Microscopic models for Fourier's law

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1

Introduction

C'est en dehors de l'équilibre que se produisent les événements les plus intéressants.

Tout phénomènes significatives, qu'ils soient biologiques, géologiques, ou encore astrophysiques, ont lieu hors de l'équilibre. Sans surprise, toute tentative de décrire le comportement des systèmes hors de l'équilibre nous oblige à reconsidérer des concepts sur lesquelles nous nous sommes appuyés pendant des décennies. Il n'est pas aisé de remettre en question notre compréhension des concepts communs tels que ceux de la thermodynamique classique, mais la majorité de la matière dans l'univers n'est pas en équilibre. Cet ouvrage poursuit un effort de longue date, qui remonte à Maxwell et Boltzmann, pour sonder la physique des systèmes déplacés hors d'équilibre. Parmi tous les phénomènes non-équilibrés, une situa-

tion commune est la conduction de chaleur, découvert par J.B.J. Fourier, qu'il a analysé dans son célèbre traité "Théorie analytique de la chaleur "([31]). Il y a deux siècles déjà, Fourier a souligné l'impossibilité de décrire le phénomène au moyen de principes fondamentaux: "Mais quelle que soit l'étendue des théories mécaniques, elles ne s'appliquent pas aux effets de la chaleur. Ils composent un ordre spécial de phénomènes qui ne peuvent s'expliquer par les principes du mouvement et de l'équilibre."

La loi de Fourier pose une question complexe et encore non résolue: comment peut-elle être dérivée à partir de la dynamique microscopique?

Il est possible de faire l'hypothèse d'une séparation nette entre les échelles microscopiques et macroscopiques en utilisant une description grossière du système. A l'échelle microscopique, les transporteurs de chaleur sont des molécules dans les gaz et les liquides ou des vibrations du réseau (les phonons) dans les solides, qui évoluent en conséquence d'une dynamique déterministe et Hamiltonienne. À l'échelle macroscopique la loi de Fourier implique un transfert diffusif d'énergie. Si l'hypothèse se vérifie, il est possible de définir sur tous les points de l'espace, à l'instant t, un champ local de température$\mathbf{T}(x,t)$ qui varie lentement à l'échelle microscopique.

Un système en contact avec une source de chaleur maintient une densité de flux $\mathbf{J}(x,t)$ proportionnelle au gradient de température $\mathbf{T}$ via un conductivité thermique k, pour laquelle la relation est donnée par:

$$\mathbf{J}(x,t) = -k\nabla\mathbf{T}(x,t). \tag{1.1}$$

Si $u(x,t)$ représente la densité d'énergie locale, l'équation de continuité est satisfaite $\partial u/\partial t + \nabla\cdot\mathbf{J} = \mathbf{0}$. En utilisant la relation$\partial u/\partial T = c$, où c est le la chaleur par unité de volume, conduit à l'équation de diffusion:

$$\frac{\partial\mathbf{T}(x,t)}{\partial t} = \frac{1}{c}\nabla\cdot[k\nabla\mathbf{T}(x,t)]. \tag{1.2}$$

La diffusion de l'énergie est conséquence de la loi de Fourier.

Il existe un grand nombre d'études et de nombreux modèles sur la conduction de la chaleur traitant de la dérivation rigoureuse de la loi de Fourier à partir de la dynamique microscopique Hamiltonienne. Pour des références sur des revues voir [13], [20], et sur des résultats exacts avec résultats numériques voir [51]. Puisque le but de ces études est de comprendre la physique fondamental sur laquelle repose le phénomène de diffusion de chaleur, on étudie des modèles simples en 1 ou 2 dimensions spatiales, dont les aspects techniques ont été écartés en faveur des caractéristiques essentielles. Une conclusion importante et surprenante émergent de ces études est la non validité de la loi de Fourier dans un et deux dimensions. Sauf lorsque le système est rattaché à un potentiel de strate. Pour les systèmes tridimensionnels, on s'attend à ce que la loi de Fourier soit vraie mais on ne sait pas encore sous quelles conditions.

La difficulté d'aborder la question de la dérivation microscopique est donnée par le manque de cadre mathématique dans le régime de non-équilibre, où la dynamique joue un rôle majeur. Tous les observables physiques impliqués dans les phénomènes de transport de la chaleur comme le flux thermique, la température et la conductivité sont définis seulement en équilibre ou très près de lui. Dans cette thèse, nous considérons les modèles en 1 dimension, électriquement isolé avec des potentiels, qui modélisent les interactions entre les particules elles-mêmes et la structure en treillis. Les systèmes considérés sont connectés à des réservoirs caractérisés par leurs potentiels chimiques ou par leurs températures. Les réservoirs sont supposés beaucoup plus grands que le système, de sorte que leur état physique n'est pas influencé par ce dernier.

L'hypothèse principale à faire est celle de *l'équilibre thermique local*: nous imaginons le système divisé en plusieurs petits cubes, chacun assez grand pour contenir un grand nombre de particules, mais qui reste assez petit à l'échelle macroscopique. On définit ensuite une température d'équilibre à un instant donné

et dans le centre du i-ème cube. Cette température varie dans le cube très lentement par rapport à l'échelle macroscopique. Le système microscopique atteint alors un équilibre local dans un temps qui est plus court que le temps typique de l'évolution macroscopique, où les observables de la thermodynamique sont bien définies. Le passage de microscopique à macroscopique est ensuite effectué au moyen de la *limite hydrodynamique*. Les équations diffusives sont obtenues à partir des modèles microscopiques comme une loi de grands nombres.

1.0.1 États stationnaires hors équilibre

L'une des approches les plus couramment utilisées consiste à étudier le transport de la chaleur à *l'état stationnaire de non-équilibre*, obtenu lorsque le système est en contact avec des sources d'énergie externes et / ou des réservoirs à différentes températures. Les états stationnaires sont caractérisés par la présence des courants qui traversent le système, et leur comportement macroscopique est codé dans les coefficients de transport. Plusieurs modèles de réservoirs sont généralement utilisés. Pour souci de simplicité, nous considérons ici uniquement des modèles à 1 dimension .

L'Hamiltonien d'un système de particules interagissant à travers un potentiel d'interaction des proches voisins U et avec un potentiel externe V est

$$H = \sum_{i=1}^{n} \left(\frac{p_i}{2m_i} + V(x_i) \right) + \sum_{i=1}^{n-1} U(x_1 - x_{i-1}). \tag{1.3}$$

Avec $\{m_i, x_i, p_i\}$ où $i = 1, 2, ..., n$ on désigne les masses (qui sont généralement considérées toutes égales à 1), les positions et les moments des n particules. Pour obtenir un courant de chaleur dans le système Hamiltonien, ce dernier doit être connecté aux réservoirs. Ceux que nous utiliserons dans cette thèse sont les réservoirs de Langevin. Ces types de réservoirs sont définis en ajoutant des termes de force supplémentaires dans la dynamique. La forme la plus simple, est

donnee' par un terme dissipatif et un terme stochastique de type bruit gaussien. Ainsi avec les réservoirs de Langevin connectés aux particules $i = 1$ et $i = n$, les équations du mouvement sont obtenues par:

$$\begin{cases} \dot{p}_1 = f_1 - \dfrac{\gamma_l}{m_1} p_1 + \eta_l(t) \\ \dot{p}_i = f_i \qquad\qquad \text{for i=2,3,...,n-1} \\ \dot{p}_n = f_n - \dfrac{\gamma_r}{m_n} p_n + \eta_r(t) \end{cases} \tag{1.4}$$

Où $f_i = -\dfrac{\partial H}{\partial x_i}$ est la force newtonienne habituelle sur la i-ème particule. Les termes des bruits $\eta_{r,l}$ sont des Gaussiens, avec zéro moyen, et dont les coefficients de dissipation $\gamma_{l,r}$ sont donnés par les covariances:

$$\begin{cases} \langle \eta_l(t)\eta_l(t') \rangle = 2k_B T_l \gamma_l \delta(t - t') \\ \langle \eta_r(t)\eta_r(t') \rangle = 2k_B T_r \gamma_r \delta(t - t') \\ \langle \eta_l(t)\eta_r(t') \rangle = 0 \end{cases} \tag{1.5}$$

où T_r, T_l sont respectivement les températures des réservoirs gauche et droit, et γ le coefficient de dissipation.

1.1 But de cette thèse

Dans cette thèse, nous considérerons des systèmes de particules en interaction qui évoluent selon deux modèles dynamiques: l'équation de Schrödinger linéaire discrète (DLSE),(chapter 3), et une chaîne anharmonique d'oscillateurs immergés dans un bain de chaleur avec un gradient de température et perturbés par une tension à une extrémité (chapter 4). Nous avons prouvé une limite hydrodynamique pour ces modelés, y compris la dérivation de la loi de Fourier pour DLSE et la dérivation microscopique d'une transformation isotherme pour la chaîne anhar-

monique perturbée.

1.1.1 Équation discrète de Schrödinger

L'équation Discrete NonLineare de Schrödinger (DNLSE) est un système particulièrement intéressant , qui a une application importante dans de nombreux domaines de la physique. Une exemple classique est le transport électronique dans les biomolécules, DNLSE décrit la propagation d'ondes non linéaires dans une couche photonique ou phononique([47], [25], [72], [42]). Au cours des dernières années, DNLSE a attiré l'attention de la communauté mathématique et physique, car elle donne la description semi-classique des bosons piégés dans des réseaux optiques périodiques: phénomène dit des *breathers*.

Les breathers sont des solutions ponctuelles et spatialement localisées de l'équation du réseau et correspondent à une particularité des systèmes discrets non linéaires qui est celle de maintenir une forte localisation de l'énergie[65]. Le mécanisme non linéaire est responsable du stockage et du transport d'emballages cohérents d'énergie et de charges localisées dans le système. Malheureusement, DNLSE pose toujours des problèmes différents tels que le global well-posedness de l'équation et comment gérer les breathers dans un cadre statistique. Vu les nombreuses difficultés rencontrées sur le chemin non linéaire, nous avons étudié le cas linéaire de l'équation (DSLE). La DLSE est l'une des équations les plus utilisées pour résoudre des problèmes dans une seule dimension de la mécanique quantique sur ordinateur et il est le modèle naturel pour les puits quantiques semi-conducteurs et les dispositifs nanoélectriques. Dans chapter 3 nous avons étudié la limite hydrodynamique de la DLSE et la compréhension du comportement en présence de thermostats, afin de démontrer la loi de Fourier.

1.1.2 Chaîne anharmonique perturbée dans un gradient de température et transformations thermodynamiques

Dans chapter 4, nous étudierons une chaîne anharmonique de$n$ particules , fixe à une extrémité et où est appliquée une tension τ à l'autre extrémité. La chaîne est en présence d'un gradient de température: chaque particule est en contact indépendamment avec un réservoir de Langevin à température différente. Le but est de prouver qu'à une échelle spatio-temporelle diffusive et de grainage grossier, les contraintes volumiques évoluent vers une équation déterministe non-linéaire diffusive. La transformation isotherme quasi statique est obtenue par une nouvelle mise à l'échelle. Le développement d'une approche dynamique rigoureuse pour prouver la transformations thermodynamique pour les états d'équilibre et de non-équilibre est le but de la dérivation microscopique des transformations thermodynamiques développées par Bertini, De Sole, Gabrielli, Jona-Lasinio et Landim [9],[11] [10][12] et mis en œuvre par Olla et Simon[54],[55] est d'étude le développement d'une approche dynamique rigoureuse pour prouver la transformations thermodynamique pour les états d'équilibre et de non-équilibre. Ce principe a été dérivé [11], à partir de l'hypothèse d'une l'évolution macroscopique décrite par des équations hydrodynamiques. L'approche utilisée dans cette thèse est le suivant : la dérivation microscopique de la transformation quasistatique par la mise en échelle appropriée pour l'espace et le temps.

La transformation thermodynamique est effectuée par des changements dans des contraintes ou des conditions externes qui entraînent un changement d'état macroscopique. Ces transformations sont classées comme réversibles ou irréversibles selon le fait que l'inversion des changements annulent ou n'annulent pas leurs effets. Bien que les transformations irréversibles soient les plus courantes, les transformations réversibles jouent un rôle central dans le développement de la théorie thermodynamique ; une des conditions de réversibilité nécessaire (mais pas suffisante) est qu'elle soit quasi-statique. En effet, pour passer d'un état d'équilibre

à un autre, le système traverse une séquence d'états de non-équilibre, caractérisée par des variations très lentes de l'environnement (où des transformations quasi-statiques sont représentées par des courbes de trajectoires lisses continues par morceaux sur la surface d'équilibre dans l'espace des paramètres.). Nous devrions imaginer des transformations quasi-statiques, comme limite à l'infinie de séquences de transformations irréversibles en non-équilibre.

La nouvelle idée dans [54] utilisée dans chapter 4,est de construire ces états sous un rééchelonnement macroscopique de l'espace et du temps de la configuration microscopique des positions et des vitesses du système. Nous devrions imaginer un système mécanique simple : un fil soumis à une tension en présence d'un gradient de température. Le fil est caractérisé par sa longueur $\mathcal{L}$, la distance entre la première et la dernière particule. Chaque particule est en contact avec un thermostat différent à une température différente et il y a un flux constant d'énergie dans le fil. La première particule est attachée à un point fixe à une de ses extrémités et il est tiré sur l'autre extrémité,par une tension τ, dont la longueur du fil est fonction de la tension et de la température: $\mathcal{L} = \mathcal{L}(\tau, \beta_1^{-1}, ..., \beta_n^{-1})$. En changent la valeur de la tension appliquée, le système convergera finalement vers un état stationnaire paramétré par la tension appliquée. A l'échelle appropriée, il s'agit d'une transformation thermodynamique isotherme à partir d'un état stationnaire à un autre, qui satisfait une inégalité de Clausius. Si nous voulons obtenir une transformation réversible isotherme quasi statique, nous devons introduire une échelle temporelle plus longue, et appliquer une tension variant lentement dans le temps $\bar{\tau}(\epsilon)$, le processus limite est si lent que le système est dans un état stationnaire à chaque instant.

1.2 Technique utilisée

Dans le premier travail (chapter 3) nous démontrons la limite hydrodynamique en utilisant des arguments standards dans la littérature [6]. Pour démontrer que

le flux de densité vérifie la loi de Fourier dans l'état stationnaire, nous avons utilisé la limite de la production d'entropie. Une fois l'entropie bornée, on peut contrôler les valeurs attendues des densités dans la mesure stationnaire. On montre que la densité totale est contrôlée proportionnellement à la taille du système. Lorsque nous étudions le comportement hydrodynamique de la chaîne dans le chapter 4, nous avons découvert que la mesure d'entropie relative utilisée dans le cas d'équilibre échoue en présence d'un gradient de température. Les états stationnaires de la dynamique donnent lieu à une production d'entropie positive, de sorte que l'entropie relative classique les méthodes ne peuvent pas être utilisées. Nous développons de nouvelles estimations basées sur l'hypocoercivité entropique, qui permet de contrôler la distribution des configurations des positions de la chaîne. Nous appliquons la méthode de Guo Papanicolau et Varadhan (GPV), précédemment développée pour une dynamique sur-amortie. Dans cette approche, l'étape principale de la clôture de l'équation macroscopique est la comparaison directe de la distribution empirique à grain grossier dans l'espace microscopique et de la densité à l'échelle macroscopique. Ceci est réalisé par un lié sur l'entropie relative et l'information de Fisher, utilisé comme fonction de Liapunov par rapport à la mesure de Gibbs non homogène. Les moyennes spatiales -temporelles des états évolués convergent vers un équilibre local canonique comme dans les arguments d'un bloc / deux blocs (chapitre 5 de [48]). La limite hydrodynamique de la chaîne d'oscillateurs en interaction donne une équation de diffusion linéaire, dont le coefficient de diffusion est naturellement exprimé en termes de fonctions thermodynamiques du système unidimensionnel. Pour justifier l'ansatz que la mesure de densité hors équilibre ressemble lentement à une famille variable d'états locaux de Gibbs, on démontre que les moyennes des quantités microscopique peuvent être remplacées par leurs valeurs macroscopiques moyennes locales. Même si le système considéré est en déséquilibre, car en présence d'un gradient macroscopique, la tension τ change très lentement et régulièrement dans

l'espace, de sorte que nous pouvons diviser la chaîne en blocs assez petits qui sont en équilibre local entre eux; en d'autres termes, dans un bloc microscopique, la température est constante. Cependant ce n'est pas la longueur de la chaine elle-même qui apparaît dans la fonction intégrale mais la fonction potentielle (une fonction locale de la configuration). Le principal problème consiste donc à remplacer $V'(r_{i+1})$ par une fonction de la longueur d'étirement afin de « fermer » l'équation. Ce remplacement est l'étape cruciale dans la démonstration et est la conséquence de certaines bornes élémentaires sur la mesure de la densité d'équilibre, obtenues pour la première fois par GPV. Ainsi, on obtient d'abord une borne de la forme de Dirichlet (appelée plus précisément Information de Fisher) à partir de la dérivée temporelle de l'entropie relative aux mesures stationnaires à l'équilibre. Cette limite implique que le système est proche de l'équilibre à l'échelle microscopique locale, et que la densité, sur un grand intervalle microscopique, est proche de la densité dans un petit intervalle macroscopique. Dans le chapter 4, on utilisera une hypocoercivité entropique, où l'information de Fisher est associée aux champs vectoriels de position et de vitesse. Les gradients de la distribution des vitesses sont très proches des gradients des positions, de sorte qu'ils peuvent être liés aux informations de Fisher sur les positions avec celui sur les vitesses, revenant à un modèle surmoulé. Ainsi, le reste de la preuve est la même que dans [37] .

2

Introduction

Out of equilibrium is where the most interesting events happen. All compelling phenomena, from biological ones to earth sciences and astrophysics significant processes take place out of equilibrium. Unsurprisingly any attempt to understand the behavior of systems removed from equilibrium forces us to reconsider ideas we have relied on for decades. It is quite undertaking to question our understanding of commonly held concepts such as classic thermodynamics, but a good part of matter in the universe, if not most of it, is not on equilibrium. So here we are pursuing a longtime effort, which dates back to Maxwell and Boltzmann themselves, to probe physics of systems displaced out of equilibrium.

Among all non equilibrium phenomena a particular situation all of us is familiar with is heat conduction. This was first discovered by J.B.J. Fourier who

analyzed the phenomenon of heat transport in his famous treatise "Théorie analytique de la chaleur" ([31]). Two centuries ago he already pointed out the impossibility of describing the phenomenon by means of first principles: "But whatever may be the range of mechanical theories, they do not apply to the effects of heat. These make up a special order of phenomena, which cannot be explained by the principles of motion and equilibria". *Fourier's law* poses a complex and yet unsolved question: how can it be derived from the underlying microscopic dynamics?

One assumption is that it is possible to have a coarse-grained description with a clear separation between microscopic and macroscopic scales. At the microscopic scale, heat carriers which are molecules in gas and liquids, lattice vibration, phonons, in solids, evolve accordingly a deterministic dynamics well accounted for an Hamiltonian description, whereas at macroscopic scale Fourier's law implies a diffusive transfer of energy. If the assumption is achieved, it is possible to define at any spatial point x in the system and at time t, a local temperature field $\mathbf{T}(x,t)$ which varies slowly both in space and time (compared to microscopic scales). A system in contact with a source of heat sustains a heat flux density $\mathbf{J}(x,t)$ proportional to the gradient of temperature $\mathbf{T}$ via a thermal conductivity k, for which the relation is given by:

$$\mathbf{J}(x,t) = -k\nabla\mathbf{T}(x,t). \tag{2.1}$$

If $u(x,t)$ represents the local energy density then this satisfies the continuity equation $\partial u/\partial t + \nabla\cdot\mathbf{J} = \mathbf{0}$. Using the relation $\partial u/\partial T = c$, where c is the specific heat per unit volume, leads to the diffusion equation:

$$\frac{\partial\mathbf{T}(x,t)}{\partial t} = \frac{1}{c}\nabla\cdot[k\nabla\mathbf{T}(x,t)]. \tag{2.2}$$

The diffusion of energy is indeed implied by Fourier's law. Microscopically we

have to think about heat carriers colliding randomly and the result is a heat diffusion. Thus the Fourier's law is a phenomenological law which provides an accurate description of heat transport as observed in experimental systems. How to rigorously derive Fourier's law from the microscopic Hamiltonian has motivated a large number of studies, and many model systems on heat conduction, see for instance for short and schematic reviews of problems [13], [20], and known exact results with numerical results [51]. Since the purpose of these studies is to understand the basic physics behind the heat diffusion phenomenon, we convey with the simple models proposed in 1 or 2 spatial dimensions, and the realistic aspects have been discarded in favor of the essential features responsible of the energy transport. One important and somewhat surprising conclusion that emerges from these studies is that Fourier's law is probably not valid in one and two dimensional systems, except when the system is attached to an external substrate potential. For three dimensional systems, one expects that Fourier's law is true in generic models, but it is not yet known as to what are the necessary conditions.

The difficulty of approaching the question of microscopic derivation is given by the lack of mathematical framework in the regime of non equilibrium, where dynamics plays a major role, yet all the physical observables involved in heat transport phenomena, heat flux, temperature and the conductivity are defined only in equilibrium or very close to it. In this thesis we consider simple lattice models in 1 dimension, electrically insulated with smooth inter-particle and pinning potentials which model interactions among particles themselves and the lattice structure. The systems are connected to reservoirs, characterized by their chemical potentials or temperatures, assumed much larger then the system so that their state is not changed by it.

The main assumption to be made is that of *local thermal equilibrium*: we imagine the system divided into many little cubes, each big enough to contain a

large number of particle but small enough on the macroscopic scale to be described by an equilibrium temperature $T(t, r_i)$ defined at a specified time t and in the center of the i-th cube r_i, which vary very slowly compared to macroscopic scale. The microscopic system reaches a local equilibrium in a time which is shorter than the typical time of the macroscopic evolution, where the thermodynamic observables are well defined. The passage from microscopic to macroscopic is then performed by means of the *hydrodynamic limit*. In the diffusive equations are obtained from the microscopic models as a law of large numbers, in the limit in which the ratio of the microscopic to the macroscopic spatial and temporal scales go to zero, it holds with probability one.

2.0.1 Non equilibrium stationary states

One of the most commonly used approach to study heat transport has been to look at the *nonequilibrium stationary state*, obtained when the system is in contact with external sources of energy and/or reservoirs at different temperatures. In the stationary states there are currents passing through the system, and their macroscopic behavior is encoded in the transport coefficients. There are severals models of reservoirs generally used. For sake of simplicity we consider here a 1-dimensional model.

The Hamiltonian of a system of n particles interacting through a nearest neighbors interaction potential U and with an external potential V is

$$H = \sum_{i=1}^{n} \left(\frac{p_i}{2m_i} + V(x_i) \right) + \sum_{i=1}^{n-1} U(x_1 - x_{i-1}) \tag{2.3}$$

where $\{m_i, x_i, p_i\}$ for $i = 1, 2, ..., n$ denotes the masses (which usually are considered all equals to 1), positions and momenta of the n particles. To drive heat current in the Hamiltonian system, we need to connect it to heat reservoirs and we describe here the one we will use in this thesis: *Langevin baths*. These partic-

ular type of reservoirs are defined by adding additional force terms in the motion equation of the particles in connection with them. In the simplest form, the additional forces consist of a dissipative term and a stochastic term, which is taken to be a Gaussian white noise. Thus with Langevin reservoirs connected to particles $i = 1$ and $i = n$, the equations of motion are given by:

$$\begin{cases} \dot{p}_1 = f_1 - \dfrac{\gamma_l}{m_1} p_1 + \eta_l(t) & \\ \dot{p}_i = f_i & \text{for i=2,3,...,n-1} \\ \dot{p}_n = f_n - \dfrac{\gamma_r}{m_n} p_n + \eta_r(t) & \end{cases} \tag{2.4}$$

where $f_i = -\dfrac{\partial H}{\partial x_i}$ is the usual Newtonian force on the i-th particle. The noise terms given by $\eta_{r,l}$ are Gaussian, with zero mean, and relater do dissipation coefficients $\gamma_{l,r}$ by the covariances:

$$\begin{cases} \langle \eta_l(t)\eta_l(t') \rangle = 2k_B T_l \gamma_l \delta(t - t') \\ \langle \eta_r(t)\eta_r(t') \rangle = 2k_B T_r \gamma_r \delta(t - t') \\ \langle \eta_l(t)\eta_r(t') \rangle = 0 \end{cases} \tag{2.5}$$

where T_r, T_l are the temperatures of the left and right reservoirs respectively, γ is the dissipation coefficient.

2.1 Aim of this thesis

In this thesis we have considered systems of interacting particles which evolve according to two dynamical models: discrete linear Schrödinger equation (DLSE), (chapter 3), and an anharmonic chain of oscillators immersed in a heat bath with a gradient of temperature and perturbed by a tension on one end of it (chapter 4). We have proved an hydrodynamic limit for the these dynamics, including the

derivation of Fourier's law for DLSE and a microscopic derivation of an isothermal transformation for the perturbed anharmonic chain.

2.1.1 Discrete Schrödinger equation

A particularly interesting system is the Discrete NonLinear Schrödinger equation (DNLSE), that has important application in many domains of physics. A classic example is electronic transport in biomolecules or in optics and acoustics it describes the propagation of nonlinear waves in a layered photonic or phononic media ([47], [25], [72], [42]). In the recent years the DNLSE has attracted the attention of the mathematics and physics community because it provides an approximate semiclassical description of bosons trapped in periodic optical lattices, the so called *breathers* phenomenon.

The breathers are a time-periodic, spatially localized solutions to the dynamical lattice equation, a particularity of discrete non linear systems, which are able to sustain strong localization of energy [65]. The non-linear mechanism is responsible for storage and transport of localized coherent packages of energy and charge in the system. Unfortunately DNLSE are still posing different issues such as local and global well-posedness of the equation and how to handle the *breathers* in a statistical frameworks. In view of the many difficulties that we encountered in the nonlinear path, we studied the linear case: the Discrete Linear Schrödinger equation (DSLE). The DLSE it's one of the most commonly employed equation for solving problems in one dimension quantum mechanics on computer and it is the natural model for semiconductor quantum wells and nanoelectric devices. In chapter 3 we study the hydrodynamic limit of the DLSE and understanding the behavior in presence of thermostats, in order to prove the Fourier's law.

2.1.2 Perturbed anharmonic chain in a gradient of temperature and thermodynamic transformations

In chapter 4 we study an anharmonic chain of n particles, which at one end is fixed, at the other end a tension τ is applied. Moreover the chain is in presence of a gradient of temperature: each particle is in contact independently with a Langevin heat bath at different temperature. The aim is to prove that after a diffusive space-time scaling and coarse-graining the volume strains evolves to a deterministic non-linear diffusive equation. Quasi-static isothermal transformations in a temperature gradient are obtained by a further time scaling.

The development of a coherent dynamical approach to prove thermodynamic transformations for both equilibrium and non-equilibrium states is the aim of the microscopic derivation of thermodynamics transformations developed by Bertini, De Sole, Gabrielli, Jona-Lasinio and Landim [9],[11] [10][12] and implemented by Olla and Simon [54],[55]. This principle has been derived [11], by an explicit construction of quasi static transformation, from the assumption that during the transformation the system in *local equilibrium* state so that the macroscopic evolution can be described by hydrodynamic equations, this is the leading idea of the *Microscopic Fluctuation Theory (MFT)*. The aim of which is to construct analogues of thermodynamic potentials and to extract from them the typical macroscopic behavior of the system. It is an extension of the Einstein equilibrium fluctuation theory to stationary non equilibrium states combined with a dynamical point of view. The other approach is the one used in this thesis: the microscopic derivation of quasistatic transformation by proper space and time scaling.

A thermodynamic transformation is effected by changes in the constraints or external conditions which result in a change of macro state, these transformations may be classified as *reversible* or *irreversible* according to the fact that reversing the changes undo or do not undo their effects. Although irreversible transforma-

tions are the most common ones, reversible transformations play a central role in the development of thermodynamic theory, and a necessary but not sufficient condition for reversibility is that the transformation be *quasi-static*. *Quasi-static* transformation is such that in order to go from one equilibrium state to another one, the system passes through a sequence of non-equilibrium states, characterized by very slow variations of the environment. (Hence, quasi-static transformations are represented by continuous piecewise smooth path curves upon the equilibrium surface, the parameter space.) We should imagine *quasi-static* transformations as happening in a *larger* time-scale, as limit of sequence of irreversible infinitesimal non-equilibrium transformations, so that the new idea in [54] and used in chapter 4, is to construct these states under a proper macroscopic rescaling of space and time of the microscopic configuration of the positions and velocities of the system. We should imagine a simple mechanical system: a wire submitted to a tension in presence of a gradient of temperature. The wire is characterized by its length $\mathcal{L}$, the distance between the first and last particle. Each particle is in contact with a different thermostat at a different temperature and there is a constant flow of energy in the wire. The first particle is attached to a fixed point on one extreme and it is pulled at the other one by a tension (force) τ, thus the length is a function of the tension and temperatures: $\mathcal{L} = \mathcal{L}(\tau, \beta_1^{-1}, ..., \beta_n^{-1})$. By changing the value of the applied tension, the system will eventually converge to a stationary state parametrized by the tension applied. On an appropriate time scale, this is an isothermal thermodynamic transformation from a stationary state to another, and it satisfies a Clausius inequality. If we want to obtain a reversible quasi-static isothermal transformation we have to introduce another larger time scale ϵt, and apply a tension slowly varying in time $\bar{\tau}(\epsilon)$, the limiting process are so slow that the system is in a stationary state at each instant of time.

2.2 Technique used

In the first work (chapter 3) we prove the hydrodynamic limit using standard arguments in the literature [6]. To demonstrate that in the stationary state the density flow verifies Fourier's law, we used the bound of the entropy production. Once the entropy is bounded, we can control the expected values of the densities with respect to the stationary measure, it is straightforward to show the total density is controlled proportionally on the size of the system.

When we investigated the hydrodynamic behavior of the chain in chapter 4, we discovered that the relative entropy measure used in the equilibrium case was failing in the presence of a temperature gradient. The stationary states of the dynamics have a positive entropy production, so the classical relative entropy methods cannot be used. We develop new estimates based on entropic hypocoercivity, that allows to control the distribution of the positions configurations of the chain. We applied the Guo Papanicolau and Varadhan (GPV) method, previously developed for over-damped dynamics. In this approach the main step in closing the macroscopic equation is the direct comparison of the coarse grained empirical density in the microscopic and macroscopic space scale. This is achieved by a bound on the Relative Entropy and the Fisher Information, used as Liapunov functions with respect to the in-homogeneous Gibbs measure. The space-time averages of the evolved state converge to a canonical local equilibrium as in the one-block/two blocks argument (chapter 5 of [48]).

The hydrodynamic limit for the interacting chain of oscillators gives us a non-linear diffusion equation, and the diffusion coefficient is naturally expressed in terms of the thermodynamic functions of the one-dimensional system. We have to justify the ansatz that the non-equilibrium density measure looks like a slowly varying family of local Gibbs states. This means that the averages of microscopic quantities can be replaced by their local macroscopic mean values. Even if our system is in non-equilibrium, because we are in presence of a macroscopic gradi-

ent, the tension τ changes very slowly and smoothly in space, so we can divide the chain in blocks small enough to have a local equilibrium for each one of them, i. e. in a microscopic block the temperature is constant. However it is not the length stretch itself that appears in the integral but the potential function, a local function of the configuration. The main problem consists therefore in replacing $V'(r_{i+1})$ by a function of the length stretch in order to "close" the equation. This replacement is the crucial step in the proof and it is the consequence of certain elementary bounds on the equilibrium density measure, obtained for the first time by GPV. They first obtained a bound of the Dirichlet form (more precisely called Fisher information) from the time derivative of the relative entropy with respect to the equilibrium stationary measures. This bound implies that the system is close to equilibrium on a local microscopic scale, and that the density on a large microscopic interval is close to the density in a small macroscopic interval. In chapter 4 it has been used an entropic hypocoercivity, where the Fisher information is associated to the vector fields of position and velocity. Obtaining that the gradients of the distribution in the velocities are very close to the gradients in the positions, so that we can bound the Fisher Information on the positions with the one on the velocities, coming back to overdamped model. So the rest of the proof is the same as in [37].

3

Diffusive limit and Fourier's law for the discrete Schrödinger equation

3.1 Introduction

Discrete Schrödinger equation, besides being viewed as a toy model for its continuous counterparts, has itself a physical application as a discrete systems: it serves as a model for electronic transport through crystals. In the realm of the physics of cold atomic gases, the equation is an approximate semiclassical description of bosons trapped in periodic optical lattices, and experimentally, discrete solitons have been observed in a nonlinear optical array [26].

In the past years much attention has been paid on the non linear case (DNLS) for which the first analysis of the equilibrium statistical mechanics has been performed in [65]. It has been osserved [63] the relaxation of localized modes (discrete breathers) in the presence of phonon baths has been discussed in. Only recently, [42], the non equilibrium properties have been explored, considering an open system that exchanges energy with external reservoirs, for which the resulting stationary states are investigated in the limit of low temperatures and large particle densities, mapping the dynamics onto a coupled rotator chain.

Here we are interested in proving the hydrodynamic limit and Fourier's law for the DS equation in the simplified linear case. The linear case equation is interesting as one of the most commonly employed methods for solving one-dimensional quantum problems, for which many characteristics are still poorly understood. The natural applications are in the context of solid-state physics, which links the discrete model to realistic semiconductor quantum wells and nanoelectric devices.

In the present paper we study a chain of particles, for which the Hamiltonian dynamics is perturbed by a random continuous phase-changing noise. The resulting total dynamics of the system is a degenerate hypoelliptic diffusion on the phase space, which assures good ergodic properties, it conserves the total norm and destroy the other conservation laws. The system is considered under periodic boundary conditions. In the first part of the article we will prove the hydrodynamic limit using standard arguments. In the second part we will add an interaction between the system and external reservoirs, modeled by Ornstein-Uhlenbeck processes at the corresponding chemical potentials. We prove that in the stationary state Fourier's law is valid for the density flow. The main tool used in the proof is the bound of the entropy production as in [6]. Then in order to obtain Fourier's law, we need to control the expected values of the densities respect to the stationary measure, which results in a bound of the expected total density proportional to the size of the system.

The article is structured in the following way. In section 4.2 we define the dynamics. In section 3.3 we state and prove the result of hydrodynamic limit. In section 3.4 we prove the Fourier's law by means of entropy bounds.

3.2 The model

Atoms are labeled by $x \in \mathbb{T}_N$ where $\mathbb{T}_N = 1, ..., N$ is the lattice torus of lenght N, corresponding to periodic boundary conditions. The configuration space is $\Omega^N = \mathbb{C}^{\mathbb{T}_N}$ and a generic element is $\{\psi(x)\}_{x\in\mathbb{T}_N}$, where $\psi(x)$ characterize the amplitude of the wave function of each particle. The Hamiltonian of the system writes

$$\mathcal{H}_N = \sum_{x=1}^{N} |\psi(x) - \psi(x+1)|^2 + \frac{1}{p+1}\sum_{x=1}^{N} |\psi(x)|^{p+1} \tag{3.1}$$

where $|\psi(x)|^2$ is the number of particle or the "mass" at site x, at the boundary the conditions are fixed: $\psi_{N+1} = \psi_0 = 0$.

The linear case is for $p = 1$:

$$\mathcal{H}_N = \sum_{x=1}^{N-1} (\psi(x)\psi(x+1)^* + \psi(x)^*\psi(x+1)) + 2\sum_{x=1}^{N} |\psi(x)|^2 \tag{3.2}$$

the corresponding equations of motion are

$$\begin{cases} \dfrac{d\psi(x)}{dt} = i\dfrac{\partial\mathcal{H}}{\partial\psi^*(x)} = -i\triangle\psi(x) \\ \dfrac{d\psi^*(x)}{dt} = -i\dfrac{\partial\mathcal{H}}{\partial\psi(x)} = +i\triangle\psi^*(x). \end{cases} \tag{3.3}$$

Here $\Delta\psi(x) = \psi(x+1) + \psi(x-1) - 2\psi(x)$.

We denote $\psi(x) = \psi_r(x) + i\psi_i(x) = |\psi(x)|e^{i\theta(x)}$, and define the operator (on local functions $F : \mathbb{T}_N \to \mathbb{C}$)

$$\partial_{\theta(x)}F(\psi) = i\psi(x)\partial_\psi F(\psi) = \psi_i(x)\partial_{\psi_r(x)}F - \psi_r(x)\partial_{\psi_i(x)}F. \tag{3.4}$$

We look for a stochastic perturbation which change randomly the phase of the wave function, such that the total "mass"

$$M_N(\psi) = \sum_{x \in \mathbb{T}_N} |\psi(x)|^2 \tag{3.5}$$

is still a conserved quantity. The total "mass" is linear in the number of particles $M_N(\psi) \sim N$.

The dynamics is described by the following system of stochastic differential equation for $x = 1, ..., N$

$$\begin{cases} d\psi(x,t) = -i\triangle\psi(x,t)dt - \dfrac{\gamma}{2}\psi(x,t)dt + i\psi(x,t)\sqrt{\gamma}dw_x \\ d\psi^*(x,t) = +i\triangle\psi^*(x,t)dt - \dfrac{\gamma}{2}\psi^*(x,t)dt - i\psi^*\sqrt{\gamma}dw_x \end{cases} \tag{3.6}$$

where $w_x(t)$ are real independent standard Brownian motions and γ is the noise intensity parameter.

Let $\mathcal{L}_N$ be the generator of the system. A core for $\mathcal{L}_N$ is given by the space $C^\infty(\Omega^N)$ of smooth functions on Ω^N endowed with the product topology. On $C^\infty(\Omega^N)$, the generator is defined by

$$\mathcal{L}_N = \mathcal{A}_N + \mathcal{S}_N \tag{3.7}$$

where

$$\mathcal{A}_N = \sum_{x \in \mathbb{T}_N} \{i\triangle\psi^*\partial_{\psi(x)} - i\triangle\psi\partial_{\psi^*(x)}\} \tag{3.8}$$

is the Liouville operator of a chain of interacting and

$$\mathcal{S}_N = \frac{\gamma}{2} \sum_{x \in \mathbb{T}_N} \partial^2_{\theta(x)} \tag{3.9}$$

is the diffusive operator corresponding to the noise part of eq. (3.6) Since the

total mass is conserved by the stochastic perturbation, we have

$$\mathcal{S}_N M_N(\psi) = 0. \tag{3.10}$$

In the infinite volume case, the family of product measures:

$$d\mu_\lambda(d\psi) = \prod_{x\in\mathbb{T}_N} \frac{e^{-\lambda|\psi(x)|^2}}{Z(\lambda)} d\psi \tag{3.11}$$

are stationary for the dynamics, the parameter $\lambda > 0$ correspond to the conserved quantity of the dynamics, the total "mass", while $Z(\lambda)$ is the normalization constant. Here $d\psi = \prod_{x=1}^{N} d\psi(x)d\psi^*(x)$.

The Lie algebra, generated by the Hamiltonian vector field and the noise fields, has full rank at every point of the state space $\mathbb{C}^N$, so the stationary measure has a smooth density. We denote by $\langle\cdot\rangle$ the expectation with respect to the stationary measure.

Let us define the density of particle x as

$$\rho_x = |\psi(x)|^2, \tag{3.12}$$

locally the conservation of mass generates an instantaneous current

$$\mathcal{L}_N \rho_x = j_{x-1,x} - j_{x,x+1} \tag{3.13}$$

with

$$j_{x,x+1} = -i\{\psi_x \psi^*_{x+1} - \psi^*_x \psi_{x+1}\}. \tag{3.14}$$

3.3 Hydrodynamic limit in the diffusive scaling

3.3.1 Notation

Let's introduce some notation and definitions.

We will denote by $(\omega^N(t))_{t\geq 0} = (\psi^N(t), \psi^{*N}(t))_{t\geq 0}$ the process on the torus $\mathbb{T}_N$ whose evolution time is given by $N^2\mathcal{L}_N$. The factor N^2 corresponds to the acceleration of time by N^2 in the stochastic differential equations (3.6). The associated semigroup is denoted by $(S_t^N)_{t\geq 0}$.

Fix a time $T > 0$. Let $\mathcal{M}_+$ be the space of finite positive measures on $\mathbb{T}_N$ endowed with the weak topology. Consider a sequence of probability measures $(Q_N)_N$ on $D([0,T], \mathcal{M}_+)$ corresponding to the Markov process π_t^N defined as the density of the empirical measure

$$\pi^N(\omega, du) := \frac{1}{N}\sum_{x\in\mathbb{T}_N} \rho_x \delta_{x/N}(du) \tag{3.15}$$

where $\delta_a(du)$ is the Dirac measure localized on the point $a \in \mathbb{T}_N$. The time evolution of the empirical measure will be

$$\pi_t^N := \pi^N(\omega_t^N) = \frac{1}{N}\sum_{x\in\mathbb{T}_N} \rho_x(t) \delta_{x/N}(du) \tag{3.16}$$

starting from $(\mu^N)_N$, a sequence of probability measures on Ω^N associated to a fixed initial deformation profile $\rho_0 : \mathbb{T}^N \to [0, \infty)$.

We will assume that the system is close to a local equilibrium. More precisely we have the following definition:

Definition 1. *A sequence $(\mu^N)_N$ of probability measures on $\mathbb{T}_N$ is associated to a deformation profile $\rho_0 : \mathbb{T}_N \to [0, \infty)$, if for every continuous function $G : \mathbb{T}_N \to$*

$[0, \infty)$ *and for every* $\delta > 0$

$$\lim_{N\to\infty} \mu^N \left[\left| \frac{1}{N} \sum_{x\in\mathbb{T}_N} G(x/N)\rho_x - \int_{\mathbb{T}_N} G(v)\rho_0(v)dv \right| > \delta \right] = 0. \tag{3.17}$$

Our goal is to show that, if at a time $t = 0$ the empirical measures are associated to some initial profile ρ_0, at a macroscopic time t they are associated to a profile ρ_t which is the solution of an hydrodynamic equation.

Theorem 3.3.1. *Let* $(\mu_N)_N$ *be a sequence of probability measures on* Ω^N *associated to a bounded initial density profile* ρ_0*. Then for every* $t > 0$*, the sequence of random measures*

$$\pi_t^N(du) = \frac{1}{N} \sum_{x\in\mathbb{T}} \rho_t(x)\delta_{x/N}(du) \tag{3.18}$$

converges in probability to the absolutely continuous measure $\pi_t(du) = \rho(t, u)du$ *whose density is the solution of the heat equation:*

$$\begin{cases} \partial_t\rho = \dfrac{1}{\gamma}\triangle\rho \\ \rho(0, \cdot) = \rho_0(\cdot). \end{cases} \tag{3.19}$$

For any function $w : \mathbb{T}_N \to \mathbb{C}$, we denote ∇w the discrete gradient of w defined by

$$(\nabla w)(x) = w(x + 1) - w(x) \tag{3.20}$$

and ∇^* is the adjoint on $\mathbb{L}^2(\mathbb{T}_N)$ endowed with the standard inner product

$$(\nabla^* w)(x) = w(x - 1) - w(x). \tag{3.21}$$

The discrete Laplacian is $\triangle = -\nabla\nabla^*$. For a discrete function w, $\triangle w$ is given by

$$(\triangle w)(x) = w(x + 1) + w(x - 1) - 2w(x). \tag{3.22}$$

If G is a smooth local function on $\mathbb{T}_N$ and $x \in \mathbb{T}_N$, the discrete gradient is related to the continuous one by:

$$(\nabla_N G)(x/N) = N\left[G(\frac{x}{N}) - G(\frac{x-1}{N})\right] = G'(x/N) + o(N^{-1}) \tag{3.23}$$

and the discrete Laplacian to the continuous one by:

$$(\triangle_N G)(x/N) = N\left[G(\frac{x+1}{N}) - 2G(\frac{x}{N}) - G(\frac{x-1}{N})\right] = G''(x/N) + o(N^{-1}). \tag{3.24}$$

3.3.2 Limit identification

Under the empirical measure Q^N for every smooth function $G : \mathbb{T}_N \to \mathbb{C}$, the quantity

$$\langle \pi_t^N, G\rangle = \frac{1}{N}\sum_{x\in\mathbb{T}_N} G(\frac{x}{N})\rho_t(x), \tag{3.25}$$

the noise conserves ponctually the density so

$$\langle \pi_t^N, G\rangle = \langle \pi_0^N, G\rangle - \int_0^t N^2\mathcal{L}_N\langle \pi_s^N, G\rangle ds. \tag{3.26}$$

We do now some manipulation on the integrand of the previous equation, first using the definition of the empirical measure we have

$$N^2\mathcal{L}_N\langle \Pi^N, G\rangle = \frac{1}{N}\sum_{x=1}^{N} G(x/N)N^2\mathcal{L}_N\rho_t(x). \tag{3.27}$$

Substituting in it the explicit continuity equation (3.13) we get

$$N^2\mathcal{L}_N\langle \Pi^N, G\rangle = \frac{1}{N}\sum_{x=1}^{N} G(x/N)N^2\mathcal{L}_N(j_{x-1,x}(t) - j_{x,x+1}(t)). \tag{3.28}$$

Now we perform a summation by part

$$N^2\mathcal{L}_N\langle\Pi^N, G\rangle = \frac{1}{N}\sum_x(\nabla_N G)(x/N)Nj_{x,x+1}. \tag{3.29}$$

A second summation by parts is also possible, substituting the current by his *fluctuation-dissipation* relation

$$j_{x,x+1} = -\frac{1}{2\gamma}\mathcal{L}_N j_{x,x+1} + \frac{1}{\gamma}(\rho_t(x+1) - \rho_t(x)) - \frac{1}{\gamma}(\mathcal{E}_{x+1,x-1} - \mathcal{E}_{x,x-2}) \tag{3.30}$$

where $\mathcal{E}_{x+1,x-1}$ is given by

$$\mathcal{E}_{x+1,x-1} = \psi(x+1)\psi^*(x-1) + \psi^*(x+1)\psi(x-1). \tag{3.31}$$

Then

$$\begin{aligned}
&\frac{1}{N}\sum_x(\nabla_N G)(x/N)Nj_{x,x+1} = -\frac{1}{N}\sum_x(\nabla G)(x/N)N\frac{1}{2\gamma}\mathcal{L}j_{x,x+1}+\\
&+\frac{1}{N}\sum_x(\nabla_N G)(x/N)N\frac{1}{\gamma}\nabla(\rho_s(x+1) - \mathcal{E}_s(x+1,x-1)) =\\
&= -\frac{1}{N}\sum_x(\nabla_N G)(x/N)N\frac{1}{2\gamma}\mathcal{L}j_{x,x+1}+\\
&-\frac{1}{N}\sum_x(\triangle_N G)(x/N)\frac{1}{\gamma}(\rho_s(x+1) - \mathcal{E}_s(x+2,x)).
\end{aligned} \tag{3.32}$$

we then obtain

$$\begin{aligned}
0 = \langle\pi_t^N, G\rangle - \langle\pi_0^N, G\rangle - \int_0^t \frac{1}{\gamma N}\sum_x(\triangle_N G)(x/N)(\rho_s(x) - \mathcal{E}_s(x+1,x-1))ds\\
-\frac{N}{2\gamma}\int_0^t \frac{1}{N}\sum_x(\nabla_N G)(x/N)\mathcal{L}j_{x,x+1}.
\end{aligned} \tag{3.33}$$

It remains to study two terms, the first one is the contribution of the energy between second neighbors and the other one is the contribution of the dissipative

term. We study now the former one which is

$$\int_0^t \frac{1}{N}\sum_x (\triangle_N G)(x/N)\frac{1}{\gamma}\mathcal{E}_s(x+1,x-1)ds, \tag{3.34}$$

we remark that

$$\mathcal{E}_s(x+1,x-1) = -\partial_{\theta(x+1)} j_{x+1,x-1} \tag{3.35}$$

and the *fluctuation-dissipation* relation for the current $j_{x+1,x-1}$ is

$$j_{x+1,x-1} = -\frac{1}{2\gamma}\mathcal{L}_N j_{x+1,x-1} + \frac{1}{\gamma}\nabla\{\mathcal{E}_{x+2,x-1} - \mathcal{E}_{x+1,x}\}. \tag{3.36}$$

The commutator $[\partial_{\theta(x+1)}, \mathcal{L}_N]$ is

$$\begin{aligned}[\partial_{\theta(x+1)}, \mathcal{L}_N] = 2\nabla \big[&(\psi_r(x+2)\partial_{\psi_r(x+1)} - \psi_r(x+1)\partial_{\psi_i(x+2)}) \\ &+ (\psi_i(x+2)\partial_{\psi_r(x+1)} - \psi_i(x+1)\partial_{\psi_r(x+2)})\big],\end{aligned} \tag{3.37}$$

which applied to $j_{x+1,x-1}$ gives

$$\begin{aligned}[\partial_{\theta(x+1)}, \mathcal{L}_N] j_{x+1,x-1} =& 4\psi_i(x-1)\left(\psi_i(x+2) + \psi_i(x)\right) \\ &- 4\psi_r(x-1)\left(\psi_r(x+2) + \psi_r(x)\right)\end{aligned} \tag{3.38}$$

The term $\partial_{\theta(x+1)}\nabla\{\mathcal{E}_{x+2,x-1} - \mathcal{E}_{x+1,x}\}$ is

$$\begin{aligned}\partial_{\theta(x+1)}\nabla\{\mathcal{E}_{x+2,x-1} - \mathcal{E}_{x+1,x}\} =& 2\psi_i(x+1)\left(\psi_i(x) + \psi_i(x-2)\right) \\ &- 2\psi_r(x+1)\left(\psi_r(x) + \psi_r(x-2)\right)\end{aligned} \tag{3.39}$$

so that

$$\mathcal{E}_s(x+1,x-1) = \frac{1}{\gamma}\mathcal{L}_N\partial_{\theta(x+1)} j_{x+1,x-1} - 2\nabla(\mathcal{F}_{x+2,x-1} - \mathcal{F}_{x+1,x}) \tag{3.40}$$

where

$$\mathcal{F}_{x+2,x-1} = 2\{\psi_r(x+2)\psi_r(x-1) - \psi_i(x+2)\psi_i(x-1)\}. \tag{3.41}$$

We substitute this last expression in (3.34) and perform some manipulations

$$\begin{aligned}\int_0^t \frac{1}{N}\sum_x (\triangle_N G)(x/N)\frac{1}{2\gamma^2}\left(\mathcal{L}_N \partial_{\theta(x+1)} j_{x+1,x-1} - 2\nabla(\mathcal{F}_{x+2,x-1} - \mathcal{F}_{x+1,x})\right) ds \\ = \frac{1}{2\gamma^2 N^2}\int_0^t \frac{1}{N}\sum_x (\triangle_N G)(x/N) N^2 \mathcal{L}_N \mathcal{E}_{x+1,x-1}(s) ds \\ - \frac{1}{2N\gamma^2}\int_0^t \frac{1}{N}\sum_x (\nabla_N G)(x/N) 2\nabla(\mathcal{F}_{x+2,x-1} - \mathcal{F}_{x+1,x}) ds \\ = \frac{1}{2N^2\gamma}\frac{1}{N}\sum_x (\nabla_N G)(x/N)\left(\mathcal{E}_{x+1,x-1}(t) - \mathcal{E}_{x+1,x-1}(0)\right) + \\ + \frac{1}{\gamma^2 N^2}\int_0^t \frac{1}{N}\sum_x (\nabla_N^3 G)(x/N)(\mathcal{F}_{x+2,x-1} - \mathcal{F}_{x+1,x}) ds + N_t^G.\end{aligned} \tag{3.42}$$

Where the quadratic variation of the martingale N_t^G is

$$\begin{aligned}[N_t^G]^2 =& \frac{N^2}{N^6}\sum_x \int_0^t \left((\triangle_N G)(x/N)\right)^2 \left(\partial_{\theta(x+1)}\mathcal{E}_{x+1,x-1}\right)^2 = \\ =& \frac{N^2}{N^6}\sum_x \int_0^t \left((\triangle_N G)(x/N)\right)^2 j_{x+1,x-1}^2.\end{aligned} \tag{3.43}$$

So then, the contribution of the total term studied here, (3.34), can be neglected considering the following bounds

$$\begin{aligned}&\frac{1}{N^3}\sum_{x\in\mathbb{T}_N} \mathcal{E}_{x,x+p}(t) \le \frac{1}{2N^3}\sum_{x\in\mathbb{T}_N}\left(|\psi(x,t)|^2 + |\psi(x+p,t)|^2\right) = \frac{M_N(\psi)}{N^3} \to 0, \\ &\frac{1}{N^2}\sum_{x\in\mathbb{T}_N} \mathcal{F}_{x,x+p}(t) \le \frac{1}{2N^2}\sum_{x\in\mathbb{T}_N}\left(|\psi(x,t)|^2 + |\psi(x+p,t)|^2\right) = \frac{M_N(\psi)}{N^2} \to 0, \\ &\frac{1}{N^4}\sum_{x\in\mathbb{T}_N} j_{x,x+p}^2(t) \le \frac{1}{N^4}\sum_{x\in\mathbb{T}_N}|\psi(x,t)|^4 \le \frac{1}{N^4}\left(\sum_{x\in\mathbb{T}_N}|\psi(x,t)|^2\right)^2 \le \frac{M_N^2(\psi)}{N^4} \to 0.\end{aligned} \tag{3.44}$$

We expect then the following characterization of the hydrodynamic limit:

$$\langle \pi_t^N, G\rangle = \langle \pi_0^N, G\rangle + \frac{1}{\gamma N}\sum_{x\in\mathbb{T}_N}\int_0^t (\triangle_N G)(x/N)\rho_s(x)ds + o(N). \tag{3.45}$$

3.3.3 A rigorous proof

Let $G \in C^2(\mathbb{T}_N)$, then under Q_N the quantity

$$\langle \pi_t^N, G\rangle = \frac{1}{N}\sum_{x\in\mathbb{T}} G(\frac{x}{N})\rho_t(x) \tag{3.46}$$

has an associated process

$$\langle \pi_t^N, G\rangle = \langle \pi_0^N, G\rangle + \int_0^t (\partial_s + N^2 L_N)\langle \pi_s^N, G\rangle ds \tag{3.47}$$

with respect to the filtration $\mathcal{F}_t = \sigma(\rho_s, s \le t)$.

In order to prove the convergence of the sequence, we need first to show its relatively compactness, then that all converging subsequences converge to the same limit.

3.3.4 Relative Compactness

To show that $(Q_N)_N$ is relatively compact, it suffices to prove that the sequence of laws of the real processes $(\langle \pi_t^N, G\rangle)_{t\ge 0}$ is relatively compact for any fixed G in $C^2(\mathbb{T}_N)$. We can repeat the same arguments as in [48] (Theorem 2.1, pag. 55). Let us denote Q_N^G the probability $Q_N G^{-1}$ on $C([0,T],\mathbb{R})$, and define for any function $x \in C([0,T],\mathbb{R})$ and any $\delta > 0$, the modulus of continuity of x by $w(x,\gamma) = \sup\{|x(s) - x(t)|; s,t \in [0,T], |s-t| \le \delta\}$. The criterion for relative compactness of probabilities is:

Lemma 3.3.2. *The sequence Q_N^G is relatively compact if*

- $\forall t \in [0,T]$, $\forall \epsilon > 0$ $\exists A = A(t,\epsilon) > 0$, $\sup_N Q_N^G[|\langle \pi_t^N, G\rangle| \ge A] \le \epsilon$

- $\limsup_{\delta\to 0}\limsup_{N\to\infty} Q_N^G[w(\langle\pi^N, G\rangle, \delta) > \epsilon] = 0$

Proof. The first condition of the lemma is satisfied thanks to the conservation of the total "mass" and the following bound

$$|\langle\pi_t^N, G\rangle| \leq \|G\|_\infty \frac{1}{N}\sum_{x\in\mathbb{T}_N}\rho_t(x) = \|G\|_\infty \frac{M_N(\psi)}{N} \leq C(G) \tag{3.48}$$

where $C(G)$ is a constant depending only on G. Then

$$\begin{aligned} Q_N^G\left[|\langle\pi_t^N, G\rangle| \geq A\right] &= Q_N^G\left[|\langle\pi_0^N, G\rangle + \frac{1}{\gamma N}\sum_{x\in\mathbb{T}_N}\int_0^t (\triangle_N G)(x/N)\rho_s(x)ds| \geq A\right] \leq \\ &\leq \frac{1}{A}E_{\mu_N}\left[|\langle\pi_0^N, G\rangle + \frac{1}{\gamma N}\sum_{x\in\mathbb{T}_N}\int_0^t (\triangle_N G)(x/N)\rho_s(x)ds|\right] \\ &\leq \frac{C(G,t)}{\gamma A}. \end{aligned} \tag{3.49}$$

The first condition is satisfied choosing $A \geq \frac{C(G,t)}{\gamma\epsilon}$. Also the second condition is verified:

$$\begin{aligned} Q_N^G[\sup_{|t-s|\leq\delta}|\langle\pi_t^N, G\rangle - \langle\pi_s^N, G\rangle|] &\leq \frac{1}{\epsilon\gamma N}E_{\mu_N}[\sup_{|t-s|\leq\delta}|\int_s^t \sum_{x\in\mathbb{T}_N}(\triangle_N G)(x/N)\rho_u(x)du|] \\ &\leq \frac{C(G)\delta M_N(\psi)}{N\gamma\epsilon} \end{aligned} \tag{3.50}$$

which goes to zero for $N\to\infty$ and $\delta\to 0$. □

3.3.5 Uniqueness of limit points

After proving the relatively compactness of $(Q_N)_N$, we want to characterize the limit points of Q_N.

Lemma 3.3.3. *Let Q^* be a limit point of the sequence $(Q_N)_N$, then Q^* is con-*

centrated on trajectories $\pi_t \in C([0,T],\mathcal{M})$ *satisfying*

$$\langle \pi_t, G\rangle = \langle \pi_0, G\rangle + \frac{1}{\gamma}\int_0^t \langle \pi_s, G''\rangle ds \tag{3.51}$$

Proof. Let Q^* be a limit point and let Q_{N_k} be a sub-sequence converging to Q^*. We can replace de discrete Laplacian by the continuous one, since $(\triangle_N G)(x/N) = G''(x/N) + o(N^{-1})$, uniformly in N, in eq. (3.47). We fix $t \in [0,T]$. The application from $C([0,T],\mathcal{M})$ to $\mathbb{R}$, which associates $|\langle \pi_t, G\rangle - \langle \pi_0, G\rangle - \frac{1}{\gamma}\int_0^t \langle \pi_s, G''\rangle ds|$ to a path $\{\pi_t; 0 \le t \le T\}$, is continuous. So

$$\begin{aligned}\liminf_{k\to\infty} Q_{N_k}\left(\langle|\pi_t, G\rangle - \langle \pi_0, G\rangle - \frac{1}{\gamma}\int_0^t \langle \pi_s, G''\rangle ds| > \epsilon\right) \\ \ge Q^*\left(\langle|\pi_t, G\rangle - \langle \pi_0, G\rangle - \frac{1}{\gamma}\int_0^t \langle \pi_s, G''\rangle ds| > \epsilon\right)\end{aligned} \tag{3.52}$$

since the set is open. Then simply observing that

$$Q_N[\sup_{0\le t\le T}|M_t^G|] = 0, \tag{3.53}$$

we can conclude that all limit points Q^* are concentrated on trajectories π_t satisfying

$$\langle \pi_t^N, G\rangle = \langle \pi_0^N, G\rangle + \frac{1}{\gamma}\int_0^t \langle \pi_s^N, G''\rangle ds \tag{3.54}$$

It remains to prove that the limit trajectories are absolutely continuous respect to the Lebesgue measure.

Lemma 3.3.4. *All limit points* Q^* *of* $(Q_N)_N$ *are concentrated on absolutely continuous measures, with respect to the Lebesgue measure,* $\pi(du) = \rho(u)du$ *such that* $\pi \in \mathbb{L}^2(\mathbb{T}_N, du)$:

$$Q^*\{\pi : \pi(du) = \rho(u)du\} = 1 \tag{3.55}$$

Proof. Since

$$Q^*\left(\langle|\pi_t, G\rangle - \langle\pi_0, G\rangle - \frac{1}{\gamma}\int_0^t \langle\pi_s, G''\rangle ds| = 0\right) = 1 \tag{3.56}$$

then choosing $\pi_0 = \rho_0(u)du$ it implies that $\pi_t = \rho_t(u)du$. □

□

3.3.6 Uniqueness of weak solutions of the heat equation and convergence in probability at fixed time

We need to show that there exists only one weak solution of the hydrodynamic equation. There are different methods to prove that there exists only one weak solution of the heat equation. We refer to [48] for the proof.

The limiting probability measure is concentrated on weakly continuous trajectories, thus π_t^N converges in distribution to the deterministic measure $\pi_t(u)du$. Since convergence in distribution to a deterministic variable implies convergence in probability, the theorem is proved.

3.4 Physical implications

The model is composed of $x \in \{1, ..., N\}$ atoms attached at their extremities to particle reservoirs of Langevin type at two different densities μ_l and μ_r. The interaction between the reservoirs is modeled by two Ornstein Uhlenbeck process at the corresponding chemical potentials.

The stationary state is given by the law of independent Gaussian variables if the two reservoirs have the same chemical potentials.

We prove that the Fourier's law is valid in the stationary state for the density flow, that the total mass is proportional to its size and that the average density

per volume, in the infinite volume limit is given by the average of the chemical potentials at the boundaries.

We attach the first particle 1 and the last N to two Langevin thermostats, the dynamics is then described by the following system of stochastic differential equation

$$\begin{cases} d\psi(x,t) = -i\triangle\psi(x,t)dt - \dfrac{\gamma}{2}\psi(x,t)dt + i\psi(x,t)\sqrt{\gamma}dw_x \\ d\psi^*(x,t) = +i\triangle\psi^*(x,t)dt - \dfrac{\gamma}{2}\psi^*(x,t)dt - i\psi^*\sqrt{\gamma}dw_x \\ \qquad x = 2,...,N-1 \\ d\psi(1,t) = -i\triangle\psi(1,t)dt - \dfrac{1}{2}(\delta+\gamma)\psi(1,t)dt + i\psi\sqrt{\gamma}dw_1 + \sqrt{\delta\mu_l}dw_{\mu_l,1} \\ d\psi^*(1,t) = +i\triangle\psi^*(1,t)dt - \dfrac{1}{2}(\delta+\gamma)\psi^*(1,t)dt - i\psi^*(1,t)\sqrt{\gamma}dw_x + \sqrt{\delta\mu_l}dw^*_{\mu_l,1} \\ d\psi(N,t) = -i\triangle\psi(N,t)dt - \dfrac{1}{2}(\delta+\gamma)\psi(N,t)dt + i\psi\sqrt{\gamma}dw_N + \sqrt{\delta\mu_r}dw_{N,\mu_r} \\ d\psi^*(N,t) = +i\triangle\psi^*(N-1,t)dt - \dfrac{1}{2}(\delta+\gamma)\psi^*(N-1,t)dt - i\psi^*(N)\sqrt{\gamma}dw_N + \sqrt{\delta\mu_r}dw^*_{N,\mu_r} \end{cases} \tag{3.57}$$

Where $w_x(t)$ are real independent standard Brownian motions, and $w_{0,1}(t)$ and $w_{N-1,N}(t)$ are complex independent standard Brownian motions.

The generator of the dynamics is $\mathcal{L} = \mathcal{L}_N + \mathcal{L}_L + \mathcal{L}_R$ where $\mathcal{L}_N$ is (3.8), and

$$\begin{aligned} \mathcal{L}_L =& + \frac{\delta}{2}\{\mu_l(\partial^2_{\psi_{r(1)}} + \partial^2_{\psi_{i(1)}}) - (\psi_{r(1)}\partial_{\psi_{r(1)}} + \psi_{i(1)}\partial_{\psi_{i(1)}})\}, \\ \mathcal{L}_R =& \frac{\delta}{2}\{\mu_r(\partial^2_{\psi_{r(N)}} + \partial^2_{\psi_{i(N)}}) - (\psi_{r(N)}\partial_{\psi_{r(N)}} + \psi_{i(N)}\partial_{\psi_{i(N)}})\} \end{aligned} \tag{3.58}$$

The currents are

$$\begin{aligned} j_{x,x+1} &= -i\{\psi_x\psi^*_{x+1} - \psi^*_x\psi_{x+1}\} \text{ for } x = 2,...,N-1, \\ j_{0,1} &= (2\mu_l - \rho_1), \\ j_{N,N+1} &= -(2\mu_r - \rho_N) \end{aligned} \tag{3.59}$$

Because of the presence of reservoirs we have stationarity, for any $x = 1,..,N-1$,

we have

$$\langle j_{x,x+1}\rangle = \langle j_{0,1}\rangle = \langle j_{N-1,N}\rangle. \tag{3.60}$$

3.4.1 Entropy production

Denote by $g_{\mu_r}(\psi_1, \psi_1^*, ...\psi_N, \psi_N^*)$ the density of the product of Gaussians with mean 0 and variance μ_r

$$g_{\mu_r}(\psi_1, \psi_1^*, ...\psi_N, \psi_N^*) = e^{-\sum_{x=1}^N \frac{|\psi(x)|^2}{2\mu_r}} \tag{3.61}$$

and by f_N the density of the stationary measure with respect to g_{μ_r}

$$\langle\cdot\rangle = \int f_N g_{\mu_r} d\psi \tag{3.62}$$

where $d\psi = \prod_{x=1}^N d\psi(x)d\psi^*(x)$, by hypoellipticity this density is smooth. By stationarity

$$\begin{aligned} 0 &= -2\langle \mathcal{L}_N \log f_N\rangle \\ &= \gamma \sum_{x=1}^N \int \frac{(\partial_{\theta(x)} f_N)^2}{f_N} g_{\mu_r} d\psi + \frac{\delta}{2}\mu_r \int \frac{(\partial_{\psi(N)} f_N)^2}{f_N} g_{\mu_r} d\psi - 2\langle \mathcal{L}_l \log f_N\rangle \end{aligned} \tag{3.63}$$

for the left thermostat entropy production, let $h = g_{\mu_l}/g_{\mu_r}$ and we rewrite the last term as

$$\begin{aligned} -2\langle \mathcal{L}_l \log f_N\rangle &= -2\int \frac{f_N}{h}\mathcal{L}_l \log(\frac{f_N}{h}) g_{\mu_l} d\psi - 2\int \frac{f_N}{h}\mathcal{L}_l \log(h) g_{\mu_r} d\psi \\ &= \frac{\delta}{2}\mu_l \int \frac{(\partial_{\psi(1)}(f_N/h))^2}{f_N/h} g_{\mu_l} d\psi + \delta(\mu_l - \mu_r)(2\mu_l - \langle\rho_1\rangle) \end{aligned} \tag{3.64}$$

Recognizing the last term as the current $\langle j_{0,1}\rangle = (2\mu_l - \langle\rho_1\rangle)$ we can have the following bound

$$\begin{aligned}
&\gamma\sum_{x=1}^{N}\int\frac{(\partial_{\theta(x)}f_N)^2}{f_N}g_{\mu_r}d\psi+\\
&+\frac{\delta}{2}\mu_r\int\frac{(\partial_{\psi(N-1)}f_N)^2}{f_N}g_{\mu_r}d\psi+\frac{\delta}{2}\mu_l\int\frac{(\partial_{\psi(1)}(f_N/h))^2}{f_N/h}g_{\mu_l}d\psi=\\
&=\delta(\mu_l-\mu_r)\langle j_{x,x+1}\rangle\geq 0
\end{aligned}\tag{3.65}$$

The right sign for the density current is then $\langle j_{x,x+1}\rangle \leq 0$ (resp. $\langle j_{x,x+1}\rangle \geq 0$) if $\mu_l \leq \mu_r$ (resp. $\mu_l \geq \mu_r$).

3.4.2 Scaling of the average current

In order to recover the Fourier's law we need to bound the instantaneous current. From the stationarity, (3.59) and (3.60), we have

$$\langle\rho_1\rangle + \langle\rho_N\rangle = 2(\mu_l+\mu_r)\tag{3.66}$$

By (3.30) we have:

$$\begin{aligned}
j_{x,x+1} &= \frac{1}{\gamma}\{(\rho_{x+1}-\rho_x)-\frac{1}{2}(\mathcal{E}_{x,x+2}-\mathcal{E}_{x-1,x+1})\}-\frac{1}{2\gamma}L_N j_{x,x+1}\quad \text{for } x=2,...,N-2,\\
j_{1,2} &= \frac{4}{4\gamma+\delta}\{(\rho_2-\rho_1)-\frac{2}{4\gamma+\delta}\mathcal{E}_{1,3}-\frac{2}{4\gamma+\delta}L_N j_{1,2}\\
j_{N-1,N} &= \frac{4}{4\gamma+\delta}(\rho_N-\rho_{N-1})+\frac{2}{4\gamma+\delta}\mathcal{E}_{N,N-2}-\frac{2}{4\gamma+\delta}L_N j_{N-1,N},
\end{aligned}\tag{3.67}$$

where

$$\mathcal{E}_{x,x+2} = \psi(x)\psi^*(x+2)+\psi^*(x)\psi(x+2).\tag{3.68}$$

Using the stationarity of the current we obtain

$$\begin{aligned}\langle j_{x,x+1}\rangle &= \frac{1}{N-3}\sum_{x=2}^{N-2}\langle j_{x,x+1}\rangle \\ &= \frac{1}{(N-3)\gamma}(\langle\rho_{N-1}\rangle - \langle\rho_2\rangle) - \frac{1}{2(N-3)\gamma}\langle(\mathcal{E}_{N-2,N} - \mathcal{E}_{1,3})\rangle\end{aligned} \tag{3.69}$$

and by the relation $\langle j_{1,2}\rangle = \langle j_{N-1,N}\rangle$, we get

$$\langle\rho_{N-1}\rangle = -\langle\rho_2\rangle + 2(\mu_l + \mu_r) + \frac{1}{2}\langle(\mathcal{E}_{N-2,N} - \mathcal{E}_{1,3})\rangle. \tag{3.70}$$

we substitute the expression for $\langle\rho_{N-1}\rangle$ in (3.69) and obtain

$$\langle j_{x,x+1}\rangle = \frac{1}{(N-3)\gamma}(2(\mu_l + \mu_r) - 2\langle\rho_2\rangle + \langle\mathcal{E}_{1,3}\rangle).$$

By (3.67) we get $\langle\mathcal{E}_{1,3}\rangle$ as function of the densities and currents

$$\langle\mathcal{E}_{1,3}\rangle = -\frac{4\gamma+\delta}{2}\langle j_{1,2}\rangle + 2(\langle\rho_2\rangle - \langle\rho_1\rangle), \tag{3.71}$$

and then

$$\begin{aligned}\langle j_{x,x+1}\rangle &= \frac{1}{(N-3)\gamma}\left(2(\mu_l+\mu_r) - 2\langle\rho_2\rangle - \frac{4\gamma+\delta}{2}\langle j_{x,x+1}\rangle + 2(\langle\rho_2\rangle - \langle\rho_1\rangle\right) \\ &= \frac{1}{(N-3)\gamma}\left(2(\mu_l+\mu_r) - \frac{4\gamma+\delta}{2}\langle j_{x,x+1}\rangle - \langle\rho_1\rangle\right) \\ &= \frac{2}{\gamma(N-3)+4\gamma+\delta}\left((\mu_l+\mu_r) - \langle\rho_1\rangle\right).\end{aligned}$$

Given that $\rho \geq 0$, we can bound the current by the external chemical potential as

$$\langle j_{x,x+1}\rangle \leq \frac{2(\mu_l+\mu_r)}{\gamma(N-3)+4\gamma+\delta}. \tag{3.72}$$

So there exists a constant C, which depends on μ_r and μ_l, such that

$$\langle j_{x,x+1} \rangle \leq \frac{C}{N}.$$

for $\mu_l > \mu_r$, and

$$\langle j_{x,x+1} \rangle \geq -\frac{C}{N}$$

for $\mu_l > \mu_r$, such that

$$|\langle j_{x,x+1} \rangle| \leq \frac{C}{N}. \tag{3.73}$$

. Thanks to this bound to the current we are able now to claim the result in the following theorems.

Theorem 1. *For any* $\gamma > 0$

$$\lim_{N\to\infty} N\langle j_{x,x+1} \rangle = \frac{2}{\gamma}(\mu_r - \mu_l) \tag{3.74}$$

Theorem 2.

$$\lim_{N\to\infty} \frac{\langle M_N(\psi) \rangle}{N} = (\mu_r + \mu_l) \tag{3.75}$$

3.4.3 Fourier's law

Proposition 3.4.1. *For* $x = 1$ *and* $x = N - 2$ *we have*

$$\lim_{N\to\infty} \langle \psi_x \psi^*_{x+2} \rangle = 0 \tag{3.76}$$

Proof. The proof for $x = 1$ and $x = N - 2$ are similar. Let's do it for $x = 1$. We

make use of Cauchy-Schwarz inequality.

$$\begin{aligned}\langle\psi_1\psi_3^*\rangle &= \int \psi_1\psi_3^*\frac{f_N}{h}g_{\mu_l}d\psi d\psi^* = \\ &= \mu_l\int \psi_3^*\partial_{\psi_1^*}(\frac{f_N}{h})g_{\mu_l}d\psi d\psi^* \\ &\leq \mu_l\sqrt{\langle\rho_3\rangle}\sqrt{\int\left(\frac{\partial_{\psi_1^*}(f_N/h)}{f_N/h}\right)^2 g_{\mu_l}d\psi d\psi^*} \\ &\leq \frac{C}{\sqrt{N}}.\end{aligned} \tag{3.77}$$

□

Proposition 3.4.2. *For $x = 1$ and $x = N - 1$*

$$\lim_{N\to\infty}(\langle\rho_x\rangle - \langle\rho_{x+1}\rangle) = 0. \tag{3.78}$$

Proof. By (3.67)

$$\gamma\langle j_{12}\rangle + \frac{1}{2}\langle(\mathcal{E}_{2,4} - \mathcal{E}_{1,3})\rangle = \langle\rho_2\rangle - \langle\rho_1\rangle \tag{3.79}$$

then by (3.73) and (3.76) we have

$$\lim_{N\to\infty}(\langle\rho_1\rangle - \langle\rho_2\rangle) = 0 \tag{3.80}$$

and similarly for $x = N - 1$. □

Then we have

$$\begin{aligned}\lim_{N\to\infty}\langle\rho_1\rangle &= 2\mu_l \\ \lim_{N\to\infty}\langle\rho_N\rangle &= 2\mu_r\end{aligned} \tag{3.81}$$

and the Fourier's law is

$$\lim_{N\to\infty} N\langle j_{x,x+1}\rangle = \frac{2}{\gamma}(\mu_r - \mu_l). \tag{3.82}$$

3.4.4 Average "mass" density

We define a function

$$\phi(x) = \frac{1}{\gamma}(\langle\rho_x\rangle - \frac{1}{2}\langle\mathcal{E}_{x-1,x+1}\rangle), \tag{3.83}$$

by the continuity equation for $x = 2, ..., N-1$

$$\mathcal{L}\rho_x = j_{x-1,x} - j_{x,x+1} \tag{3.84}$$

and the fluctuation-dissipation equation

$$\langle j_{x,x+1}\rangle = -\nabla^*\phi(x) \tag{3.85}$$

we can write

$$\triangle\phi(x) = 0 \ \text{ for } x = 2, ..., N-1. \tag{3.86}$$

By the discrete maximum principle $|\phi(x)| \leq max\{\phi(2), \phi(N-1)\}$ and using the definition of currents (3.67)

$$\begin{aligned} \phi(2) &= (\frac{4\gamma+\delta}{4\gamma})\langle j_{12}\rangle + \langle\rho_1\rangle \\ \phi(N-1) &= -(\frac{4\gamma+\delta}{4\gamma})\langle j_{N-1,N}\rangle + \langle\rho_N\rangle \end{aligned} \tag{3.87}$$

both with (3.66), so, given that $\langle\rho_x\rangle \leq 2(\mu_l + \mu_r)$ for $x = 1, N-1$ it follows

$$|\phi(x)| \leq \frac{4\gamma+\delta}{4\gamma}|\langle j_{x,x+1}\rangle| + 2(\mu_l + \mu_r)$$

In view of (3.73), it follows that

$$|\phi(x)| \leq \frac{C}{N} + 2(\mu_l + \mu_r) \text{ for } x = 1, ..., N-1. \tag{3.88}$$

Furthermore, given the results of the previous section, propositions 3.76 and 3.78, and the explicit expression of ϕ

$$\lim_{N\to\infty} \frac{1}{N} \sum_{x=1}^{N-1} \phi(x) = \frac{1}{\gamma}(\mu_l + \mu_r) : \tag{3.89}$$

then for

$$M_N(\psi) = \sum_{x=1}^{N-1} \rho_x$$

we obtain the result

$$\lim_{N\to\infty} \frac{1}{N} \sum_{x=1}^{N-1} \langle M_N(\psi) \rangle = (\mu_l + \mu_r). \tag{3.90}$$

We can verify that, at equilibrium, the two thermostats must have the same chemical potentials.

Proposition 3.4.3. *If* $\langle j_{x,x+1} \rangle = 0$ *then* $\mu_l = \mu_r$.

Proof. By the stationarity and by (3.59), we can write the average densities at the extremities in $x = 1$ and $x = N$

$$\begin{aligned} \langle \rho_1 \rangle &= 2\mu_l \\ \langle \rho_N \rangle &= 2\mu_r \end{aligned} \tag{3.91}$$

and by (3.67) in the bulk, $x = 1, ..., N-1$

$$\langle \rho_{x+1} \rangle - \langle \rho_x \rangle = \frac{1}{2} \left(\langle \mathcal{E}_{x,x+2} \rangle - \langle \mathcal{E}_{x-1,x+1} \rangle \right) \tag{3.92}$$

Then substituting recursively the extremity density value in 1, we find

$$\langle \rho_x \rangle = 2\mu_r + \frac{1}{2}\langle \mathcal{E}_{x-1,x+1} \rangle \tag{3.93}$$

and similarly when substituting the N density value

$$\langle \rho_x \rangle = 2\mu_l + \frac{1}{2}\langle \mathcal{E}_{x-1,x+1} \rangle \tag{3.94}$$

so that $\mu_r = \mu_l$. □

3.4.5 Non Linear Case

When the Hamiltonian is nonlinear, $p > 1$, the current doesn't decompose in *fluctuation-dissipation* terms:

$$j_{x,x+1} = -\mathcal{L}_N j_{x,x+1} + \nabla \rho_x + \mathcal{E}_{x-1,x+1} + \mathcal{E}_{x,x+1} + \mathcal{E}_{x,x+1}|\psi_x|^{p-1}. \tag{3.95}$$

Being a non gradient system a correction term in the second order approximation of a local Gibbs measure in the relative entropy method should be added. Unfortunately the non linearity made it for us impossible to find the proper correction term which would gauge the system in the local averages.

4

Non-equilibrium Isothermal transformations in a temperature gradient from a microscopic dynamics

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4.1 Introduction

Macroscopic isothermal thermodynamic transformations can be modeled microscopically by putting a system in contact with Langevin heat bath at a given temperature β^{-1}. In [54] a chain of n anharmonic oscillators is *immersed* in

a heat bath of Langevin thermostats acting independently on each particle. A macroscopically equivalent isothermal dynamics is obtained by elastic collisions with an external gas of independent particles with Maxwellian random velocities with variance β^{-1}. The effect is to quickly renew the velocities distribution of the particles, so that at any given time it is very close to a Maxwellian at given temperature. The chain is pinned only on one side, while at the opposite site a force (tension) τ is acting. The equilibrium distribution is characterized by the two control parameters β^{-1}, τ (temperature and tension). The total length and the energy of the system in equilibrium are in general non-linear functions of these parameters given by the standard thermodynamic relations.

By changing the tension τ applied to the system, a new equilibrium state, with the same temperature β^{-1}, will be eventually reached. For large n, while the heat bath equilibrates the velocities at the corresponding temperature at time of order $\tilde{1}$, the system converges to this global equilibrium length at a time scale of order $n^2 t$. In [54] it is proven that the length stretch of the system evolves in a diffusive space-time scale, i.e. after a scaling limit the empirical distribution of the interparticle distances converges to the solution of a non-linear diffusive equation governed by the local tension. Consequently this diffusive equation describes the non-reversible isothermal thermodynamic transformation from one equilibrium to another with a different tension. By a further rescaling of the time dependence of the changing tension, a so called *quasi-static* or *reversible* isothermal transformation is obtained. Corresponding Clausius equalities/inequalities relating work done and change in free energy can be proven.

The results of [54] summarized above concern isothermal transformations from an *equilibrium* state to another, by changing the applied tension. In this chapter we are interested in transformations between *non-equilibrium* stationary states. We now consider the chain of oscillators immersed in a heat bath with a *macroscopic gradient* of temperature: each particle is in contact with thermostats at a

different temperature. These temperatures slowly change from a particle to the neighboring one. A tension τ is again applied to the chain. In the stationary state, that is now characterized by the tension τ and the profile of temperatures $\beta_1^{-1}, \ldots, \beta_n^{-1}$, there is a continuous flow of energy through the chain from the hot thermostats to the cold ones. Unlike the equilibrium case, the probability distribution of the configurations of the chain in the stationary state cannot be computed explicitly.

By changing the applied tension we can obtain transitions from a non-equilibrium stationary state to another, that will happen in a diffusive space-time scale as in the equilibrium case. The main result in the present chapter is that these transformations are again governed by a diffusive equation that takes into account the local temperature profile. The free energy can be computed according to the local equilibrium rule and its changes during the transformation satisfy the Clausius inequality with respect to the work done. This provides a mathematically precise example for understanding non-equilibrium thermodynamics from microscopic dynamics.

The results in [54] where obtained by using the relative entropy method, first developed by H.T.Yau in [84] for the Ginzburg-Landau dynamics, which is just the over-damped version of the bulk dynamics of the oscillators chain. The relative entropy method is very powerful and flexible, and was already applied to interacting Ornstein-Uhlenbeck particles [76] as well as many other cases, in particular in the hyperbolic scaling limit for Euler equation in the smooth regime [58, 14]. This method consists in looking at the time evolution of the relative entropy of the distribution of the particle with respect to the local Gibbs measure parametrized by the non-constant tension profile corresponding to the solution of the macroscopic diffusion equation. The key point of the method is in proving that the time derivative of such relative entropy is small, so that the relative entropy itself remains small with respect to the size of the system and local

equilibrium, in a weak but sufficient form, propagates in time. In the particular applications to interacting Ornstein-Uhlenbeck particles [76, 54], the local Gibbs measure needs to be corrected by a small recentering of the damped velocities due to the local gradient of the tension.

The relative entropy method seems to fail when the stationary measures are not the equilibrium Gibbs measure, like in the present case. The reason is that when taking the time derivative of the relative entropy mentioned above, a large term, proportional to the gradient of the temperature, appears. This term is related to the *entropy production* of the stationary measure. Consequently we could not apply the relative entropy method to the present problem.

A previous method was developed by Guo, Papanicolaou and Varadhan in [37] for over-damped dynamics. In this approach the main step in closing the macroscopic equation is the direct comparison of the coarse grained empirical density in the microscopic and macroscopic space scale. They obtain first a bound of the Dirichlet form (more precisely called Fisher information) from the time derivative of the relative entropy with respect to the equilibrium stationary measures. This bound implies that the system is close to equilibrium on a local microscopic scale, and that the density on a large microscopic interval is close to the density in a small macroscopic interval (the so called *one* and *two block estimates*, see [48] chapter 5).

In the over-damped dynamics considered in [37], the Dirichlet form appearing in the time derivative of the relative entropy controls the gradients of the probability distributions with respects to the position of the particles. In the damped models, the Dirichlet form appearing in the time derivative of the relative entropy controls only the gradients on the velocities of the probability distribution of the particles. In order to deal with damped models a different approach for comparing densities on the different scales was developed in [57], after the over-damped case in [81], based on Young measures. Unfortunately this approach requires a control

of higher moments of the density that are difficult to prove for lattice models. Consequently we could not apply this method either in the present situation.

The main mathematical novelty in the present work is the use of entropic hypocoercivity, inspired by [82]. We introduce a Fisher information form I_n associated to the vector fields $\{\partial_{p_i} + \partial_{q_i}\}_{i=1,\dots,n}$, defined by (4.27). By computing the time derivative of this Fisher information form on the distribution at time t of the configurations, we obtain a uniform bound $I_n \leq Cn^{-1}$. This implies that, at the macroscopic diffusive time scale, velocity gradients of the distribution are very close to positions gradients. This allows to obtain a bound on the Fisher information on the positions from the bound on the Fisher information on the velocities. At this point we are essentially with the same information as in the over-damped model, and we proceed as in [37]. Observe that the Fisher information I_n we introduce in (4.27) is more specific and a bit different from the distorted Fisher information used by Villani in [82], in particular I_n is more degenerate. On the other hand the calculations, that are contained in appendix D are less *miraculous* than in [82], and they are stable enough to control the effect of the boundary tension and of the gradient of temperature. This also suggests that entropic hypocoercivity seems to be the right tool in order to obtain explicit estimates uniform in the dimension of the system.

Adiabatic thermodynamic transformations are certainly more difficult to be obtained from microscopic dynamics, for some preliminary results see [58, 14, 8, 55]. Equilibrium fluctuations for the dynamics with constant temperature can be treated as in [56]. The fluctuations in the case with a gradient of temperature are non-equilibrium fluctuation, and we believe that can be treated with the techniques of the present work together with those developed in the over-damped case in [16].

Large deviations for the stationary measure also require some further mathematical investigations, but we conjecture that the corresponding quasi-potential

functional ([11]) is given by the free energy associated to the local Gibbs measure, without any non-local terms, unlike the case of the simple exclusion process.

The chapter is structured in the following way. In section 4.2 we define the dynamics and we state the main result (Theorem 4.2.1). In section 4.3 we discuss the consequences for the thermodynamic transformations from a stationary state to another, the Clausius inequality and the quasi-static limit. In section 4.4 are obtained the bounds on the entropy and the various Fisher informations needed in the proof of the hydrodynamic limit. In section 4.5 we show that any limit point of the distribution of the empirical density on strain of the volume is concentrated in the weak solutions of the macroscopic diffusion equation. The compactness, regularity and uniqueness of the corresponding weak solution, necessary to conclude the proof, are proven in the first three appendices. Appendix D contains the calculations and estimates for the time derivative of the Fisher information I_n.

4.2 The dynamics and the results

We consider a chain of n coupled oscillators in one dimension. Each phase space is described by $\{q_i, p_i, i = 1, \dots, n\} \in \mathbb{R}^{2n}$. The interaction between two particles i and $i-1$ is described by the potential energy $V(q_i - q_{i-1})$ of an anharmonic spring. The chain is attached on the left to a fixed point, so we set $q_0 = 0, p_0 = 0$. We call $\{r_i = q_i - q_{i-1}, i = 1, \dots, n\}$ the interparticle distance.

We assume V to be a positive smooth function, satisfying the following assumptions:

i)

$$\lim_{|r|\to\infty} \frac{V(r)}{|r|} = \infty, \tag{4.1}$$

ii) there exists a constant $C_2 > 0$ such that:

$$\sup_r |V''(r)| \leq C_2, \tag{4.2}$$

iii) there exists a constant $C_1 > 0$ such that:

$$V'(r)^2 \leq C_1 \left(1 + V(r)\right). \tag{4.3}$$

In particular these conditions imply $|V'(r)| \leq C_0 + C_2|r|$ for some constant C_0. Notice that these conditions allow potentials growing like $V(r) \sim |r|^\alpha$ for large r, with $1 < \alpha \leq 2$.

The energy is defined by the following Hamiltonian function:

$$\mathcal{H} := \sum_{i=1}^{n} \left(\frac{p_i^2}{2} + V(r_i) \right). \tag{4.4}$$

The particle dynamics is subject to an interaction with an environment given by Langevin heat bath at different temperatures β_i^{-1}. We choose β_i as slowly varying on a macroscopic scale, i.e. $\beta_i = \beta(i/n)$ for a given smooth strictly positive function $\beta(x)$, $x \in [0,1]$ such that $\inf_{y\in[0,1]} \beta(y) \geq \beta_- > 0$.

The equations of motion are given by

$$\begin{cases} dr_i(t) = n^2(p_i(t) - p_{i-1}(t))dt \\ dp_i(t) = n^2(V'(r_{i+1}(t)) - V'(r_i(t)))\, dt - n^2\gamma p_i(t)dt + n\sqrt{\dfrac{2\gamma}{\beta_i}}dw_i(t), \quad i = 1, .., N-1 \\ dp_n(t) = n^2(\bar{\tau}(t) - V'(r_n(t)))\, dt - n^2\gamma p_n(t)\, dt + n\sqrt{\dfrac{2\gamma}{\beta_n}}dw_n(t). \end{cases} \tag{4.5}$$

Here $\{w_i(t)\}_i$ are n-independent Wiener processes, $\gamma > 0$ is the coupling parameter with the Langevin thermostats. The time is rescaled according to the diffusive space-time scaling, i.e. t is the macroscopic time. The tension $\tilde{\tau} = \tilde{\tau}(t)$ changes at the macroscopic time scale (i.e. very slowly in the microscopic time scale).

The generator of the diffusion is given by

$$\mathcal{L}_n^{\bar{\tau}(t)} := n^2 \mathcal{A}_n^{\bar{\tau}(t)} + n^2 \gamma \mathcal{S}_n, \tag{4.6}$$

where $\mathcal{A}_n^{\bar{\tau}}$ is the Liouville generator

$$A_n^{\bar{\tau}} = \sum_{i=1}^{n} (p_i - p_{i-1}) \partial_{r_i} + \sum_{i=1}^{n-1} (V'(r_{i+1}) - V'(r_i)) \partial_{p_i} + (\bar{\tau} - V'(r_n)) \partial_{p_n} \tag{4.7}$$

while S_n is the operator

$$S_n = \sum_{i=1}^{n} \left(\beta_i^{-1} \partial_{p_i}^2 - p_i \partial_{p_i} \right). \tag{4.8}$$

4.2.1 Gibbs measures

For $\bar{\tau}(t) = \tau$ constant, and $\beta_i = \beta$ homogeneous, the system has a unique invariant probability measure given by a product of invariant Gibbs measures $\mu_{\tau,\beta}^n$:

$$d\mu_{\tau,\beta}^n = \prod_{i=1}^{n} e^{-\beta(\mathcal{E}_i - \tau r_i) - \mathcal{G}(\tau,\beta)} \, dr_i dp_i \tag{4.9}$$

where $\mathcal{E}_i$ is the energy of the particle i:

$$\mathcal{E}_i = \frac{p_i^2}{2} + V(r_i). \tag{4.10}$$

The function $\mathcal{G}(\tau, \beta)$ is the Gibbs potential defined as:

$$\mathcal{G}(\tau, \beta) = \log \left[\sqrt{2\pi\beta^{-1}} \int e^{-\beta(V(r) - \tau r)} dr \right]. \tag{4.11}$$

Notice that, thanks to condition (4.1), $\mathcal{G}(\tau, \beta)$ is finite for any $\tau \in \mathbb{R}$ and any $\beta > 0$. Furthermore it is strictly convex in τ.

The free energy of the equilibrium state (r, β) is given by the Legendre trans-

form of $\beta^{-1}\mathcal{G}(\tau,\beta)$:

$$\mathcal{F}(r,\beta) = \sup_{\tau}\{\tau r - \beta^{-1}\mathcal{G}(\tau,\beta)\} \tag{4.12}$$

The corresponding convex conjugate variables are the equilibrium average length

$$\mathfrak{r}(\tau,\beta) = \beta^{-1}\partial_\tau \mathcal{G}(\tau,\beta) \tag{4.13}$$

and the tension

$$\boldsymbol{\tau}(r,\beta) = \partial_r \mathcal{F}(r,\beta). \tag{4.14}$$

Observe that

$$\mathbb{E}_{\mu^n_{\tau,\beta}}[r_i] = \mathfrak{r}(\tau,\beta), \qquad \mathbb{E}_{\mu^n_{\tau,\beta}}[V'(r_i)] = \tau. \tag{4.15}$$

4.2.2 The hydrodynamic limit

We assume that for a given initial profile $r_0(x)$ the initial probability distribution satisfies:

$$\frac{1}{n}\sum_{i=1}^{n} G(i/n) r_i(0) \underset{n\to\infty}{\longrightarrow} \int_0^1 G(x) r_0(x) dx \qquad \text{in probability} \tag{4.16}$$

for any continuous test function $G \in \mathcal{C}_0([0,1])$. We expect that this same convergence happens at the macroscopic time t:

$$\frac{1}{n}\sum_{i=1}^{n} G(i/n) r_i(t) \longrightarrow \int_0^1 G(x) r(x,t) dx \tag{4.17}$$

where $r(x,t)$ satisfies the following diffusive equation

$$\begin{cases} \partial_t r(x,t) = \dfrac{1}{\gamma}\partial_x^2 \boldsymbol{\tau}(r(x,t),\beta(x)) \qquad \text{for} \qquad x \in [0,1] \\ \partial_x \boldsymbol{\tau}(r(t,x),\beta(x))|_{x=0} = 0, \quad \boldsymbol{\tau}(r(t,x),\beta(x))|_{x=1} = \bar{\tau}(t), \quad t > 0 \\ r(0,x) = r_0(x), \quad x \in [0,1] \end{cases} \tag{4.18}$$

We say that $r(x,t)$ is a weak solution of (4.18) if for any smooth function $G(x)$ on $[0,1]$ such that $G(1) = 0$ and $G'(0) = 0$ we have

$$\int_0^1 G(x)\left(r(x,t) - r_0(x)\right)dx = \gamma^{-1}\int_0^t ds\left[\int_0^1 G''(x)\tau(r(x,s),\beta(x))dx - G'(1)\bar{\tau}(s)\right]. \tag{4.19}$$

In appendix C we prove that the weak solution is unique in the class of functions such that:

$$\int_0^t ds \int_0^1 \left(\partial_x \tau(r(x,s),\beta(x))\right)^2 dx < +\infty. \tag{4.20}$$

Let $\nu_{\beta\cdot}^n$ the inhomogeneous Gibbs measure

$$d\nu_{\beta\cdot}^n = \prod_{i=1}^n \frac{e^{-\beta_i \mathcal{E}_i}}{Z_{\beta_i}} \tag{4.21}$$

Observe that this is **not** the stationary measure for the dynamics defined by (4.5) and (4.6) for $\bar{\tau} = 0$.

Let f_t^n the density, with respect to $\nu_{\beta\cdot}^n$, of the probability distribution of the system at time t, i.e. the solution of

$$\partial_t f_t^n = \mathcal{L}_n^{\bar{\tau}(t),*} f_t^n, \tag{4.22}$$

where $\mathcal{L}_n^{\bar{\tau}(t),*}$ is the adjoint of $\mathcal{L}_n^{\bar{\tau}(t)}$ with respect to $\nu_{\beta\cdot}^n$, i.e. explicitly

$$\mathcal{L}_n^{\bar{\tau}(t),*} = -n^2 \mathcal{A}_n^{\tau(t)} - n\sum_{i=1}^{n-1} \nabla_n \beta(i/n) p_i V'(r_{i+1}) + n^2 \beta(1) p_n \bar{\tau} + n^2 \gamma \mathcal{S}_n, \tag{4.23}$$

where

$$\nabla_n \beta(i/n) = n\left(\beta\left(\frac{i+1}{n}\right) - \beta\left(\frac{i}{n}\right)\right), \qquad i = 1, \ldots, n-1. \tag{4.24}$$

Define the relative entropy of $f_t^n d\nu_{\beta\cdot}^n$ with respect to $d\nu_{\beta\cdot}^n$ as:

$$H_n(t) = \int f_t^n \log f_t^n d\nu_{\beta\cdot}^n. \tag{4.25}$$

We assume that the initial density f_0^n satisfy the bound

$$H_n(0) \leq Cn. \tag{4.26}$$

We also need some regularity of f_0^n: define the hypercoercive Fisher information functional:

$$I_n(t) = \sum_{i=1}^{n-1} \beta_i^{-1} \int \frac{((\partial_{p_i} + \partial_{q_i}) f_t^n)^2}{f_t^n} d\nu_{\beta\cdot} \tag{4.27}$$

where $\partial_{q_i} = \partial_{r_i} - \partial_{r_{i+1}}, i = 1, \ldots, n-1$, and $\nu_{\beta\cdot} := \nu_{\beta\cdot}^n$. We assume that

$$I_n(0) \leq K_n \tag{4.28}$$

with K_n growing less than exponentially in n. We will show in Appendix D that for any $t > 0$ we have $I_n(t) \leq Cn^{-1}$.

Furthermore we assume that

$$\lim_{n\to\infty} \int \left| \frac{1}{n} \sum_{i=1}^{n} G\left(\frac{i}{n}\right) r_i - \int_0^1 G(x) r_0(x) dx \right| f_0^n d\nu_{\beta\cdot} = 0 \tag{4.29}$$

for any continuous test function $G \in \mathcal{C}_0([0,1])$.

Theorem 4.2.1. *Assume that the starting initial distribution satisfy the above*

conditions. Then

$$\lim_{n\to\infty} \int \left| \frac{1}{n} \sum_{i=1}^{n} G\left(\frac{i}{n}\right) r_i - \int_0^1 G(x) r(x,t) dx \right| f_t^n d\nu_{\beta\cdot} = 0, \tag{4.30}$$

where $r(x,t)$ is the unique weak solution of (4.18) satisfying (4.20)*.*

Furthermore a local equilibrium result is valid in the following sense: consider a local function $\phi(\mathbf{r},\mathbf{p})$ such that for some positive finite constants C_1, C_2 we have the bound

$$|\phi(\mathbf{r},\mathbf{p})| \leq C_1 \sum_{i\in\Lambda_\phi} (p_i^2 + V(r_i))^\alpha + C_2, \qquad \alpha < 1 \tag{4.31}$$

where Λ_ϕ is the local support of ϕ. Let k_ϕ the length of Λ_ϕ, and let $\theta_i\phi$ be the shifted function, well defined for $k_\phi < i < n - k_\phi$, and define

$$\hat{\phi}(r,\beta) = \mathbb{E}_{\mu_{\boldsymbol{\tau}(r,\beta),\beta}}(\phi)\,. \tag{4.32}$$

Corollary 4.2.2. *It holds*

$$\lim_{n\to\infty} \int \left| \frac{1}{n} \sum_{i=k_\phi+1}^{n-k_\phi} G\left(\frac{i}{n}\right) \theta_i\phi(\mathbf{r},\mathbf{p}) - \int_0^1 G(x) \hat{\phi}(r(x,t),\beta(x)) dx \right| f_t^n d\nu_{\beta\cdot} = 0. \tag{4.33}$$

4.3 Non-equilibrium thermodynamics

We collect in this section some interesting consequences of the main theorem for the non-equilibrium thermodynamics of this system. All statements contained in this section can be proven rigorously, except for one that will require more investigation in the future. The aim is to build a non equilibrium thermodynamics in the spirit of [12, 11]. The equilibrium version of these results has been already proven in [54].

As we already mentioned, stationary states of our dynamics are not given by Gibbs measures if a gradient in the temperature profile is present, but they are still characterized by the tension $\bar{\tau}$ applied. We denote these stationary distributions as *non-equilibrium stationary states* (NESS). Let us denote $f^n_{ss,\tau}$ the density of the stationary distribution with respect to $\nu_{\beta.}$.

It is easy to see that

$$\int V'(r_i) f^n_{ss,\tau} \nu_{\beta.} = \tau, \qquad i = 1, \dots, n. \tag{4.34}$$

In fact, since $\int p_i f^n_{ss,\tau} \nu_{\beta.} = 0$ and

$$\begin{aligned} n^{-2}\mathcal{L}^\tau_n p_i &= V'(r_{i+1}) - V'(r_i) - \gamma p_i, \quad i = 1, \dots, n-1, \\ n^{-2}\mathcal{L}^\tau_n p_n &= \tau - V'(r_n) - \gamma p_n, \end{aligned}$$

we have

$$0 = \int (V'(r_{i+1}) - V'(r_i)) f^n_{ss,\tau} \nu_{\beta.} = \int (\tau - V'(r_n)) f^n_{ss,\tau} \nu_{\beta.}.$$

By the main theorem 4.2.1, there exists a stationary profile of stretch $r_{ss,\tau}(y) = \mathfrak{r}(\tau, \beta(y))$ (defined by (4.13)) such that for any continuous test function G:

$$\lim_{n\to\infty} \int \left| \frac{1}{n} \sum_{i=1}^{n} G\left(\frac{i}{n}\right) r_i - \int_0^1 G(x) r_{ss,\tau}(x) dx \right| f^n_{ss,\tau} d\nu_{\beta.} = 0, \tag{4.35}$$

In order to study the transition from one stationary state to another with different tension, we start the system at time 0 with a stationary state with tension τ_0, and we change tension with time, setting $\bar{\tau}(t) = \tau_1$ for $t \geq t_1$. The distribution of the system will eventually converge to a stationary state with tension τ_1. Let $r(x,t)$ be the solution of the macroscopic equation (4.19) starting with $r_0(x) = r_{ss,\tau_0}(x)$. Clearly $r(x,t) \to r_1(x) = r_{ss,\tau_1}(x)$, as $t \to \infty$.

4.3.1 Excess Heat

The (normalized) total internal energy of the system is defined by

$$U_n := \frac{1}{n}\sum_{i=1}^{n}\left(\frac{p_i^2}{2} + V(r_i)\right) \tag{4.36}$$

It evolves as:

$$U_n(t) - U_n(0) = \mathcal{W}_n(t) + Q_n(t)$$

where

$$\mathcal{W}_n(t) = \int_0^t \bar{\tau}(s) n p_n(s) ds = \int_0^t \bar{\tau}(s)\frac{dq_n(s)}{n}$$

is the (normalized) work done by the force $\bar{\tau}(s)$ up to time t, while

$$Q_n(t) = \gamma\, n\sum_{j=1}^{n}\int_0^t ds\left(p_j^2(s) - \beta_j^{-1}\right) + \sum_{j=1}^{n}\sqrt{2\gamma\beta_j^{-1}}\int_0^t p_j(s)dw_i(s). \tag{4.37}$$

is the total flux of energy between the system and the heat bath (divided by n). As a consequence of theorem 4.2.1 we have that

$$\lim_{n\to\infty}\mathcal{W}_n(t) = \int_0^t \bar{\tau}(s)d\mathcal{L}(s)$$

where $\mathcal{L}(t) = \int_0^1 r(x,t)dx$, the total macroscopic length at time t. While for the energy difference we expect that

$$\lim_{n\to\infty}\left(U_n(t) - U_n(0)\right) = \int_0^1 \left[u(\boldsymbol{\tau}(r(x,t),\beta(x)),\beta(x)) - u(\tau_0,\beta(x))\right]dx \tag{4.38}$$

where $u(\tau,\beta)$ is the average energy for $\mu_{\beta,\tau}$, i.e.

$$u(\tau,\beta) = \int \mathcal{E}_1 d\mu^1_{\tau,\beta} = \frac{1}{2\beta} + \int V(r)e^{-\beta(V(r)-\tau r)-\tilde{\mathcal{G}}(\tau,\beta)}dr$$

with $\tilde{\mathcal{G}}(\tau,\beta) = \log \int e^{-\beta(V(r)-\tau r)} dr$. Unfortunately (4.38) does not follow from (4.33), since (4.31) is not satisfied. Consequently at the moment we do not have a rigorous proof of (4.38). In the constant temperature profile case, treated in [54], this limit can be computed rigorously thanks to the use on the relative entropy method [84] that gives a better control on the local distribution of the energy.

Since $\boldsymbol{\tau}(r(x,t),\beta(x)) \to \tau_1$ as $t \to \infty$, it follows that

$$u(\boldsymbol{\tau}(r(x,t),\beta(x)),\beta(x)) \to u(\tau_1,\beta(x))$$

and the energy change will become

$$\int_0^1 \left(u(\tau_1,\beta(x)) - u(\tau_0,\beta(x))\right) dx = \int_0^{+\infty} \bar{\tau}(s) d\mathcal{L}(s) ds + Q = \mathcal{W} + Q \qquad (4.39)$$

where Q is the limit of (4.37), which is called *excess heat*. So equation (4.39) is the expression of the first principle of thermodynamics in this *isothermal* transformation between non–equilibrium stationary states. Here *isothermal* means that the profile of temperature does not change in time during the transformation.

4.3.2 Free energy

Define the *free energy* associated to the macroscopic profile $r(x,t)$:

$$\widetilde{\mathcal{F}}(t) = \int_0^1 \mathcal{F}(r(x,t),\beta(x)) dx. \qquad (4.40)$$

Correspondingly the free energy associated to the macroscopic stationary state is:

$$\widetilde{\mathcal{F}}_{ss}(\tau) = \int_0^1 \mathcal{F}(r_{ss,\tau}(x),\beta(x)) dx \qquad (4.41)$$

A straightforward calculation using (4.19) gives

$$\widetilde{\mathcal{F}}(t) - \widetilde{\mathcal{F}}_{ss}(\tau_0) = \mathcal{W}(t) - \gamma^{-1} \int_0^t ds \int_0^1 \left(\partial_x \boldsymbol{\tau}(r(x,s),\beta(x))\right)^2 dx \tag{4.42}$$

and after the time limit $t \to \infty$

$$\begin{aligned} \widetilde{\mathcal{F}}_{ss}(\tau_1) - \widetilde{\mathcal{F}}_{ss}(\tau_0) = \mathcal{W} - \gamma^{-1} \int_0^{+\infty} dt \int_0^1 \left(\partial_x \boldsymbol{\tau}(r(x,t),\beta(x))\right)^2 dx \\ \leq \mathcal{W} \end{aligned} \tag{4.43}$$

i.e. Clausius inequality for NESS. Notice that in the case β_j constant, this is just the usual Clausius inequality (see [54]).

4.3.3 Quasi-static limit and reversible transformations

The thermodynamic transformation obtained above from the stationary state at tension τ_0 to the one at tension τ_1 is an irreversible transformation, where the work done on the system by the external force is strictly bigger than the change in free energy.

In thermodynamics the *quasi-static* transformations are (vaguely) defined as those processes where changes are so slow such that the system is in *equilibrium* at each instant of time. In the spirit of [12] and [54], these quasi static transformations are precisely defined as a limiting process by rescaling the time dependence of the driving tension $\bar{\tau}$ by a small parameter ε, i.e. by choosing $\bar{\tau}(\epsilon t)$. Of course the right time scale at which the evolution appears is $\varepsilon^{-1}t$ and the rescaled solution $\tilde{r}^\varepsilon(x,t) = r(x,\varepsilon^{-1}t)$ satisfy the equation

$$\begin{cases} \partial_t \tilde{r}^\varepsilon(x,t) = \dfrac{1}{\epsilon\gamma} \partial_x^2 \boldsymbol{\tau}(\tilde{r}^\varepsilon(x,t),\beta(x)) \qquad \text{for} \qquad x \in [0,1] \\ \partial_x \boldsymbol{\tau}(\tilde{r}^\varepsilon(t,x),\beta(x))|_{x=0} = 0, \quad \boldsymbol{\tau}(\tilde{r}^\varepsilon(t,x),\beta(x))|_{x=1} = \bar{\tau}(t), \quad t > 0 \\ \tau(\tilde{r}^\varepsilon(0,x),\beta(x)) = \tau_0, \quad x \in [0,1] \end{cases} \tag{4.44}$$

By repeating the argument above, equation (4.43) became:

$$\widetilde{\mathcal{F}}_{ss}(\tau_1) - \widetilde{\mathcal{F}}_{ss}(\tau_0) = \mathcal{W}^{\varepsilon} - \frac{1}{\epsilon\gamma}\int_0^{+\infty} dt \int_0^1 \left(\partial_x \boldsymbol{\tau}(\tilde{r}^{\varepsilon}(x,t),\beta(x))\right)^2 dx \qquad (4.45)$$

By the same argument used in [54] for β constant, it can be proven that the last term on the right hand side of (4.45) converges to 0 as $\varepsilon \to 0$, and that $\boldsymbol{\tau}(\tilde{r}^{\varepsilon}(x,t),\beta(x)) \to \bar{\tau}(t)$ for almost any $x \in [0,1]$ and $t \geq 0$. Consequently in the quasi-static limit we have the Clausius equality

$$\widetilde{\mathcal{F}}_{ss}(\tau_1) - \widetilde{\mathcal{F}}_{ss}(\tau_0) = \mathcal{W}$$

This implies the following equality for the heat in the quasi-static limit:

$$Q = \int_0^1 \beta^{-1}(x)\left(S(r_{ss}(x,\tau_1),u_{ss}(x,\tau_1)) - S(r_{ss}(x,\tau_0),u_{ss}(x,\tau_0))\right) dx \qquad (4.46)$$

analogous of the equilibrium equality $Q = T\Delta S$.

In [53] a direct quasi-static limit is obtained form the microscopic dynamics without passing through the macroscopic equation (4.19), by choosing a driving tension $\bar{\tau}$ that changes at a slower time scale.

4.4 Entropy and hypercoercive bounds

In this section we prove the bounds on the relative entropy and the different Fisher information that we need in the proof of the hydrodynamic limit in section section 4.5. These bounds provide a quantitative information on the closeness of the local distributions of the particles to some equilibrium measure.

In order to shorten formulas, we introduce here some vectorial notation. Given

two vectors $u = (u_1, \dots, u_n), v = (v_1, \dots, v_n)$, define

$$u \odot v = \sum_{i=1}^{n} \beta_i^{-1} u_i v_i, \qquad u \tilde{\odot} v = \sum_{i=1}^{n-1} \beta_i^{-1} u_i v_i, \qquad |u|^2_{\odot} = u \odot u, \quad |u|^2_{\tilde{\odot}} = u \tilde{\odot} u.$$

We also use the notations

$$\begin{aligned} \partial_p = (\partial_{p_1}, \dots, \partial_{p_n}) \qquad \partial_p^* = (\partial^*_{p_1}, \dots, \partial^*_{p_n}), \qquad \partial^*_{p_i} = \beta_i p_i - \partial_{p_i} \\ \partial_q = (\partial_{q_1}, \dots, \partial_{q_n}), \qquad \partial_{q_i} = \partial_{r_i} - \partial_{r_{i+1}}, \quad \partial_{q_n} = \partial_{r_n}. \end{aligned} \tag{4.47}$$

Observe that with this notations we can write

$$\mathcal{S}_n = -\partial_p^* \odot \partial_p, \qquad \mathcal{A}_n^{\tau} = p \cdot \partial_q - \partial_q \mathcal{V} \cdot \partial_p + \tau \partial_{p_n} \tag{4.48}$$

where $\mathcal{V} = \sum_i V(r_i)$ and the $\cdot$ denotes the usual scalar product in $\mathbb{R}^n$. Then we define the following Fisher informations forms on a probability density distribution (with respect to $\nu_{\beta \cdot}$):

$$\begin{aligned} \mathcal{D}_n^p(f) &= \int \frac{|\partial_p f|^2_{\odot}}{f} d\nu_{\beta \cdot}, \qquad \tilde{\mathcal{D}}_n^p(f) = \int \frac{|\partial_p f|^2_{\tilde{\odot}}}{f} d\nu_{\beta \cdot} \\ \mathcal{D}_n^r(f) &= \int \frac{|\partial_q f|^2_{\tilde{\odot}}}{f} d\nu_{\beta \cdot} \\ I_n(f) &= \int \frac{|\partial_p f + \partial_q f|^2_{\tilde{\odot}}}{f} d\nu_{\beta \cdot} = \tilde{\mathcal{D}}_n^p(f) + \mathcal{D}_n^r(f) + 2 \int \frac{\partial_q f \tilde{\odot} \partial_p f}{f} d\nu_{\beta \cdot} \geq 0 \end{aligned} \tag{4.49}$$

Proposition 4.4.1. *Let f_t^n the solution of the forward equation* (4.22)*. Then there exist a constant C such that*

$$H_n(t) \leq Cn, \qquad \int_0^t \mathcal{D}_n^p(f_s^n) ds \leq \frac{C}{n}, \qquad \int_0^t \mathcal{D}_n^r(f_s^n) ds \leq \frac{C}{n}. \tag{4.50}$$

Proof. Taking the time derivative of the entropy we obtain:

$$\frac{d}{dt} H_n(t) = \int (\mathcal{L}_n^{\bar{\tau}(t)})^* f_t^n \log f_t^n d\nu_{\beta \cdot} \tag{4.51}$$

So that, using (4.23), we have

$$\frac{d}{dt}H_n(t) = \int f_t^n \mathcal{L}_n^{\bar\tau(t)} \log f_t^n d\nu_{\beta.} = \int n^2 \mathcal{A}_n^{\bar\tau(t)} f d\nu_{\beta.} - \gamma n^2 \mathcal{D}_n^p(f_t^n)$$
$$= -n\sum_{i=1}^{n-1} \nabla_n \beta(i/n) \int V'(r_{i+1}) p_i f_t^n d\nu_{\beta.} + n^2 \beta_n \bar\tau(t) \int p_n f_t^n d\nu_{\beta.} - \gamma n^2 \mathcal{D}_n^p(f_t^n) \tag{4.52}$$

Recall that $q_n = \sum_{i=1}^{n} r_i$, then the time integral of the second term on the RHS of (4.52) gives

$$n^2\beta_n \int_0^t ds\ \bar\tau(s) \int p_n f_s^n d\nu_{\beta.} = \beta_n \int_0^t ds\ \bar\tau(s) \int \mathcal{L}_n^{\bar\tau(s)} q_n f_s^n d\nu_{\beta.}$$
$$= \beta_n \bar\tau(t) \int q_n f_t^n d\nu_{\beta.} - \beta_n \bar\tau(0) \int q_n f_0^n d\nu_{\beta.} - \beta_n \int_0^t ds\ \bar\tau'(s) \int q_n f_s^n d\nu_{\beta.} \tag{4.53}$$

By the entropy inequality, for any $a_1 > 0$, using the first of the conditions (4.1),

$$\int |q_n| f_s^n d\nu_{\beta.} \le \frac{1}{a_1} \log \int e^{a_1|q_n|} d\nu_{\beta.} + \frac{1}{a_1} H_n(s) \le \frac{1}{a_1} \log \int \prod_{i=1}^{n} e^{a_1|r_i|} d\nu_{\beta.} + \frac{1}{a_1} H_n(s)$$
$$\le \frac{1}{a_1} \sum_{i=1}^{n} \log \int \left(e^{a_1 r_i} + e^{-a_1 r_i}\right) d\nu_{\beta.} + \frac{1}{a_1} H_n(s)$$
$$= \frac{1}{a_1} \sum_{i=1}^{n} \left(\mathcal{G}(a_1, \beta_i) + \mathcal{G}(-a_1, \beta_i) - 2\mathcal{G}(0, \beta_i)\right) + \frac{1}{a_1} H_n(s) \le nC(a_1, \beta.) + \frac{1}{a_1} H_n(s) \tag{4.54}$$

We apply (4.54) to the three terms of the RHS of (4.53). So after this time integration we can estimate, for any $a_1 > 0$,

$$n^2\beta(1) \left| \int_0^t ds\ \bar\tau(t) \int p_n f_t^n d\nu_{\beta.} \right| \le \frac{\beta(1) K_{\bar\tau}}{a_1} \left(H_n(t) + H_n(0) + \int_0^t H_n(s) ds \right)$$
$$+ n(2+t)\beta(1) K_{\bar\tau} C(a_1, \beta.) \tag{4.55}$$

where $K_{\bar\tau} = \sup_{s>0}(|\bar\tau(s)| + |\bar\tau'(s)|)$.

By integration by part and Schwarz inequality, for any $a_2 > 0$ we have

$$\left| n\sum_{i=1}^{n-1} \nabla_n\beta(i/n) \int V'(r_{i+1}) p_i f_t^n d\nu_{\beta.} \right| = \left| n\sum_{i=1}^{n-1} \frac{\nabla_n\beta(i/n)}{\beta(i/n)} \int V'(r_{i+1}) \partial_{p_i} f_t^n d\nu_{\beta.} \right|$$
$$\leq \frac{1}{2a_2}\sum_{i=1}^{n-1} \frac{(\nabla_n\beta(i/n))^2}{\beta_i} \int V'(r_{i+1})^2 f_t^n d\nu_{\beta.} + \frac{a_2 n^2}{2}\tilde{\mathcal{D}}_n^p(f_t^n)$$

By our assumptions on $\beta(\cdot)$ and assumption (4.3) on V, we have that for some constant $C_{\beta.} > 0$ depending on $\beta(\cdot)$ and V,

$$\sum_{i=1}^{n-1} \frac{(\nabla_n\beta(i/n))^2}{\beta_i} V'(r_{i+1})^2 \leq C_{\beta.} \sum_{i=1}^{n-1} V'(r_{i+1})^2 \leq C_{\beta.} C_1 \sum_{i=1}^{n} (V(r_i) + 1) \quad (4.56)$$

By the entropy inequality, for any δ such that $0 < \delta < \inf_y \beta(y)$, there exists a finite constant $C_{\delta,\beta.}$ depending on V, δ and $\beta(\cdot)$ such that:

$$\sum_{i=1}^{n} \int V(r_i) f_t^n d\nu_{\beta.} \leq \frac{1}{\delta}\log \int e^{\delta\sum_{i=1}^n \int V(r_i) d\nu_{\beta.}} + \frac{1}{\delta} H_n(t)$$
$$= \frac{1}{\delta}\sum_{i=1}^{n} (\mathcal{G}(0, \beta_i - \delta) - \mathcal{G}(0, \beta_i)) + \frac{1}{\delta} H_n(t) \leq C_{\delta,\beta.} n + \frac{1}{\delta} H_n(t) \quad (4.57)$$

At this point we have obtained the following inequality, for some constant C not depending on n,

$$H_n(t) - H_n(0) \leq -n^2\left(\gamma - \frac{a_2}{2}\right)\int_0^t \mathcal{D}_n^p(f_s^n) ds + \left(\frac{C_{\beta.}}{2a_2\delta} + \frac{\beta(1)K_{\bar\tau}}{a_1}\right)\int_0^t H_n(s) ds$$
$$+ \frac{\beta(1)K_{\bar\tau}}{a_1}(H_n(t) + H_n(0)) + nc(a_1, a_2, \delta, \bar\tau, \beta.). \quad (4.58)$$

As a consequence, choosing $a_2 = \gamma$ and $a_1 = 2\beta(1)K_{\bar{\tau}}$, we have

$$H_n(t) \leq 3H_n(0) + C' \int_0^t H_n(s)ds + cn - n^2\gamma \int_0^t \mathcal{D}_n^p(f_s^n)ds \tag{4.59}$$

where C' and c are constants independent of n. Given the initial bound on $H_n(0) \leq cn$, by Gronwall inequality we have for some c'' independent on n:

$$H_n(t) \leq c'' e^{C't} n. \tag{4.60}$$

Inserting this in (4.59) we obtain, for some $\tilde{C}$ independent of n,

$$\gamma \int_0^t \mathcal{D}_n^p(f_s^n)ds \leq \frac{\tilde{C}}{n} \tag{4.61}$$

The bound (4.61) gives only information about the distribution of the velocities. We also need a bound of the distribution of the positions.

In appendix D we prove that, as a consequence of (4.61), we have

$$I_n(t) \leq \frac{C}{n} \qquad \forall t > 0. \tag{4.62}$$

Consequently

$$\begin{aligned}
\mathcal{D}_n^r(f_t^n) = I_n(f_t^n) - \tilde{\mathcal{D}}_n^p(f_t^n) - 2\int \frac{\partial_q f_t^n \tilde{\odot} \partial_p f_t^n}{f_t^n} d\nu_{\beta\cdot} \\
\leq \frac{C}{n} - \tilde{\mathcal{D}}_n^p(f_t^n) - 2\int \frac{\partial_q f_t^n \tilde{\odot} \partial_p f_t^n}{f_t^n} d\nu_{\beta\cdot} \\
\leq \frac{C}{n} - \tilde{\mathcal{D}}_n^p(f_t^n) + 2\tilde{\mathcal{D}}_n^p(f_t^n) + \frac{1}{2}\mathcal{D}_n^r(f_t^n)
\end{aligned}$$

that gives

$$\mathcal{D}_n^r(f_t^n) \leq 2\tilde{\mathcal{D}}_n^p(f_t^n) + \frac{2C}{n}$$

Since we have already the bound (4.61), (4.50) follows. □

4.5 Characterization of the limit points

Now we investigate the hydrodynamic behavior of our model. Let us define the empirical measure

$$\pi_t^n(dx) := \frac{1}{n}\sum_{i=1}^{n} r_i(t)\delta_{i/n}(dx).$$

We also use the following notation, for a given smooth function $G : [0,1] \to \mathbb{R}$,

$$\langle \pi_t^n, G\rangle := \frac{1}{n}\sum_{i=1}^{n} G\left(\frac{i}{n}\right) r_i(t)$$

Computing the time derivative we have:

$$\langle \pi_t^n, G\rangle - \langle \pi_0^n, G\rangle = \int_0^t \frac{1}{n}\sum_{i=1}^{n} G\left(\frac{i}{n}\right) \mathcal{L}_n^{\tilde{\tau}(t)} r_i(t) \tag{4.63}$$

Since

$$\mathcal{L}_n^{\tilde{\tau}(t)} r_i = n^2(p_i - p_{i-1}), \qquad i = 1, \ldots, n, \quad p_0 = 0,$$

after performing a summation by parts, we obtain

$$\mathcal{L}_n^{\bar{\tau}(t)} \langle \pi_t^n, G\rangle = -\sum_{i=1}^{n-1} \nabla_n G\left(\frac{i}{n}\right) p_i(t) + n p_n(t) G(1), \tag{4.64}$$

where $\nabla_n G$ is defined by (4.24). We define also

$$\nabla_n^* G\left(\frac{i}{n}\right) = n\left[G\left(\frac{i-1}{n}\right) - G\left(\frac{i}{n}\right)\right] \qquad i = 2, \ldots, n.$$

Now observe that

$$\begin{aligned}
\mathcal{L}_n^{\bar\tau(t)}\left[\frac{1}{n^2}\sum_{i=1}^{n-1}\nabla_n G\left(\frac{i}{n}\right)p_i-\frac{1}{n}p_nG(1)\right] &= -\gamma\sum_{i=1}^{n-1}\nabla_n G\left(\frac{i}{n}\right)p_i+\gamma np_nG(1)\\
&+\sum_{i=1}^{n-1}\nabla_n G\left(\frac{i}{n}\right)\left(V'(r_{i+1})-V'(r_i)\right)-nG\left(1\right)\left(\bar\tau(t)-V'(r_n)\right)\\
=&-\gamma\sum_{i=1}^{n-1}\nabla_n G\left(\frac{i}{n}\right)p_i+\gamma np_nG(1)\\
&+\frac{1}{n}\sum_{i=2}^{n-1}\nabla_n^*\nabla_n G\left(\frac{i}{n}\right)V'(r_{i+1})+\nabla_n G\left(\frac{n-1}{n}\right)V'(r_n)-\nabla_n G\left(\frac{1}{n}\right)V'(r_1)\\
&-nG\left(1\right)\left(\bar\tau(t)-V'(r_n)\right)
\end{aligned}\tag{4.65}$$

Recall that, by the weak formulation of the macroscopic equation, cf. (4.19), it is enough to consider test functions G such that $G(1)=0$ and $G'(0)=0$. This takes care of the last term on the RHS of the above expression and in (4.64), and putting these two expression together and dividing by γ, we obtain

$$\begin{aligned}
\mathcal{L}_n^{\bar\tau(t)}\langle\pi^n,G\rangle=\frac{1}{\gamma n}\sum_{i=2}^{n-1}(-\nabla_n^*\nabla_n)G\left(\frac{i}{n}\right)V'(r_{i+1})-\gamma^{-1}\nabla_n G\left(\frac{n-1}{n}\right)V'(r_n)\\
+\gamma^{-1}\nabla_n G\left(\frac{1}{n}\right)V'(r_1)+\mathcal{L}_n^{\bar\tau(t)}\left[\frac{1}{\gamma n^2}\sum_{i=1}^{n-1}\nabla_n G\left(\frac{i}{n}\right)p_i\right]
\end{aligned}\tag{4.66}$$

It is easy to show, by using the entropy inequality, that the last two terms are negligible. In fact, since $G'(0)=0$ we have that $|\nabla_n G\left(\frac{1}{n}\right)|\le C_G n^{-1}$. Furthermore

$$\int e^{\alpha|V'(r)|-\beta_1 V(r)}dr<+\infty\qquad\forall\alpha>0.$$

Then, using the entropy inequality we have for any $\alpha > 0$:

$$\begin{aligned}\int \left|\gamma^{-1}\nabla_n G\left(\frac{1}{n}\right) V'(r_1)\right| f_s^n d\nu_{\beta\cdot} &\leq \frac{C_G}{n\gamma}\int |V'(r_1)| f_s^n d\nu_{\beta\cdot} \\ &\leq \frac{C_G}{n\gamma\alpha}\int e^{\alpha|V'(r_1)|} d\nu_{\beta\cdot}^n + \frac{C_G}{n\gamma\alpha} H_n(s) \leq \frac{C(\alpha)}{n} + \frac{C'}{\alpha}\end{aligned} \tag{4.67}$$

that goes to 0 after taking the limit as $n \to \infty$ then $\alpha \to \infty$. About the last term of the RHS in (4.66), after time integration we have to estimate

$$\int \frac{1}{\gamma n^2}\sum_{i=1}^{n-1}\left|\nabla_n G\left(\frac{i}{n}\right)\right| |p_i| f_s^n d\nu_{\beta\cdot}$$

for $s = 0, t$. By similar use of the entropy inequality it follows that this term also disappears when $n \to \infty$.

To deal with the second term of the RHS of (4.66), we need the following lemma:

Lemma 4.5.1.

$$\lim_{n\to\infty} \mathbb{E}\left(\left|\int_0^t \left(V'(r_n(s)) - \bar{\tau}(s)\right) ds\right|\right) = 0 \tag{4.68}$$

Proof. Observe that

$$V'(r_n) - \bar{\tau}(s) = -\frac{1}{n^2}\mathcal{L}^{\bar{\tau}(s)} p_n - \gamma p_n = -\frac{1}{n^2}\mathcal{L}^{\bar{\tau}(s)}(p_n + \gamma q_n). \tag{4.69}$$

Then after time integration:

$$\int_0^t \left(V'(r_n(s)) - \bar{\tau}(s)\right) ds = \frac{1}{n^2}\left(p_n(0) - p_n(t)\right) - \frac{\gamma}{n^2}(q_n(t) - q_n(0)) + \frac{\sqrt{2\gamma\beta_n}}{n} w_n(t).$$

It is easy to show that, using similar estimate as (4.53) and (4.54), the expectation of the absolute value of the right hand side of the above expression converges to 0 as $n \to \infty$. □

It follows that

$$\lim_{n\to\infty} \mathbb{E}\left(\left|\int_0^t \left(\nabla_n G\left(\frac{n-1}{n}\right) V'(r_n(s)) - G'(1)\bar{\tau}(s)\right) ds\right|\right) = 0. \tag{4.70}$$

We are finally left to deal with the first term of the RHS of (4.66). We will proceed as in [37]. For any $\varepsilon > 0$ define

$$\bar{r}_{i,\varepsilon} = \frac{1}{2n\varepsilon + 1} \sum_{|j-i|\le n\varepsilon} r_j, \qquad n\varepsilon < i < n(1-\varepsilon). \tag{4.71}$$

We first prove that the boundary terms are negligible:

Lemma 4.5.2.

$$\lim_{\varepsilon\to 0}\lim_{n\to\infty} \int_0^t \int \left|\frac{1}{\gamma n}\left(\sum_{i=2}^{[n\varepsilon]} + \sum_{i=[n(1-\varepsilon)]+1}^{[n-1]}\right)(-\nabla_n^*\nabla_n)G\left(\frac{i}{n}\right)V'(r_{i+1})\right| f_s^n \, d\nu_{\beta\cdot}\, ds = 0 \tag{4.72}$$

Proof. For simplicity of notation let us estimate just one side. Since our conditions on V imply that $|V'(r)| \le C_2|r| + C_0$, we only need to prove that for any $t \ge 0$:

$$\lim_{\varepsilon\to 0}\lim_{n\to\infty} \int \frac{1}{n}\sum_{i=2}^{[n\varepsilon]} |r_i| \, f_t^n \, d\nu_{\beta\cdot} = 0 \tag{4.73}$$

By the entropy inequality we have:

$$\begin{aligned}\int \frac{1}{n}\sum_{i=2}^{[n\varepsilon]} |r_i| \, f_t^n \, d\nu_{\beta\cdot} &\le \frac{1}{n\alpha}\log\int \prod_{i=2}^{[n\varepsilon]} e^{\alpha|r_i|} d\nu_{\beta\cdot} + \frac{H_n(t)}{\alpha n} \\ &\le \frac{1}{n\alpha}\sum_{i=2}^{[n\varepsilon]} \left(\mathcal{G}(\alpha,\beta_i) + \mathcal{G}(-\alpha,\beta_i) - 2\mathcal{G}(0,\beta_i)\right) + \frac{C}{\alpha}\end{aligned}$$

Since $\mathcal{G}(\alpha,\beta_i) + \mathcal{G}(-\alpha,\beta_i) - 2\mathcal{G}(0,\beta_i) \le C'\alpha^2$, for a constant C' independent on i, we have

$$\int \frac{1}{n}\sum_{i=2}^{[n\varepsilon]} |r_i| \, f_t^n \, d\nu_{\beta\cdot} \le C'\varepsilon\alpha + \frac{C}{\alpha},$$

and by choosing $\alpha = \varepsilon^{-1/2}$ (4.73) follows. □

We are only left to show that

$$\lim_{\varepsilon\to 0}\lim_{n\to\infty}\int_0^t\int\left|\frac{1}{\gamma n}\sum_{i=[n\varepsilon]+1}^{[n(1-\varepsilon)]}(-\nabla_n^*\nabla_n)G\left(\frac{i}{n}\right)\left(V'(r_{i+1})-\boldsymbol{\tau}(\bar r_{i,\varepsilon},\beta_i)\right)\right| f_s^n\,d\nu.\,ds = 0 \tag{4.74}$$

Thanks to the bound (4.50), we are now in the same position as in the proof of the over-damped dynamics, as considered in [37], and by using similar argument as used there (the so called one-block/two blocks) (4.74) follows. A slight difference is due to the dependence of $\boldsymbol{\tau}$ on β_i, but since this changes very slowly and smoothly in space it is easy to consider microscopic blocks of size k with constant temperature inside.

At this point the proof of theorem 4.2.1 follows by standard arguments. Let Q_n the probability distribution of $\pi_\cdot^n$ on $\mathcal{C}([0,T],\mathcal{M}([0,1]))$, where $\mathcal{M}([0,1])$ are the signed measures on $[0,1]$. In appendix B we prove that the sequence Q_n is compact. Then, by the above results any limit point Q of Q_n is concentrated on absolutely continuous measures with densities $\bar r(y,t)$ such that for any $0\le t\le T$,

$$\mathbb{E}^Q\Big|\int_0^1 G(y)\left(\bar r(y,t)-\bar r(y,0)\right)dy - \gamma^{-1}\int_0^t ds\left[\int_0^1 G''(y)\boldsymbol{\tau}(\bar r(y,s),\beta(y))dy - G'(1)\bar\tau(s)\right]\Big| = 0 \tag{4.75}$$

Furthermore in appendix A we prove that Q is concentrated on densities that satisfy the regularity condition to have uniqueness of the solution of the equation.

4.6 Appendix A: Proof of the regularity bound 4.20

Proposition 4.6.1. *There exists a finite constant C such that for any limit point distribution Q we have the bound:*

$$\mathbb{E}^Q\left(\int_0^t ds\int_0^1 dx\left(\partial_x\boldsymbol{\tau}(\bar{r}(s,x),\beta(x))\right)^2\right)<C. \tag{4.76}$$

Proof. It is enough to prove that for any function $F\in\mathcal{C}^1([0,1])$ such that $F(0)=0$ the following inequality holds:

$$\mathbb{E}^Q\left(\int_0^t ds\left[\int_0^1 dxF'(x)\boldsymbol{\tau}(\bar{r}(s,x),\beta(x))-F(1)\bar{\tau}(s)\right]\right)\leq C\left(\int_0^1 F(x)^2dx\right)^{1/2}. \tag{4.77}$$

In fact by a duality argument, since $\boldsymbol{\tau}(\bar{r}(s,1),\beta(1))=\bar{\tau}(s)$, we have:

$$\int_0^1 dx\left(\partial_x\boldsymbol{\tau}(\bar{r}(s,x),\beta(x))\right)^2=\sup_{F\in\mathcal{C}^1([0,1])}\frac{\int_0^1 dxF'(x)\boldsymbol{\tau}(\bar{r}(s,x),\beta(x))-F(1)\bar{\tau}(s)}{\int_0^1 F(x)^2dx}.$$

Observe that (4.77) corresponds to a choice of test functions $G(x)$ in (4.19) such that $G'=F$. In order to obtain (4.77), compute

$$\begin{aligned}\frac{1}{n^2}\mathcal{L}_n^{\bar{\tau}}\sum_{i=1}^n F(i/n)(p_i+\gamma q_i)&=\sum_{i=1}^n F(i/n)A_n^{\bar{\tau}}p_i\\ =\sum_{i=1}^{n-1}F(i/n)\left(V'(r_{i+1})-V'(r_i)\right)&+F(1)\left(\bar{\tau}-V'(r_n)\right)\\ =\frac{1}{n}\sum_{i=2}^n\nabla_n^*F(i/n)V'(r_i)&+F(1)\bar{\tau}-F(1/n)V'(r_1)\end{aligned}$$

and after time integration and averaging over trajectories we have

$$\begin{aligned}
&\frac{1}{n^2}\int \sum_{i=1}^{n} F(i/n)(p_i+\gamma q_i)(f_t^n - f_0^n)d\nu_{\beta.} \\
&= \int_0^t ds \int \frac{1}{n}\sum_{i=2}^{n} \nabla_n^* F(i/n) V'(r_i) f_s^n d\nu_{\beta.} + F(1)\int_0^t \bar{\tau}(s)\, ds \\
&\qquad -F(1/n)\int_0^t ds \int V'(r_1) f_s^n d\nu_{\beta.}.
\end{aligned} \tag{4.78}$$

It is easy to see that, since $F(0) = 0$ and differentiable, the last term of the right hand side is negligible as $n \to \infty$, by the same argument used in (4.67).

About the first term on the RHS of (4.78), by the results of section 4.5, it converges,upon extracting subsequences, to

$$-\mathbb{E}^Q\left(\int_0^t ds \int_0^1 dx F'(x)\boldsymbol{\tau}(\bar{r}(s,x),\beta(x))\right).$$

About the left hand side of (4.78), one can see easily that

$$\frac{1}{n^2}\int \sum_{i=1}^{n} F(i/n) p_i (f_t^n - f_0^n) d\nu_{\beta.} \underset{n\to\infty}{\longrightarrow} 0.$$

Using the inequality $\sum_i q_i^2 \le n^2 \sum_i r_i^2$, we can bound the other term of the LHS of (4.78) by observing that, for $s = 0, t$,

$$\begin{aligned}
&\left|\frac{\gamma}{n}\int \sum_{i=1}^{n} F(i/n)\frac{q_i}{n} f_s^n d\nu_{\beta.}\right| \le \gamma\left(\frac{1}{n}\sum_{i=1}^{n} F(i/n)^2\right)^{1/2}\left(\int \frac{1}{n}\sum_{i=1}^{n}\frac{q_i^2}{n^2} f_s^n d\nu_{\beta.}\right)^{1/2} \\
&\le \gamma\left(\frac{1}{n}\sum_{i=1}^{n} F(i/n)^2\right)^{1/2}\left(\int \frac{1}{n}\sum_{i=1}^{n} r_i^2 f_s^n d\nu_{\beta.}\right)^{1/2} \le C\gamma\left(\frac{1}{n}\sum_{i=1}^{n} F(i/n)^2\right)^{1/2}.
\end{aligned}$$

Since F is a continuous function on $[0,1]$ the rhs of the above expression is bounded in n and converges to the L^2 norm of F as $n \to \infty$. Thus (4.77) follows. □

4.7 Appendix B: Compactness

We prove in this section that the sequence of probability distributions Q_n on $\mathcal{C}([0,t],\mathcal{M})$ induced by π_n is tight. Here $\mathcal{M}$ is the space of the signed measures on $[0,1]$ endowed by the weak convergence topology. This tightness is consequence of the following statement.

Proposition 4.7.1. *For any function $G \in \mathcal{C}^1([0,1])$ such that $G(1) = 0$, $G'(0) = 0$ and any $\varepsilon > 0$ we have*

$$\lim_{\delta\to 0}\limsup_{n\to\infty} \mathbb{P}^{\mu_0}\left[\sup_{0\le s<t\le T, |s-t|<\delta} |\langle \pi_n(t), G\rangle - \langle \pi_n(s), G\rangle| \ge \varepsilon\right] = 0 \tag{4.79}$$

Proof. By doing similar calculations as done in section 4.5 (see (4.64) and following ones)

$$\begin{aligned}
&< \pi_n(t), G > - < \pi_n(s), G >= -\int_s^t du \sum_{i=1}^{n-1} \nabla_n G\left(\frac{i}{n}\right) p_i(u) \\
&= \int_s^t du \frac{1}{\gamma n}\sum_{i=2}^{n-1}(-\nabla_n^*\nabla_n)G\left(\frac{1}{n}\right)V'(r_{i+1}(u)) - \int_s^t du\frac{1}{\gamma}\nabla_n G\left(\frac{n-1}{n}\right)V'(r_n(u)) \\
&\quad + \int_s^t du\frac{1}{\gamma}\nabla_n G\left(\frac{1}{n}\right)V'(r_1(u)) + \frac{1}{\gamma n^2}\sum_{i=2}^{n-1}\nabla_n G\left(\frac{i}{n}\right)(p_i(t)-p_i(s)) \\
&\quad + \frac{1}{n}\sum_{i}^{n}\sqrt{2\gamma\beta_j^{-1}}\nabla_n G\left(\frac{i}{n}\right)(w_i(t)-w_i(s)) \\
&\quad := I_1(s,t) + I_2(s,t) + I_3(s,t) + I_4(s,t) + I_5(s,t)
\end{aligned}$$

We treat the corresponding 5 terms separately. The term $I_3 = \int_s^t du\frac{1}{\gamma}\nabla_n G\left(\frac{1}{n}\right)V'(r_1(u))$

is the easiest to estimate, since $G'(0) = 0$, and using Schwarz inequality we have

$$\begin{aligned}\sup_{0\le s<t\le T,|s-t|<\delta} |I_3(s,t)| &\le \sup_{0\le s<t\le T,|s-t|<\delta} \frac{C}{n\gamma}\int_s^t |V'(r_1(u))|du \\ &\le \sup_{0\le s<t\le T,|s-t|<\delta} \frac{C}{n\gamma}|t-s|^{1/2}\left(\int_s^t |V'(r_1(u))|^2 du\right)^{1/2} \\ &\le \frac{C\delta^{1/2}}{n\gamma}\left(\int_0^T |V'(r_1(u))|^2 du\right)^{1/2}.\end{aligned}$$

Since, by entropy inequality,

$$\begin{aligned}\mathbb{E}\left[\left(\int_0^T |V'(r_1(u))|^2 du\right)^{1/2}\right] &\le \left[\int_0^T \mathbb{E}\left(|V'(r_1(u))|^2\right) du\right]^{1/2} \\ &\le C\left[\int_0^T \mathbb{E}\left(\sum_{i=1}^n (V(r_i(u))+1)\right) du\right]^{1/2} \le CT^{1/2}n^{1/2}\end{aligned}$$

so that

$$\mathbb{E}\left[\sup_{0\le s<t\le T,|s-t|<\delta} |I_3(s,t)|\right] \le \frac{C\delta^{1/2}T^{1/2}}{\gamma n^{1/2}} \underset{n\to\infty}{\longrightarrow} 0.$$

About I_2, this is equal to

$$-\frac{1}{\gamma}\nabla_n G\left(\frac{n-1}{n}\right)\int_s^t du\,(V'(r_n(u)) - \bar\tau(u)) - \frac{1}{\gamma}\nabla_n G\left(\frac{n-1}{n}\right)\int_s^t du\bar\tau(u) \quad (4.80)$$

The second term of the above expression is trivially bounded by $C\delta$ since $|t-s| \le \delta$. For the first term on the right hand side of (4.80), by (4.69), we have

$$\int_s^t du\,(V'(r_n(u)) - \bar\tau(u)) = \frac{p_n(s)-p_n(t)}{n^2} - \gamma\int_s^t p_n(u)du + \frac{\sqrt{2\gamma\beta_n^{-1}}}{n}(w_n(t)-w_n(s))$$

The last term of the right hand side of the above is estimated by the standard modulus of continuity of the Wiener process w_n. For the second term of the right

hand side, this is bounded by

$$\mathbb{E}\left[\sup_{0\le s<t\le T,|s-t|<\delta}\gamma\left|\int_s^t p_n(u)du\right|\right] \le \gamma\delta^{1/2}\mathbb{E}\left[\left(\int_0^T p_n^2(u)du\right)^{1/2}\right]$$
$$\le \gamma\delta^{1/2}\left[\int_0^T \mathbb{E}(p_n^2(u))du\right]^{1/2} = \gamma\delta^{1/2}\left[\int_0^T \mathbb{E}(p_n^2(u)-\beta_n^{-1})du + T\beta_n^{-1}\right]^{1/2}$$
$$\le C\gamma\delta^{1/2}\left[\int_0^T\int p_n\partial_{p_n}f_u^n d\nu_{\beta\cdot}du + T\beta_n^{-1}\right]^{1/2}$$
$$\le C\gamma\delta^{1/2}\left[\left(\int_0^T\int p_n^2 f_u^n d\nu_{\beta\cdot}du\right)^{1/2}\left(\int_0^T\int\frac{(\partial_{p_n}f_u^n)^2}{f_u^n}d\nu_{\beta\cdot}du\right)^{1/2} + T\beta_n^{-1}\right]^{1/2}$$
$$\le C'\gamma\delta^{1/2}$$

where the last inequality is justified by the inequalities:

$$\int p_n^2 f_u^n d\nu_\cdot \le Cn$$
$$\int_0^T\int\frac{(\partial_{p_n}f_u^n)^2}{f_u^n}d\nu_\cdot du \le \frac{C}{n}$$

To deal with the first term we have to prove that

$$\lim_{n\to\infty}\mathbb{E}\left(\sup_{0\le t\le T}\frac{1}{n^2}|p_n(t)|\right) = 0 \tag{4.81}$$

Since

$$\frac{p_n(t)}{n^2} = \frac{1}{n^2}p_n(0)e^{-\gamma n^2 t} + \int_0^t e^{-\gamma n^2(t-u)}\left[\bar\tau(u) - V'(r_n(u))\right]du + \sqrt{2\gamma\beta_n^{-1}}\frac{1}{n}\int_0^t e^{-\gamma n^2(t-u)}dw_n(u) \tag{4.82}$$

The stochastic integral is easy to estimate by Doob's inequality:

$$\mathbb{E}\left(\sup_{0\le t\le T}\left|\sqrt{2\gamma\beta_n^{-1}}\frac{1}{n}\int_0^t e^{-\gamma n^2(t-u)}dw_n(u)\right|^2\right) \le \frac{CT}{n^2}$$

About the second term, by Schwarz inequality we have that

$$\mathbb{E}\sup_{0\le t\le T}\left|\int_0^t e^{-\gamma n^2(t-u)}\left[\bar{\tau}(u)-V'(r_n(u))\right]du\right| \\ \le \frac{1}{n\sqrt{2\gamma}}\left(\int_0^T \mathbb{E}\left(\left[\bar{\tau}(u)-V'(r_n(u))\right]^2\right)du\right)^{1/2}$$

and by the entropy bound we have

$$\mathbb{E}\left(\left[\bar{\tau}(u)-V'(r_n(u))\right]^2\right)\le Cn$$

so that this term goes to zero like $n^{-1/2}$. The first term in (4.82) is trivial to estimate. This conclude the estimate of I_2.

The estimation of I_4 is similar to the proof of (4.81), but require a little extra work. We need to prove that

$$\lim_{n\to\infty}\mathbb{E}\sup_{0\le t\le T}\left|\frac{1}{n^2}\sum_{i=2}^{n-1}\nabla_n G\left(\frac{i}{n}\right)p_i(t)\right|=0. \tag{4.83}$$

By the evolution equations we have

$$\frac{1}{n^2}\sum_{i=2}^{n-1}\nabla_n G\left(\frac{i}{n}\right)p_i(t)=\frac{1}{n^2}\sum_{i=2}^{n-1}\nabla_n G\left(\frac{i}{n}\right)p_i(0)e^{-\gamma n^2 t} \\ +\int_0^t ds\; e^{-\gamma n^2(t-s)}\frac{1}{n}\sum_{i=3}^{n-1}\nabla_n^*\nabla_n G\left(\frac{i}{n}\right)V'(r_i(s)) \\ +\int_0^t ds\; e^{-\gamma n^2(t-s)}\left(\nabla_n G\left(1\right)V'(r_n(s))-\nabla_n G\left(\frac{2}{n}\right)V'(r_2(s))\right)$$

and all these terms can be estimated as in the proof of (4.81), so that (4.83) follows.

Also I_5 can be easily estimated by Doob inequality and using the independence of $w_i(t)$.

Finally estimating I_1, notice that since G is a smooth function, it can be

bounded by

$$\begin{aligned}\sup_{0\le s<t\le T,|s-t|<\delta}|I_1(s,t)| &\le \frac{C}{\gamma n}\sup_{0\le s<t\le T,|s-t|<\delta}\int_s^t du\sum_{i=2}^{n-1}|V'(r_{i+1}(u))| \\ &\le \frac{C\delta^{1/2}}{\gamma}\left(\int_0^T\frac{1}{n}\sum_{i=2}^{n-1}|V'(r_{i+1}(u))|^2du\right)^{1/2}\end{aligned} \tag{4.84}$$

and, by entropy inequality

$$\mathbb{E}\left[\left(\int_0^T\frac{1}{n}\sum_{i=2}^{n-1}|V'(r_{i+1}(u))|^2du\right)^{1/2}\right]\le\left[\int_0^T\frac{1}{n}\sum_{i=2}^{n-1}\mathbb{E}\left(|V'(r_{i+1}(u))|^2\right)du\right]^{1/2}\le C,$$

so that the expression in (4.84) is negligible in the limit $\delta\to 0$. □

4.8 Appendix C: Uniqueness of weak solutions

Proposition 4.8.1. *The weak solution of* (4.19) *is unique in the class of function such that*

$$\int_0^t ds\int_0^1\left(\partial_x\tau(r(x,s),\beta(x))\right)^2dx<+\infty \tag{4.85}$$

Proof. Let $g(x)\ge 0$ a smooth function with compact support contained in $[-1/4,1/4]$ such that $\int_{\mathbb{R}}g(y)dy=1$. Then for $\lambda>0$ large enough, define the function

$$G_\lambda(y,x)=1-\int_{-\infty}^y\lambda g(\lambda(z-x))dz$$

Then for $1/(4\lambda)<x<1-1/(4\lambda)$, we have $G_\lambda(0,x)=0$ and $\partial_yG_\lambda(1,x)=0$, and it can be used as test function in (4.19). So if $r(x,t)$ is a solution in the given class, we have

$$\int_0^1 G_\lambda(y,x)\left(r(y,t)-r_0(y)\right)dx=\gamma^{-1}\int_0^t ds\left[\int_0^1\lambda g(\lambda(y-x))\partial_y\tau(r(y,s),\beta(y))dy\right].$$

Letting $\lambda \to +\infty$ we obtain:

$$\int_0^x (r(y,t) - r_0(y))\, dx = \gamma^{-1} \int_0^t ds \partial_y \tau(r(x,s), \beta(x)), \qquad \forall x \in (0,1).$$

Let $r_1(x,t), r_2(x,t)$ two solutions in the class considered, and define

$$R_j(x,t) = \int_0^x r_j(y,t) dy, \qquad j = 1, 2.$$

By the approximation argument done at the beginning of the proof, we have that

$$\partial_t R_j(x,t) = \gamma^{-1} \partial_x \tau(r_j(x,s), \beta(x))$$

for every $x \in (0,1)$ and $t > 0$.

Since $\tau(r_j(1,t), \beta(1)) = \bar{\tau}(t)$, and since $\tau(r, \beta)$ is a strictly increasing function of r,

$$\begin{aligned}
&\frac{d}{dt} \int_0^1 (R_1(x,t) - R_2(x,t))^2\, dx \\
&= 2\gamma^{-1} \int_0^1 (R_1(x,t) - R_2(x,t))\, \partial_x \left(\tau(r_1(x,t), \beta(x)) - \tau(r_2(x,t), \beta(x))\right) dx \\
&= -2\gamma^{-1} \int_0^1 (r_1(x,t) - r_2(x,t)) \left(\tau(r_1(x,t), \beta(x)) - \tau(r_2(x,t), \beta(x))\right) dx \leq 0.
\end{aligned}$$

□

4.9 Appendix D: proof of the entropic hypocoercive bound (4.16)

We will prove in this appendix that there exists constants $\lambda > 0$ and $C > 0$ independent of n such that

$$\frac{d}{dt} I_n(f) \leq -\lambda n^2 I_n(f) + Cn. \tag{4.86}$$

We will use the following commutation relations:

$$[\partial_{p_i}, \beta_j^{-1}\partial^*_{p_j}] = \delta_{i,j}, \qquad [\partial_{p_i}, \mathcal{A}_n^\tau] = \partial_{q_i}, \qquad [\partial_{q_i}, \mathcal{A}_n^\tau] = -(\partial_q^2 \mathcal{V}\ \partial_p)_i \tag{4.87}$$

where $\partial_q^2\mathcal{V}$ is the corresponding hessian matrix of $\mathcal{V} = \sum_{i=1}^n V(r_n)$.

Denote $g_t = \sqrt{f_t^n}$ and observe that

$$I_n(g_t^2) = 4\int \left(|\partial_p g_t|^2_{\tilde{\odot}} + |\partial_q g_t|^2_{\tilde{\odot}} + 2\ \partial_q g_t \tilde{\odot} \partial_p g_t\right) d\nu_{\beta\cdot} \tag{4.88}$$

Recall that

$$n^2 \mathcal{A}_n^{\tau,*} = -n^2 \mathcal{A}_n^\tau + B_n^\tau \tag{4.89}$$

where

$$B_n^\tau = -n\sum_{i=1}^{n-1} \nabla_n \beta(i/n) p_i V'(r_{i+1}) + n^2 \beta(1) p_n \tau$$

Consequently g_t solves the equation:

$$\partial_t g = -n^2 \mathcal{A}_n^{\bar\tau(t)} g_t + n^2\gamma \mathcal{S}_n g_t + n^2\gamma \frac{|\partial_p g_t|^2_\odot}{g_t} + \frac{1}{2} B_n^{\bar\tau(t)} g_t$$

We then compute the time derivative of $I_n(g_t^2)$ by considering the three terms separately. The first one gives:

$$\begin{aligned}
\frac{d}{dt}\int |\partial_p g_t|^2_{\tilde\odot}\ d\nu_{\beta\cdot} =& -2n^2 \int \partial_p g_t \tilde\odot \partial_p (\mathcal{A}^{\bar\tau(t)} g_t)\ d\nu_{\beta\cdot} \\
&- 2n^2\gamma \int \partial_p g_t \tilde\odot \partial_p (\partial_p^* \odot \partial_p g_t)\ d\nu_{\beta\cdot} \\
&+ 2n^2\gamma \int \partial_p g_t \tilde\odot \partial_p \left(\frac{|\partial_p g_t|^2_\odot}{g_t}\right)\ d\nu_{\beta\cdot} \\
&+ \int \partial_p g_t \tilde\odot \partial_p (B_n^{\bar\tau(t)} g_t)\ d\nu_{\beta\cdot}.
\end{aligned} \tag{4.90}$$

By the commutation relations (4.87), and using (4.89), the first term on the RHS of (4.90) is equal to

$$\begin{aligned}&-2n^2\int \partial_p g_t \tilde{\odot} \partial_q g_t \; d\nu_{\beta.} - 2n^2 \int \partial_p g_t \tilde{\odot} \mathcal{A}^{\bar{\tau}(t)} \partial_p g_t \; d\nu_{\beta.} \\ &= -2n^2 \int \partial_p g_t \tilde{\odot} \partial_q g_t \; d\nu_{\beta.} - \int \partial_p g_t \tilde{\odot} B_n^{\bar{\tau}(t)} \partial_p g_t \; d\nu_{\beta.}\end{aligned}$$

Then the RHS of (4.90) is equal to

$$\begin{aligned}&- 2n^2 \int \partial_p g_t \tilde{\odot} \partial_q g_t \; d\nu_{\beta.} - 2n^2\gamma \int \partial_p g_t \tilde{\odot} \partial_p (\partial_p^* \odot \partial_p g_t) \; d\nu_{\beta.} \\ &+ 2n^2\gamma \int \partial_p g_t \tilde{\odot} \partial_p \left(\frac{|\partial_p g_t|^2_{\odot}}{g_t} \right) \; d\nu_{\beta.} + \int g_t \partial_p g_t \tilde{\odot} \partial_p B_n^{\bar{\tau}(t)} \; d\nu_{\beta.}.\end{aligned}$$

The last term of the above equation is equal to

$$\int g_t \partial_p g_t \tilde{\odot} \partial_p B_n \; d\nu_{\beta.} = -n \int g_t \sum_{i=1}^{n-1} \beta_i^{-1} \nabla_n \beta(\frac{i}{n}) V'(r_{i+1}) \partial_{p_i} g_t \; d\nu_{\beta.} \tag{4.91}$$

Notice that the term involving $n^2 \tau p_n$ does not appear in the above expression, because the particular definition of $\tilde{\odot}$. For any $\alpha_1 > 0$, using Schwarz inequality, (4.56) and (4.57), (4.91) is bounded by

$$\begin{aligned}&\frac{1}{2\alpha_1} \int g_t^2 \sum_{i=1}^{n-1} \frac{(\nabla_n \beta(\frac{i}{n}))^2}{\beta_i} V'(r_{i+1})^2 \; d\nu_{\beta.} + \frac{\alpha_1 n^2}{2} \int |\partial_p g_t|^2_{\tilde{\odot}} \; d\nu_{\beta.} \\ &\qquad\qquad \leq \frac{Cn}{\alpha_1} + \frac{\alpha_1 n^2}{2} \int |\partial_p g_t|^2_{\tilde{\odot}} \; d\nu_{\beta.}\end{aligned}$$

for a constant C depending on $\beta.$ and the initial entropy, but independent of n.

Computing the second term of the RHS of (4.90) we have:

$$\begin{aligned}\int \partial_p g_t \tilde{\odot} \partial_p (\partial_p^* \odot \partial_p g_t) \; d\nu_{\beta.} &= \int \sum_{j=1}^{n-1} \beta_j^{-1} |\partial_p \partial_{p_j} g|^2_{\odot} \; d\nu_{\beta.} + \int |\partial_p g|^2_{\tilde{\odot}} \; d\nu_{\beta.} \\ &= \int \sum_{i=1}^{n} \sum_{j=1}^{n-1} \beta_j^{-1} \beta_i^{-1} (\partial_{p_i} \partial_{p_j} g)^2 \; d\nu_{\beta.} + \int |\partial_p g|^2_{\tilde{\odot}} \; d\nu_{\beta.}\end{aligned}$$

About the third term on the RHS:

$$\partial_p g_t \tilde{\odot} \partial_p \left(\frac{|\partial_p g_t|^2_{\odot}}{g_t} \right) = \frac{2 \sum_{j=1}^{n-1} \sum_{i=1}^{n} \beta_j^{-1} \beta_i^{-1} \, \partial_{p_j} g_t \, \partial_{p_i} g_t \, \partial_{p_i} \partial_{p_j} g_t}{g_t} - \frac{|\partial_p g|^2_{\odot} |\partial_p g|^2_{\tilde{\odot}}}{g_t^2}$$

Summing all together we have obtained

$$\begin{aligned} \frac{d}{dt} \int |\partial_p g_t|^2_{\tilde{\odot}} \, d\nu_{\beta\cdot} = -2n^2 \int \partial_p g_t \tilde{\odot} \partial_q g_t \, d\nu_{\beta\cdot} - n^2 \left(2\gamma - \frac{\alpha_1}{2} \right) \int |\partial_p g_t|^2_{\tilde{\odot}} \, d\nu_{\beta\cdot} \\ -2n^2 \gamma \int \sum_{j=1}^{n-1} \sum_{i=1}^{n} \beta_j^{-1} \beta_j^{-1} \left(\partial_{p_i} \partial_{p_j} g_t - g_t^{-1} \partial_{p_i} g_t \partial_{p_j} g_t \right)^2 \, d\nu_{\beta\cdot} + \frac{Cn}{\alpha_1}. \end{aligned} \tag{4.92}$$

Now we deal with the derivative of the second term:

$$\begin{aligned} \frac{d}{dt} \int |\partial_q g_t|^2_{\tilde{\odot}} \, d\nu_{\beta\cdot} = -2n^2 \int \partial_q g_t \tilde{\odot} \partial_q (\mathcal{A}^{\bar{\tau}(t)} g_t) \, d\nu_{\beta\cdot} - 2n^2 \gamma \int \partial_q g_t \tilde{\odot} \partial_q (\partial_p^* \odot \partial_p g_t) \, d\nu_{\beta\cdot} \\ +2n^2 \gamma \int \partial_q g_t \tilde{\odot} \partial_q \left(\frac{|\partial_p g_t|^2_{\odot}}{g_t} \right) \, d\nu_{\beta\cdot} + \int \partial_q g_t \tilde{\odot} \partial_q (B_n g_t) \, d\nu_{\beta\cdot} \\ = -2n^2 \int \partial_q g_t \tilde{\odot} \partial_q (\mathcal{A}^{\bar{\tau}(t)} g_t) \, d\nu_{\beta\cdot} - 2n^2 \gamma \int \sum_{j=1}^{n-1} \sum_{i=1}^{n} \beta_i^{-1} \beta_j^{-1} \left(\partial_{p_i} \partial_{q_j} g - g_t^{-1} \partial_{p_i} g \partial_{q_j} g \right)^2 \, d\nu_{\beta\cdot} \\ + \int \partial_q g_t \tilde{\odot} \partial_q (B_n g_t) \, d\nu_{\beta\cdot}. \end{aligned} \tag{4.93}$$

The first and the last term give:

$$\begin{aligned} -2n^2 \int \partial_q g_t \tilde{\odot} \partial_q (\mathcal{A}^{\bar{\tau}(t)} g_t) \, d\nu_{\beta\cdot} + \int \partial_q g_t \tilde{\odot} \partial_q (B_n g_t) \, d\nu_{\beta\cdot} \\ = 2n^2 \int \partial_q g_t \tilde{\odot} (\partial_q^2 \mathcal{V} \partial_p) g_t \, d\nu_{\beta\cdot} + \int g_t \partial_q g_t \tilde{\odot} \partial_q B_n \, d\nu_{\beta\cdot} \end{aligned}$$

The last term on the RHS of the above expression is equal to

$$\begin{aligned}
&\int g_t \partial_q g_t \tilde{\odot} \partial_q B_n \, d\nu_{\beta.} \\
=&n \sum_{i=2}^{n-1} \int \beta_i^{-1} g_t (\partial_{q_i} g_t) \left[\nabla_n \beta \left(\frac{i}{n} \right) V''(r_{i+1}) p_i - \nabla_n \beta \left(\frac{i-1}{n} \right) V''(r_i) p_{i-1} \right] \, d\nu_{\beta.} \\
&+ n \int \beta_1^{-1} g_t (\partial_{q_1} g_t) \nabla_n \beta \left(\frac{1}{n} \right) V''(r_2) p_1.
\end{aligned}$$

Since V'' and $\nabla_n \beta$ are bounded and $\beta(\cdot)$ is positive bounded away from 0, this last quantity is bounded for any $\alpha_2 > 0$ by

$$n^2 \alpha_2 \int |\partial_q g_t|^2_{\tilde{\odot}} d\nu_{\beta.} + C \alpha_2^{-1} \int \sum_{i=1}^{n-1} p_i^2 g_t^2 d\nu_{\beta.} \leq n^2 \alpha_2 \int |\partial_q g_t|^2_{\tilde{\odot}} d\nu_{\beta.} + C' \alpha_2^{-1} n.$$

Since V'' is bounded, for any $\alpha_3 > 0$ we have

$$2n^2 \int \partial_q g_t \tilde{\odot} (\partial_q^2 \mathcal{V} \partial_p) g_t \, d\nu_{\beta.} \leq \alpha_3 n^2 \int |\partial_q g_t|^2_{\tilde{\odot}} \, d\nu_{\beta.} + \frac{|V''|^2_\infty n^2}{\alpha_3} \int |\partial_p g_t|^2_{\tilde{\odot}} \, d\nu_{\beta.}$$

Putting all the terms together, the time derivative of the second term is bounded by

$$\begin{aligned}
\frac{d}{dt} \int |\partial_q g_t|^2_{\tilde{\odot}} \, d\nu_{\beta.} \leq (\alpha_2 + \alpha_3) n^2 \int |\partial_q g_t|^2_{\tilde{\odot}} \, d\nu_{\beta.} + \frac{C n^2}{\alpha_3} \int |\partial_p g_t|^2_{\tilde{\odot}} \, d\nu_{\beta.} \\
- 2n^2 \gamma \int \sum_{j=1}^{n-1} \sum_{i=1}^{n} \beta_i^{-1} \beta_j^{-1} \left(\partial_{p_i} \partial_{q_j} g - g_t^{-1} \partial_{p_i} g \partial_{q_j} g \right)^2 \, d\nu_{\beta.} + C' \alpha_2^{-1} n
\end{aligned} \tag{4.94}$$

About the derivative of the third term, using the third of the commutation

relations (4.87), gives

$$\begin{aligned}
\frac{d}{dt}2\int \partial_q g_t \tilde{\odot} \partial_p g_t d\nu_{\beta\cdot} &= -2n^2 \int \left[\partial_q(\mathcal{A}^{\tau(t)} g_t)\tilde{\odot}\partial_p g_t + \partial_q g_t \tilde{\odot}\partial_p(\mathcal{A}^{\tau(t)} g_t)\right] d\nu_{\beta\cdot} \\
&\quad + \int \left[\partial_q(B_n g_t)\tilde{\odot}\partial_p g_t + \partial_q g_t \tilde{\odot}\partial_p(B_n g_t)\right] d\nu_{\beta\cdot} \\
&\quad -2n^2\gamma \int \left[\partial_q g_t \tilde{\odot}\partial_p(\partial_p^* \odot \partial_p g_t) + \partial_q(\partial_p^* \odot \partial_p g_t)\tilde{\odot}\partial_p g_t\right] d\nu_{\beta\cdot} \\
&\quad +2n^2\gamma \int \left[\partial_q g_t \tilde{\odot}\partial_p \left(\frac{|\partial_p g_t|^2_{\odot}}{g_t}\right) + \partial_q \left(\frac{|\partial_p g_t|^2_{\odot}}{g_t}\right)\tilde{\odot}\partial_p g_t\right] d\nu_{\beta\cdot} \\
&= 2n^2 \int (\partial_q^2 \mathcal{V}\partial_p) g_t \tilde{\odot}\partial_p g_t d\nu_{\beta\cdot} - 2n^2 \int |\partial_q g_t|^2_{\tilde{\odot}} d\nu_{\beta\cdot} \\
&\quad + \frac{1}{2}\int g_t \left[\partial_q B_n \tilde{\odot}\partial_p g_t + \partial_q g_t \tilde{\odot}\partial_p B_n\right] d\nu_{\beta\cdot} \\
&\quad -4n^2\gamma \int \sum_{j=1}^{n-1}\sum_{i=1}^{n} \beta_i^{-1}\beta_j^{-1} \left[\left(\partial_{p_i}\partial_{q_j} g\right)\left(\partial_{p_i}\partial_{p_j} g\right)\right] d\nu_{\beta\cdot} \\
+2n^2\gamma \int \sum_{j=1}^{n-1}\sum_{i=1}^{n} 2\beta_i^{-1}\beta_j^{-1} g_t^{-1} &\left[(\partial_{p_i}\partial_{p_j} g)(\partial_{p_i} g_t)(\partial_{q_j} g_t) + (\partial_{q_j}\partial_{p_i} g)(\partial_{p_j} g_t)(\partial_{p_i} g_t)\right] d\nu_{\beta\cdot} \\
&\quad -4n^2\gamma \int \sum_{j=1}^{n-1}\sum_{i=1}^{n} \beta_i^{-1}\beta_j^{-1} g^{-2}(\partial_{p_i} g_t)^2(\partial_{q_j} g_t)(\partial_{p_j} g_t) d\nu_{\beta\cdot}
\end{aligned} \tag{4.95}$$

The last three terms of the RHS of the (4.95) can be written as

$$-4n^2\gamma \int \sum_{j=1}^{n-1}\sum_{i=1}^{n} \beta_i^{-1}\beta_j^{-1} \left[\left(\partial_{p_i}\partial_{q_j} g_t - g_t^{-1}\partial_{p_i} g_t \partial_{q_j} g_t\right)\left(\partial_{p_i}\partial_{p_j} g_t - g_t^{-1}\partial_{p_i} g_t \partial_{p_j} g_t\right)\right] d\nu_{\beta\cdot}$$

so they combine with the corresponding terms coming from the time derivative of the first two terms of I_n giving an exact square.

The second term of (4.95), by the same arguments used before, can be bounded by

$$n^2\alpha_4 \int |\partial_q g_t|^2_{\tilde{\odot}} d\nu_{\beta\cdot} + n^2\alpha_5 \int |\partial_p g_t|^2_{\tilde{\odot}} d\nu_{\beta\cdot} + Cn(\alpha_4^{-1} + \alpha_5^{-1})$$

About the first term of (4.95), since V'' is bounded, it is bounded by $V''_\infty n^2 \int |\partial_p g_t|^2_{\tilde{\odot}} d\nu_{\beta\cdot}$.

Putting all these bounds together we obtain that

$$\frac{d}{dt} I_n(f_t) \leq -n^2 \kappa_p \int |\partial_p g_t|^2_{\tilde{\odot}} d\nu_{\beta\cdot} - n^2 \kappa_q \int |\partial_q g_t|^2_{\tilde{\odot}} d\nu_{\beta\cdot} - 2n^2 \int \partial_p g_t \tilde{\odot} \partial_q g_t d\nu_{\beta\cdot} + Cn$$
$$-2N^2\gamma \int \sum_{j=1}^{n-1} \sum_{i=1}^{n} \beta_i^{-1} \beta_j^{-1} \left[\left(\partial_{p_i} \partial_{q_j} g_t - g_t^{-1} \partial_{p_i} g_t \partial_{q_j} g_t \right) + \left(\partial_{p_i} \partial_{p_j} g_t - g_t^{-1} \partial_{p_i} g_t \partial_{p_j} g_t \right) \right]^2 d\nu_{\beta\cdot}$$

with

$$\kappa_p = 2\gamma - \frac{\alpha_1}{2} - \frac{C}{\alpha_3} - \alpha_5 - V''_\infty$$
$$\kappa_q = 2 - \alpha_2 - \alpha_3 - \alpha_4$$

By choosing $\alpha_2 + \alpha_3 + \alpha_4 \leq 1$ we have obtained that for some constants $C_1, C_2 > 0$ independent of n

$$\frac{d}{dt} I_n(f_t) \leq -n^2 I_n(f_t) + C_1 n + C_2 \int |\partial_p g_t|^2_{\tilde{\odot}} d\nu_{\beta\cdot}.$$

By recalling 4.61

$$\int_0^t ds \int |\partial_p g_s|^2_{\tilde{\odot}} d\nu_{\beta\cdot} \leq \frac{C'}{n}$$

after time integration we have for some constant C_3:

$$I_n(f_t) \leq e^{-n^2 t} I_n(f_0) + \frac{C_3}{n}(1 - e^{-n^2 t})$$

that implies

$$I_n(f_t) \leq \frac{C_4}{n} \tag{4.96}$$

for any reasonable initial conditions such that $I_n(f_0)$ is finite and not growing too fast with n.

Remark 4.9.1. *An important example for understanding the meaning of a den-*

sity with small I_n functional, consider the inhomogeneous Gibbs density:

$$f = \exp\left(\sum_{i=1}^{n} \beta_i \tau_i r_i + \sum_{i=1}^{n-1} \frac{1}{n} \nabla_n(\beta_i \tau_i) p_i\right) / \mathcal{N} \tag{4.97}$$

where $\mathcal{N}$ is a normalization constant. In the case of constant temperature these densities play an important role in the relative entropy method (cf [76, 54]), as to a non-constant profile of tension corresponds a profile of small damped velocities averages. Computing I_n on f we have

$$I_n(f) = \sum_{i=1}^{n-1} \left[\beta_i \tau_i - \beta_{i+1} \tau_{i+1} + \frac{1}{n} \nabla_n(\beta_i \tau_i)\right] = 0.$$

5

CEMRACS Project: Turbulent

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5.1 Introduction

Since the early work of Pope [62], the so-called probability density function (PDF) approach has proved to be an efficient tool for predicting turbulent flows. In this approach, one derives and solves a modeled transport equation for the one-point PDF of the fluctuating velocity field and, when necessary, of additional variables

describing the state of the flow, such as concentration, temperature or density. In the modeling process of the flow one-point statistics, closures must be applied to the turbulent acceleration as well as to molecular diffusion terms. Most of these closures yield a PDF transport equation of the Langevin type [62, 60, 61, 32]. In this work, we will only focus on this class of models.

While mostly used to predict turbulent reactive flows, the PDF approach has also demonstrated its utility for solving incompressible inert flows. In this context, Langevin PDF models have been shown [60] to be connected to simpler turbulent models which focus solely on the second-order one-point correlation tensor of the velocity field, also called Reynolds stress tensor. These Reynolds stress models (RSM) revert to the well known $k - \varepsilon$ model when turbulence is isotropic. The PDF/RSM equivalence encompasses most physical processes at work in incompressible flows, including production, non-linear redistribution and dissipation effects. However, strong differences exist in the way both approaches deal with the transport of the turbulent kinetic energy and of its anisotropy.

In RSM, turbulent transport is usually modeled by a gradient diffusion assumption. Many variants of this closure exist, but most are found to yield similar results in practical situations [85, 79]. In the PDF approach, the situation is different. The advection term appearing in the Navier-Stokes equations does not require any closure. In that sense, turbulent advection is often said to be treated "exactly" or "without assumption" [80, 32]. However, such statements might be somewhat misleading. Indeed, the overall process of turbulent transport is not exact since the statistics of the velocity field are affected by the Langevin closures used in the remaining parts of the PDF transport equation.

Thus, turbulent transport and Langevin closures are interacting in PDF models. This interaction is flow-dependent and cannot be made explicit in the general case. Yet, when non-equilibrium/production effects become negligible, the PDF equation is expected to degenerate and to yield a gradient diffusion formulation

for the transport of Reynolds stresses. This is suggested by several works, for instance [60, 38, 85], which focus on triple velocity correlations and on their expression in the absence of production. As a consequence, in this diffusion limit, a PDF/RSM equivalence should exist for the turbulent transport term. Then, significant knowledge could be gained by comparing the two families of models, just as it was done in the homogeneous case by Pope [60].

However, the diffusion limit of PDF models has never been looked at thoroughly. The precise conditions under which it occurs have not been explicited. Besides, the influence of dissipation processes are usually discarded while they are expected to play a significant role. Finally and more importantly, the study of the diffusion limit has been limited to considerations on the sole triple velocity correlations and not on the PDF itself.

Thus, the purpose of this work is to study the diffusion limit of PDF Langevin models and to explicit the connection with RSM models in that particular case. To this end, we consider a simplified setting in which diffusion and dissipation are the only active physical mechanisms. Then, we look for an asymptotic expansion of the Langevin PDF equation in terms of the ratio of the integral to the mean gradient length. The relevance of this expansion is verified on several simulations. Finally, its implications in terms of physical models are discussed.

5.2 Simplified Langevin PDF model applied to a turbulent zone

Throughout this work, we will consider a canonical turbulent flow consisting in a 1D slab of turbulence that decays and diffuses with time. This flow is sketched in figure 5-1 and will be refered to as turbulent zone (TZ). The inhomogeneous direction is denoted by x_1 and the length of the TZ by L_{TZ}. Our interest lies in finding the properties of the PDF $f(\mathbf{u}; x_1, t)$ of the velocity field $\mathbf{u} = (u_1, u_2, u_3)$

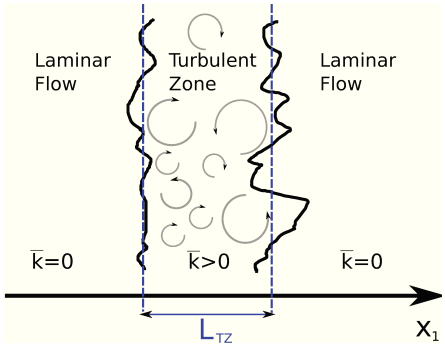


Figure 5-1: Sketch of a turbulent zone as studied in this work.

at point x_1 and time t when modelled by the simplified Langevin model (SLM) [62]. In the TZ configuration and with the SLM, the evolution of f is given by:

$$\frac{\partial f}{\partial t} + u_1 \frac{\partial f}{\partial x_1} = -\frac{\partial}{\partial u_j}\left[\left(\frac{\partial R_{1j}}{\partial x_1} - \frac{C_1}{2}\overline{\omega} u_j\right) f\right] + \frac{C_0}{2}\overline{\varepsilon}\frac{\partial^2 f}{\partial u_j u_j} \ , \tag{5.1}$$

where C_0 and C_1 are model constants, $R_{ij} = \overline{u_i u_j}$ is the Reynolds stress tensor, $\overline{k}$ is the mean turbulent kinetic energy, $\overline{\omega}$ is the mean dissipation frequency and $\overline{\varepsilon}$ is the mean dissipation rate. The Reynolds stress tensor R_{ij} and $\overline{k}$ are obtained directly from the PDF by the relations:

$$\overline{k}(x_1,t) = \frac{1}{2}R_{ii}(x_1,t) = \frac{1}{2}\overline{u_i u_i}(x_1,t) \quad \text{and} \quad R_{ij}(x_1,t) = \overline{u_i u_j}(x_1,t) = \int_{\mathbb{R}^3} u_i u_j f(\mathbf{u}; x_1, t) d\mathbf{u} \tag{5.2}$$

The dissipation rate and frequency are linked by the relation:

$$\overline{\omega}(x_1,t) = \frac{\overline{\varepsilon}(x_1,t)}{\overline{k}(x_1,t)} \tag{5.3}$$

An additional equation for the dissipation is required to close the system. As in standard $\overline{k} - \overline{\varepsilon}$ models, this equation is obtained by direct analogy with the

equation of $\overline{k}$. The evolution of $\overline{k}$ deduced from the PDF equation (5.1) is:

$$\frac{\partial \overline{k}}{\partial t} + \frac{\partial}{\partial x_1}\left(\overline{u_1 k}\right) = -\overline{\varepsilon} \tag{5.4}$$

The evolution of $\overline{\varepsilon}$ is then set to:

$$\frac{\partial \overline{\varepsilon}}{\partial t} + \frac{\partial}{\partial x_1}\left(C_\varepsilon \overline{\omega}\ \overline{u_1 k}\right) = -C_{\varepsilon_2} \overline{\omega}\ \overline{\varepsilon} \tag{5.5}$$

where C_ε and C_{ε_2} are model constants and where $\overline{u_i k}$ is the following triple velocity correlation:

$$\overline{u_i k} = \frac{1}{2}\overline{u_i u_p u_p}$$

The values of the different constants appearing in the above equations are given in table 5.1. These values are taken from the litterature [62, 60, 61, 32].

C_0	C_1	C_ε	C_{ε_2}
$\frac{2}{3}(C_1 - 1)$	1.5–5	1	1.9

Table 5.1: Model constants

Note that C_0 and C_1 are not independent: in order to ensure that $\overline{\varepsilon}$ is the dissipation rate of $\overline{k}$ one must have $C_0 = \frac{2}{3}(C_1 - 1)$. As noted in [60], the value of C_1 varies significantly in the litterature. It mostly depends on whether the SLM is used to model both the non-linear redistribution of energy and the rapid contribution of the pressure gradient, or whether it is associated with an additional component modelling the rapid pressure part. In the former case, the value of C_1 is usually set to higher values, typically $C_1 = 4.15$. In the latter case, it is set to lower values, typically $C_1 = 1.8$. In the absence of production, as in the TZ case considered here, there is no rapid pressure term and both low and high values of C_1 are acceptable.

5.3 Weakly inhomogeneous limit and diffusion regime

5.3.1 Main assumption

Two main lengths characterize the turbulent field in the TZ configuration, the integral length ℓ and the gradient length L. They are respectively defined as:

$$\ell = \frac{\overline{k}^{3/2}}{\overline{\varepsilon}} \quad \text{and} \quad L = \left[\frac{1}{\overline{k}}\frac{\partial \overline{k}}{\partial x_1}\right]^{-1}$$

The integral length ℓ is representative of the size of the turbulent eddies present in the turbulent zone, while L measures the inhomogeneity of the turbulent field and is expected to be roughly on the order of the turbulent zone size L_{TZ}.

We now make the assumption that the flow is weakly inhomogeneous, i.e. that turbulent eddies are much smaller than L. More precisely, we assume that:

$$\frac{\ell}{L} \sim \epsilon_a \ll 1 \tag{5.6}$$

Anticipating on a configuration where the PDF remains close to a Gaussian, this assumption can be incorporated in the equation (5.1) and (5.5) as:

$$\frac{\partial f}{\partial t} + \epsilon_a u_1 \frac{\partial f}{\partial x_1} = -\frac{\partial}{\partial u_j}\left[\left(\epsilon_a \frac{\partial R_{1j}}{\partial x_1} - \frac{C_1}{2}\overline{\omega} u_j\right) f\right] + \frac{C_0}{2}\overline{\varepsilon}\frac{\partial^2 f}{\partial u_j u_j} \tag{5.7}$$

$$\frac{\partial \overline{\varepsilon}}{\partial t} + \epsilon_a \frac{\partial}{\partial x_1}\left(C_\varepsilon \overline{\omega}\ \overline{u_1 k}\right) = -C_{\varepsilon_2}\overline{\omega}\ \overline{\varepsilon} \tag{5.8}$$

5.3.2 Asymptotic expansion

We look for a solution of equations (5.7) and (5.8) in the form of an expansion along the small parameter ϵ_a:

$$f = f^{(0)} + \epsilon_a f^{(1)} + \epsilon_a^2 f^{(2)} + \dots\ , \tag{5.9}$$

$$\overline{\varepsilon} = \overline{\varepsilon}^{(0)} + \epsilon_a \overline{\varepsilon}^{(1)} + \epsilon_a^2 \overline{\varepsilon}^{(2)} + \dots\ , \tag{5.10}$$

where we impose $\int_{\mathbb{R}^3} f^{(0)}(\mathbf{u}; x_1, t) d\mathbf{u} = 1$ and $\int_{\mathbb{R}^3} f^{(i)}(\mathbf{u}; x_1, t) d\mathbf{u} = 0, \forall i \geq 1$, without loss of generality.

The zeroth order of the expansion for f obeys a Fokker-Planck equation. Its asymptotic solution is an isotropic Gaussian of variance $\sigma^2 = \frac{2}{3}\overline{k}^{(0)}$. We will assume that the time is large enough so that this asymptotic solution is reached. Then, we have:

$$f^{(0)}(\mathbf{u}; x_1, t) = \frac{e^{-\frac{u_i u_i}{2\sigma^2}}}{(2\pi\sigma^2)^{3/2}} \quad \text{with} \quad \sigma^2 = \frac{2}{3}\overline{k}^{(0)}$$

where the zeroth order kinetic energy and its dissipation evolve according to:

$$\frac{\partial \overline{k}^{(0)}}{\partial t} = -\overline{\varepsilon}^{(0)} \quad , \quad \frac{\partial \overline{\varepsilon}^{(0)}}{\partial t} = -C_{\varepsilon_2} \frac{\overline{\varepsilon}^{(0)^2}}{\overline{k}^{(0)}}$$

The variance $\overline{u_i u_j}^{(1)}$ and $\overline{\varepsilon}^{(1)}$ obey an autonomous system of equations. Zero being a particular solution of it, the choice we retain is

$$\overline{u_i u_j}^{(1)} = 0 \text{ and } \overline{\varepsilon}^{(1)} = 0$$

With this condition, we obtain:

$$f^{(1)} = C_g \frac{\sigma}{\omega} \frac{\partial_{x_1} \sigma^2}{\sigma^2} \ \frac{u_1}{\sigma} \left(5 - \frac{u_i u_i}{\sigma^2}\right) f^{(0)} \qquad \text{with } C_g = \frac{1}{3C_1 + 2C_{\varepsilon_2} - 6}$$

As explained above, $f^{(1)}$ does not contribute to the Reynolds stresses ($\overline{u_i u_j}^{(1)} = 0$). However, it yields the main contribution to the third order moments. From the previous formula, one has:

$$\overline{u_i u_j u_k}^{(1)} = -2C_g \frac{\sigma^2}{\omega} \frac{\partial \sigma^2}{\partial x_1} \left(\delta_{1i}\delta_{jk} + \delta_{1j}\delta_{ik} + \delta_{1k}\delta_{ij}\right) \tag{5.11}$$

In particular, the flux of kinetic energy is given by:

$$\overline{u_i k}^{(1)} = -5C_g \frac{\sigma^2}{\omega} \frac{\partial \sigma^2}{\partial x_1} \delta_{i_1} \tag{5.12}$$

The second order is not detailed here. It yields an anisotropic contribution to the Reynolds stresses and an even contribution to the PDF, with a dependency on the gradient of σ^2 and on its Laplacian.

5.3.3 Main result: approximate PDF solution in the weakly inhomogeneous regime

By collecting the main orders of the asymptotic expansion, we obtain that:

$$f(\mathbf{u}; x_1, t) = \left[1 + \sqrt{2/3} C_g \, \ell \frac{1}{\overline{k}} \frac{\partial \overline{k}}{\partial x_1} \, \frac{u_1}{2\overline{k}/3} \left(5 - \frac{u_i u_i}{2\overline{k}/3}\right)\right] \frac{e^{-u_i u_i / (4\overline{k}/3)}}{(4\pi \overline{k}/3)^{3/2}} \tag{5.13}$$

where $\overline{k}$ is solution of a $\overline{k} - \overline{\varepsilon}$-like system:

$$\frac{\partial \overline{k}}{\partial t} = \frac{\partial}{\partial x_1} \left(C_k \frac{\overline{k}^2}{\overline{\varepsilon}} \frac{\partial \overline{k}}{\partial x_1} \right) - \overline{\varepsilon} \tag{5.14}$$

$$\frac{\partial \overline{\varepsilon}}{\partial t} = \frac{\partial}{\partial x_1} \left(C_\varepsilon C_k \frac{\overline{k}^2}{\overline{\varepsilon}} \left(\frac{\partial \overline{\varepsilon}}{\partial x_1} - \overline{k} \frac{\partial \overline{\omega}}{\partial x_1} \right) \right) - C_{\varepsilon_2} \overline{\omega} \, \overline{\varepsilon} \tag{5.15}$$

with:

$$C_k = \frac{20}{9} C_g = \frac{20}{9\,(3C_1 + 2C_{\varepsilon_2} - 6)}$$

To obtain these expressions, we used the relations $\ell = \overline{k}^{3/2}/\overline{\varepsilon}$ and $\sigma^2 = 2\overline{k}/3$. We also injected relation (5.12) into the evolution equations (5.4)-(5.5) of $\overline{k}$ and $\overline{\varepsilon}$.

When $C_\varepsilon = 1$, as chosen in this study, the above $\overline{k} - \overline{\varepsilon}$ system admits an asymptotic self-similar solution, first found by Barenblatt & co-workers [3] and

later by Cherfils & Harrison [19]. It is given by:

$$\overline{k}(x_1,t) = \overline{k}_0 \left(1 + {}^{t}\!/_{\tau_0}\right)^{-2+2\beta} \left(1 - \left[{}^{x_1}\!/_{\Lambda(t)}\right]^2\right) \quad , \quad \varepsilon(x_1,t) = \overline{\varepsilon}_0 \left(1 + {}^{t}\!/_{\tau_0}\right)^{-3+2\beta} \left(1 - \left[{}^{x_1}\!/_{\Lambda(t)}\right]^2\right) \ , \tag{5.16}$$

$$\text{with } \Lambda(t) = \Lambda_0 \left(1 + {}^{t}\!/_{\tau_0}\right)^{\beta} \quad \text{and} \quad \beta = \frac{2C_{\varepsilon_2} - 3}{3(C_{\varepsilon_2} - 1)} \tag{5.17}$$

The values of $\overline{k}$ and $\overline{\varepsilon}$ at $t = 0$ and $x_1 = 0$ are related to the two free parameters defining the initial length of the profile Λ_0 and the initial turbulent time τ_0:

$$\tau_0 = \frac{1}{C_{\varepsilon_2} - 1} \frac{\overline{k}_0}{\overline{\varepsilon}_0} \quad , \quad \Lambda_0 = \sqrt{\frac{2C_k}{\beta(C_{\varepsilon_2} - 1)}} \frac{\overline{k}_0^{3/2}}{\overline{\varepsilon}_0} \tag{5.18}$$

Equations (5.13)-(5.15), with their analytic solution (5.16)-(5.18), are the main result of this work. They show that, in the weakly inhomogeneous regime, the simplified Langevin PDF model behaves as a standard $\overline{k} - \overline{\varepsilon}$ model. In particular, turbulent transport is given on first order by a diffusion term which coefficient depends explicitely on two model constants: C_1 and C_{ε_2}. The physical implications of this finding will be discussed in section 5.5.

5.4 Numerical validation

In order to gain confidence in the solution derived in section 5.3.2, we would like to provide, *a posteriori*, the numerical evidence that the derived PDF shapes (5.13) are observed and correspond to the diffusion regime described by equations (5.14)-(5.15). To do so, we use two different numerical solvers.

- The first one is a Eulerian Monte Carlo (EMC) solver and is applied to solve equations (5.1) and (5.5). EMC methods have been introduced in [78, 71] and have been extended to include the velocity field in [75].

- The second one is a direct deterministic solver based on finite volume ap-

proximations and described in appendix 5.6. Given the high number of dimensions of equation (5.1), the computational cost of a deterministic method is too expensive. Hence, we decide to apply the deterministic method to a simplified version of equations (5.1) and (5.5). This simplified system is described in section 5.4.2.

5.4.1 Eulerian Monte Carlo simulations

First, we solve equations (5.1) and (5.5) with a Eulerian Monte Carlo (EMC) solver. The parameters of the simulation are the following. The computational domain $[x_{min}, x_{max}]$ is set to $[-80, 80]$. It is discretized with $N_x = 256$ points. The number of stochastic fields is set to $N_f = 16000$. The initial conditions are set according to the expected solution (5.16):

$$\overline{k}(x_1, t=0) = \overline{k}_0 \left(1 - \left[\frac{x_1}{\Lambda_0}\right]^2\right) \quad , \quad \varepsilon(x_1, t=0) = \overline{\varepsilon}_0 \left(1 - \left[\frac{x_1}{\Lambda_0}\right]^2\right)$$

where we set the values $\Lambda_0 = 10$ and $\overline{k}_0 = 1.5$ and where the values of τ_0 and $\overline{\varepsilon}_0$ are given by formula (5.18). Two calculations are done: one with $C_1 = 4.15$ and one with $C_1 = 1.8$. For $C_1 = 1.8$, one has $\tau_0 = 2.0$ and $\overline{\varepsilon}_0 = 0.84$ and for $C_1 = 4.15$, one has $\tau_0 = 3.6$ and $\overline{\varepsilon}_0 = 0.47$.

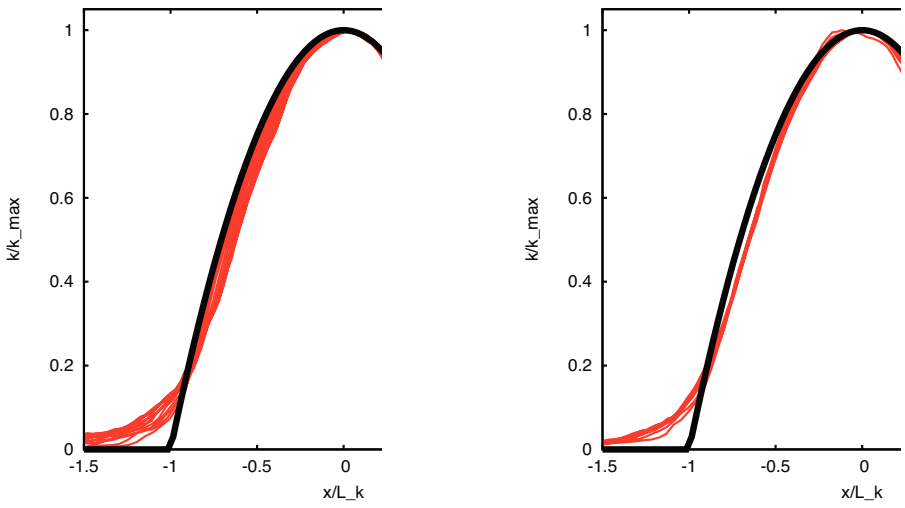
Self-similarity

In order to assess the self-similarity of the solution, we focus on the following three parameters:

$$\overline{k}_{max}(t) = \max_{x_1 \in \mathbb{R}} \left(\overline{k}(x_1, t)\right) \quad , \quad \overline{\varepsilon}_{max}(t) = \max_{x_1 \in \mathbb{R}} \left(\overline{\varepsilon}(x_1, t)\right) \quad \text{and} \quad L_k = \frac{3}{4} \frac{\int \overline{k}(x_1, t) dx_1}{k_{max}}$$

The ratio $\overline{k}/k_{max}$ taken at different times is displayed on figure 5-2 as a function of x_1/L_k and for two values of C_1. It can be seen that the respective profiles of

the two ratios fall approximately on a single curve. This indicates that $\overline{k}$ is close to a self-similar state. Besides, the collapsed curves remain close to parabolas as predicted by solution (5.14)-(5.15). The main difference with this solution occurs at the edges of the turbulent zone : while equations (5.14)-(5.15) predict a compact support for $\overline{k}$, the simulation yields a non-compact one. While not displayed here, the same conclusions also apply to $\overline{\varepsilon}$.



(a) $C_1 = 1.8$ (b) $C_1 = 4.15$

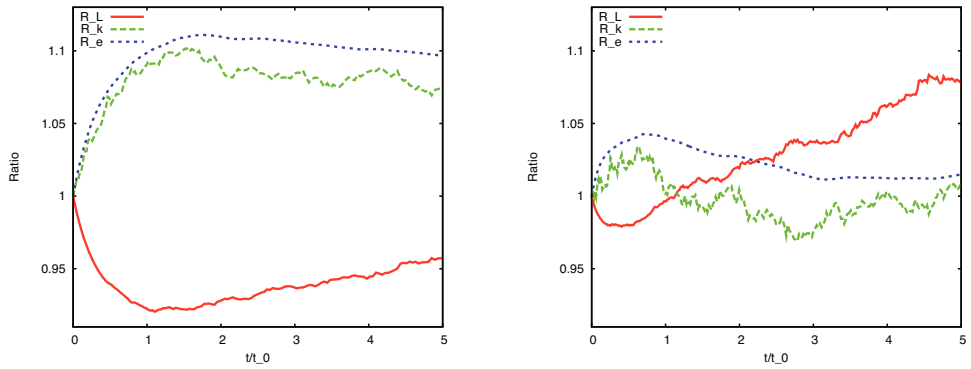
Figure 5-2: $\overline{k}/\overline{k}_{max}$ as a function of x_1/L_k at different times from $t/t_0 = 0.3$ to $t/t_0 = 5$

We now consider the time evolutions of the three parameters $\overline{k}_{max}$, $\overline{\varepsilon}_{max}$ and L_k and compare them against their predicted values given by the self-similar solution (5.14)-(5.15). To this end, we introduce the three ratios R_k, R_ε and R_L defined by:

$$R_k = \frac{\overline{k}_{max}}{\overline{k}_0 \left(1 + t/\tau_0\right)^{-2+2\beta}} \quad , \quad R_\varepsilon = \frac{\overline{\varepsilon}_{max}}{\overline{\varepsilon}_0 \left(1 + t/\tau_0\right)^{-3+2\beta}} \quad , \quad R_L = \frac{L_k}{\Lambda_0 \left(1 + t/\tau_0\right)^{\beta}}$$

If the self-similar solution (5.14)-(5.15) applies, then R_k, R_ε and R_L should become independent of time. Besides, given that the initial condition was chosen close to a self-similar solution, one should have $R_k = R_\varepsilon = R_L \approx 1$. A strict equality is not expected since the initial is not fully coherent with the self-similar state. In particular, the initial PDF is a Gaussian, whereas the self-similar PDF deviates from Gaussianity.

The three ratios R_k, R_ε and R_L are displayed in figure 5-3. It can be seen that they indeed remain approximately constant and stay close to one for the two simulations respectively performed with $C_1 = 1.8$ and $C_1 = 4.15$. As a conclusion,



(a) $C_1 = 1.8$ (b) $C_1 = 4.15$

Figure 5-3: Evolution of R_k, R_ε and R_L as a function of time.

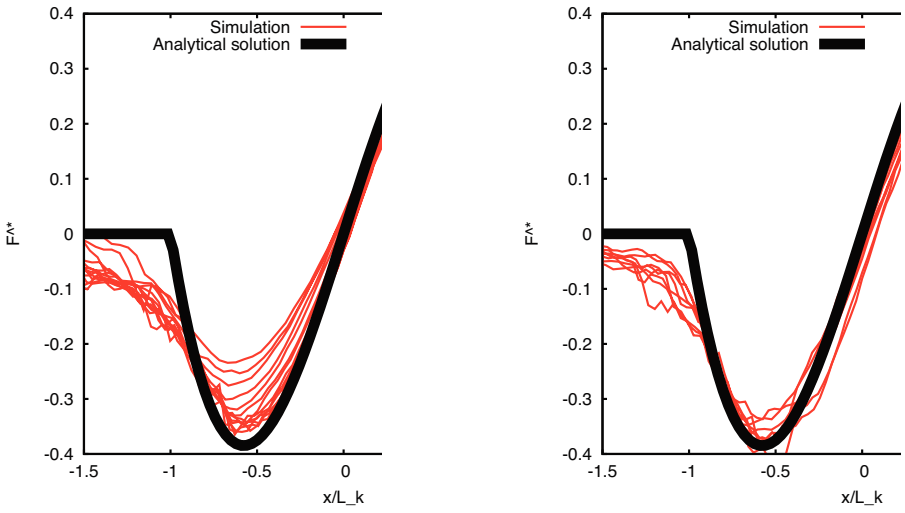
the self-similar solution (5.14)-(5.15) appears to be in good agreement with the simulation results.

Flux of kinetic energy

The existence and properties of the self-similar solution arise from the approximation of the flux of kinetic energy given by formula (5.12). To check this approximation, we introduce the non-dimensional flux :

$$F^*(x_1, t) = \frac{\overline{u_1 k}}{\overline{k}_{max}^{3/2} \sqrt{2\beta C_k (C_{\varepsilon_2} - 1)}}$$

According to formula (5.12), F^* should be equal to $x_1/L_k(1-[x_1/L_k]^2)$. The comparison between the two functions is displayed in figure 5-4 at different times. It can be seen that both simulation and prediction are in good agreement in the central part of the mixing zone, from $x_1/L_k \in [-0.7, 0.7]$. Outside, the gradient diffusion assumption ceases to be relevent: the predicted flux of kinetic energy becomes much smaller than the simulated flux. This observation is consistent with the one made on the non-compactness of the $\overline{k}-\overline{\varepsilon}$ profiles observed in figure 5-2.



(a) $C_1 = 1.8$ (b) $C_1 = 4.15$

Figure 5-4: F^* as a function of x_1/L_k at different times from $t/t_0 = 1$ to $t/t_0 = 5$.

5.4.2 Deterministic finite volume simulations

The Eulerian Monte Carlo method has allowed to study some properties of the second and third order moments of the velocity field. However, its intrisic noise is too high to directly study the PDF. To circumvent this deficiency, we propose

to use a deterministic solver.

Simplification of system (5.1)-(5.5)

As explained above, equations (5.1)-(5.5) have a high number of dimenions : 1 in time and 4 in velocity and physical space. The computational cost of a deterministic method is too expensive so that we propose to simplify these equations in order to reduce their dimensionality. More precisely, we focus on the the marginal PDF f_1 of u_1. By integrating equation (5.1) over u_2 and u_3, one obtains that f_1 evolves as:

$$\frac{\partial f_1}{\partial t} + u_1 \frac{\partial f_1}{\partial x_1} = -\frac{\partial}{\partial u_1}\left[\left(\frac{\partial \overline{u_1^2}}{\partial x_1} - \frac{C_1}{2}\overline{\omega} u_1\right) f_1\right] + \frac{C_1 - 1}{2}\overline{\varepsilon}^* \frac{\partial^2 f_1}{\partial u_1 u_1} \ , \qquad (5.19)$$

where $\overline{\varepsilon}^* = \dfrac{2}{3}\overline{\varepsilon}$ is the dissipation of $\overline{u_1^2}$. This equation is closed provided the evolution of $\overline{\varepsilon}^*$ is known in terms of the statistics of u_1. This is not the case of equation (5.5) which is related to $\overline{k}$. Hence, we propose to simplify this equation. Namely, we assume that the Reynolds stresses are strictly isotropic. Then, the turbulent frequency can be related to $\overline{u_1^2}$ according to: $\omega = \overline{\varepsilon}/\overline{k} = \overline{\varepsilon}^*/\overline{u_1^2}$. Besides, we assume that $\overline{u_1 u_i u_j}$ is also an isotropic tensor, which yields $\overline{u_1 k} = 3\overline{u_1^3}/2$. With these assumptions, one deduces from equation (5.5) the following simplified evolution for $\overline{\varepsilon}^*$:

$$\frac{\partial \overline{\varepsilon}^*}{\partial t} + \frac{\partial}{\partial x_1}\left(C_\varepsilon \overline{\omega}\ \overline{u_1^3}\right) = -C_{\varepsilon_2}\overline{\omega}\ \overline{\varepsilon}^* \qquad (5.20)$$

Equations (5.19)-(5.20) are three dimensional and can be solved with the deterministic solver. They share the same properties as equations (5.1)-(5.5) but present a slight variation in the weakly inhomogeneous limit. The limit of f_1 is,

as expected, the integral of the limit of f (5.13) over u_2 and u_3:

$$f_1(u_1;x_1,t) = \frac{e^{-u_1^2/(2\overline{u_1^2})}}{\sqrt{2\pi\overline{u_1^2}}}\left(1 + C_g\left(\frac{1}{\sqrt{\overline{u_1^2}}\omega}\frac{\partial\overline{u_1^2}}{\partial x_1}\right)\frac{u_1}{\sqrt{\overline{u_1^2}}}\left(3 - \frac{u_1^2}{\overline{u_1^2}}\right)\right) \quad , \qquad (5.21)$$

However, the value of $\overline{u_1^3}$ is not given by formula (5.11) but by:

$$\overline{u_1^3} = -C_k\frac{\overline{u_1^2}}{\omega}\frac{\partial\overline{u_1^2}}{\partial x_1}$$

with $C_k = 6C_g$. The notation C_k has been retained here because in the diffusion limit, $\overline{u_1^2}$ and $\overline{\varepsilon}^*$ obey a $\overline{k} - \overline{\varepsilon}$ like system similar to equations (5.14)-(5.15). The solution of this system is then obtained directly from equations (5.16) by replacing $\overline{k}$ by $\overline{u_1^2}$ and $\overline{\varepsilon}$ by $\overline{\varepsilon}^*$.

Set-up

The computational domain is defined by $[x_{min}, x_{max}] = [-30, 30]$ and $[u_{min}, u_{max}] = [-6, 6]$. It is discretized with $(n_x, n_{vx}) = 256^2$ points and the time step is set to $dt = 2 \cdot 10^{-3}$. The initial conditions are set according to

$$\overline{u_1^2}(x_1, t=0) = \overline{k}_0\left(1 - \left[\frac{x_1}{\Lambda_0}\right]^2\right) + \overline{k}_{min} \quad , \quad \varepsilon^*(x_1, t=0) = \overline{\varepsilon}_0\left(1 - \left[\frac{x_1}{\Lambda_0}\right]^2\right)$$

where $\overline{k}_0 = 1$ and $\Lambda_0 = 10$ and where the values of τ_0 and $\overline{\varepsilon}_0$ are given by formula (5.18). The additional parameter $\overline{k}_{min}$ is set to $\overline{k}_{min} = 10^{-2}$. It is required because Diracs cannot be represented in a deterministic method. They are here replaced by a Gaussian with a variance sufficiently small for the PDF to approximate a Dirac, and sufficiently large to obtain a numerical resolution of the PDF with a reasonable number of velocity points.

The coefficients of the model are set such as $C_1 = 2.73$, in order to recover $C_k = 1$.

Comparison with analytical PDF solutions

For the TMZ configuration described in section 5.4.2, we first compare the diffusion solution (5.16), and the numerical solution of the equations (5.19)-(5.20). In the figures 5-5 and 5-6, we observe a good agreement between the numerical and the analytical solutions, for the second and third moments of the PDF. Moreover, in figure 5-7, the self-similality of the solution is checked, with respect to the quantities R_k, R_ϵ and R_L (that are defined in section 5.4.1). This shows that the PDF solution operates close to the diffusion regime, for which asymptotic PDF solutions have been derived in section 5.3.2.

Then, we can legitimately analyse the anisotropic, odd part of the PDF, with respect to the analytical one (denoted as $\epsilon_a f^1$ in section 5.3.2). The comparison between the numerical and analytical PDF is shown in figure 5-8, respectively at the center and at the edge of the TMZ. At the end of the simulation, the anisotropy of the PDF is greater at the edge than at the center of the TMZ. This can be seen *via* the value of the small expansion parameter, which stabilizes at $\epsilon_a = 5.10^{-3}$ at the center of the TMZ, and $\epsilon_a = 0.8$ at the edge of the TMZ. The validity range of the expansion is therefore not verified *a posteriori* at all points of the domain. However the PDF shapes are qualitatively the same, and the TMZ diffuses at the correct rate. This gives confidence in the asymptotic expansion derived in section 5.3.2.

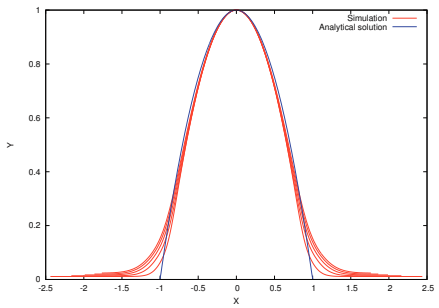


Figure 5-5: Turbulent kinetic energy from $t/t_0 = 1$ to $t/t_0 = 5$. Comparison between Barenblatt analytical solution [3] and the numerical PDF solution.

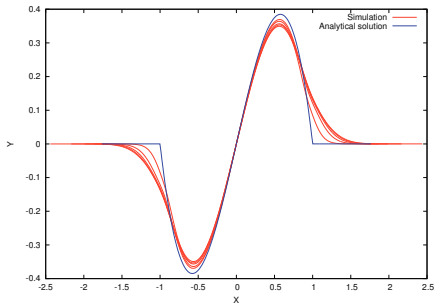


Figure 5-6: Normalized third order moment from $t/t_0 = 1$ to $t/t_0 = 5$. Comparison between Barenblatt analytical solution [3] and the numerical PDF solution.

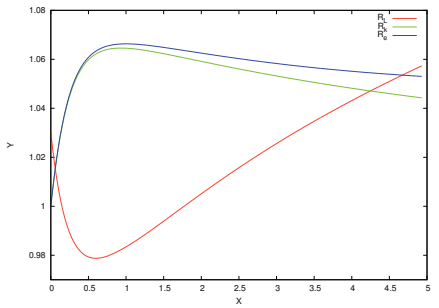
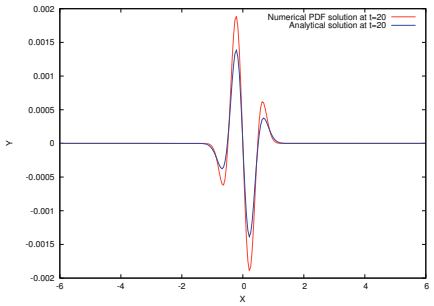
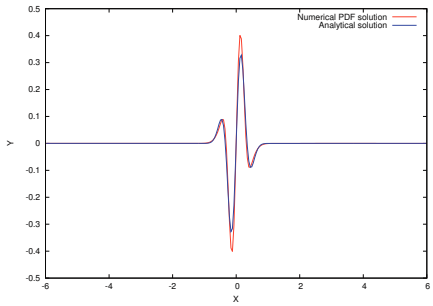


Figure 5-7: Evolution of R_k, R_ϵ, and R_L as a function of time.



(a) PDF at the TMZ center



(b) PDF at the point where $\frac{\partial \overline{u^2}}{\partial x}$ is maximum

Figure 5-8: Even part of the PDF. Comparison bewteen the numerical PDF and the solution obtained from the asymptotic development, at $t/t_0 = 5$.

5.5 Discussion and conclusions

In section 5.3, we showed that, in the weakly inhomogeneous limit, the simplified Langevin PDF model gives rise to diffusion approximation for turbulent transport and behaves as a standard $\overline{k} - \overline{\varepsilon}$ model. In section 5.4, we performed numerical simulations of a turbulent mixing zone and showed that the weakly inhomogeneous limit and the diffusion approximation were relevent to describe the diffusion and decay of turbulence in this configuration.

These results raise a number of questions concerning the way turbulent transport is effectively modelled in Langevin PDF models. First, the transport of kinetic energy is given on first order by a gradient diffusion approximation. The corresponding diffusion coefficient C_k is found to depend explicitely on two model constants: C_1 and C_{ε_2}. We recall that the constant C_{ε_2} is set in order to reproduce the correct decay of kinetic energy in homogeneous isotropic turbulence. As for the constant C_1, it is set in order to specify the decay of the anisotropy tensor $b_{ij} = R_{ij} - 2\overline{k}/3\delta_{ij}$ in homogeneous turbulence. Hence, one is faced with an apparent contradiction : the coefficient controlling turbulent transport in Langevin PDF methods is set by observations and reasonings made in homogeneous tur-

bulence, which by definition is devoid of turbulent transport.

Second, the value of C_1 varies in the litterature and so does the value of the diffusion coefficient C_k. For $C_1 = 1.8$, one has $C_k = 0.7$ and for $C_1 = 4.15$, one has $C_k = 0.22$. These values have to be compared with the usual value retained in $\overline{k} - \overline{\varepsilon}$ models $C_k^{\overline{k}-\overline{\varepsilon}} = 0.15 - 0.22$. Thus, if one wants to obtain results close to a standard $\overline{k} - \overline{\varepsilon}$ model in the diffusion-dissipation regime, one should rather choose a value of $C_1 = 4.15$. However, as explained in section 5.2, higher values of C_1 are usually associated with simpler models discarding the rapid contribution of the pressure gradient. For more realistic models, it is the value $C_1 = 1.8$ which is relevant. Hence, one is left to choose between a value of C_1 that captures correctly turbulent transport and a value that is compatible with the presence of a rapid pressure model. In addition to the first comment, this second remark tends to indicate that the definition of C_1 and the term it controls in the simplified Langevin model is overloaded. It looks as if the C_1 term in equation (5.1) had to represent two distinct physical mechanisms: return to isotropy and turbulent transport.

Finally, a last remark must be made. While the Langevin PDF and $\overline{k} - \overline{\varepsilon}$ models behave alike in the diffusion limit, there is still a fundamental difference between the two. In the $\overline{k}-\overline{\varepsilon}$ model, the gradient diffusion term models turbulent advection and also turbulent transport by the pressure: $-C_k^{\overline{k}-\varepsilon}\dfrac{\overline{k}^2}{\overline{\varepsilon}}\partial_{x_i}\overline{k} = \overline{u_i k} + \overline{u_i p}$. By contrast, in the simplified Langevin PDF model, pressure transport is neglected. This can be seen in equation (5.4) where only the flux of $\overline{k}$ appears. For the simplified Langevin model, one has: $-C_k\dfrac{\overline{k}^2}{\overline{\varepsilon}}\partial_{x_i}\overline{k} = \overline{u_i k}$. This relation could be justified if $\overline{u_i p}$ was negligible. However, this is not the case. In isotropic turbulence, one has exactly: $\overline{u_i p} = -2/5\overline{u_i k}$ [52]. Therefore, an important part of turbulent transport is missing in PDF models. Still, the fact that $\overline{u_i p}$ and $\overline{u_i k}$ are proportional allows for an effective definition of C_k which accounts for the missing term and give an overall correct transport in the diffusion regime. In

that case, the value of $\overline{u_i k}$ is overestimated by a factor $5/3 \approx 1.7$.

All these remarks point to some deficiencies in the way turbulent transport is represented in PDF models. We hope to adress some of these deficiencies in a forthcoming paper.

5.6 Deterministic direct method

We propose here a Finite Volume numerical method to discretize the equation (5.19), where the space, velocity fluctuation and time dimensions are discretized to yield a unique value of the PDF $f_1(u_1; x_1, t)$. This numerical scheme should allow to statisfy the following constraints:

$$f_1(u_1; x_1, t) \geq 0 \ , \tag{5.22}$$

$$\int_{\mathbb{R}} f_1(u_1; x_1, t) du_1 = 1 \ , \tag{5.23}$$

$$\int_{\mathbb{R}} u_1 f_1(u_1; x_1, t) du_1 = 0 \ . \tag{5.24}$$

To simplify notations, we will hereafter drop the index 1 from x_1 and f_1.

We introduce a cartesian, uniform mesh, defined by the control volumes $\mathcal{C}_{i,j} = \left[x_{i-1/2}, x_{i+1/2}\right] \left[u_{j-1/2}, u_{j+1/2}\right]$, where $(i, j) \in I \times J \subset \mathbb{N} \times \mathbb{Z}$. We define Δx and Δv as the sizes of the space and velocity control volumes, respectively. $x_i = i\Delta x$ and $u_j = j\Delta v$ here refer to the cell centers, whereas $x_{i+1/2} = (i + 1/2)\Delta x$ and $u_{j+1/2} = (j + 1/2)\Delta u$ refer to the volume control boundaries.
Let $f_{i,j}^n$ be an average approximation of the PDF on the control volume at time $t^n = n\Delta t$, $n \in \mathbb{N}$,

$$f_{i,j}^n = \frac{1}{\Delta x \Delta v} \int_{\mathcal{C}_{i,j}} f(x, u, t^n) \, du dx \ . \tag{5.25}$$

We start from the Finite Volume scheme originally derived in [29]. We recall the

basic steps leading to its construction on the simplified advection equation

$$\frac{\partial f}{\partial t} + u\frac{\partial f}{\partial x} = 0 \ , u > 0 \ , \tag{5.26}$$

for the sake of simplicity. Its extension by symmetry to the negative velocity space is straighforward. Its application to the right-hand side, velocity drift terms, in equation (5.19), will be discussed herebelow.

First, a time explicit Euler scheme is employed to discretize the equation (5.26) as

$$f_i^{n+1} = f_i^n + u\frac{\Delta t}{\Delta x}\left(F_{i+1/2}^n - F_{i-1/2}^n\right) \ , \tag{5.27}$$

where $F_{i+1/2}^n = F(x_{i+1/2}, t^n)$ stands as a discrete conservative approximation of $f(x,t)$ on the boundary of the control volume $\left[x_{i-1/2}, x_{i+1/2}\right]$. Second, following [29], a second order MUSCL reconstruction technique (by primitive), leads to the approximation

$$F(x,t^n) = \left[f_i^n + \epsilon^+ \frac{x - x_i}{\Delta x}\left(f_{i+1}^n - f_i^n\right)\right] \ , \ \forall x \in \left[x_{i-1/2}, x_{i+1/2}\right] \ . \tag{5.28}$$

The slope limiter ϵ^+ is introduced in order to recover the maximum priciple $0 \leq f_i^n \leq \|f\|_\infty$ under the CFL condition $u\dfrac{\Delta t}{\Delta x} \leq 1$. Its expression, given by

$$\epsilon^+ = \begin{cases} 0 \ , \text{if } \left(f_{i+1}^n - f_i^n\right)\left(f_i^n - f_{i-1}^n\right) < 0 \\ \min\left(1, \dfrac{2\left(\|f\|_\infty - f_i^n\right)}{f_i^n - f_{i+1}^n}\right) \ , \text{if } \left(f_{i+1}^n - f_i^n\right) < 0 \\ \min\left(1, \dfrac{2f_i^n}{f_{i+1}^n - f_i^n}\right) \ , \text{else} \end{cases} \tag{5.29}$$

leads to a nonlinear expression for the numerical flux.

This approximation procedure can be further extended to evaluate the velocity drift term in the right hand side of equation (5.19), which involves the velocity

variance gradient $\dfrac{\partial \overline{u^2}}{\partial x}$. This drift term should balance with the advection term in the left hand side of equation (5.19), in order to guarantee the zero mean velocity conservation (5.24). At the discrete level, this requirement is met with a re-definition of $\left.\dfrac{\partial \overline{u^2}}{\partial x}\right|_i^n$ as a function of the discrete, reconstructed, numerical flux obtained for the advection term (left hand side of equation (5.19))

$$\left.\frac{\partial \overline{u^2}}{\partial x}\right|_i^n = \sum_j u_j^2 \frac{F^n_{i+1/2,j} - F^n_{i-1/2,j}}{\Delta x}\Delta v \Bigg/ \left(-\sum_j u_j \frac{F^n_{i,j+1/2} - F^n_{i,j-1/2}}{\Delta v}\Delta v \right) , \tag{5.30}$$

which is the analogous of the continuous relation, obtained by integration by parts,

$$\frac{\partial \overline{u^2}}{\partial x} = \int_{\mathbb{R}} du u^2 \frac{\partial f}{\partial x} \Bigg/ \left(-\int_{\mathbb{R}} du u \frac{\partial f}{\partial u} \right) . \tag{5.31}$$

The chosen discrete definition (5.30) mimics the integration by part (5.31) required to satisty the zero mean velocity conservation (5.24), that is $\overline{u} = 0$.
A similar procedure is now applied to the C_1 term in the right hand side of equation (5.19), which is rewritten as

$$\frac{\partial}{\partial u}\left(\frac{C_1}{2}\omega u f\right) \rightarrow \frac{\partial}{\partial u}\left(\frac{C_1}{2}\omega \left(u - \overline{u}\right) f\right) . \tag{5.32}$$

An extension of the Finite Volume scheme (5.27)-(5.28)-(5.29) is employed here, to the more general case where the fluxes depend on the drift variable u. This dependance is treated with a conservative centered discretization of the velocity variable in the flux uf. A discrete definition for $\overline{u}$ is required at this point in (5.32). We introduce an approximation that satisfies the zero mean velocity conservation in a discrete manner on the discrete analogous of the equation (5.32)

$$\overline{u}_i^n = \sum_j u_j \frac{F^n_{i,j+1/2} - F^n_{i,j-1/2}}{\Delta v}\Delta v \Bigg/ \left(\sum_j u_j \frac{u_{j+1/2}F^n_{i,j+1/2} - u_{j-1/2}F^n_{i,j-1/2}}{\Delta v}\Delta v \right) , \tag{5.33}$$

which is the discrete analoguous of the continuous expression

$$\overline{u} = \int_{\mathbb{R}} du u \frac{\partial f}{\partial u} \Bigg/ \int_{\mathbb{R}} du \frac{\partial}{\partial u}\left(uf\right) = 0 \ . \tag{5.34}$$

We finally obtain un unsplit discretization for all the advection terms in equation (5.19). The discrete analogous of the probability density conservation (5.23) is satisfied if the slope limiters are not active for the advection term $u\dfrac{\partial f}{\partial x}$. In this case, we indeed obtain a centered discretization whatever the sign of the velocity is. We accept a small deviation from the probability density conservation, where the limiters are active to guarantee the maximum principle.

We now turn to the discretization of the C_0 operator in the right hand side of equation (5.19). This term is splitted and discretized with an centered, implicit scheme, with net flux boundary conditions on the velocity space. This ensures the respect of the conservations (5.23) and (5.24), at the discrete level. Moreover, we obtain a M-matrix with a positive right hand side, leading to a positive PDF. Finally, we remark that the splitting of the C_0 operator is convenient in the sense that it allows both the implicitation of this term and an easy implementation of a parallelisation on the space dimension x with good expected scalability. We have made use of the MPI parallelisation protocol to do so.

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Résumé

Cette thèse réalisée sous la direction du Professeur Stefano Olla, est consacrée à l'étude des modèles microscopiques pour la derivation de la conduction de la chaleur. Démontrer rigoureusement une equation diffusive macroscopique à partir d'une description microscopique du système est à aujourd'hui encore une problème ouvert. Le premier model consideré est une système décrit par l'equation de Schrödinger linéaire discrete (DLS) en dim 1, perturbé par une dynamique stochastique conservative. La phase de chaque particule change mais la norme totale (ou le nombre de particules) est conservée. La dynamique résultante est une diffusion hypoelliptique dégénérée qui converge vers un état stationnaire régulier. On peut montrer que le système a un limite hydrodynamique donné par la solution de l'equation de la chaleur. Quand le système est rattaché aux bords à deux reservoirs de Langevin à deux différents potentiels chimiques, on peut montrer que l'état stationnaire, dans la limite vers l'infinie, satisfait la loi de Fourier. On étudie une chaine des oscillateurs anharmonique immergée en un reservoir de chaleur avec un gradient de temperature. On exerce une tension, variable dans le temps, à une des deux extrémités de la chaine, et l'autre reste fixe. On montre que sous un changement d'échelle diffusive dans l'espace et dans le temps, la distribution d'étirement de la chaine évolue selon un equation diffusive non-lineaire. Les états stationnaires de la dynamique sont hors-équilibre et ils ont une production d'entropie positive, donc les techniques classiques comme le méthode de l'entropie relative ne peuvent pas être utilisés directement. On developpe des estimations qui reposent sur l'hypocoercitivité entropique.La limite macroscopique peut être utilisé pour modéliser les transformations thermodynamique isothermiques entre états stationnaire de non-équilibre.

Mots Clés

Loi de Fourier, mécanique statistique, thermodynamique hors équilibre , hypocoercitivité, limite hydrodynamique, equation diffusive

Abstract

The object of research of this thesis is the derivation of heat equation from the underlying microscopic dynamics of the system. Two main models have been studied: a microscopic system described by the discrete Schrödinger equation and an anharmonic chain of oscillators in presence of a gradient of temperature. The first model considered is the one-dimensional discrete linear Schrödinger (DLS) equation perturbed by a conservative stochastic dynamics, that changes the phase of each particles, conserving the total norm (or number of particles). The resulting total dynamics is a degenerate hypoelliptic diffusion with a smooth stationary state. It has been shown that the system has a hydrodynamical limit given by the solution of the heat equation. When it is coupled at the boundaries to two Langevin thermostats at two different chemical potentials, it has been proven that the stationary state, in the limit to infinity, satisfies the Fourier's law. The second model considered is a chain of anharmonic oscillators immersed in a heat bath with a temperature gradient and a time varying tension applied to one end of the chain while the other side is fixed to a point. We prove that under diffusive space-time rescaling the volume strain distribution of the chain evolves following a non-linear diffusive equation. The stationary states of the dynamics are of non-equilibrium and have a positive entropy production, so the classical relative entropy methods cannot be used. We develop new estimates based on entropic hypocoercivity, that allows to control the distribution of the positions configurations of the chain. The macroscopic limit can be used to model isothermal thermodynamic transformations between non-equilibrium stationary states.CEMRACS project on simulating Rayleigh- Taylor and Richtmyer-Meshkov turbulent mixing zones with a probability density function method at last.

Keywords

Fourier's law, statistical mechanics, thermodynamics, non equilibrium thermodynamics, hypocoercivity, hydrodynamic limit, diffusive equation.