beta(f^\eta)$ is a weak solution of:

$$\begin{cases} \eta\partial_t\beta(f^\eta)_k + v\cdot\nabla_x\beta(f^\eta)_k - \nabla_x\epsilon_k^\eta\cdot\nabla_v\beta(f^\eta)_k = \dfrac{Q^\eta(f^\eta)_k}{\eta}\beta'(f^\eta)_k, \\ \beta(f^\eta)_k(t=0) = \beta(f^{in})_k. \end{cases}$$

(ii) $\forall\,\lambda>0$, $\Theta^\eta_{k,\lambda} := (f^\eta_k + \lambda\exp(-\frac{1}{2}(v^2+k^2)))^{1/2}$ *satisfies*

$$\eta\partial_t\Theta^\eta_{k,\lambda} + v\cdot\nabla_x\Theta^\eta_{k,\lambda} - \nabla_v(\nabla_x\epsilon^\eta_k\;\Theta^\eta_{k,\lambda}) = \frac{Q^\eta(f^\eta)_k}{2\eta\Theta^\eta_{k,\lambda}} + \lambda\nabla_x\epsilon^\eta_k\,\frac{ve^{-\frac{1}{2}(v^2+k^2)}}{2\Theta^\eta_{k,\lambda}}.$$

(iii) We have the local mass conservation

$$\partial_t N^\eta_s + \nabla_x\cdot J^\eta = 0, \qquad \textit{where} \quad J^\eta = \frac{1}{\eta}\sum_{k\geq 1}\int_{\mathbb{R}^2} v f^\eta_k\,dv.$$

(iv) We have the entropy inequality :

$$\forall\, t\in[0,T], \quad 0\leq W^\eta(t) + \frac{\alpha_1}{2\eta^2}\int_0^t \mathcal{R}^\eta(s)\,ds \leq C_T, \tag{7.1.8}$$

where the entropy of the system is defined by

$$W^\eta(t) = \sum_k \iint_{\omega\times\mathbb{R}^2}\left(f^\eta_k\log\frac{f^\eta_k}{M_k} - f^\eta_k + M_k\right)dxdv + \frac{1}{2}\iint_\Omega |\nabla_{x,z}V^\eta|^2\,dxdz$$

and the dissipation rate by

$$\mathcal{R}^\eta(t) = \frac{1}{2}\sum_k\iint_{\omega\times\mathbb{R}^2}\left(\sqrt{f^\eta_k} - \sqrt{N^\eta_s\mathcal{M}^\eta_k}\right)^2 dxdv.$$

The result presented here is the diffusive limit :

Theorem 7.1.4 *Let, for $\eta>0$, $(V^\eta,(f^\eta_k,\epsilon^\eta_k,\chi^\eta_k)_{k\geq1})$ be the renormalized solution of the Boltzmann-Schrödinger-Poisson system defined in Theorem 7.1.3. Then as $\eta\to0$, this solution converges to the solution $(V,N_s,(\epsilon_k,\chi_k)_{k\geq1})$ of the drift-diffusion-Schrödinger-Poisson system defined by*

$$\partial_t N_s + \mathrm{div}_x\,J = 0, \qquad J = -\mathbb{D}(\nabla_x N_s + N_s\nabla_x V_s), \tag{7.1.9}$$

$$\begin{cases} -\dfrac{1}{2}\,\partial_{zz}\chi_k + V\chi_k = \epsilon_k\chi_k & (k\geq1),\\ \chi_k(t,x,\cdot)\in H^1_0(0,1), & \displaystyle\int_0^1 \chi_k\,\chi_\ell\,dz = \delta_{k\ell}\,, \end{cases} \tag{7.1.10}$$

$$-\Delta_{x,z}V = N, \tag{7.1.11}$$

where the density N and the effective potential V_s are defined by

$$N = N_s\sum_k \frac{e^{-\epsilon_k}}{\sum_\ell e^{-\epsilon_\ell}}\,|\chi_k|^2\,, \qquad V_s = -\log\sum_k e^{-\epsilon_k}. \tag{7.1.12}$$

And this system is completed with an initial condition $N_s(0,x) = N^0_s(x)$ and with the following conservative boundary conditions:

$$\begin{cases} J(t,x)\cdot\nu(x) = 0, \quad \partial_\nu V(t,x,z) = 0 & \textit{for } x\in\partial\omega, \quad z\in(0,1),\\ V(t,x,0) = V(t,x,1) = 0 & \textit{for } x\in\omega. \end{cases}$$

We have up to an extraction of a subsequence, as $\eta \to 0$,

$$\|f_k^\eta - N_s \mathcal{M}_k\|_{\ell^1(L^1([0,T]\times\omega\times\mathbb{R}^2))} \to 0 \qquad \text{and} \qquad \|V^\eta - V\|_{L^2([0,T],H^1(\Omega))} \to 0.$$

We will not give the proof of this result in detail because most of results used have been established in the previous chapter. The main difficulty here is the fact that we do not have anymore the imbedding $H^1(\Omega) \hookrightarrow L^\infty_x L^2_z(\Omega)$. Therefore we do not conserve the uniqueness of the solution of the quasistatic Schrödinger-Poisson system. To overcome this difficulty, we will use the Trudinger and Young inequalities presented in the Appendix of chapter 4. The idea is that with these inequalities the set of the square of functions in $H^1(\omega)$ is in duality with $L\log L$. In fact in the previous chapter, we have only used the L^1 bound of the occupation factor whereas the entropy inequality (7.1.8) gives a bound in $L\log L$. With this technique, we are able to pass to the limit $\eta \to 0$ but not to establish the existence of solutions. In a full classical problem, we do not have this difficulty and we can find a rigorous derivation of a drift-diffusion-Poisson system from a Boltzmann-Poisson system for a 2D transport in [4].

This chapter is organized as follows

In section 7.2 we analyze the Schrödinger-Poisson system when the occupation factors are assumed to be given in $L\log L$. In section 7.3, we follows the development of the previous chapter to prove Theorem 7.1.4.

7.2 The Schrödinger-Poisson system for ρ in $L\log L$

The main problem which does not allow us to prove Theorem 7.1.3 is the fact that we are not able to establish the uniqueness of the solution of the Shcrödinger-Poisson system for ρ_k in $L\log L$ and $\Omega \subset \mathbb{R}^3$. In fact in section 6.3 this property relies strongly on lemma 6.2.3 which is not true in 3D. However we can establish an existence result whose proof is given in this section. Namely, we consider the Schrödinger-Poisson system (7.1.3)–(7.1.4) (in which we omit to write the exponents η) for $\rho = (\rho_k)_{k\geq 1}$ given in $L^\infty(0,T;\ell^1(L^1(\omega)))$ and completed by the following boundary conditions :

$$\partial_\nu V(t,x,z) = 0 \text{ on } \partial\omega \times (0,1), \qquad V(t,x,0) = V(t,x,1) = 0 \text{ for } x \in \omega.$$

Assumption 7.2.1 *We assume that the given* ρ *is such that* $\forall\, k \geq 1$, $\rho_k \geq 0$ *and there exists a nonnegative constant* C_T *such that :*

$$\forall\, t \in [0,T], \qquad \sum_k \int_\omega \rho_k(1 + k^2 + |\log \rho_k|)\, dx \leq C_T, \tag{7.2.13}$$

In the sequel we will use the functional space

$$H^1_{01} = \{V \in H^1(\Omega)\ :\ V(x,0) = V(x,1) = 0\}.$$

Proposition 7.2.2 (Existence) *Let us suppose that* $\rho = (\rho_k)_{k\geq 1}$ *is given in* $L^\infty(0,T;\ell^1(L^1(\omega)))$ *and satisfies Assumption 7.2.1. Then the Schrödinger-Poisson system* (7.1.3)–(7.1.4) *admits a solution in* H^1_{01}.

As in the previous chapter (and see [5, 1]), we consider the functional defined on H^1_{01} by

$$J_\rho(V) = \frac{1}{2}\iint_\Omega |\nabla V|^2\,dxdz - \sum_{k\geq 1}\int_\omega \rho_k \epsilon_k[V]\,dx = J_0(V) + J_1(V,\rho). \tag{7.2.14}$$

We first prove that this functional has a minimizer and that this minimizer defines a solution of (7.1.3)–(7.1.4). The main idea is the fact that we only use the L^1 bound of ρ_k in section 6.3 whereas the entropy estimate gives more regularity. As in chapter 5, we will then use the Young and Trudinger inequalities to prove the following result :

Lemma 7.2.3 *Assume that $\rho \in L^\infty(0,T;\ell^1(L^1(\omega)))$ and satisfies Assumption 7.2.1. Then the functional J_ρ defined in (7.2.14) is continuous, locally Lipschitz and weakly lower semi-continuous on H^1_{01}. It is coercive : there exists nonnegative constants C_1, C_2 and C_3 such that*

$$J_\rho(V) \geq C_1\|V\|^2_{H^1(\Omega)} - C_2\|V\|^{4/3}_{H^1(\Omega)} - C_3. \tag{7.2.15}$$

Thus the system (7.1.3)–(7.1.4) admits a solution $(V,(\epsilon_k,\chi_k)_{k\geq 1})$ such that $V \in H^1_{01}$.

Proof. The functional J_0 is clearly continuous and strongly convex on H^1_{01}. For the functional J_1, we use the properties of $\epsilon_k[V]$ stated in (B.0.14) to prove

$$\begin{aligned}|J_1(V,\rho) - J_1(\widetilde{V},\rho)| &\leq \sum_{k\geq 1}\int_\omega \rho_k|\epsilon_k[V] - \epsilon_k[\widetilde{V}]|\,dx \\ &\leq C\sum_{k\geq 1}\int_\omega \rho_k(k^{1/2} + \|V\|^{1/3}_{L^2_z(0,1)} + \|\widetilde{V}\|^{1/3}_{L^2_z(0,1)})\|V-\widetilde{V}\|_{L^2_z(0,1)}\,dx.\end{aligned} \tag{7.2.16}$$

Moreover after an interpolation we have

$$\sum_k\int_\omega \rho_k k^{1/2}\|V-\widetilde{V}\|_{L^2_z(0,1)}\,dx \leq \left(\sum_k\int_\omega \rho_k k^2\,dx\right)^{1/4}\left(\int_\omega N_s\|V-\widetilde{V}\|^{4/3}_{L^2_z(0,1)}\,dx\right)^{3/4}.$$

Using the Young inequality given in (A.1.1), we have

$$\begin{aligned}\int_\omega N_s\|V-\widetilde{V}\|^{4/3}_{L^2_z(0,1)}\,dx &= \int_\omega N_s\frac{\|V-\widetilde{V}\|^{4/3}_{L^2_z(0,1)}}{\|V-\widetilde{V}\|^{4/3}_{H^1(\Omega)}}\,dx\|V-\widetilde{V}\|^{4/3}_{H^1(\Omega)} \\ &\leq \int_\omega\left(N_s\log N_s - N_s + \exp\frac{\|V-\widetilde{V}\|^{4/3}_{L^2_z(0,1)}}{\|V-\widetilde{V}\|^{4/3}_{H^1(\Omega)}}\right)dx\ \|V-\widetilde{V}\|^{4/3}_{H^1(\Omega)}.\end{aligned}$$

Therefore, the Trudinger inequality (A.2.3) and (7.2.13) lead to

$$\sum_{k\geq 1}\int_\omega \rho_k k^{1/2}\|V-\widetilde{V}\|_{L^2_z(0,1)}\,dx \leq C_T\|V-\widetilde{V}\|_{H^1(\Omega)}. \tag{7.2.17}$$

Doing the same for the others term, we have

$$\int_\omega N_s \|V\|^{1/3}_{L^2_z(0,1)} \|V-\widetilde{V}\|_{L^2_z(0,1)}\,dx \le C\|V\|^{1/3}_{H^1(\Omega)}\|V-\widetilde{V}\|_{H^1(\Omega)} \times \int_\omega \left(N_s \log N_s - N_s + \exp \frac{\gamma \|V\|^{1/3}_{L^2_z(0,1)} \|V-\widetilde{V}\|_{L^2_z(0,1)}}{\|V\|^{1/3}_{H^1(\Omega)}\|V-\widetilde{V}\|_{H^1(\Omega)}} \right) dx.$$

An interpolation gives

$$\int_\omega \exp \frac{\gamma \|V\|^{1/3}_{L^2_z(0,1)} \|V-\widetilde{V}\|_{L^2_z(0,1)}}{\|V\|^{1/3}_{H^1(\Omega)}\|V-\widetilde{V}\|_{H^1(\Omega)}}\,dx \le \le \left(\int_\omega \exp \frac{\gamma \|V\|^{2/3}_{L^2_z(0,1)}}{\|V\|^{2/3}_{H^1(\Omega)}}\,dx \right)^{1/2} \left(\int_\omega \exp \frac{\gamma \|V-\widetilde{V}\|^2_{L^2_z(0,1)}}{\|V-\widetilde{V}\|^2_{H^1(\Omega)}}\,dx \right)^{1/2} \le C,$$

thanks to the Trudinger inequality (A.2.3) and (7.2.13). Thus,

$$\sum_{k\ge 1} \int_\omega \rho_k \|V\|^{1/3}_{L^2_z(0,1)} \|V-\widetilde{V}\|_{L^2_z(0,1)}\,dx \le C_T \|V\|^{1/3}_{H^1(\Omega)}\|V-\widetilde{V}\|_{H^1(\Omega)}. \tag{7.2.18}$$

Obviously we have the same estimate (7.2.18) if we change V to $\widetilde{V}$ and $\widetilde{V}$ to V. Thus (7.2.17) and (7.2.18) injected in (7.2.16) prove

$$|J_1(V,\rho) - J_1(\widetilde{V},\rho)| \le C_T(1 + \|V\|^{1/3}_{H^1(\Omega)} + \|\widetilde{V}\|^{1/3}_{H^1(\Omega)})\|V-\widetilde{V}\|_{H^1(\Omega)}. \tag{7.2.19}$$

Hence $J_1(\cdot,\rho)$ is Lipschitz and weakly continuous on H^1_{01}. Now if we take $\widetilde{V}=0$ in (7.2.19), from (7.2.13) we have that $0 \ge J_1(0,\rho) \ge -C_T$. Thus,

$$J_\rho(V) \ge \frac{1}{2}\|\nabla V\|^2_{L^2(\Omega)} - C(1+\|V\|^{1/3}_{H^1(\Omega)})\|V\|_{H^1(\Omega)} - C'.$$

We apply the Poincaré inequality in H^1_{01} to find (7.2.15). Hence the functional J_ρ admits a minimizer in H^1_{01}. Moreover, from the properties of the spectrum of the Hamiltonian (see Lemma B.0.3), it is clear that J_ρ is Gâteaux differentiable on H^1_{01} and for any $W \in H^1(\Omega)$,

$$d_V J_\rho(V)\cdot W = \iint_\Omega \nabla V \cdot \nabla W\,dxdz - \sum_k \int_\omega \rho_k \langle |\chi_k[V]|^2 W\rangle\,dx.$$

Thus each minimizer of the functional J_ρ is a weak solution of the Schrödinger-Poisson system (7.1.3)–(7.1.4). □

7.3 Diffusive limit

This section is devoted to the proof of Theorem 7.1.4. We follow the analysis of the previous chapter and only detail the changes.

7.3.1 Convergence of the density

Lemma 7.3.1 *Let f^η be the renormalized solution of the Boltzmann-Schrödinger-Poisson system defined in Theorem 7.1.3. Then $\rho^\eta = \int_{\mathbb{R}^2} f^\eta\, dv$ is strongly relatively compact in $\ell^1(L^1((0,T)\times\omega))$.*

We skip the proof which is exactly the same as in the previous chapter. Thus with this result, we can extract a subsequence (still denoted ρ^η) converging towards ρ in $\ell^1(L^1((0,T)\times\omega))$. The Fatou lemma and the entropy inequality (7.1.8) imply that for a.e. $t\in[0,T]$,

$$\sum_k \int_\omega \rho_k(1+k^2+|\log\rho_k|)\,dx \le C_T. \tag{7.3.20}$$

Proposition 7.3.2 *Under assumptions of Theorem 7.1.3, if (f^η, V^η) is a solution of (7.1.1)-(7.1.3)–(7.1.7) as defined in Theorem 7.1.3. Then there exist V in $L^\infty(0,T;H^1(\Omega))$ and N_s in $L^\infty(0,T;L^1(\omega))$ such that, up to an extraction,*

$$V^\eta \to V \text{ in } L^2(0,T;H^1(\Omega)) \text{ and } f^\eta \to N_s\mathcal{M} \text{ in } \ell^1(L^1([0,T]\times\omega\times\mathbb{R}^2)).$$

Proof. With Lemma 7.2.2 and (7.3.20) there exists $V\in L^\infty(0,T;H^1(\Omega))$ weak solution of the Schrödinger-Poisson system (7.1.3)–(7.1.4) for the given ρ. Since we do not have the imbedding $H^1(\Omega)\hookrightarrow L^\infty_x L^2_z(\Omega)$, we must be more precise than before to establish the convergence of V^η towards this solution V.

If we multiply the Poisson equation by $(V-V^\eta)$ and integrate, we use the same decomposition as before

$$\int_0^T \iint_\Omega |\nabla(V^\eta - V)|^2\,dxdzdt = I + II + III,$$

where

$$I = \sum_k \int_0^T \int_\omega (\rho_k - \rho_k^\eta)\langle |\chi_k[V]|^2 (V-V^\eta)\rangle\,dxdt,$$

$$II = \sum_k \int_0^T \iint_{\omega\times\mathbb{R}^2} (f_k^\eta - N_s^\eta\mathcal{M}_k^\eta)\langle (|\chi_k[V]|^2 - |\chi_k[V^\eta]|^2)(V-V^\eta)\rangle\,dxdvdt,$$

$$III = \sum_k \int_0^T \iint_{\omega\times\mathbb{R}^2} N_s^\eta\mathcal{M}_k^\eta\langle (|\chi_k[V]|^2 - |\chi_k[V^\eta]|^2)(V-V^\eta)\rangle\,dxdvdt,$$

We will used techniques based on the Trudinger and Young inequalities to treat the first and second term as in the proof of Proposition 7.2.2. Moreover, as before, the decay of the Maxwellian with respect to k insures that the third term is nonpositive.

For the first term, as in the proof of Proposition 7.2.2, we can show that

$$|I| \le C_1 \|\rho_k - \rho_k^\eta\|^{1/4}_{\ell^1(L^1_{t,x})}. \tag{7.3.21}$$

For the second term, we use Lemma (B.0.5) to write

$$|II| \leq C_2 \sum_k \int_0^T \iint_{\omega\times\mathbb{R}^2} |f_k^\eta - N_s^\eta \mathcal{M}_k^\eta| (1 + \|V\|_{L_z^2}^{1/2} + \|V^\eta\|_{L_z^2}^{1/2}) \|V - V^\eta\|_{L_z^2}\, dxdvdt.$$

Doing the same calculations as for I, we get the estimate

$$|II| \leq C_3 \left(\sum_k \int_0^T \iint_{\omega\times\mathbb{R}^2} |f_k^\eta - N_s^\eta \mathcal{M}_k^\eta|\, dxdvdt \right)^{1/4}. \tag{7.3.22}$$

We show that the entropy inequality (7.1.8) implies the convergence towards 0 of this term. Indeed, by a Cauchy-Schwarz inequality

$$\sum_k \int_0^T \iint_{\omega\times\mathbb{R}^2} |f_k^\eta - N_s^\eta \mathcal{M}_k^\eta|\, dxdvdt \leq 2\sqrt{2} \|N_s^\eta\|_{L_{t,x}^1}^{1/2} \left(\int_0^T \mathcal{R}^\eta(t)\, dt \right)^{1/2}.$$

Thanks to the properties of the eigenvalues of the Hamiltonian, we have, with the injection of $H^1(\Omega) \hookrightarrow L_x^p L_z^2(\Omega)$ for all $1 \leq p < +\infty$, that

$$\|\epsilon_k[V^\eta] - \epsilon_k[V]\|_{L^2([0,T],L^p(\omega))} \to 0 \quad \text{as } \eta \to 0, \quad \text{for all } 1 \leq p < +\infty.$$

Moreover, using properties of the eigenvalues of the Hamiltonian, we have

$$|\mathcal{M}_k^\eta - \mathcal{M}_k| \leq C(1 + \|V^\eta\|_{L_z^2} + \|V\|_{L_z^2}) \|V - V^\eta\|_{L_z^2} \int_0^1 M(v)\, \frac{e^{-\epsilon_k^s}}{\mathcal{Z}^s}\, ds, \tag{7.3.23}$$

where we use the notation $f^s = f[sV^\eta + (1-s)V]$. Thus $\mathcal{M}^\eta \to \mathcal{M}$ as $\eta \to 0$ in $L^2([0,T], \ell^p(L^p(\omega\times\mathbb{R}^2)))$ for all $p < +\infty$. Furthermore,

$$\|N_s\mathcal{M} - N_s^\eta \mathcal{M}^\eta\|_{\ell^1(L_{t,x,v}^1)} \leq \|N_s - N_s^\eta\|_{L_{t,x}^1} + \|N_s^\eta(\mathcal{M} - \mathcal{M}^\eta)\|_{\ell^1(L_{t,x,v}^1)}. \tag{7.3.24}$$

The bound (7.3.23) provides

$$\|N_s^\eta(\mathcal{M} - \mathcal{M}^\eta)\|_{\ell^1(L_{t,x,v}^1)} \leq \int_0^T \int_\omega N_s^\eta (1 + \|V^\eta\|_{L_z^2} + \|V\|_{L_z^2}) \|V - V^\eta\|_{L_z^2}\, dxdt.$$

We will use the same techniques as before based on the Young and Trudinger inequalities to bound the right hand side. In fact we have for instance with (A.1.1)

$$\int_0^T \int_\omega N_s^\eta \|V\|_{L_z^2} \|V - V^\eta\|_{L_z^2}\, dxdt \leq \int_0^T \|V\|_{H^1(\Omega)} \|V - V^\eta\|_{H^1(\Omega)}\, dt \times$$
$$\sup_{t\in[0,T]} \left\{ \int_\omega N_s^\eta \log N_s^\eta - N_s^\eta + C \exp\left(\gamma \frac{\|V\|_{L_z^2}^2}{\|V\|_{H^1(\Omega)}^2} \right) \exp\left(\gamma \frac{\|V - V^\eta\|_{L_z^2}^2}{\|V - V^\eta\|_{H^1(\Omega)}^2} \right) dx \right\}.$$

Thus the Trudinger inequality (A.2.3) and the entropy inequality (7.1.8) imply that there exists a nonnegative constant C such that

$$\|N_s^\eta(\mathcal{M} - \mathcal{M}^\eta)\|_{\ell^1(L_{t,x,v}^1)} \leq C \|V - V^\eta\|_{L^2([0,T],H^1(\Omega))}^{1/2}.$$

This last estimate combines with the strong convergence of N_s^η in $L^1_{t,x}$ imply thanks to (7.3.24) that

$$\|N_s\mathcal{M} - N_s^\eta \mathcal{M}^\eta\|_{\ell^1(L^1_{t,x,v})} \to 0 \quad \text{as } \eta \to 0.$$

Moreover, the entropy estimate (7.1.8) implies a control of the dissipation rate:

$$\int_0^T \mathcal{R}^\eta(t)\,dt = \frac{1}{2}\sum_{k\geq 1}\int_0^T \iint_{\omega\times\mathbb{R}^2}\left(\sqrt{f_k^\eta} - \sqrt{N_s^\eta \mathcal{M}_k^\eta}\right)^2 dxdvdt \leq C_T\eta^2.$$

Thus, by a Cauchy-Schwarz inequality,

$$\begin{aligned}\|f^\eta - N_s\mathcal{M}\|_{\ell^1(L^1_{t,x,v})} &\leq \|f^\eta - N_s^\eta\mathcal{M}^\eta\|_{\ell^1(L^1_{t,x,v})} + \|N_s^\eta\mathcal{M}^\eta - N_s\mathcal{M}\|_{\ell^1(L^1_{t,x,v})}\\ &\leq 4\|N_s^\eta\|^{1/2}_{L^1_{t,x}}\left(\int_0^T \mathcal{R}^\eta(t)\,dt\right)^{1/2} + \|N_s^\eta\mathcal{M}^\eta - N_s\mathcal{M}\|_{\ell^1(L^1_{t,x,v})}.\end{aligned}$$

Thus $f^\eta \to N_s\mathcal{M}$ strongly in $\ell^1(L^1_{t,x,v})$.

□

7.3.2 The limit equation

By a straightforward adaptation of the previous chapter (using the Young and Trudinger inequalities when it is useful) we can prove :

Proposition 7.3.3 *Let (f^η, V^η) be a solution of the renormalized system defined in Theorem 7.1.3, then the current J^η, defined by*

$$J^\eta := \frac{1}{\eta}\sum_k \int_{\mathbb{R}^2} v f_k^\eta\,dv, \tag{7.3.25}$$

satisfies

$$\begin{cases} J^\eta \rightharpoonup J = -\mathbb{D}(\nabla_x N_s + N_s\nabla_x V_s) & \text{in weak} - L^1_{t,x},\\ J\cdot\nu = 0 & \text{for } x\in\partial\omega,\end{cases}$$

where $\mathbb{D}$ is the diffusion matrix defined in the previous chapter and the autoconsistant potential is $V_s = -\log(\sum_{k\geq 1} e^{-\epsilon_k[V]})$.

Thus the limit (N_s, V) satisfies the drift-diffusion-Schrödinger-Poisson system. This ends the proof of Theorem 7.1.4.

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PART III

Simulations numériques

Chapter 8

Simulation d'un transistor double grille avec le modèle DDSP

Joint work with P. Pietra [1].

8.1 Introduction

Nowadays, the improve of the technology allows us to realize electronic components at nanometer scales. Such components increase speed and functionality of electronic devices. The nanotechnology becomes a major center of interest for future electronic. In this task, modeling and numerical simulations play an important role to estimate the behaviour of devices whose electrons transport properties are mainly based on quantum effects [3, 10, 12]. In these ultimate size devices like ultrashort channel double gate MOSFETs [1], electrons might be extremely confined in one or several directions, which are referred to the confining directions.

This article proposes to handle with nanoscale semiconductor devices using a general subband decomposition approach. This approach consists of a diagonalisation of the Hamiltonian thanks to a separation of the confinement and the transport directions. The computational gain is significant by the reduction of the dimension of the transport problem [19, 6]. The model presented in this article is defined by a self-consistent process between the calculation of the electron density and the space charge effects using the Poisson equation. In the device, electrons are in a mixed state with given statistics. They are like point particles in the transport direction while they behave like waves in the transverse one. The elementary states are obtained thanks to the resolution of a classical transport equation.

Such a coupled classical-quantum model is presented in this work to obtain the modelling and the numerical simulation of a double gates nanoMOSFET. A model of a purely

[1] IMATI del CNR, Pavia, Italy.

ballistic quantum transport of Schrödinger type and its numerical treatment relying on the subband decomposition approach are presented in [17, 19]. Here transport properties are not expected to be based on quantum effects but the design of the device is assumed to be such that the transport can be considered as classical. The main mechanism driving the electrons towards a local equilibrium in a diffusive regime is collisions with phonons (vibrations of the lattice) [15, 21]. The transport is then well described by a fluid model. One of the most used equation is the drift-diffusion equation [16, 22, 11, 2] which present the advantages to be of low numerical cost.

In the following section we present an overview of the model and of the equations used. In section 3 we explain the Gummel process implemented with the aim to obtain a numerical simulation of a double gate MOSFET. Finally, the numerical results are presented in the last section.

8.2 Presentation of the model

In this section we will present more precisely the model used and implemented in this work. We denote the space variable (x, y, z). We assume that the problem is invariant by translation in the y direction. Thus it is equivalent to consider that we have a 2D device occupying the interval $[0, L]$ with a width ℓ. Then the transport variable x is assumed to lie in $[0, L]$, while in the confined direction the variable z belongs to $[0, \ell]$.

8.2.1 The subband decomposition method

In the subband decomposition approach the system is viewed as a statistical mixture of eigenstates of the Schrödinger operator in the transverse direction. The occupation number of each state is given by a statistic function : for Boltzmann statistics it is $\exp(\frac{\epsilon_F - \epsilon}{k_B T})$, for Fermi-Dirac statistics it is $1/(1 + \exp(\frac{\epsilon - \epsilon_F}{k_B T}))$. In these expressions ϵ is the energy of the considered staten, k_B is the Boltzmann constant, T is the temperature of the lattice and ϵ_F is the so-called Fermi energy which, at zero temperature, represents the threshold between occupied and unoccupied states [18, 23].

In the transversal direction, the system is assumed to be at the equilibrium with a local Fermi level ϵ_F which depends on the transport variable x. At a position (x, z), the particle density $N(x, z)$ for Boltzmann statistics is given by

$$N(x,z) = \sum_{k=1}^{+\infty} e^{\beta(\epsilon_F(x) - \epsilon_k(x))} |\chi_k(x,z)|^2, \tag{8.2.1}$$

where $\beta = 1/(k_B T)$ and $(\chi_k, \epsilon_k)_{k \geq 1}$ is the complete set of eigenfunctions and eigenvalues of the Schrödinger operator in the z variable

$$\begin{cases} -\dfrac{\hbar^2}{2} \dfrac{d}{dz} \left(\dfrac{1}{m_*(z)} \dfrac{d}{dz} \chi_k \right) + (U + U_c)\chi_k = \epsilon_k \chi_k. \\ \chi_k(x, \cdot) \in H_0^1(0, \ell), \quad \displaystyle\int_0^\ell \chi_k \, \chi_{k'} \, dz = \delta_{kk'} \, . \end{cases} \tag{8.2.2}$$

In this equation $\hbar$ is the Planck constant, m_* the effective mass, e the elementary charge and U_c is a given potential barrier between the silicon and the oxyde in the nanotransistor. The electrostatic energy generated by the electrons themselves $V = U/e$ is the solution of the Poisson equation

$$-\text{div}_{\,x,z}(\varepsilon_R \nabla_{x,z} U) = \frac{e}{\varepsilon_0}(N - N_D), \tag{8.2.3}$$

where ε_R is the relative permittivity, ε_0 the permittivity constant in vacuum and N_D is the doping density.

8.2.2 The diffusive regime

In the transport direction, we consider that the transport is purely classical in the diffusive regime. This motion is described thanks to the stationary drift-diffusion equation :

$$-\text{div}_x \, J(x) = 0, \tag{8.2.4}$$

$$J(x) = \mathbb{D}(\nabla_x N_s(x) + \beta N_s(x) \nabla_x U_s(x)), \tag{8.2.5}$$

where N_s is the surface density, $\mathbb{D}$ denotes the diffusion coefficient $\mathbb{D} = \mu k_B T$ for a constant mobility μ and the effective energy U_s is given by

$$U_s = -k_B T \log\left(\sum_{k=1}^{+\infty} e^{-\beta\epsilon_k}\right). \tag{8.2.6}$$

If we note the repartition function $\mathcal{Z}$ by

$$\mathcal{Z}(x) = \sum_{k=1}^{+\infty} e^{-\beta\epsilon_k(x)}, \tag{8.2.7}$$

then we remark easily from (8.2.1) that the surface density satisfy

$$N_s(x) = \int_0^\ell N(x,z)\, dz = e^{\beta\epsilon_F}\mathcal{Z}(x).$$

Therefore we can choose the unknow N_s instead of ϵ_F in the modelling. We have then

$$N(x,z) = \frac{N_s(x)}{\mathcal{Z}(x)} \sum_{k=1}^{+\infty} e^{-\beta\epsilon_k(x)} |\chi_k(x,z)|^2. \tag{8.2.8}$$

If we introduce the slotboom variable u defined by

$$u(x) = e^{\beta\epsilon_F} = \frac{N_s(x)}{\mathcal{Z}(x)}, \tag{8.2.9}$$

then we remark easily that the drift-diffusion equation (8.2.4) reads

$$-\text{div}_{\,x}(\mathbb{D}\mathcal{Z}(x)\nabla_x u(x)) = 0.$$

Thus the invariance of the problem in the y direction implies that this last equation can be written $-\frac{d}{dx}(\mathbb{D}\mathcal{Z}(x)\frac{du}{dx}) = 0$, which shows that the slotboom variable u is constant.

The drift-diffusion equation can be derived from kinetic theory when the mean free path is small compared to the system length-scale [20, 13]. Such a derivation from the Boltzmann equation of semiconductors is derived formally in chapter 2 and a rigorous proof of it is done in chapter 6.

The unknowns of the overall system are the surface density $N_s(x)$, the eigenenergies $\epsilon_k(x)$, the eigenfunctions $\chi_k(x, z)$ and the electrostatic potential $V(x, z)$.

If we assume that the electrostatic potential V is given. Then a diagonalization of the one dimensional Schrödinger operator (8.2.2) provides the eigenvalues and eigenvectors (ϵ_k, χ_k). The effective energy U_s can be computed from (8.2.6). This allows us to obtain the surface density N_s by solving the drift-diffusion problem (8.2.4). Thus we have all the knowledge to find the density N (8.2.8) and therefore to compute a new potential thanks to the resolution of the Poisson equation (8.2.3).

8.3 Numerical implementation

8.3.1 The modeled device

Here we are interested in a Double-Gate MOSFET (Metal Oxyde Semiconductor Field Effect Transistor). This nanotransistor is a very small structure Si/SiO_2. The charge carriers are sent out from the Source to the Drain. The transport takes place in the canal which is the active region between the Source and the Drain. This MOSFET has two gates which are insulated from the canal by a layer of dioxyde of Silicium SiO_2 and where we can apply a voltage.

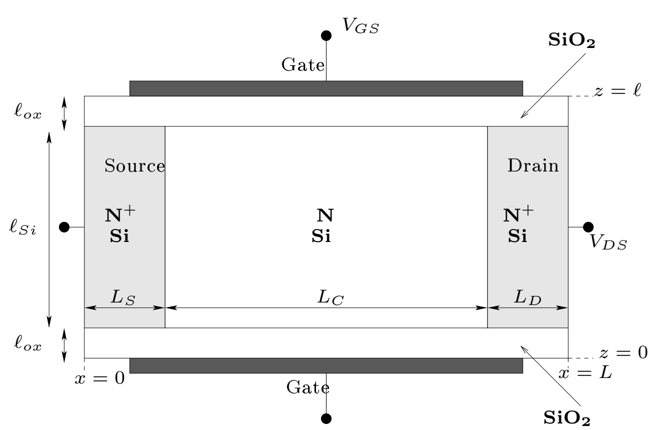

Figure 8.1: Schematic representation of the modeled device. The Drain and the Source are large doped by a density N^+.

We assume that the model is invariant in the y direction (infinite boundary conditions) and the problem is then studied in the x, z domain. The device occupies a region of a 2D domain denoted by $[0, L] \times [0, \ell]$. A schematic representation of the device is presented in Figure 8.1. Moreover the high doping regions at the source and at the drain contacts imply that these contacts can be considered as small electron reservoirs in which we assume that the potential does not depend on the transport direction. And the physic of the frontier implies mixed boundary conditions : Dirichlet boundary conditions at the ohmic contacts of the Drain, Source and gate contacts, Neumann boundary conditions everywhere else.

8.3.2 General scheme of the Gummel iterations

We mesh the domain $[0, L]\times[0, \ell]$ by finite elements, and obtain the nodes x_i, $i = 1, \cdots, N_x$ and z_j, $j = 1, \cdots, N_z$. The procedure is decomposed in three main steps using Gummel iterations [14].

First we consider the boundary conditions at the drain and at the source contact. As we saw before, the high doping profile at these regions implies that the potential does not depend on the transport direction. Thus the surface density at the Drain and Source contact is equal to $N^+ \times \ell_{Si}$. It remains then to solve in the z direction a 1D Schrödinger-Poisson system. To this aim we use a Gummel iteration and find $(\chi_k(x_1, z), \epsilon_k(x_1))_k$ and the potential energy that we will denote $U_b(z)$.

Secondly, we consider the whole system when there is no applied voltage. The results obtained in the first step allows us to determinate the slotboom variable u thanks to (8.2.9). In fact, since u is constant, it suffices to determine it on the boundary (for $x = x_1$ for instance). It remains to calculate a 2D Schrödinger-Poisson system. The boundary conditions for the Poisson equation are $U(x = 0, z) = U(x = L, z) = U_b(z)$ at the Drain and Source contacts, $U(x, z = 0) = U(x, z = \ell) = U_{gate}$ for $x \in [L_1, L_2]$ at the Gate contact (if we assume that the Gates occupy the position $[L_1, L_2]$) and Neumann boundary condition everywhere else $\frac{dU}{dz}(x, z = 0) = \frac{dU}{dz}(x, z = 1) = 0$ for $x \in [0, L_1] \cup [L_2, L]$.

Finally, we consider the resolution of the drift-diffusion-Schrödinger-Poisson system when there is an applied Drain-Source voltage U_{DS}. We start from the obtained potential and density and increment by step of $0.02V$ in order to avoid too big gap for the accuracy of the computer. We impose Dirichlet boundary conditions for the drift-diffusion equation at $x = 0$ and $x = L$. For the potential, we impose Dirichlet boundary conditions at the Gate and at the Source and Drain contacts : $U(x = 0, z) = U_b(z)$ and $U(x = L, z) = U_b(z)+U_{DS}$.

The Gummel iteration for the drift-diffusion-Schrödinger-Poisson system is summarized in the following steps :

1. For a given potential U_{old} in the whole domain $[0, L] \times [0, \ell]$, we solve the eigenvalue problem (8.2.2) on each slices of the device by diagonalization of the Hamiltonian. Thus we obtain N_x sets of eigenfunctions $\{\chi_k(x_i, z)\}_{i=1,\cdots,N_x}$ and eigenvectors $\{\epsilon_k\}$. The eigenfunctions have then to be normalized.

2. We compute then the effective energy U_s from (8.2.6). We are then able to solve the 1D stationary drift-diffusion equation (8.2.4) with Dirichlet boundary condition. The method used is the one described in [8].

3. We have then all the ingredients to compute the density N thanks to the expression (8.2.8).

4. The Poisson equation is solved in the 2D domain using Dirichlet boundary conditions for the interfaces with the gates and on the source and drain interfaces, and Neumann boundary conditions everywhere else. The system is solved using the preconditioned conjugate gradient method. A new potential energy U_{new} is then obtained.

5. We repeat the four previous steps until the difference $\|U_{new} - U_{old}\|_{L^\infty}$ be sufficiently small.

We end the description of the iterations by a remark on the resolution of the Poisson equation. Following the idea of Caussignac et al. [9], we implement a quasi-Newton method such that we solve

$$-\nabla(\varepsilon_R \nabla U_{new}) + \frac{e}{\varepsilon_0} \frac{U_{new}}{U_{ref}} = \frac{e}{\varepsilon_0} \left(N(x,z) \left(1 - \frac{U_{old}}{U_{ref}} \right) - N_D \right),$$

with $U_{ref} = k_B T$. This method can be viewed as a linearization of the Newton method. This is the method used in [19] where a ballistic 2D Schrödinger-Poisson system is implemented.

8.3.3 The three valleys

The silicon presents the particularity to have three different electron configurations in the band structure (Figure 8.2). The electrons are distributed among six ellipsoids which present some symmetry properties. Due to anisotropic effects in the band structure we define for the electron a transverse effective mass m_t^* and a longitudinal effective mass m_ℓ^*. If we use the notation (m_x^*, m_y^*, m_z^*) to define the effective mass in the direction (x, y, z),

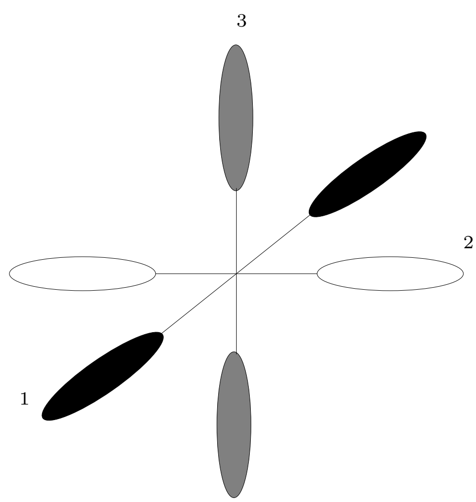

Figure 8.2: Constant energy surface for the first conduction band in silicon (six ellipsoids and three different configurations for the electrons due to the symmetry properties).

then we have three different configuration for the Silicon : (m_t^*, m_t^*, m_ℓ^*), (m_t^*, m_ℓ^*, m_t^*) and (m_ℓ^*, m_t^*, m_t^*).

Table 8.1: Table of the main value used

Parameter	Value	Length	Value
N^+	$10^{20}cm^{-3}$	L_S	$15nm$
N	$10^{15}cm^{-3}$	L_C	$20nm$
U_c	$3\ eV$	L_D	$15nm$
$\varepsilon_R[Si]$	11.7	ℓ_{ox}	$2nm$
$\varepsilon_R[SiO_2]$	3.9	ℓ_{Si}	$8nm$

If we take into account these configurations, then we have to solve two different Schrödinger equations one to define the transversal eigenfunctions $(\chi_k^t)_k$ and the transversal eigenvalues $(\epsilon_k^t)_k$

$$-\frac{\hbar^2}{2}\frac{d}{dz}\left(\frac{1}{m_t^*}\frac{d}{dz}\chi_k^t\right) + (U+U_c)\chi_k^t = \epsilon_k^t\chi_k^t, \qquad \chi_k^t \in H_0^1(0,\ell),$$

whereas the diagonalization of the following Schrödinger operator

$$-\frac{\hbar^2}{2}\frac{d}{dz}\left(\frac{1}{m_\ell^*}\frac{d}{dz}\chi_k^\ell\right) + (U+U_c)\chi_k^\ell = \epsilon_k^\ell\chi_k^\ell, \qquad \chi_k^\ell \in H_0^1(0,\ell)$$

allows us to construct the longitudinal eigenfunctions $(\chi_k^\ell)_k$ and the longitudinal eigenvalues $(\epsilon_k^\ell)_k$.

Moreover the expression of the density N is changed into

$$N = \frac{N_s}{\mathcal{Z}}\sum_k\left(e^{-\epsilon_k^\ell}|\chi_k^\ell|^2 + 2\sqrt{\frac{m_\ell^*}{m_t^*}}e^{-\epsilon_k^t}|\chi_k^t|^2\right),$$

where the repartition function is defined by

$$\mathcal{Z} = 2\pi m_t^*\left(\sum_k e^{-\epsilon_k^\ell} + 2\sqrt{\frac{m_\ell^*}{m_t^*}}\sum_k e^{-\epsilon_k^t}\right).$$

We explain in Section 2.4 how to obtain these new expression thanks to the formal derivation of the equation from the Boltzmann equation.

The implementation still remains the same as the one described in the previous section with the small modifications described before : two diagonalizations of the Schrödinger operator and a different definition of the density.

8.4 Numerical results

In this section we apply the model and the procedure described before to the Double-Gate-MOSFET. We denote by L and ℓ the length and respectively the width of the device. The thickness of the oxyde layer under the two gates is defined by ℓ_{ox} (see Figure 8.1). We recall that N_D is the doping profile which is equal to N^+ in the Drain and Source and N in the channel. All the values used are given in Table 8.1. Denoting m_e the electron mass, then the transverse and longitudinal effective mass in silicon are $m_t^* = 0.19m_e$ and $m_\ell^* = 0.98m_e$. The features of the grid mesh are $N_x = 50$ and $N_y = 50$.

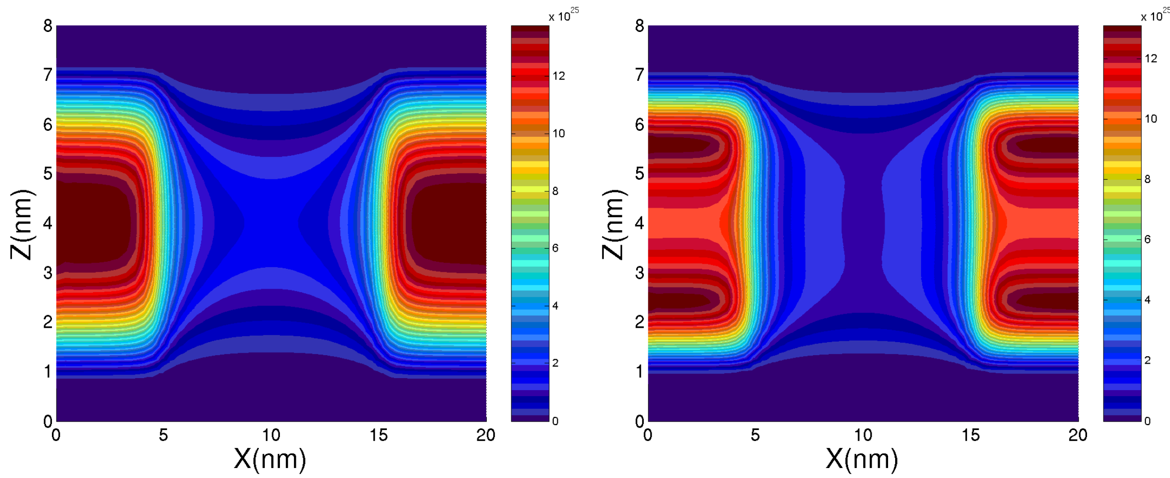

Figure 8.3: Evolution of the electron density at the equilibrium state. On the left we plot the one valley case while we plot the three valley case on the right.

Fig. 8.3 shows the obtained electron density in the device at the equilibrium for the one valley case when $m_z^* = m_t^*$ and for the three valleys case. We remark that the configuration of the electron density and thus the confinement are not the same. Figure 8.4 shows the evolution of the electron density when we apply a Drain-Source voltage $V_{DS} = 0.2V$ and $V_{DS} = 0.5V$. Because of this bias, the density does not remain symmetric but the concentration of electrons is bigger in the source.

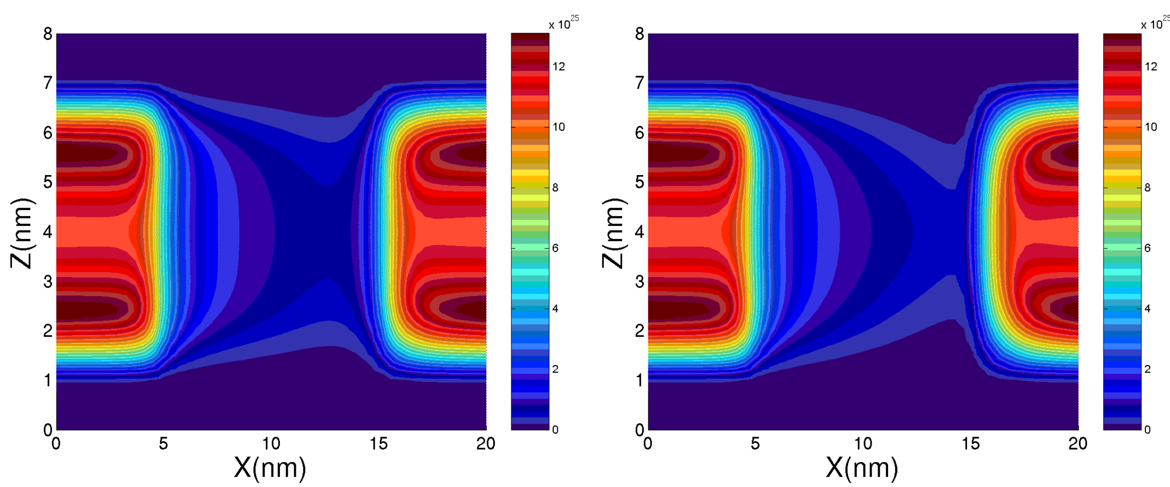

Figure 8.4: Electron density for an applied Drain-Source potential $V_{DS} = 0.2V$ on the left and $V_{DS} = 0.5V$ on the right.

In Fig. 8.5 we present the variation of the first energy levels $\epsilon_k(x)$ along the transport direction x for the two configurations of the effective mass in the confined direction z. We present the results at the equilibrium for $V_{DS} = 0V$ and for $V_{DS} = 0.5V$. We recall that the eigenvalues of the Hamiltonian form an increasing sequence of real valued numbers. We notice that the eigenvalues are closer from each other in the configuration $m_z^* = m_\ell^*$ than when $m_z^* = m_t^*$. This explains why the confinement is so different between the two configurations. In fact, if we compute the occupation factor of each state (see Figure 8.6), we notice that four modes are visible when $m_z^* = m_\ell^*$ and only two when $m_z^* = m_t^*$, because of the exponential dependence of the ϵ_k. That is the reason why we only consider a finite number of modes in our computation. Here we have taken 12 modes, but we can chose less for a faster computation.

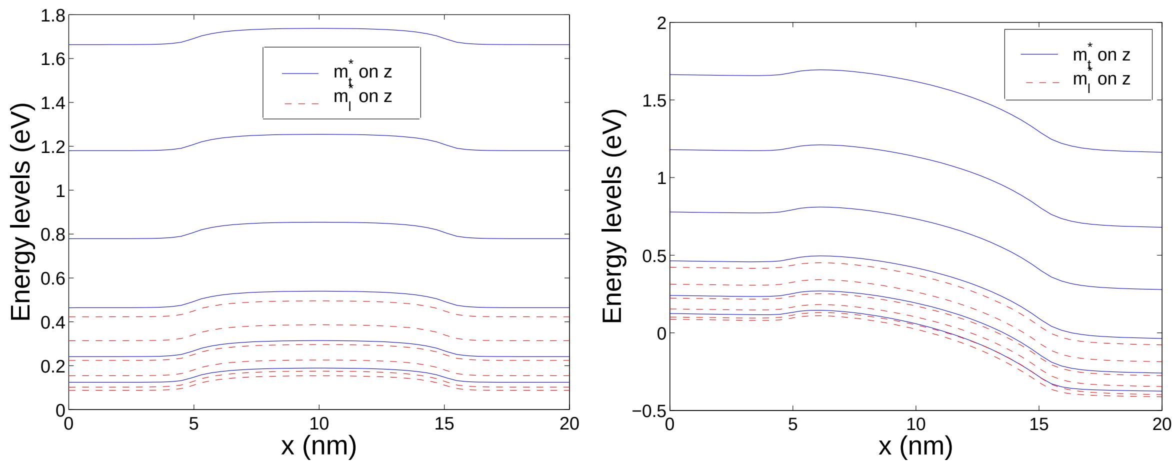

Figure 8.5: Energy levels $\epsilon_k(x)$ along the x transport direction for the two effective mass configurations in the z direction, at $V_{DS} = 0V$ (on the left) and $V_{DS} = 0.5V$ (on the right).

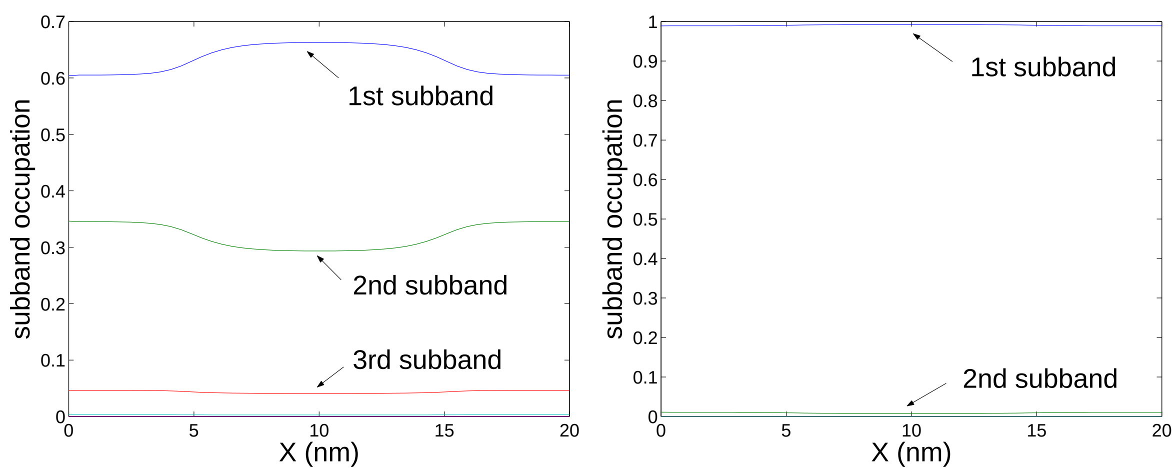

Figure 8.6: Occupation of each subband in the case $m_z^* = m_\ell^*$ (left) and $m_z^* = m_t^*$ (right). The confinement is much more important in the second case.

Moreover, in Fig. 8.5 on the right, we present the same energy levels $\epsilon_k(x)$ for an applied bias voltage at the drain. This involves a shift in the energy levels at the drain contact which is expected to be equal to the amplitude of the associated drain bias voltage.

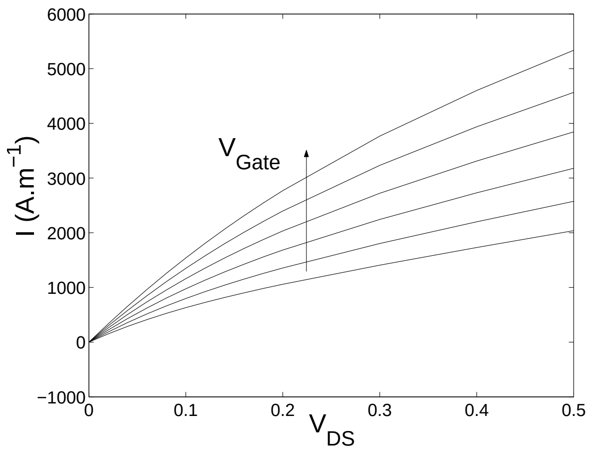

Figure 8.7: $I - V$ characteristics for the device with different Gate-Source voltage V_{GS}

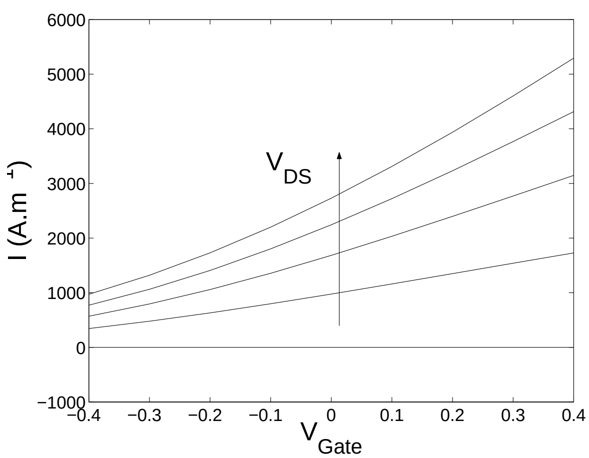

Figure 8.8: $I - V_{gate}$ characteristics for the device with different Drain-Source voltage V_{DS}

The current is defined by the quantity J in (8.2.5). The diffusion coefficient is calculated thanks to the Einstein relation : $\mathbb{D} = \mu k_B T$ where the mobility μ is equal to $\mu = 0.12 m^2 V^{-1} s^{-1}$. In Figure 8.7 we present some results on the $I - V$ characteristics of the Double-Gate-MOSFET for different gate potential V_{GS}. We notice that the numerical value of the current in the transistor increases with the gate potential. We can see more precisely this remark by looking at Figure 8.8 where the current is considered as a function of the gate potential.

Finally, in Fig. 8.9, we plot the potential energy observed in the device. The energy potential barrier between the source and the channel is visible. The gate potential V_{GS} modulates the height of this barrier and thus the number of free electrons in the channel.

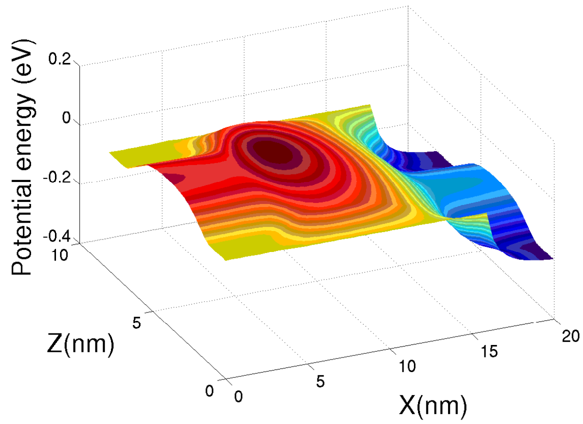

Figure 8.9: Potential energy when there is no applied gate voltage and $V_{DS} = 0.2V$.

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Chapter 9

Couplage de DDSP avec un modèle complètement quantique

Acknowledgment: The author would like to thank C. Negulescu for its help and explanation on the WKB method.

9.1 Introduction

In this work, we present a hybrid classical-quantum stationary model for the transport of charged particles confined in a nanostrucutre. In the previous chapter we have introduced a modeling and a numerical simulation for the transport in a double-gate MOSFET. This model assumes that the transport is classical in a fluid regime and the confinement in the transverse direction is described by the subband method which involves a diagonalization of the 1D Schrödinger operator in the transverse direction. It is a good alternative for the Schrödinger-Poisson model describing a purely ballistic quantum transport which numerical treatment is very expensive. However, in many semiconductor devices quantum effects take place in a localized region e.g. around the double barrier in resonant tunneling diodes, whereas in the rest of the device domain transport can be considered as classical. Thus it makes sense to follow a hybrid strategy : use a quantum model in regions where quantum effects are strong and couple it to a classical model in the rest of the device domain. Therefore a particular attention is given in the derivation of the interface conditions between these two models.

The fact is that quantum transport simulations are complex and computationally expensive. They require the self-consistent resolution of a quantum transport model with the Poisson equation. By using the subband decomposition method, the numerical cost can be reduced [7, 6] by a reduction of the dimensionality. This model does not take into account collisions of the charged particles along the transport. If the quantum region is small enough, using a collisionless model may be an acceptable approximation. In this chapter, we focus on a hybrid model in which a Schrödinger-Poisson model for the subband is coupled to the drift-diffusion-Schrödinger-Poisson model presented in the beginning of this PhD. In the large doped region of the drain and the source, the transport is expected to be classical in a highly collisional regime. Therefore the drift-diffusion model is used whereas the active zone between the source and the drain is described by a fully quantum model of Schrödinger type.

In [2], a coupled kinetic-quantum model has been introduced where the Schrödinger equation was used to define the density in the quantum zone. In the classical region a Boltzmann equation was used to compute the density in the rest of the device. At the classical-quantum interface, reflection-transmission conditions have been defined which give boundary conditions for the Boltzmann equation. Then the distribution functions solving this equation was taken as "alimentation function" to construct the density in the quantum zone. The electrostatic potential was self-consistent and therefore the model was completed by the resolution of the Poisson equation. It was shown that the reflection-transmission conditions are current flux preserving. In [5, 1], the Boltzmann equation together with the reflection-transmission conditions was replaced by the drift-diffusion equation and corresponding connection conditions were derived. In [5], these conditions were obtained by using the diffusion approximation method and a boundary layer analysis of the reflection-transmission conditions of [2]. The strategy of [1] is quite different : by aiming at a direct coupling of drift-diffusion and quantum model, the authors get analytic expression for the connection conditions by writing the continuity of the current at the interface.

Here we follow the method of [1] and operate to a direct coupling of our classical model to the quantum one. The difficulty in the subband decomposition method is that we have to take into account interactions between different subbands and the transmission or the reflection of particles can operate in different subbands. In the next section, we briefly recall the two models used and derive the interface conditions. In section 3 we present the numerical treatment of the model.

9.2 The coupling

In this section, we will present the strategy to couple the diffusive transport with the quantum transport for a confined gas.

We assume that the device domain in the transport direction x is divided into a quantum zone $\Sigma = (x_1, x_2)$, with $0 < x_1 < x_2 < L$, and a classical region $\Omega = (0, L) \setminus \Sigma$.

9.2.1 The quantum region

In a first approach, we assume that the electrostatic potential V is given on the whole domain. Thus by a diagonalization of the Hamiltonian, the set $(\epsilon_k, \chi_k)_{k\geq 1}$ is known. We consider the potential $\widetilde{V}$ defined by

$$\widetilde{V}(x) = \begin{cases} V_1 := V(x_1) & x \leq x_1, \\ V(x) & x_1 \leq x \leq x_2, \\ V_2 := V(x_2) & x \geq x_2. \end{cases}$$

This is an extension of the potential V continuously on the whole real line by a constant outside the quantum region Σ. We define the energy E_1 and E_2 on the interface $x = x_1$ and respectively on $x = x_2$ by

$$E_1(k) := \frac{p^2}{2m} + \epsilon_k(x_1) \quad ; \qquad E_2(k) := \frac{p^2}{2m} + \epsilon_k(x_2),$$

where p is the momentum variable and ϵ_k is the kth eigenvector of the Hamiltonian. The wave vector is given by

$$p_j^\ell(E_i(k)) := \sqrt{2m|E_i(k) - \epsilon_\ell(x_j)|} = \sqrt{|p^2 + 2m(\epsilon_k(x_i) - \epsilon_\ell(x_j)|},$$

where i and j take the value 1 or 2.

The Schrödinger operator is defined by

$$H = -\frac{\hbar^2}{2}\left(\frac{1}{m}\frac{d^2}{dx^2}\right) - \frac{\hbar^2}{2}\frac{\partial}{\partial z}\left(\frac{1}{m}\frac{\partial}{\partial z}\right).$$

The wave functions $\psi_k^\pm$ are solutions of the Schrödinger equation with open boundary conditions [3, 7]:

$$\begin{cases} H\psi_k^+ + \widetilde{V}\psi_k^+ = E_1\psi_k^+, \qquad \text{for } (x,z) \in [x_1, x_2] \times (0,1). \\ \psi_k^+(x,0) = \psi_k^+(x,1) = 0, \\ \hbar\dfrac{\partial \psi_k^+}{\partial x}(x_1, z) = 2\mathbf{i}p\chi_k(x_1,z) - \displaystyle\sum_{\ell=1}^{M^1(E_1(k))} \mathbf{i}p_1^\ell(E_1(k)) \left\langle \psi_k^+(x_1,\cdot)\chi_\ell(x_1,\cdot)\right\rangle \chi_\ell(x_1,z) \\ \qquad + \displaystyle\sum_{\ell=M^1(E_1(k))+1}^{\infty} p_1^\ell(E_1(k)) \left\langle \psi_k^+(x_1,\cdot)\chi_\ell(x_1,\cdot)\right\rangle \chi_\ell(x_1,z), \\ \hbar\dfrac{\partial \psi_k^+}{\partial x}(x_2, z) = \displaystyle\sum_{\ell=1}^{M^2(E_1(k))} \mathbf{i}p_2^\ell(E_1(k)) \left\langle \psi_k^+(x_2,\cdot)\chi_\ell(x_2,\cdot)\right\rangle \chi_\ell(x_2,z) \\ \qquad - \displaystyle\sum_{\ell=M^2(E^1(k))+1}^{\infty} p_2^\ell(E_1(k)) \left\langle \psi_k^+(x_2,\cdot)\chi_\ell(x_2,\cdot)\right\rangle \chi_\ell(x_2,z), \end{cases} \tag{9.2.1}$$

where

$$M^j(E_i(k)) = \sup\{\ell \in \mathbb{N}^* \text{ such that } \epsilon_\ell(x_j) \leq E_i(k)\}.$$

And

$$\begin{cases} H\psi_k^- + \widetilde{V}\psi_k^- = E_2\psi_k^-, & \text{for } (x,z)\in[x_1,x_2]\times(0,1). \\ \psi_k^-(x,0) = \psi_k^-(x,1) = 0, & \\ \hbar\dfrac{\partial\psi_k^-}{\partial x}(x_1,z) = -\displaystyle\sum_{\ell=1}^{M^1(E_2(k))} \mathbf{i}p_1^\ell(E_2(k))\left\langle\psi_k^-(x_1,\cdot)\chi_\ell(x_1,\cdot)\right\rangle\chi_\ell(x_1,z) & \\ \qquad + \displaystyle\sum_{\ell=M^1(E_2(k))+1}^{\infty} p_1^\ell(E_2(k))\left\langle\psi_k^-(x_1,\cdot)\chi_\ell(x_1,\cdot)\right\rangle\chi_\ell(x_1,z), & \\ \hbar\dfrac{\partial\psi_k^-}{\partial x}(x_2,z) = -2\mathbf{i}p\chi_k(x_2,z) - \displaystyle\sum_{\ell=1}^{M^2(E_2(k))} \mathbf{i}p_2^\ell(E_2(k))\left\langle\psi_k^-(x_2,\cdot)\chi_\ell(x_2,\cdot)\right\rangle\chi_\ell(x_2,z) & \\ \qquad + \displaystyle\sum_{\ell=M^2(E_2(k))+1}^{\infty} p_2^\ell(E_2(k))\left\langle\psi_k^-(x_2,\cdot)\chi_\ell(x_2,\cdot)\right\rangle\chi_\ell(x_1,z). & \end{cases} \tag{9.2.2}$$

The reflexion and transmission coefficients are defined by

$$\begin{cases} R^1_{k\to\ell} = \dfrac{p_1^\ell(E_1(k))}{p}\left|\delta_{k\ell} - \langle\chi_\ell(x_1,\cdot)\psi_k^+(x_1,\cdot)\rangle\right|^2 & \text{if } \ell \le M^1(E_1(k)), \\ R^1_{k\to\ell} = 0 & \text{if } \ell > M^1(E_1(k)), \end{cases}$$

$$\begin{cases} T^1_{k\to\ell} = \dfrac{p_2^\ell(E_1(k))}{p}\left|\langle\chi_\ell(x_2,\cdot)\psi_k^+(x_2,\cdot)\rangle\right|^2 & \text{if } \ell \le M^2(E_1(k)), \\ T^1_{k\to\ell} = 0 & \text{if } \ell > M^2(E_1(k)), \end{cases}$$

and respectively

$$\begin{cases} R^2_{k\to\ell} = \dfrac{p_2^\ell(E_2(k))}{p}\left|\delta_{k\ell} - \langle\chi_\ell(x_2,\cdot)\psi_k^-(x_2,\cdot)\rangle\right|^2 & \text{if } \ell \le M^2(E_2(k)), \\ R^2_{k\to\ell} = 0 & \text{if } \ell > M^2(E_2(k)), \end{cases}$$

$$\begin{cases} T^2_{k\to\ell} = \dfrac{p_1^\ell(E_2(k))}{p}\left|\langle\chi_\ell(x_1,\cdot)\psi_k^-(x_1,\cdot)\rangle\right|^2 & \text{if } \ell \le M^1(E_2(k)), \\ T^2_{k\to\ell} = 0 & \text{if } \ell > M^1(E_2(k)). \end{cases}$$

In other words, the open boundary conditions express the fact that a wave coming from a reservoir and penetrating the quantum region at $x = x_1$ or $x = x_2$ is partially reflected and transmitted by the potential barrier. The transmitted part can be an evanescent wave. A simplified scheme is presented in Figure 9.1

We have the following reciprocity relations

$$R^1_{k\to\ell} = R^1_{\ell\to k} \tag{9.2.3}$$

$$R^2_{k\to\ell} = R^2_{\ell\to k} \tag{9.2.4}$$

$$T^2_{\ell\to k}(-p_2^\ell(E_1(k))) = T^1_{k\to\ell}(p) \tag{9.2.5}$$

$$T^1_{\ell\to k}(p_1^\ell(E_2(k))) = T^2_{k\to\ell}(-p) \tag{9.2.6}$$

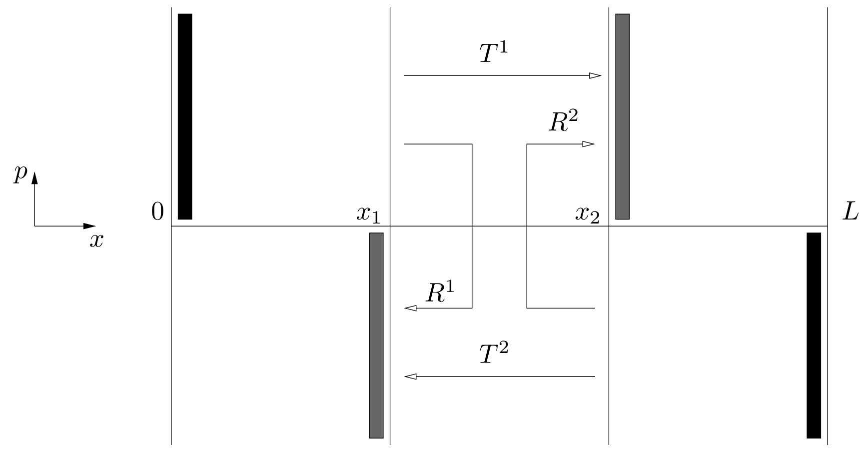

Figure 9.1: Scheme of the transmission and reflexion at the classical/quantum interface.

We denote by

$$R_k^1 = \sum_\ell R_{k\to\ell}^1 \quad ; \qquad R_k^2 = \sum_\ell R_{k\to\ell}^2,$$
$$T_k^1 = \sum_\ell T_{k\to\ell}^1 \quad ; \qquad T_k^2 = \sum_\ell T_{k\to\ell}^2.$$

Moreover we can prove [6] that we have

$$R_k^1 + T_k^1 = 1 \quad \text{for } 1 \le k \le M^1(E_1(k)), \tag{9.2.7}$$
$$R_k^2 + T_k^2 = 1 \quad \text{for } 1 \le k \le M^2(E_2(k)). \tag{9.2.8}$$

If we assume temporarily that the the distribution function $(f_k(x,p))_{k\ge1}$ of electrons entering the quantum region is known : its values are $(f_k(x_1,p))_{k\ge1}$ for $p > 0$ and $(f_k(x_2,p))_{k\ge2}$ for $p < 0$. Then, following [2], these values allow us to construct the electron density :

$$N(x,z) = \sum_{k=1}^{+\infty} \int_{p>0} f_k(x_1,p)|\psi_k^+(x,z)|^2\,dp + \sum_{k=1}^{+\infty} \int_{p<0} f_k(x_2,p)|\psi_k^-(x,z)|^2\,dp. \tag{9.2.9}$$

And the particle current is given by :

$$\begin{aligned} J_Q(x) = \ & \frac{\hbar}{m}\sum_{k=1}^{+\infty}\int_0^1\int_{p>0} f_k(x_1,p)\mathcal{I}m\,(\overline{\psi_k^+}(x,z)\nabla_x\psi_k^+(x,z))\,dpdz \\ & +\frac{\hbar}{m}\sum_{k=1}^{+\infty}\int_0^1\int_{p<0} f_k(x_2,p)\mathcal{I}m\,(\overline{\psi_k^-}(x,z)\nabla_x\psi_k^-(x,z))\,dpdz. \end{aligned} \tag{9.2.10}$$

9.2.2 The classical region

In the classical region, the transport is diffusive. We consider a stationary drift-diffusion model on the disconnected domain Ω :

$$-\frac{d}{dx}J(x) \ = \ 0, \tag{9.2.11}$$

$$J(x) \quad = \quad \mathbb{D}(\frac{d}{dx}N_s(x) + \beta N_s(x)\frac{d}{dx}U_s(x)), \tag{9.2.12}$$

where N_s is the surface density, $\mathbb{D}$ denotes the diffusion coefficient $\mathbb{D} = \mu k_B T$ for a constant mobility μ, T is the temperature of the lattice, k_B is the Boltzmann constant and β is defined by $\beta = 1/(k_B T)$. The effective energy U_s is given by

$$U_s = -k_B T \log\left(\sum_{k=1}^{+\infty} e^{-\beta\epsilon_k}\right). \tag{9.2.13}$$

We note the repartition function $\mathcal{Z}$ by

$$\mathcal{Z}(x) = \sum_{k=1}^{+\infty} e^{-\beta\epsilon_k(x)}. \tag{9.2.14}$$

Introducing the slotboom variable $u(x) = N_s(x)/\mathcal{Z}(x)$, the Fermi level is then defined by $\epsilon_F(x) = k_B T \log u(x)$ and the current (9.2.12) can be rewritten :

$$J(x) = \mathbb{D}(\mathcal{Z}(x)\frac{d}{dx}u(x)). \tag{9.2.15}$$

In order to have a well-posed problem, we have to indicate suitable boundary conditions. Following [1, 5], we impose Dirichlet boundary conditions at $x = 0$ and $x = L$,

$$N_s(0) = n_D \; ; \qquad N_s(L) = n_D, \tag{9.2.16}$$

where n_D is a doping concentration which is given. The two open sets $(0, x_1)$ and $(0, x_2)$ are connected through the conditions :

$$J(x_1) = J(x_2) := J, \tag{9.2.17}$$
$$u(x_1) - u(x_2) = e^{\beta\epsilon_F(x_1)} - e^{\beta\epsilon_F(x_2)} = \theta_Q J, \tag{9.2.18}$$

where the positive number θ_Q depends on the reflexion-transmission coefficient. This dependence will be clarify below. It is easy to show that the stationary problem (9.2.11)-(9.2.12) coupled with the boundary condition (9.2.16)-(9.2.17)-(9.2.18) is well-posed for a positive θ_Q.

From the surface density, we construct a distribution function in the classical region by assuming that we are at the thermal equilibrium and then the distribution function is Maxwellian :

$$f_k(x,p) = N_s(x)\mathcal{M}_k(p) \; ; \qquad \mathcal{M}_k(p) = \frac{1}{\sqrt{2\pi m}\mathcal{Z}} \exp\left(-\beta\frac{p^2}{2m} - \beta\epsilon_k(x)\right). \tag{9.2.19}$$

The occupation number of the kth subband is then obtained by

$$\rho_k(x) = \int_{\mathbb{R}} f_k(x,p)\,dp = u(x)e^{-\beta\epsilon_k(x)}.$$

Finally the total density is

$$N(x,z) = \sum_{k=1}^{+\infty} \rho_k(x) |\chi_k(x,z)|^2 = u(x) \sum_{k=1}^{+\infty} e^{-\beta\epsilon_k(x)} |\chi_k(x,z)|^2. \qquad (9.2.20)$$

The electrostatic potential generated by the electrons themselves V is the solution of the Poisson equation

$$-\mathrm{div}_{\,x,z}(\varepsilon_R \nabla_{x,z} V) = \frac{e}{\varepsilon_0}(N - N_D), \qquad (9.2.21)$$

where ε_R is the relative permittivity, ε_0 the permittivity constant in vacuum and N_D is the doping density.

9.2.3 The connection conditions

We explain here the condition (9.2.18) and the constant θ_Q. Following [1], this condition and the constant θ_Q provide from the continuity of the current through the interfaces. In fact, (9.2.11) implies that the current is constant on the classical region and with (9.2.17) we impose that this constant is the same. The continuity of the current is a classical property of semiconductors [2, 1]. Let us rewrite the expression (9.2.10).

From the Schrödinger equation satisfied by ψ_k^+ (9.2.1) and ψ_k^- (9.2.2),

$$\frac{d}{dx} \mathcal{I}m\,(\overline{\psi_k^{\pm}}(x,z) \frac{d}{dx} \psi_k^{\pm}(x,z)) = 0.$$

Thus we deduce from (9.2.10) that the current J_Q is constant on the quantum region. By integrating on $[x_1, x_2] \times [0,1]$, we find

$$\int_0^1 \mathcal{I}m\,(\overline{\psi_k^{\pm}}(x_1,z) \frac{d}{dx} \psi_k^{\pm}(x_1,z)\, dz = \int_0^1 \mathcal{I}m\,(\overline{\psi_k^{\pm}}(x_2,z) \frac{d}{dx} \psi_k^{\pm}(x_2,z)\, dz.$$

Using this last identity and the open boundary conditions satisfied by $\psi_k^{\pm}$ (9.2.1)–(9.2.2), we obtain after straightforward calculations

$$J_Q = \sum_{k=1}^{+\infty} \int_0^{+\infty} (\frac{p}{m} T_k^1(p) f_k(x_1,p) - \frac{p}{m} T_k^2(p) f_k(x_2,-p))\, dp.$$

We recall that we assume to be at the thermal equilibrium and then the distribution functions for $x = x_1$ and $x = x_2$ are Maxwellian :

$$f_k(x,p) = u(x) M(p) e^{-\beta\epsilon_k(x)}\ ; \qquad \text{where} \quad M(p) = \frac{1}{\sqrt{2\pi m}} e^{-\beta p^2/(2m)}.$$

Taking advantage of this Maxwellian dependence of the distribution functions and of the reciprocity relation (9.2.5) and (9.2.7) we have

$$J_Q = (u(x_1) - u(x_2)) \sum_{k=1}^{+\infty} \int_0^{+\infty} \frac{p}{m} T_k^1(p) M(p) e^{-\beta\epsilon_k(x_1)}\, dp. \qquad (9.2.22)$$

Thus if we set

$$(\theta_Q)^{-1} = \sum_{k=1}^{+\infty} \int_0^{+\infty} \frac{p}{m} T_k^1(p) M(p) e^{-\beta \epsilon_k(x_1)}\, dp, \qquad (9.2.23)$$

then the condition (9.2.18) expresses the continuity of the current at the interface.

9.3 Numerical resolution

9.3.1 Algorithmic approach

Our typical devices of interest are very small double-gate MOSFET presented in Chapter 8. A schematic representation of the device is given in Figure 8.1. We assume that the model is invariant in the y direction and the problem is then reduced to the domain $[0, L] \times [0, \ell]$ of the (x, z) domain. The larged doped region of the drain and the source are assumed to be small electrons reservoirs. The source and the drain composed the classical zone. In the vicinity of the contact, the potential does not depend of the transport direction. The active zone is then modeled by the Schrödinger-Poisson model for the subband. A schematic representation of the different regions of the device is given in Figure 9.2.

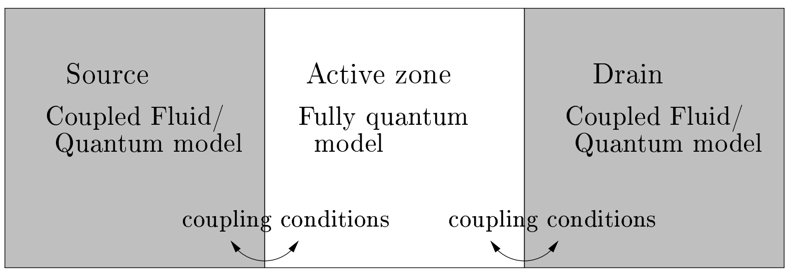

Figure 9.2: Schematic representation of the different regions of the description.

A algorithm for the coupled problem is the following. First, let assume that the potential V is given. We diagonalize the 1D Schrödinger operator in the transversal direction and find the eigenvectors $\chi_k[V]$ and the eigenvalues $\epsilon_k[V]$ of the Hamiltonian. We compute then the scattering states $\psi_k^{\pm}$ thanks to the SDM/WKB method and the reflection and transmission coefficients of the quantum region for the potential $\widetilde{V}$. Therefore a value of the coupling constant θ_Q is deduced from (9.2.23). The knowledge of this value allows us to solve the drift-diffusion problem (9.2.11) with the transmission conditions (9.2.16)–(9.2.18). An alimentation function is deduced from (9.2.19), which together with the scattering states, allows us to construct a quantum density according to (9.2.9). Then we can solve the Poisson equation and find a new value of the potential V. The iteration can then be continued.

9.3.2 Numerical results

We present here the first results obtained with the simulation. These results are close to the one observed in the previous section. For instance, Fig. 9.3 presents the evolution of the density of the charge carriers and Fig. 9.4 the potential energy. We notice that these profiles are really similar to those obtained in the previous chapter. But we remark a higher value of the electron density in the canal in this case.

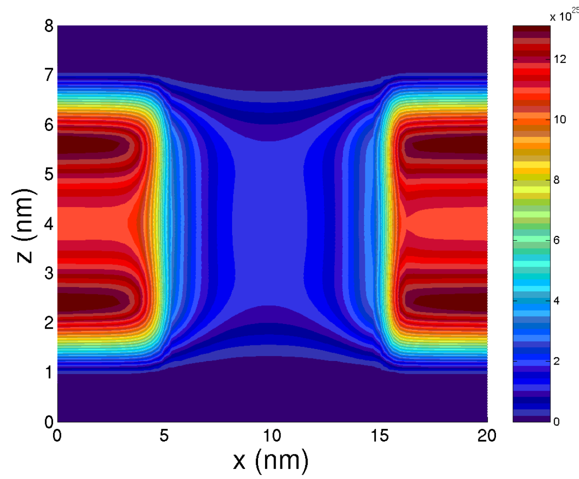

Figure 9.3: Electron density for an applied Drain-Source potential $V_{DS} = 0V$.

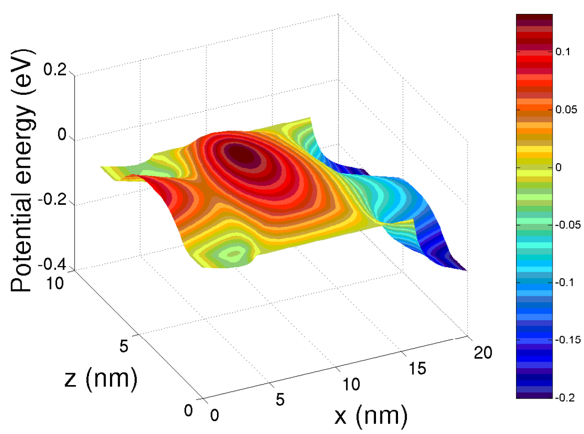

Figure 9.4: Potential energy when there is no applied gate voltage and $V_{DS} = 0.2V$. The energy potential barrier between the source and the channel is visible.

However, the values of the current are bigger than those calculated in the previous chapter. The I-V characteristic is presented in Fig. 9.5. In fact, by using the Schrödinger equation, we assume that the transport is ballistic in the canal whereas the drift-diffusion equation used in the previous section is a fluid model which describes a highly collisional motion.

Fig. 9.6 gives the evolution of the three first energy levels $\epsilon_k(x)$ for an applied drain source voltage $V_{DS} = 0.1$V. These energy levels present a small difference in the canal

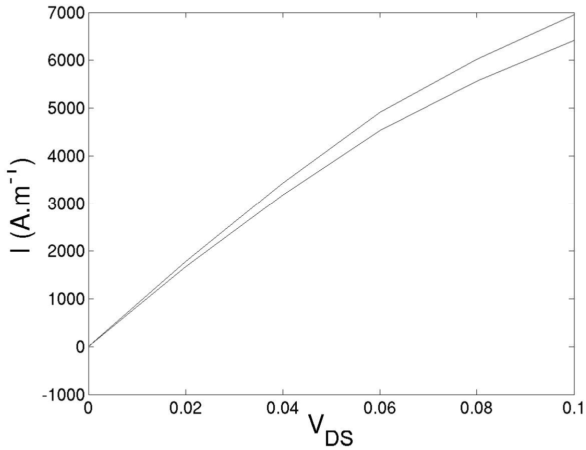

Figure 9.5: I-V characteristics of the device for $V_{GS} = 0$V and $V_{GS} = 0.1$V.

with the profiles observed in Fig. 8.5. We can make the same remarks as in the previous chapter concerning the difference between the transversal and the longitudinal case.

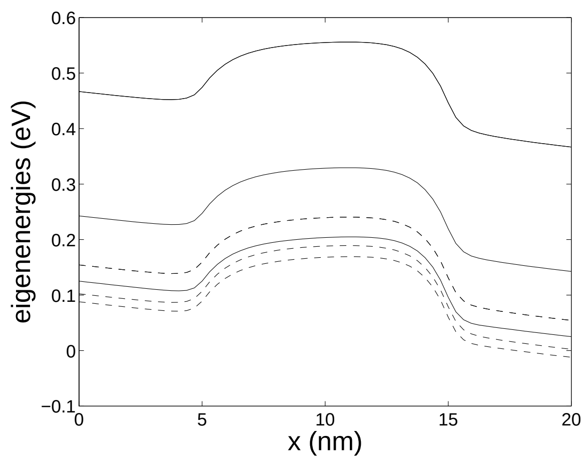

Figure 9.6: The 3 first energy levels $\epsilon_k(x)$ for $V_{DS} = 0.1$V for $m_z^* = m_t^*$ and $m_z^* = m_t^*$ (dotted line).

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Appendix

Appendix A

Technical inequalities

In this first appendix, we just recall, for the convenient of the reader, without any proof some usefull inequality used all along this work.

A.1 Young inequality

For a given function h, if we consider the Legendre transform h^*, we have for all positive numbers x and y, $xy \leq h(x) + h^*(y)$. Taking $h(z) = z\log z - z$, we deduce:

$$\forall\, x > 0,\ y \geq 0, \quad xy \leq x\log x - x + e^y. \tag{A.1.1}$$

Thus, for all $\varepsilon > 0$, we have

$$\forall\, x > 0,\ y \geq 0, \quad xy = \varepsilon(\frac{x}{\varepsilon}y) \leq x\log x - x(1 + \log\varepsilon) + \varepsilon e^y. \tag{A.1.2}$$

A.2 Trudinger inequality

We recall here the Trudinger inequality in 2D [3]. Let $\omega \subset \mathbb{R}^2$ be a regular bounded domain. There exists a constant $\gamma > 0$ depending only on ω such that, for all $u \in H^1(\omega)$, we have

$$\int_\omega e^{\gamma \frac{u(x)^2}{\|u\|^2_{H^1(\omega)}}}\, dx < \infty. \tag{A.2.3}$$

A.3 Csiszàr-Kullback inequality

Finally we present a form of the wellknown Csiszàr-Kullback inequalities. This inequality is very usefull for the analysis of the long time behaviour with a logarithmic entropy [1, 2, 5]. Let ω be a regular domain of $\mathbb{R}^d$, $d \in \mathbb{N}^*$. Let n_1 and n_2 be two nonnegative functions in $L^1(\omega)$ such that $\int_\omega n_1\, dx = \int_\omega n_2\, dx = N_0$. We have

$$\|n_1 - n_2\|^2_{L^1(\omega)} \leq 2N_0 \int_\omega n_1 \log\frac{n_1}{n_2}\, dx. \tag{A.3.4}$$

Appendix B

Spectral properties of the Hamiltonian

In this appendix, we give some properties of eigenfunctions and eigenvalues of the Schrödinger operator in the z variable. Most of these properties, which are used along the paper are either proved or can be proved by straightforwardly adapting the techniques of the book of Pöschel and Trubowitz [6]. Therefore, very few proofs are provided in this appendix.

For a given real valued function V in $L^2(0,1)$, let $H[V]$ be the Schrödinger operator

$$H[V] := -\frac{1}{2}\frac{d^2}{dz^2} + V(z)$$

defined on the domain $D(H[V]) = H^2(0,1) \cap H_0^1(0,1)$.

This operator admits a strictly increasing sequence of real eigenvalues $(\epsilon_k[V])_{k\geq 1}$ going to $+\infty$. The corresponding eigenvectors,denoted by $(\chi_k[V](z))_{k\geq 1}$ (chosen such that $\chi_k'(0) > 0$), form an orthonormal basis of $L^2(0,1)$. They satisfy of course

$$\begin{cases} -\dfrac{1}{2}\dfrac{d^2}{dz^2}\chi_k + V\chi_k = \epsilon_k\chi_k\,, \\ \chi_k \in H_0^1(0,1), \qquad \displaystyle\int_0^1 \chi_k\chi_\ell\, dz = \delta_{kl}. \end{cases} \tag{B.0.1}$$

Obviously, for $V = 0$, we have $\epsilon_k[0] = \frac{1}{2}\pi^2k^2$ and $\chi_k[0](z) = \sqrt{2}\sin(\pi k z)$. Moreover an immediat consequence of the Min-Max formula [4] is

$$\text{if } U \leq V \text{ a.e. in } (0,1) \quad \text{then} \quad \forall\, k \geq 1, \quad \epsilon_k[U] \leq \epsilon_k[V].$$

In the sequel we will use the standard notation $\langle f \rangle = \int_0^1 f(z)\,dz$ and when there is no confusion possible ϵ_k will stand for $\epsilon_k[V]$ and χ_k for $\chi_k[V]$.

Lemma B.0.1 *Let U and V be two real-valued functions in $L^2(0,1)$ such that $U - V \in L^\infty(0,1)$. Then the corresponding eigenvalues verify*

$$|\epsilon_k[U] - \epsilon_k[V]| \leq \|U - V\|_{L^\infty(0,1)}. \tag{B.0.2}$$

In particular, the case $V = 0$ gives $|\epsilon_k[U] - \dfrac{1}{2}\pi^2k^2| \leq \|U\|_{L^\infty(0,1)}$.

Moreover, following the study of the spectral properties of $H[V]$ in Chapter 2 of [6], we have the following lemma:

Lemma B.0.2 *There exists a positive constant C_V depending only on $\|V\|_{L^2(0,1)}$ such that*

$$|\epsilon_k[V] - \frac{1}{2}\pi^2 k^2| \leq C_V \quad ; \quad \|\chi_k[V] - \sqrt{2}\,\sin(\pi k z)\|_{L^\infty(0,1)} \leq C_V.$$

Moreover the constant C_V can be chosen such that $C_V \leq C_1 \exp(C_2\|V\|_{L^2(0,1)})$, where the constants C_1 and C_2 are independent of V and k.

Lemma B.0.3 *Let $V = V(\lambda, z) \in L^\infty_{loc}(\lambda, L^2_z(0,1))$ where λ is a real parameter (typically $\lambda = t$ or $\lambda = x_i$). Let us shortly denote ϵ_k instead of $\epsilon_k[V(\lambda,\cdot)]$ and χ_k instead of $\chi_k[V(\lambda,\cdot)]$. Assume that $\partial_\lambda V \in L^1_{loc}(\lambda, L^2_z(0,1))$. Then*
(i) $\partial_\lambda \epsilon_k \in L^1_{loc}$ and

$$\partial_\lambda \epsilon_k = \langle |\chi_k|^2 \partial_\lambda V\rangle.$$

(ii) $\partial_\lambda \chi_k \in L^1_{loc}(\lambda, L^\infty_z(0,1))$ and we have

$$\partial_\lambda \chi_k = \sum_{\ell \neq k} \frac{\langle \chi_k\, \chi_\ell\, \partial_\lambda V\rangle}{\epsilon_k - \epsilon_\ell}\chi_\ell.$$

Lemma B.0.4 *Let V and $\widetilde{V}$ be two real-valued functions in $L^2(0,1)$. Then there exist two positive constants C_1 and C_2 independent of k, V and $\widetilde{V}$ such that*

$$|\epsilon_k[V] - \epsilon_k[\widetilde{V}]| \leq C_1 \exp(C_2(\|V\|_{L^2(0,1)} + \|\widetilde{V}\|_{L^2(0,1)}))\|V - \widetilde{V}\|_{L^1(0,1)}\,. \qquad \text{(B.0.3)}$$

And,

$$\|\chi_k[V] - \chi_k[\widetilde{V}]\|_{L^\infty(0,1)} \leq C_1 \exp(C_2(\|V\|_{L^2(0,1)} + \|\widetilde{V}\|_{L^2(0,1)}))\|V - \widetilde{V}\|_{L^1(0,1)}\,. \qquad \text{(B.0.4)}$$

Proof. The estimate (B.0.3) is an easy consequence of Lemmata B.0.2 and B.0.3.

Let us prove (B.0.4). Without loss of generality, we assume that $\epsilon_k[V] > 0$ (by shifting V and $\widetilde{V}$ by the same constant). Let us denote

$$u_k = \frac{\chi_k[\widetilde{V}]'(0)}{\chi_k[V]'(0)}\chi_k[V] \quad ; \quad \widetilde{u_k} = \chi_k[\widetilde{V}], \qquad \text{(B.0.5)}$$

so that $u_k'(0) = \widetilde{u_k}'(0)$. Writing the equation satisfied by $u_k - \widetilde{u_k}$ and proceeding like in the proof of Lemma 1, Chapter 1 of [6], we have

$$\begin{aligned} u_k(z) - \widetilde{u_k}(z) = \; & 2\int_0^z s(z-t)V(t)(u_k - \widetilde{u_k})(t)\,dt \\ & +2\int_0^z s(z-t)\widetilde{u_k}(t)((V-\widetilde{V})(t) - (\epsilon_k[V] - \epsilon_k[\widetilde{V}]))\,dt, \end{aligned}$$

where,

$$s(t) = \frac{\sin(\sqrt{2\epsilon_k[V]}\,t)}{\sqrt{2\epsilon_k[V]}}.$$

By a Gronwall argument, we prove (B.0.4) for the difference $u_k - \widetilde{u_k}$. We finally deduce the result for $\chi_k[V] - \chi_k[\widetilde{V}]$ by using the property $\displaystyle\int_0^1 |\chi_k|^2 \, dz = 1$. □

Lemma B.0.5 *Let $V \in L^2(0,1)$ such that $V \geq 0$, then the eigenvectors of the Schödinger operator satisfy*

$$\|\chi_k[V]\|_{L^\infty(0,1)} \leq C(1 + \|V\|^{1/2}_{L^2(0,1)}).$$

Proof. The result of Lemma 1 Chapter 1 of [6] provides :

$$\chi_k(z) = A_k \sin(\sqrt{2\epsilon_k} z) + 2 \int_0^z \frac{\sin(\sqrt{2\epsilon_k}(z-t))}{\sqrt{2\epsilon_k}} V(t)\chi_k(t)\, dt, \tag{B.0.6}$$

where A_k is a nonnegative constant to be determined. Thanks to a Cauchy-Schwarz inequality, we deduced

$$\left| \int_0^z \frac{\sin(\sqrt{2\epsilon_k}(z-t))}{\sqrt{2\epsilon_k}} V(t)\chi_k(t)\, dt \right| \leq \frac{\int_0^1 V(t)|\chi_k(t)|\, dt}{\sqrt{2\epsilon_k}} \leq \frac{\langle |\chi_k|^2 V\rangle^{1/2}}{\sqrt{2\epsilon_k}} \|V\|^{1/2}_{L^2(0,1)}.$$

Moreover, from (B.0.1),

$$\epsilon_k = \frac{1}{2}\langle |\partial_z \chi_k|^2\rangle + \langle |\chi_k|^2 V\rangle \geq \langle |\chi_k|^2 V\rangle$$

Thus,

$$\left| \int_0^z \frac{\sin(\sqrt{2\epsilon_k}(z-t))}{\sqrt{2\epsilon_k}} V(t)\chi_k(t)\, dt \right| \leq \frac{1}{\sqrt{2}} \|V\|^{1/2}_{L^2(0,1)}. \tag{B.0.7}$$

Thus from (B.0.6) we have for all $z \in [0,1]$

$$|\chi_k(z)| \leq A_k + \sqrt{2}\, \|V\|^{1/2}_{L^2(0,1)}. \tag{B.0.8}$$

Now, we will use the condition $\|\chi_k\|_{L^2(0,1)} = 1$ to bound A_k. If we use the expression of χ_k (B.0.6) in the identity $\int_0^1 \chi_k^2 \, dz = 1$, we obtain

$$1 \geq A_k^2 \int_0^1 \sin(\sqrt{2\epsilon_k} z)^2 \, dz + 4A_k \int_0^1 \sin(\sqrt{2\epsilon_k} z) \int_0^z \frac{\sin(\sqrt{2\epsilon_k}(z-t))}{\sqrt{2\epsilon_k}} V(t)\chi_k(t)\, dt dx. \tag{B.0.9}$$

For the second term we have from (B.0.7)

$$\left| \int_0^1 \sin(\sqrt{2\epsilon_k} z) \int_0^z \frac{\sin(\sqrt{2\epsilon_k}(z-t))}{\sqrt{2\epsilon_k}} V(t)\chi_k(t)\, dt dx \right| \leq \frac{1}{\sqrt{2}} \|V\|^{1/2}_{L^2(0,1)}.$$

And we can calculate

$$\int_0^1 [\sin(\sqrt{2\epsilon_k} z)]^2 \, dz = \frac{1}{2} - \frac{\sin(2\sqrt{2\epsilon_k})}{4\sqrt{2\epsilon_k}}.$$

We have assumed that $V \geq 0$. It implies $\epsilon_k[V] \geq \epsilon[0] = \frac{1}{2}\pi^2 k^2$, for all $k \geq 1$. Thus we can inject these remarks in (B.0.9), it leads to

$$1 \geq A_k^2 \left(\frac{1}{2} - \frac{1}{4\pi}\right) - 2\sqrt{2}\, A_k \|V\|_{L^2(0,1)}^{1/2}.$$

This implies that there exists a nonnegative contant C such that

$$A_k \leq C(1 + \|V\|_{L^2(0,1)}^{1/2}), \forall\, k \geq 1.$$

It remains to inject this last estimate in (B.0.8) to conclude the proof. □

Lemma B.0.6 *Let V be in $L^2(0,1)$. Then the corresponding eigenvectors satisfy*

$$\forall\, k \geq 1, \qquad \|\chi_k\|_{H^1(0,1)} \leq C(k + \|V\|_{L^2(0,1)}^{2/3}). \tag{B.0.10}$$

Proof. From (B.0.1) we deduce

$$\frac{1}{2}\langle|\partial_z \chi_k|^2\rangle = \epsilon_k - \langle|\chi_k|^2 V\rangle.$$

Moreover from Lemma B.0.3 and the fact that $\epsilon_k[0] = \frac{1}{2}\pi^2 k^2$, we have

$$\epsilon_k[V] = \frac{1}{2}\pi^2 k^2 + \int_0^1 \langle|\chi_k[sV]|^2 V\rangle\, ds.$$

The Gagliardo-Nirenberg inequality gives

$$\|\chi_k\|_{L^4(0,1)}^2 \leq C\|\chi_k\|_{L^2(0,1)}^{3/2}\|\chi_k\|_{H^1(0,1)}^{1/2} = C\|\chi_k\|_{H^1(0,1)}^{1/2}. \tag{B.0.11}$$

Therefore,

$$\|\chi_k[V]\|_{H^1(0,1)}^2 \leq C(k^2 + \|V\|_{L^2(0,1)} \int_0^1 \|\chi_k[sV]\|_{H^1(0,1)}^{1/2}\, ds + \|V\|_{L^2(0,1)}^{4/3}), \tag{B.0.12}$$

where we have used the wellknown Young inequality: $xy \leq \frac{1}{4}x^4 + \frac{3}{4}x^{4/3}$. If we replace V by σV for $\sigma \in [0,1]$ and integrate over σ on $(0,1)$, we find

$$\int_0^1 \|\chi_k[\sigma V]\|_{H^1(0,1)}^2 \leq C(k^2 + \int_0^1 \int_0^1 \|\sigma V\|_{L^2(0,1)}\|\chi_k[s\sigma V]\|_{H^1(0,1)}^{1/2}\, ds d\sigma + \|V\|_{L^2(0,1)}^{4/3}).$$

The second term of the right hand side can be rewrite as

$$\int_0^1 \int_0^\sigma \|V\|_{L^2(0,1)}\|\chi_k[tV]\|_{H^1(0,1)}^{1/2}\, dt d\sigma \leq C_\delta \|V\|_{L^2(0,1)}^{4/3} + \delta \int_0^1 \int_0^1 \|\chi_k[tV]\|_{H^1(0,1)}^2\, dt d\sigma,$$

for all $\delta > 0$. Thus, if we fix δ small enough there exists a nonnegative constant still denoted C such that

$$\int_0^1 \|\chi_k[\sigma V]\|_{H^1(0,1)}^2 \leq C(k^2 + \|V\|_{L^2(0,1)}^{4/3}). \tag{B.0.13}$$

We can then inject (B.0.13) in (B.0.12). □

This last two lemmata allow us to improve the estimate B.0.3

Lemma B.0.7 *Let V and $\widetilde{V}$ be two given nonnegative potentials in $L^2(0,1)$. Then there exists a nonnegative constant C such that*

$$|\epsilon_k[V] - \epsilon_k[\widetilde{V}]| \leq C(1 + \|V\|^{1/2}_{L^2_z(0,1)} + \|\widetilde{V}\|^{1/2}_{L^2_z(0,1)})\|V - \widetilde{V}\|_{L^2_z(0,1)}. \tag{B.0.14}$$

And

$$|\epsilon_k[V] - \epsilon_k[\widetilde{V}]| \leq C(k^{1/2} + \|V\|^{1/3}_{L^2_z(0,1)} + \|\widetilde{V}\|^{1/3}_{L^2_z(0,1)})\|V - \widetilde{V}\|_{L^2_z(0,1)}. \tag{B.0.15}$$

Proof. This is an easy consequence of Lemma B.0.5 and B.0.3. Indeed, if we denote for $\lambda \in [0,1]$, $W(\lambda, z) = \widetilde{V} + \lambda(V - \widetilde{V})$ and $\epsilon_k(\lambda) = \epsilon_k[W(\lambda,\cdot)]$, we have

$$\epsilon_k[V] - \epsilon_k[\widetilde{V}] = \int_0^1 \partial_\lambda \epsilon_k(\lambda)\, d\lambda = \int_0^1 \langle |\chi_k[W(\lambda,\cdot)](z)|^2 (V - \widetilde{V})\rangle\, d\lambda.$$

Thus, we have

$$|\epsilon_k[V] - \epsilon_k[\widetilde{V}]| \leq \|V - \widetilde{V}\|_{L^2(0,1)} \int_0^1 \|\chi_k[W(\lambda,\cdot)]\|^2_{L^4(0,1)}\, d\lambda.$$

The estimate (B.0.14) follows then from Lemma B.0.5 and the interpolation:

$$\|\chi_k[W(\lambda,\cdot)]\|^2_{L^4(0,1)} \leq \|\chi_k[W(\lambda,\cdot)]\|_{L^2(0,1)} \|\chi_k[W(\lambda,\cdot)]\|_{L^\infty(0,1)}.$$

The estimate (B.0.15) is a consequence of (B.0.11) and (B.0.10). □

Now, we give two technical lemmata, where the potential is defined on Ω. We recall that $(x,z) \in \Omega = \omega \times (0,1)$ where ω is a bounded regular domain of $\mathbb{R}^2$.

Lemma B.0.8 *Assume that $V \in H^1(\Omega)$ and let ϵ_k be the eigenvalues defined by (4.1.3). Then, for all $\alpha \geq 0$ and $q \in [1, +\infty)$, we have*

$$I_\alpha := \frac{1}{\mathcal{Z}} \sum_k |\epsilon_k|^\alpha\, e^{-\epsilon_k} \in L^q(\omega),$$

where $\mathcal{Z} = \sum_k e^{-\epsilon_k}$. The L^q norm of I_α is bounded by a constant only depending on α, q and $\|V\|_{H^1}$.

Proof. Lemma B.0.2 states that the eigenvalues and eigenvectors of (4.1.3) satisfy the (uniform in p) estimate

$$\left|\epsilon_k(x) - \frac{\pi^2}{2}k^2\right| + \|\chi_k(x,\cdot)\|_{L^\infty_z} \leq C_1\, e^{C_2 \|V(x,\cdot)\|_{L^2_z}}. \tag{B.0.16}$$

It is enough to show that

$$I_\alpha(x) \leq C_3\, e^{\alpha C_2 \|V(x,\cdot)\|_{L^2_z}}. \tag{B.0.17}$$

Indeed, since $\|V(x,\cdot)\|_{L^2_z}$ is bounded in $H^1(\omega)$, the Trudinger inequality,

$$\int_{\mathcal{O}} \exp(|u|^{N/(N-1)}) < +\infty \ , \qquad \forall u \in W^{1,N}(\mathcal{O}), \qquad \mathcal{O} \subset \mathbb{R}^N \tag{B.0.18}$$

implies that $e^{\|V(x,\cdot)\|^2_{L^2_z}} \in L^1(\omega)$, which ensures that $e^{\alpha C_2 \|V(x,\cdot)\|_{L^2_z}} \in L^q(\omega)$ for all $q < +\infty$ thus leading to the result.

Let us now prove (B.0.17). To this aim, we treat differently low and high energies. More precisely, we have

$$\begin{aligned} I_\alpha &= \frac{1}{\mathcal{Z}} \sum_{|\epsilon_k| \leq KA} |\epsilon_k|^\alpha e^{-\epsilon_k} + \frac{1}{\mathcal{Z}} \sum_{|\epsilon_k| \geq KA} |\epsilon_k|^\alpha e^{-\epsilon_k} \\ &\leq (KA)^\alpha + \frac{1}{\mathcal{Z}} \sum_{|\epsilon_k| \geq KA} |\epsilon_k|^\alpha e^{-\epsilon_k} \end{aligned} \tag{B.0.19}$$

where K is chosen larger than 2 ($K > 2$) and A is such that $|\epsilon_k - \frac{1}{2}\pi^2 k^2| < A$. This choice implies that

$$\frac{1}{2}k^2\pi^2 - A < \epsilon_k < \frac{1}{2}k^2\pi^2 + A$$

and, for high energies ($|\epsilon_k| \geq KA$), that we have

$$A < \frac{1}{2(K-1)}\, k^2\pi^2 \, .$$

Hence, the high energy contribution can be estimated as follows:

$$\begin{aligned} \sum_{|\epsilon_k| \geq KA} |\epsilon_k|^\alpha e^{-\epsilon_k} &\leq \sum_{k > \sqrt{2(K-1)A}/\pi} \left(\frac{1}{2}k^2\pi^2 + A\right)^\alpha e^{-k^2\pi^2/2}\, e^A \\ &\leq \left(1 + \frac{1}{K-1}\right)^\alpha e^A \sum_{k > \sqrt{2(K-1)A}/\pi} \left(\frac{1}{2}k^2\pi^2\right)^\alpha e^{-k^2\pi^2/2} \\ &\leq C_\alpha \left(1 + \frac{1}{K-1}\right)^\alpha e^A \int_{\sqrt{2(K-1)A}/\pi}^{\infty} \left(\frac{1}{2}\pi^2 x^2\right)^\alpha e^{-\pi^2 x^2/2}\, dx, \end{aligned}$$

where we used the elementary property:

$$\lim_{n \to +\infty} \frac{\displaystyle\sum_{k \geq n} f(k)}{\displaystyle\int_n^{+\infty} f(x)\, dx} = 1,$$

for any nonnegative function decaying at infinity and such that the following integral $\int_0^{+\infty} f(x)\, dx$ converges. Assuming that $\alpha \neq 0$ (the case $\alpha = 0$ is trivial), an integration by parts leads to the estimate

$$\int_{\sqrt{2(K-1)A}/\pi}^{\infty} \left(\frac{1}{2}\pi^2 x^2\right)^\alpha e^{-\pi^2 x^2/2}\, e^A\, dx \leq C((K-1)A)^{\alpha - 1/2} e^{-(K-1)A}\, e^A,$$

which leads to

$$\sum_{|\epsilon_k|\geq KA} |\epsilon_k|^\alpha e^{-\epsilon_k} \leq C_\alpha A^{\alpha-1/2} e^{-(K-1)A}\, e^A.$$

Besides, thanks to the choice of A, we obviously have

$$\sum_k e^{-\epsilon_k} \geq Ce^{-A}.$$

Therefore, going back to (B.0.19), we have

$$I_\alpha \leq (KA)^\alpha + C_\alpha A^{\alpha-1/2} e^{(3-K)A}.$$

Setting $K = 4$, we have a bound on $A^{-1/2}e^{(3-K)A}$ for large A. Thus we proved that $I \leq C_\alpha A^\alpha$ and (B.0.17) follows thanks to (B.0.16) by taking $A = C_1 \exp(C_2\|V(x,.)\|_{L^2_z})$.

□

Lemma B.0.9 *The map* $V \mapsto V_s = -\log(\sum_k e^{-\epsilon_k[V]})$ *is locally Lipschitz continuous from* $H^2(\Omega)$ *to* $H^2(\omega)$*, where* $(\epsilon_k[V])_k$ *denotes the whole set of eigenvalues of the Hamiltonian* $-\frac{1}{2}\frac{d^2}{dz^2} + V$*.*

Proof. Since the summation over k can be done easily, it is enough to show the result for the map $V \mapsto \epsilon_k[V]$. Let U, V be two bounded potentials of $H^2(\Omega)$. From Lemma B.0.1, we deduce easily that $\|\epsilon_k[U] - \epsilon_k[V]\|_{L^2(\omega)} \leq C\|U - V\|_{H^2(\Omega)}$. For the first derivative, we write with Lemma B.0.3 :

$$\begin{aligned}\int_\omega |\nabla_x \epsilon_k[U] - \nabla_x \epsilon_k[V]|^2\,dx \leq\ & 2\int_\Omega |\nabla_x(U-V)|^2 |\chi_k[U]|^4\,dxdz \\ & +2\int_\Omega |\nabla_x V|^2 (|\chi_k[U]|^2 - |\chi_k[V]|^2)^2\,dxdz.\end{aligned}$$

The Sobolev embedding of $H^2(\Omega)$ into $L^\infty(\Omega)$ implies that for all nonnegative constant C_2,

$$\exp(C_2(\|U\|_{L^2_z(0,1)} + \|V\|_{L^2_z(0,1)})) \in L^\infty(\omega).$$

Thus, with Lemma B.0.2 we have a bound of $\chi_k[U]$ in $L^\infty(\Omega)$ and with Lemma B.0.4,

$$\|\chi_k[U] - \chi_k[V]\|_{L^\infty(\Omega)} \leq C\|U - V\|_{H^2(\Omega)}. \tag{B.0.20}$$

We deduce,

$$\int_\omega |\nabla_x \epsilon_k[U] - \nabla_x \epsilon_k[V]|^2\,dx \leq C\|U - V\|^2_{H^1(\Omega)} + C\|U - V\|^2_{H^2(\Omega)}.$$

Now it remains to estimate the difference of the second derivative of $\epsilon_k[U] - \epsilon_k[V]$. We recall that from Lemma B.0.1, we deduce easily

$$\|\epsilon_k[U] - \epsilon_k[V]\|_{L^\infty(\omega)} \leq C\|U - V\|_{H^2(\Omega)}. \tag{B.0.21}$$

If $i = 1$ or 2, $j = 1$ or 2, by the expression of the derivatives stated in Lemma B.0.3, we have

$$\partial_{x_i x_j} \epsilon_k[V] = \int_0^1 \partial_{x_i x_j} V |\chi_k[V]|^2 \, dz + 2 \int_0^1 \chi_k[V] \partial_{x_i} \chi_k[V] \partial_{x_j} V \, dz.$$

As before, we can show the Lipschitz dependency in $V \in H^2(\Omega)$ of the first term of the right hand side. For the second one, we need the following result, which is proved below : there exists a positive constant δ_V depending only on $\|V\|_{H^2(\Omega)}$ such that

$$\forall\, (k, l) \in (\mathbb{N}^*)^2 \qquad |\epsilon_k[V] - \epsilon_\ell[V]| \geq \delta_V |k - l|^2. \tag{B.0.22}$$

Since $\chi_k[V]$ is bounded in $L^\infty(\Omega)$, using the expression of $\partial_{x_i} \chi_k[V]$ in Lemma B.0.3 and (B.0.22), we have $|\partial_{x_i} \chi_k[V]| \leq C \langle |\partial_{x_i} V| \rangle$. Therefore,

$$\begin{aligned} |\chi_k[U] \partial_{x_i} \chi_k[U] \partial_{x_j} U - \chi_k[V] \partial_{x_i} \chi_k[V] \partial_{x_j} V| &\leq C \, |\chi_k[U] - \chi_k[V]| \, \langle |\partial_{x_i} U| \rangle \, |\partial_{x_i} U| + \\ &+ C \, |\partial_{x_i} U| \, |\partial_{x_i} \chi_k[U] - \partial_{x_i} \chi_k[V]| + C \, \langle |\partial_{x_i} V| \rangle \, |\partial_{x_i} (U - V)|. \end{aligned}$$

Thus, it remains to see the Lipschitz dependency in V of $\partial_{x_i} \chi_k[V]$. We have

$$\begin{aligned} \partial_{x_i} (\chi_k[U] - \chi_k[V]) &= \sum_{\ell \neq k} \left(\frac{\langle \chi_k[U] \, \chi_\ell[U] \, \partial_{x_i} U \rangle}{\epsilon_k[U] - \epsilon_\ell[U]} \chi_\ell[U] - \frac{\langle \chi_k[V] \, \chi_\ell[V] \, \partial_{x_i} V \rangle}{\epsilon_k[V] - \epsilon_\ell[V]} \chi_\ell[V] \right) \\ &= \sum_{\ell \neq k} \frac{\langle \chi_k[U] \, \chi_\ell[U] \, \partial_{x_i} U - \chi_k[V] \, \chi_\ell[V] \, \partial_{x_i} V \rangle}{\epsilon_k[U] - \epsilon_\ell[U]} \chi_\ell[U] \\ &+ \sum_{\ell \neq k} \frac{\langle \chi_k[V] \, \chi_\ell[V] \, \partial_{x_i} V \rangle}{\epsilon_k[V] - \epsilon_\ell[V]} (\chi_\ell[U] - \chi_\ell[V]) \\ &+ \sum_{\ell \neq k} \langle \chi_k[V] \, \chi_\ell[V] \, \partial_{x_i} V \rangle \chi_\ell[V] \frac{\epsilon_k[V] - \epsilon_k[U] + \epsilon_\ell[U] - \epsilon_\ell[V]}{(\epsilon_k[U] - \epsilon_\ell[U])(\epsilon_k[V] - \epsilon_\ell[V])}. \end{aligned}$$

From (B.0.20), (B.0.21) and (B.0.22), we deduce that :

$$\|\partial_{x_i} \chi_k[U] - \partial_{x_i} \chi_k[V]\|_{L^2(\Omega)} \leq C(1 + \|\partial_{x_i} U\|_{L^2(\Omega)} + \|\partial_{x_i} V\|_{L^2(\Omega)}) \|U - V\|_{H^2(\Omega)}.$$

With the Sobolev embedding of $H^1(\Omega)$ into $L^2(\Omega)$, $\|\partial_{x_i} V\|_{L^2(\Omega)} \leq C \|V\|_{H^2(\Omega)}$. This concludes the proof of the Lipschitz dependency with respect to V of the second derivative.

Proof of (B.0.22). If $k = \ell$, this inequality is obvious. Let us first prove that there exists a constant δ_V depending only on $\|V\|_{H^2(\Omega)}$, such that

$$\min_{k \neq l} |\epsilon_k[V] - \epsilon_\ell[V]| \geq \delta_V. \tag{B.0.23}$$

If not, by the compact embedding of $H^2(\Omega)$ into $L^\infty(\Omega)$ it would be possible to find a sequence (V^n) converging to V in the L^∞ strong topology and a sequence k^n of integers such that $\epsilon_{k^n+1}[V^n] - \epsilon_{k^n}[V^n]$ converges to zero as n tends to $+\infty$. The asymptotic behaviour of the ϵ_k's deduced from Lemma B.0.1 implies that the sequence (k^n) is bounded, thus, up to an extraction, it is stationary : $k^n = k$. Besides, (B.0.2) implies that $\epsilon_k[V^n]$ converges to $\epsilon_k[V]$ and $\epsilon_{k+1}[V^n]$ to $\epsilon_{k+1}[V]$. Hence $\epsilon_k[V] = \epsilon_{k+1}[V]$, which is a contradiction with the fact that the eigenvalues are strictly increasing. Moreover, by (B.0.2), we have

$$\frac{\pi^2}{2}k^2 - \|V\|_{L^\infty(\Omega)} \leq \epsilon_k[V] \leq \frac{\pi^2}{2}k^2 + \|V\|_{L^\infty(\Omega)}.$$

Therefore, for any (k, l) :

$$|\epsilon_k[V] - \epsilon_\ell[V]| \geq \frac{\pi^2}{2}|k-\ell|^2 + \pi^2|k-\ell| - 2\|V\|_{L^\infty(\Omega)}.$$

Hence, if $\pi^2|k-\ell| \geq 2\|V\|_{L^\infty(\Omega)}$, then $|\epsilon_k[V] - \epsilon_\ell[V]| \geq \frac{\pi^2}{2}|k-\ell|^2$. From this inequality and (B.0.23) we deduce easily (B.0.22) (up to a change of δ_V). □

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Conclusion et Perspectives

L'objectif principal de cette thèse est de présenter et d'analyser des modèles décrivant le transport de particules confinées dans des dispositifs nanométriques à semiconducteurs. En utilisant la méthode de décomposition en sous-bandes, les modèles de Boltzmann-Schrödinger-Poisson et dérive-diffusion-Schrödinger-Poisson ont été introduits et étudiés. Ce dernier modèle a été utilisé pour réaliser une simulation numérique du transport des électrons dans un nanotransistor de type MOSFET. Ce découplage adiabatique des variables spatiales permet de réduire considérablement le coût numérique en utilisant une description classique peu onéreuse dans la direction de transport et en réstreignant la résolution de l'équation de Schrödinger à une seule dimension. Les applications sont nombreuses en nanotechnologies par exemple pour la détermination à moindre coût des caractéristiques électroniques de dispositifs nanométriques ou du design de nouveaux dispositifs où les électrons sont fortement confinés dans une direction.

Nous allons proposer quelques enrichissements qui peuvent être apportés dans la continuité de ces travaux. Tout d'abord, les études mathématiques rigoureuses de la limite de diffusion et des résultats d'existence n'ont été effectuées que dans le cas d'une statistique de Boltzmann. Il s'agit d'une approximation de la statistique de Fermi-Dirac. La limite de diffusion formelle de l'équation de Boltzmann des semiconducteurs pour une statistique de Fermi-Dirac est présentée au Chapitre 2. Les résultats d'existence et la limite rigoureuse des modèles avec une statistique de Fermi-Dirac restent encore à établir. On peut espérer grâce aux techniques développées dans cette thèse étendre les résultats dans le cas de la statistique de Boltzmann au cas Fermi-Dirac. Bien évidemment le problème d'existence pour le problème de Boltzmann-Schrödinger-Poisson dans le cas d'une dimension totale égale à 3 reste encore une question ouverte. Il serait également intéressant de comparer les simulations numériques pour les deux statistiques.

Par ailleurs, nous avons supposé dans la première partie et la troisième partie que la matrice de diffusion $\mathbb{D}$ était une donnée du problème et la résolution du modèle fluide quantique s'est effectué en utilisant certaines hypothèses sur cette matrice. Nous avons aussi vu au chapitre 5 que la prise en compte de la matrice de diffusion complique considérablement l'analyse. Cependant, lors de l'établissement de la limite de diffusion dans la seconde partie, il apparait clairement que la matrice de diffusion n'est pas une donnée mais dépend de quantités macroscopiques du problème. Cette dépendance reste à éclaicir pour une meilleure compréhension du système et une amélioration des simulations numériques.