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Ouassim FELIACHI

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From Particles to Fluids: A Large Deviation Theory Approach to Kinetic and Hydrodynamical Limits

THÈSE DIRIGÉE PAR :

Julien BARRÉ	Professeur, Université d'Orléans
Freddy BOUCHET	Directeur de recherche, Ecole Normale supérieure

RAPPORTEURS :

Gregory L. EYINK	Professeur, The Johns Hopkins University
Hugo TOUCHETTE	Professeur, Stellenbosch University

JURY :

Julien BARRÉ	Professeur, Université d'Orléans
Nils BERGLUND	Professeur, Université d'Orléans
Freddy BOUCHET	Directeur de recherche, Ecole Normale supérieure
Gregory L. EYINK	Professeur, The Johns Hopkins University
Isabelle GALLAGHER	Professeure, Ecole Normale supérieure
Vivien LECOMTE	Chargé de recherche, Université Grenoble-Alpes
Laure SAINT-RAYMOND	Professeure, Institut des Hautes Études Scientifiques
Hugo TOUCHETTE	Professeur, Stellenbosch University

PRÉSIDÉ PAR :

Isabelle GALLAGHER	Professeure, Ecole Normale supérieure

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Ouassim Feliachi

Université d'Orléans
Institut Denis Poisson

Contents

Abstract 1

1. Introduction 5
- 1.1. Equations of motion and hydrodynamic equations . . . 5
- 1.2. Importance of the statistical physics approach to hydrodynamics . . . 6
- 1.3. From particles to hydrodynamics: a derivation that implies two limits . . . 7
- 1.4. Kinetic theory: the large N limit . . . 8
- 1.5. From kinetic equations to hydrodynamic equations . . . 10
- 1.6. Fluctuations in the kinetic and hydrodynamic limits . . . 12
- 1.7. Applications of fluctuating hydrodynamics . . . 14
- 1.8. Contents of the manuscript . . . 15

2. Introduction en français 17
- 2.1. Equations du mouvement pour les particules et équations hydrodynamiques . . . 17
- 2.2. Intérêts et importance d'une approche statistique de l'hydrodynamique . . . 19
- 2.3. Des particules à l'hydrodynamique : une dérivation qui implique deux limites . . . 20
- 2.4. La théorie cinétique : la limite "grand N" . . . 21
- 2.5. Des équations cinétiques aux équations hydrodynamiques . . . 23
- 2.6. Fluctuations dans les limites cinétiques et hydrodynamiques . . . 24
- 2.7. Quelques applications des équations hydrodynamiques fluctuantes . . . 26
- 2.8. Contenu du manuscrit . . . 27

I. Dynamical large deviations for kinetic theories 31

3. Introduction to the dynamical large deviations for kinetic theories 33
- 3.1. Beyond equilibrium statistics and relaxation to equilibrium: dynamical fluctuations . . . 33
- 3.2. Short introduction to large deviation theory . . . 34
- 3.3. Large deviation for kinetic theories: a natural framework for the statistical mechanics of trajectories . . . 38
- 3.4. Expected properties of a dynamical large deviation principle for a kinetic theory . . . 39
- 3.5. Some motivations to study large deviations for kinetic theories . . . 43
- 3.6. A few ways to compute the large deviation Hamiltonian . . . 45

3.7. Derivation of the kinetic large deviation principle for two toy-models . . 48

4. Dynamical large deviations for the kinetic theory of long-range interacting particles: beyond the Balescu-Guernse-Lenard equation 59
4.1. Introduction: particles with long-range interaction, kinetic theory, and large deviations . . . 59
4.2. Dynamics of particles with long range interactions . . . 62
4.3. Large deviations for N diffusions with mean field coupling . . . 69
4.4. Derivation of the large deviation principle from the quasi-linear dynamics 70
4.5. Computation of the large deviation Hamiltonian . . . 74
4.6. Properties of the large deviation Hamiltonian . . . 80
4.7. Perspectives . . . 84

5. Dynamical large deviations for the kinetic theory of plasmas: beyond the Landau equation 87
5.1. The dynamics of the Coulomb plasma . . . 87
5.2. Kinetic description of the Coulomb plasma within the Landau approximation . . . 89
5.3. Large deviations associated with the Landau kinetic theory from the Boltzmann kinetic theory . . . 90
5.4. From the Balescu-Guernsey-Lenard large deviation Hamiltonian to the Landau Hamiltonian . . . 99
5.5. Large deviations for the Landau equation when $L < \lambda_D$ . . . 100
5.6. Large deviations for the Landau equation expressed in physical variables 101
5.7. Inhomogeneous systems: astrophysics, plasma physics . . . 103
5.8. Perspectives and conclusions of the first part . . . 103

II. Large deviations in the hydrodynamical limit 105

6. From the kinetic to the hydrodynamic scales: a large deviation perspective 107
6.1. The example of the fluctuating diffusion equation for N independent Run-and-Tumbling particles . . . 109
6.2. Hydrodynamic scaling . . . 111
6.3. Conservation laws, hydrodynamic modes, and local equilibria of the kinetic equation . . . 112
6.4. From the kinetic equation to hydrodynamics . . . 113
6.5. Toward fluctuating hydrodynamics: the SPDE approach . . . 115
6.6. Convergence of the large deviation functionals and contraction principle 119
6.7. Outline of the part . . . 125

7. Microscopical derivation of the fluctuating (in)compressible Navier-Stokes equations **127**
7.1. Path large deviations for the empirical measure and the Boltzmann equation . . . 128
7.2. Derivation of the fluctuating compressible Navier–Stokes and Euler equations . . . 135
7.3. Derivation of the fluctuating incompressible Navier–Stokes equations . . 140
7.4. Connection between the microscopic non-dimensional and the macroscopic set of units . . . 143
7.5. Gradient-flow structure for the Navier–Stokes equation . . . 145
7.6. Conclusion . . . 152

8. Fluctuating hydrodynamics for dilute active gases **153**
8.1. Introduction: hydrodynamical theories for active matter . . . 153
8.2. Definition of the particle-based model, kinetic theory and dynamical large deviations . . . 155
8.3. Fluctuating hydrodynamics in the ordered phase . . . 159
8.4. Conclusions . . . 167

9. Large deviations for scalar conservation laws **169**
9.1. Introduction: scalar conservation laws . . . 170
9.2. Microscopic and kinetic model . . . 173
9.3. Fluctuating hydrodynamics from the kinetic LDP (without shocks) . . . 179
9.4. Jensen-Varadhan large deviation functional . . . 181
9.5. Weight of an antishock directly from the kinetic LDP . . . 184
9.6. Conclusions . . . 187

10. Conclusions **189**
10.1. Summary . . . 189
10.2. Prospects . . . 190

Acknowledgments **193**

A. Appendices relative to the first part **195**
A.1. The relative entropy for N independent diffusions solves the stationary Hamilton–Jacobi equation . . . 195
A.2. Long time large deviations for quadratic observables of Gaussian processes, functional determinants and the Szegö–Widom theorem for Fredholm determinants . . . 197
A.3. Computation of the determinant of the operator $u_{\mathbf{k},\omega}$ . . . 199
A.4. Current formulation of the large deviation principle . . . 200
A.5. Consistence of the two definitions of the tensor $\mathbf{B}$ . . . 202
A.6. Symmetries and conservation laws associated with the collision kernels . 203

A.7. Asymptotic expansions leading to the Landau equation and its large deviation Hamiltonian . . . 204
A.8. From the Balescu–Guernsey–Lenard Hamiltonian to the Landau Hamiltonian . . . 206

B. Appendices relative to the second part **211**
B.1. Properties of the kinetic noise and the linearized kinetic operator . . . 211
B.2. Computation of the viscous and noise terms for the compressible Navier–Stokes equations . . . 212
B.3. Derivation of the gradient-flow structure for the Navier-Stokes equations 218

Bibliography **225**

Abstract

The central problem of statistical physics is to understand how to describe a system with macroscopic equations, which are usually deterministic, starting from a microscopic description, which may be stochastic. This task requires taking at least two limits: a "large N" limit and a "local equilibrium" limit. The former allows a system of N particles to be described by a phase-space distribution function, while the latter reflects the separation of time scales between the fast approach to local equilibrium and the slow evolution of hydrodynamic modes. When these two limits are taken, a deterministic macroscopic description is obtained. For both theoretical and modeling reasons (N is large but not infinite, the time-scale separation is not perfect), it is sometimes important to understand the fluctuations around this macroscopic description. Fluctuating hydrodynamics provides a framework for describing the evolution of macroscopic, coarse-grained fields while taking into account finite-particle-number induced fluctuations in the hydrodynamic limit.

This thesis discusses the derivation of fluctuating hydrodynamics from the microscopic description of particle dynamics. The derivation of the fluctuating hydrodynamics is twofold. First, the "large N" limit must be refined to account for fluctuations beyond the average behavior of the system. This is done by using large deviation theory to establish kinetic large deviation principles that describe the probability of any evolution path for the empirical measure beyond the most probable path described by the kinetic equation. Then, the fluctuating hydrodynamics is derived by studying the hydrodynamical limit of the kinetic large deviation principle, or the associated fluctuating kinetic equation. This thesis is structured in two parts, reflecting the two steps of this program.

The main original result of the first part is the derivation of kinetic large deviation principles for Hamiltonian systems of particles coupled by a long-range interaction potential, extending the classical Landau and Balescu-Guernsey-Lenard kinetic theories. We also provide a general introduction to the interplay between large deviation theory and kinetic theory. In the second part of the thesis, we review methods to bridge from the kinetic large deviation principle to the fluctuating hydrodynamics description. We apply them to derive the fluctuating compressible and incompressible Navier-Stokes equations starting from the kinetic large deviation principle associated with the Boltzmann equation. We also derive, for the first time, a fluctuating hydrodynamics description of a dilute system of aligning active particles interacting through binary collisions from microscopic dynamics. Finally, we discuss the relevance of these methods in the special case where the hydrodynamical limit is a scalar conservation law. In particular, we emphasize their inability to assess the probability of non-regular hydrodynamic profiles.

Résumé

Comprendre comment décrire un système avec des équations macroscopiques, qui sont généralement déterministes, en partant d'une description microscopique, qui peut être stochastique est le problème fondamental de la physique statistique. Souvent, cette tâche implique au moins deux limites : une limite "grand N" et une limite "d'équilibre local". La première permet de décrire un système de N particules par une fonction de distribution dans l'espace des phases, tandis que la seconde reflète la séparation des échelles de temps entre l'approche rapide de l'équilibre local et l'évolution lente des modes hydrodynamiques. En supposant ces deux limites, on obtient une description macroscopique déterministe. Pour des raisons à la fois théoriques et de modélisation (N est grand mais pas infini, la séparation des échelles de temps n'est pas parfaite), il est parfois important de comprendre les fluctuations autour de cette description macroscopique. L'hydrodynamique fluctuante fournit un cadre pour décrire l'évolution des champs macroscopiques tout en prenant en compte les fluctuations induites par le nombre de particules finies dans la limite hydrodynamique.

Cette thèse traite de la dérivation de l'hydrodynamique fluctuante à partir de la description microscopique de la dynamique des particules. La dérivation de l'hydrodynamique fluctuante se fait en deux étapes. Premièrement, la limite "grand N" doit être affinée pour prendre en compte les fluctuations au-delà du comportement moyen du système. Pour ce faire, nous utilisons la théorie des grandes déviations pour établir des principes de grandes déviations qui décrivent la probabilité de tout chemin d'évolution pour le système de particule au-delà du chemin le plus probable décrit par l'équation cinétique. Ensuite, nous dérivons la l'hydrodynamique fluctuante en étudiant la limite hydrodynamique du principe de grande déviation cinétique, ou l'équation cinétique fluctuante associée. Cette thèse est structurée en deux parties, reflétant les deux étapes de ce programme.

Le principal résultat original de la première partie est la dérivation des principes de grandes déviations cinétiques pour les systèmes Hamiltoniens de particules couplées par un potentiel d'interaction à longue portée, étendant les théories cinétiques classiques de Landau et de Balescu-Guernsey-Lenard. Nous fournissons également une introduction générale à l'interaction entre la théorie des grandes déviations et la théorie cinétique. Dans la deuxième partie de cette thèse, nous discutons plusieurs méthodes permettant de passer du principe de grandes déviations cinétique à l'hydrodynamique fluctuante. Nous les appliquons pour dériver les équations de Navier-Stokes fluctuantes compressibles et incompressibles à partir du principe de grandes déviations associé à l'équation de Boltzmann. Nous déduisons également, pour la première fois, une description hydrodynamique fluctuante d'un système dilué de particules actives s'alignant via des collisions binaires, à partir de la dynamique microscopique. Enfin, nous discutons de la perti-

nence de ces méthodes dans le cas particulier où la limite hydrodynamique est une loi de conservation scalaire. Dans ce contexte, nous soulignons leur incapacité à évaluer la probabilité de profils hydrodynamiques non réguliers.

1. Introduction

This dissertation delves into the study of the hydrodynamic limit of particle systems, utilizing the framework of large deviation theory. The primary objective is to investigate the derivation of fluid equations that can depict matter as a continuum at a macroscopic scale, starting from the discrete microscopic dynamics of particles. A significant focus of this manuscript is on the study of fluctuations within the hydrodynamical limit, which involves quantifying the error in describing a particle system as a continuum and accounting for finite numbers of particle effects in the fluid description. While historically, the statistical mechanics techniques presented in this manuscript were developed to bridge the molecular description of gases to their fluid description [157, 158, 69, 14], they are also applicable to a wide range of systems. For instance, they can be used to investigate large conglomerate of stars [41, 124, 68], synchronization in the firing of large assemblies of neurons [193], and even collective motion of bird flocks or bacteria [40, 12, 23]. Hence, the terms "particle" and "microscopic dynamics" do not necessarily refer to physically small objects but rather to the fundamental entities of a system composed of a large number of them. This dissertation begins by introducing the concept of particle dynamics, kinetic theory, and hydrodynamic equations, and the connections between these different levels of description.

1.1. Equations of motion and hydrodynamic equations

A way to describe the evolution of a classical particle systems is through equations of motion. In this dissertation, we consider the equations of motion as the starting point, whether they are a consequence of Newton's laws of motion, or if they are phenomenologically postulated. We label $\{\mathbf{r}_n(t), \mathbf{v}_n(t)\}_{1\leq n\leq N}$ the positions and velocities of the N particles at a given time $t \in [0, T]$. Typically, $\mathbf{r}_n \in \mathbb{R}^3$ or $\mathbb{T}^3$ which means that the particles evolve in a continuum space of dimension 3, that might be infinite or periodic. These equations can be Ordinary Differential Equations (ODEs) or Stochastic Differential Equations (SDEs). For instance, in the case of a Hamiltonian dynamics, with Hamiltonian

$$\mathcal{H} = \frac{1}{2}m\sum_{n=1}^{N}\mathbf{v}^2 + \frac{1}{2}\sum_{p\neq n} W\left(\mathbf{r}_n - \mathbf{r}_p\right),$$

the equations of motion are ODEs:

$$\begin{cases} \dfrac{\mathrm{d}\mathbf{r}_n}{\mathrm{d}t} & = \mathbf{v}_n, \\ m\dfrac{\mathrm{d}\mathbf{v}_n}{\mathrm{d}t} & = -\displaystyle\sum_{p\neq n} \nabla W\left(\mathbf{r}_n - \mathbf{r}_p\right), \end{cases} \tag{1.1}$$

where W is the pairwise interaction potential, prescribing the interaction of a particle with another, and m is the mass of a particle. Equations (1.1) are nothing else than a reformulation of Newton's second law. In principle, it is possible to predict the trajectories of particles given the initial conditions for equations (1.1), through numerical integration for instance. However, there are two inherent limitations in this approach. Firstly, an accurate prediction of trajectories can only be achieved with infinitely precise knowledge of the initial data, especially if the system is sensitive to initial conditions, i.e. if the system is chaotic. Secondly, if N the number of particles is large, the time required to numerically integrate (1.1) is at least[1] proportional to N. For example, if we wanted to model the airflow around the wing of an airplane, we would not go to the trouble of solving (1.1) for every molecule of nitrogen or oxygen surrounding the airplane, assuming we knew how they interacted individually. In the 19th century, despite widespread skepticism about the existence of atoms and molecules, great advances were made in fluid dynamics. Obviously, at that time the equations of motion of the molecules were never used to describe fluid dynamics. Instead, engineers and physicists used fluid equations. The incompressible Navier-Stokes system is probably the most widely used set of fluid equations in physics and engineering:

$$\begin{cases} \partial_t \mathbf{u} + \mathbf{u}\cdot\nabla\mathbf{u} + \nabla\left(\frac{P}{\rho_0}\right) = \nu\Delta\mathbf{u}, \\ \nabla\cdot\mathbf{u} = 0. \end{cases} \tag{1.2}$$

It is a set of Partial Differential Equations (PDEs) that describe the time-evolution of the velocity field $\mathbf{u}\left(\mathbf{r},t\right)$ and pressure field $P\left(\mathbf{r},t\right)$ of an incompressible and viscous fluid, characterized by its viscosity ν and density ρ_0. Although mathematical questions about the existence and smoothness of solutions to the Navier-Stokes equations remain open [149, 62, 143, 188], their direct numerical simulation provided a breakthrough in a number of applications such as aerodynamics and weather forecasting [185, 174, 6].

1.2. Importance of the statistical physics approach to hydrodynamics

By definition, the velocity field in (1.2) is defined at all points in space and describes matter as a continuum. A common way to understand the origin of (1.2) is to see it as

[1] If W is a long-range potential, meaning that each particle is interacting with all others, the calculation time could be proportional to $N\log N$ or N^2 depending on the solver [129].

the conservation of momentum equation for the fluid. More specifically, the hydrodynamical equations can be obtained as a consequence of Newton's second law applied to a control volume: *"a region of space through which fluid flows"* as explained in [211], of size conveniently chosen to obtain a simple result. A control volume is an abstract object that can neither be observed nor precisely defined. For many applications, including educational ones, this justification of the Navier-Stokes equations is useful. From the statistical physicist's point of view however, it is intriguing to try to explain how the Navier-Stokes equation can be related to the Newton's equations (1.1) that govern the behavior of the fluid at the molecular scale. "[Connecting] the atomistic view to the laws of motion of continua" is part of Hilbert's Sixth Problem [81, 212], which states goals for the axiomatization of physics, including the clear definition of the asymptotic processes that lead to the descriptions of matter from the atomic scale to the macroscopic scale.

Understanding the microscopic derivation of fluid equations does not only have an axiomatic purpose. It also allows a better understanding of the range of validity of the fluid description. How many particles is enough to describe a system as a continuum fluid? How can we assert the accuracy of the fluid description of a discrete system? Why is the macroscopic evolution of the system predicted by hydrodynamics irreversible while its microscopic dynamics is not? These are key questions that not only require a precise understanding of the derivation of hydrodynamical equations, but also imply the need for new tools to assert their accuracy. As is common in statistical physics, the key point is that when the number of particles in a system is large, we can treat them in a statistical way, rather than having to track the behavior of each particle individually. In this sense, the fluid equations can be seen as a Law of Large Numbers (LLN): when there are many particles, it is sufficient to describe their average behavior; for example, their average velocity at a certain point in space, which is given by the data of a velocity field. However, this approach does not allow to quantify possible deviations from the average behavior. Although very rare, such deviations can have drastic effects on the system (triggering a phase transition for instance). The appropriate probabilistic tool to deal with the study of such rare events is called Large Deviation Theory. It is used extensively in this manuscript not only to derive the hydrodynamical equations from the particle dynamics, but also to quantify the probability that the actual behavior of the particle system deviates from the average evolution path predicted by the hydrodynamics. To better understand where the LLN comes into play in the derivation of hydrodynamics and how to take into account fluctuations in the hydrodynamical limit, we heuristically introduce the notion of hydrodynamical limit in the next section.

1.3. From particles to hydrodynamics: a derivation that implies two limits

Let us first try to imagine how a description in terms of trajectories $\{\mathbf{r}_n(t), \mathbf{v}_n(t)\}$ can be linked to a velocity field description $\mathbf{u}(\mathbf{r}, t)$. Naively, we can try to compute the velocity field at a certain point in space $\mathbf{u}(\mathbf{r}, t)$ by computing a local average of the velocity

particles nearby:

$$\mathbf{u}(\mathbf{r},t) \approx \frac{1}{|B(\mathbf{r},l)|} \sum_{\mathbf{r}_n \in B(\mathbf{r},l)} \mathbf{v}_n(t), \tag{1.3}$$

where $B(\mathbf{r},l)$ is a ball of center $\mathbf{r}$ and radius l, and $|B(\mathbf{r},l)|$ is the number of particles in such a ball. Then, since we know the equations (1.1) ruling the time evolution of the $\mathbf{v}_n$ and $\mathbf{r}_n$, we can compute the time evolution of the velocity field $\mathbf{u}$. However, there are two main issues with guessing the velocity field through (1.3).

1. For equation (1.3) to make sense, we must ensure that within any ball of radius l of the system, we can find at least one particle. Then, since the velocity field is computed as a local average, we also have to ensure there is not only one but many particles in such a ball. If $\rho_0 = N/L^3$ is the average density of the system, and L the size of the system, this requirement can be mathematically translated as $\rho_0 l^3 \gg 1$. This assumption is in some sense a LLN assumption: when $\rho_0 l^3 \gg 1$, the empirical average computed in (1.3) is close to the statistical average.

2. However, the radius of the ball l cannot be too large. If l has the same order of magnitude as the system size L, then $\mathbf{u}(\mathbf{r},t)$ would globally have the same value at any point in the system $\mathbf{r}$, and would correspond to the global average velocity of all the particles in the system, rather than to a velocity field. A way to ensure that the velocity field constructed from (1.3) does not suffer this issue is to choose a radius l much smaller than the size of the system: $l \ll L$. This is necessary but not sufficient depending on the nature of the particle system.

These two points reveal that the derivation of the fluid equations from the equations of motion of the particles involves two limits. As can be easily guessed, the first limit is related to the LLN and is a large N limit called the *kinetic limit*. Less obviously, for the hydrodynamical equations to make sense, the system must also exhibit a large separation of scales between the scale of the particle dynamics and the scale at which we observe the macroscopic system. This limit of large scale separation is called the *hydrodynamical limit*.

1.4. Kinetic theory: the large N limit

A first step toward the derivation of hydrodynamics starting from a particle dynamics is to obtain a kinetic description. The main idea of kinetic theory is, in the spirit of a LLN, that when the particle number N is large, instead of describing the trajectories $\{\mathbf{r}_n(t), \mathbf{v}_n(t)\}_{1\leq n\leq N}^{0\leq t\leq T}$ of every particles, it is sufficient to describe the statistics of their positions and velocities. This is done by introducing the distribution function f. The distribution function f is a function that depends on the velocity and the position variable, and also on time. Its physical interpretation is that

$$f(\mathbf{r},\mathbf{v},t)\,\mathbf{dr}\mathbf{dv}$$

is the average number of particles that have a position $\mathbf{r}$ up to d$\mathbf{r}$, a velocity $\mathbf{v}$ up to d$\mathbf{v}$ at a certain time t. The goal is to establish a PDE that rules the time evolution of the distribution function. Such a PDE is called the kinetic equation. For a dynamics such as (1.1), the kinetic equation generally reads

$$\partial_t f + \underbrace{\mathbf{v}\cdot\nabla f}_{\text{transport term}} = \underbrace{Q(f)}_{\text{collision term}}, \tag{1.4}$$

where the transport term accounts for transport of the particles due to their own velocities, and the collision[2] term generically accounts for the effect of the interactions on the velocity distribution. A common way to obtain an evolution equation for the distribution function f is to start from Liouville's theorem, that states that the N particles joint distribution function $f_{\text{N part}}(\mathbf{r}_1, \mathbf{v}_1, \cdots, \mathbf{r}_N, \mathbf{v}_N, t)$ is conserved by the Hamiltonian dynamics (1.1). Then, by successive integration of the Liouville equation, one can express the time evolution of the distribution function f as a function of the two-particle joint distribution in phase space $f_2(\mathbf{r}_1, \mathbf{v}_1, \mathbf{r}_2, \mathbf{v}_2, t)$. This method is known as the BBGKY hierarchy. A way to close this hierarchy is to assume that at leading order, $f_2(\mathbf{r}_1, \mathbf{v}_1, \mathbf{r}_2, \mathbf{v}_2, t) \approx f(\mathbf{r}_1, \mathbf{v}_1, t) f(\mathbf{r}_2, \mathbf{v}_2, t)$. This is exactly true when there is no interaction between the N particles and when they are initially uncorrelated. Otherwise, the accuracy of this approximation is not only linked to the number of particles in the system, but also to the strength of the interaction. There are two main scenarios where we can justify this approximation, at least from a theoretical physics point of view. First, when the interactions between particle are rare enough so that we can consider them almost statistically independent. This is the case for the dilute gas, i.e. when the interaction potential W in (1.1) is short-ranged, that is described at the kinetic level by the Boltzmann equation, namely (1.4) where the collision term is defined by

$$Q(f)(\mathbf{r},\mathbf{v}) = \iiint \mathrm{d}\mathbf{v}_2 \mathrm{d}\mathbf{v}_1' \mathrm{d}\mathbf{v}_2'\, w(\mathbf{v}_1', \mathbf{v}_2'; \mathbf{v}, \mathbf{v}_2)\, \left[f(\mathbf{r},\mathbf{v}_1') f(\mathbf{r},\mathbf{v}_2') - f(\mathbf{r},\mathbf{v}) f(\mathbf{r},\mathbf{v}_2)\right]. \tag{1.5}$$

Another important situation is when all the particles are interacting with every other one, but with a weak interaction potential. This corresponds to the case where W is long-ranged but proportional to $1/N$ so that the sum of the forces exerted on a particle is still of order one. In this case, when the system is homogeneous in space, it can be described by the Balescu-Guernsey-Lenard kinetic equation

$$\partial_t f = \frac{\partial}{\partial \mathbf{v}} \cdot \left(\int \mathrm{d}\mathbf{v}_2\, \mathbf{B}[f](\mathbf{v}, \mathbf{v}_2) \cdot \left(-\frac{\partial f}{\partial \mathbf{v}_2} f(\mathbf{v}) + f(\mathbf{v}_2) \frac{\partial f}{\partial \mathbf{v}} \right) \right), \tag{1.6}$$

with

$$\mathbf{B}[f](\mathbf{v}_1, \mathbf{v}_2) = \frac{\pi}{L^3} \int_{-\infty}^{+\infty} \mathrm{d}\omega \sum_{\mathbf{k}\in(2\pi/L)\mathbb{Z}^3} \frac{\hat{W}(\mathbf{k})^2\, \mathbf{k}\otimes\mathbf{k}}{|\varepsilon[f](\mathbf{k},\omega)|^2} \delta(\omega - \mathbf{k}.\mathbf{v}_1)\, \delta(\omega - \mathbf{k}.\mathbf{v}_2), \tag{1.7}$$

[2] The terminology "collision term" is historical and refers to the interaction term of the Boltzmann equation accounting for the effect of actual elastic collisions between particles on the distribution function. We still use the term collisions even if the interaction between particle is not collisional.

where this time f only depends on the velocity variable as a consequence of spatial homogeneity, $\hat{W}$ is the Fourier transform of the potential, and ε is the dielectric function, that depends nonlinearly on f and will be introduced in detail in chapter 4.

The dilute gas, described by the Boltzmann equation, and the systems of particles with long-range interactions, described by the Balescu-Guernsey-Lenard equation will be discussed at length throughout this thesis, as they constitute paradigmatic examples of kinetic theories. The specific asymptotic regime in which they are valid will be clarified later in the manuscript, but both of them require the number of particles in the system to go to infinity. In both cases, the distribution function f is obtained as LLN for the μ-space empirical measure

$$f_N(\mathbf{r}, \mathbf{v}, t) = \frac{1}{N} \sum_{n=1}^{N} \delta(\mathbf{r} - \mathbf{r}_n(t)) \, \delta(\mathbf{v} - \mathbf{v}_n(t)),$$

a distribution on the μ-space (the one-particle phase space) that depends on the exact N particle trajectories, that allows to bridge from particle to kinetic description in the large N limit.

The interest in uncovering such kinetic theories is twofold. First, kinetic equations such as the Boltzmann and the Balescu-Guernsey-Lenard (1.6) equations give physical information about the system that was not obvious from the equations of motion. A striking example is that both equations describe the relaxation to equilibrium, i.e. that the velocity distribution relaxes toward a Gaussian distribution, the so-called Maxwell-Boltzmann equation. More interestingly, the Boltzmann equation is also the first step in deriving hydrodynamic equations such as the Navier-Stokes equations starting from the molecular dynamics.

1.5. From kinetic equations to hydrodynamic equations

Once we established a kinetic equation describing the time evolution of the distribution function f in some asymptotic regime linked to a large N limit, it is possible to investigate the time evolution of hydrodynamical fields. Such fields are typically linked to moments of the distribution function with respect to the velocity variable. For instance, the zeroth, first, and second moment

$$\rho(\mathbf{r}, t) = \int \mathrm{d}\mathbf{v} \, f(\mathbf{r}, \mathbf{v}, t),$$

$$\rho \mathbf{u}(\mathbf{r}, t) = \int \mathrm{d}\mathbf{v} \, \mathbf{v} f(\mathbf{r}, \mathbf{v}, t),$$

$$\rho e(\mathbf{r}, t) = \int \mathrm{d}\mathbf{v} \, \frac{v^2}{2} f(\mathbf{r}, \mathbf{v}, t),$$

can be interpreted as the average number of particles ρ, the average velocity $\mathbf{u}$, and the average kinetic energy e at a given point in space $\mathbf{r}$ and time t. In general, it is not possible to obtain evolution equations for the hydrodynamic fields by simple integration of the kinetic equation over the velocity variable. Without further assumptions, the evolution of the hydrodynamic fields depends on the whole distribution function and not only on the other hydrodynamic fields. This problem can be overcome by a precise study of the conservation laws associated with the particle dynamics and its relationship with local equilibria of the kinetic equation, i.e. distribution functions that cancels the collision operator $Q(f) = 0$. Assuming that the kinetic equation relaxes toward its local equilibria on time scales much shorter than the macroscopic observation time scale, it is possible to obtain closed equations on the hydrodynamic fields. For the Boltzmann equation for instance, a way to achieve this program is to look for a solution of the Boltzmann equation as a Chapman-Enskog expansion close to a local equilibrium of the Boltzmann equation, which is nothing else than a Gaussian distribution (the Maxwell-Boltzmann distribution). This procedure is an asymptotic one and is associated with a small parameter: the Knudsen number, that is the ratio between the microscopic and macroscopic (time or length) scales of the system. Depending on the scaling we chose between the time and length scales of the system, it allows to recover the compressible or incompressible Euler and Navier-Stokes equations from the Boltzmann equation.

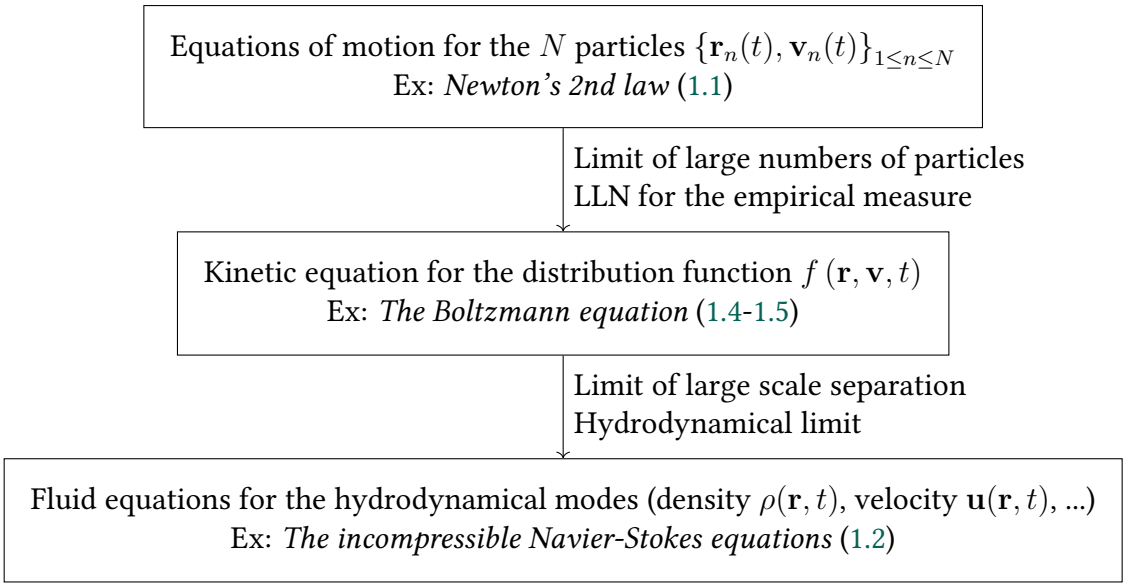


Figure 1.1.: Asymptotic procedures that bridge molecular and fluid descriptions.

1.6. Fluctuations in the kinetic and hydrodynamic limits

The fluid equations derived following the steps detailed in figure 1.1 are valid in the limit as N goes to infinity. Hence, they fall short at describing finite N effects. For example, by running a molecular dynamics simulation using the equations of motion (1.1) and numerically reconstructing the empirical velocity field (1.3), we can observe that the resulting evolution of the field is a noisy one. More precisely, the empirical velocity field should look like the solution of the deterministic fluid equations (with appropriate initial conditions) up to some random fluctuations around it. The noisiness is eventually smoothed out as the number of particles increases. This is analogous to the fact that if we sample N realizations of identically normally distributed random variables and represent the sampling in a histogram, the histogram appears smoother and closer to the normal distribution as the number of realizations increases. From this observation, it has been postulated than in a large N regime, it is reasonable to assume that the evolution of the empirical hydrodynamical fields can be seen as the one of a deterministic field derived from the LLN, plus a random noise that becomes smaller as N increases. This is for instance what is predicted by the fluctuating incompressible Navier-Stokes system (also known as the Landau-Lifshitz-Navier-Stokes system) first derived in [147, 113, 42, 137]:

$$\begin{cases} \partial_t \mathbf{u} + \mathbf{u} \cdot \nabla \mathbf{u} + \nabla \left(\frac{P}{\rho_0} \right) = \nu \Delta \mathbf{u} + \nabla \cdot \mathbf{J}, \\ \nabla \cdot \mathbf{u} = 0. \end{cases} \tag{1.8}$$

where $\mathbf{J}$ is a random Gaussian tensor whose components J_{ij} satisfy

$$\mathbb{E}\left(J_{ij}\left(\mathbf{r},t\right) J_{kl}\left(\mathbf{r}',t'\right)\right) = \frac{2\nu k_B T_0}{\rho_0} \left(\delta_{ik}\delta_{jl} + \delta_{il}\delta_{jk} - \frac{2}{3}\delta_{ij}\delta_{kl} \right) \delta(t-t')\delta(\mathbf{r}-\mathbf{r}'), \tag{1.9}$$

where T_0 is the average temperature, ρ_0 the average density, and k_B is the Boltzmann constant. From the variance of the noise term (1.9), we recover than in the large N limit (at fixed volume), the noise term vanishes and we recover the incompressible Navier-Stokes equation as a LLN[3]. Even if the Landau-Lifshitz-Navier-Stokes system is widely used in its nonlinear form (1.8), most works dedicated to its derivation are restricted to the linearized case [147, 113, 42, 137]. Those derivations either rely on adding a noise term to the linearized Navier-Stokes equations on the basis of thermodynamics considerations[4], or using the Mori-Zwanzig formalism [161, 42, 128]. Such a technique allows to add a noise term to the linearized Boltzmann kinetic equation, whose average

[3] It should be noted that the interpretation of the Navier-Stokes equations as a law of large numbers must be treated with caution. For instance, the dynamics of a passive scalar advected by the incompressible Navier-Stokes equations and subjected to thermal fluctuations seems to remain stochastic even in the vanishing diffusion and thermal noise limit [103, 28]. This phenomenon is essentially related to the roughness of the advection term and is called *spontaneous stochasticity*. In this manuscript, the denomination "law of large numbers" comes from the fact we derive the fluid equation from the kinetic equation which is actually a law of large numbers for the empirical measure.

[4] Here, "thermodynamics considerations" means a priori knowledge of the stationary state distribution of probability of the macrostate. This is obviously granted though not restricted to thermodynamical equilibrium situations.

value and correlation structure is based on fluctuation-dissipation relations. A first-principle derivation of the nonlinear fluctuating Navier-Stokes equations is proposed in [100, 101, 162], based on [214] that obtained a generalized functional Fokker-Planck equation for the hydrodynamic fields. In the mathematical literature, the characterization of fluctuations beyond the Navier-Stokes equations were notably discussed by Quastel and Yau. In [182], they established a large deviation result for the incompressible Navier-Stokes equations starting from the stochastic dynamics of a lattice gas, in an effort to understand how to establish rigorous results about the microscopic derivation of the Navier-Stokes equations without assumption on the regularity of its solutions.

The consistence of the fluctuating Navier-Stokes equations with molecular dynamics approaches have been numerically assessed and confirmed in [118, 119, 153]. It should be noted that the fluctuation-dissipation relations based derivations of the fluctuating Navier-Stokes equations assume the expression of the noise term either at the kinetic or hydrodynamic level from fluctuation-dissipation relations rather than deriving it from the microscopic dynamics. Notably, their starting point is the deterministic Boltzmann equation, that somehow already assumes a large N limit. Their validity is restricted to cases where the underlying microscopic system has a time-reversible dynamics. This assumption is valid for the dilute gas dynamics, from which we can derive (1.8), but fall short to describe more generic, out-of-equilibrium systems. Another question stemming from those derivations comes from their starting point: a fluctuating Boltzmann equation with a Gaussian noise term. Given the dynamics of the underlying particle system there is no reason for this noise to be Gaussian, and a priori, no reason either for the noise term in the fluctuating hydrodynamics to be Gaussian.

The more general and microscopic approach taken in [100, 101, 162] allows for derivations that could be extended in out-of-equilibrium contexts. These derivations rely on the manipulation of Stochastic Partial Differential Equations (SPDEs) which are the right tool to describe small fluctuations driven by finite N effects.

In this dissertation, we take a different but complementary approach to the derivation of fluctuating hydrodynamics, also starting from the particle dynamics but leveraging large deviation theory instead of SPDEs. As explained in section 2.4, finite N effects disappear in the kinetic equation through a LLN approximation. Hence, we aim to refine the large N asymptotics at this level to keep track of fluctuations within the hydrodynamic limit. Rather than simply describing the evolution of the average of the empirical measure, namely the distribution function at the kinetic level, we introduce large deviation principles to quantify the probability of large fluctuations of the empirical measure in the large N limit. In some cases, these fluctuations can be represented by a fluctuating kinetic equation with a small noise term that describes finite N effects, with some prescriptions that will be explained in the next chapter. We then consider the hydrodynamical limit to derive fluctuating hydrodynamics equations either as SPDEs, such as (1.8) or as large deviation principles for the empirical hydrodynamical fields. Large deviation theory has been widely used to describe fluctuations in macroscopic field descriptions of particle systems, notably including the Macroscopic Fluctuation Theory (MFT) describing fluctuations of the density field beyond its diffusive dynamics [32] for a wide range of particle systems, including the celebrated lattice exclusion processes. For

these systems, there is no notion of velocity (particles hop from a node to a neighboring one at fixed rates), there is no kinetic theory and the route to obtain fluctuating hydrodynamics is slightly different. Here, we recall the main works that precisely focused on establishing large deviations principles for kinetic theories that describe large N behavior particle systems whose dynamics is given by differential equations on their positions and velocities as in (1.1). The literature includes works that have formally understood large deviations for the Boltzmann equation [50], mathematically for Boltzmann-like toy-models [184, 126, 18]; recently rigorous large deviations results were established starting from the hard sphere dynamics for short times [46, 45]. Central limit theorem results were already understood and coincide with the large deviations ones for small fluctuations [191, 192]. For weakly interacting particles (through a mean-field interaction), we refer to the pioneering work of Dawson and Gartner [82], who established a large deviation result for the empirical measure of N Ito diffusions coupled in a mean-field way. This result was reinterpreted as a fluctuating kinetic equation known as the Dean-Kawasaki equation by physicists [86, 136].

1.7. Applications of fluctuating hydrodynamics

Before diving into the outline of this dissertation, we discuss here some of the motivations driving us to study finite N fluctuations within the hydrodynamical and kinetic limits. So far, we mainly focused on theoretical ones. These theoretical motivations are detailed in chapter 3, but the main point is that by constructing a statistical approach of trajectories rather than static (equilibrium) configurations, large deviations for kinetic theories and fluid equations naturally generalizes to out of equilibrium systems. Here, we focus on a few possible applications of fluctuating hydrodynamics. Generally speaking, finite N fluctuations, or thermal fluctuations as they are referred to in the historical literature, become prominent when the molecular nature of matter cannot be ignored. This is the case when dealing with a fluid at micro or nanoscales [43], with surface interactions, and when biological [165, 178, 91] or chemical processes are implied. As a consequence, the development of numerical schemes to simulate fluctuating hydrodynamics such as the Landau-Lifshitz-Navier-Stokes (LLNS) system (1.8) allowed major breakthrough in these fields [9, 39, 96]. Notably, in [170], the authors numerically predict through the LLNS system the *giant concentration fluctuations*[5] observed in the diffusive mixing of water and glycerol in molecular dynamics simulations [95] and experiments [204, 80, 203]. Another field of application of the fluctuating Navier-Stokes equations is the study of turbulence. As suggested by the seminal work of Betchov [35, 36, 37], thermal fluctuations seems to modify the spectrum of the kinetic energy cascade in turbulence. These effects have been numerically [117] and analytically [102, 13, 19] studied starting from the fluctuating hydrodynamics description.

[5] When studying the mixing of two liquids in the absence of gravity (with microgravity techniques for instance), it is known that the spectrum of the intensity of the concentration fluctuations scales like k^{-4} with the wavenumber k [85], yielding thermally sourced propagative macroscopic fluctuations at small wavenumbers.

All these works starts from the fluctuating Navier-Stokes equations, for which the noise terms were already characterized from thermodynamics consideration. More interestingly, the microscopical derivation of fluctuating hydrodynamics becomes crucial when the noise term cannot be assumed from equilibrium thermodynamics. An important example is the one of active matter. Active systems are composed of units able to extract non-thermal energy from the environment and dissipate it to self-propel. Bacteria or mammals can be example of such units. The modeling of such system usually starts from particle dynamics that explicitly breaks detailed balance, as in the paradigmatic case of the Vicsek model [209]. Fluctuating hydrodynamics descriptions of such systems are crucial, given that in the biological applications, the particle number remains relatively small. Given the absence of thermodynamics argument, the noise term in such description is usually added ad hoc [199, 200, 198].

1.8. Contents of the manuscript

This manuscript deals with the derivation of fluctuating hydrodynamics from the particle dynamics. Its organization naturally follows the two steps of such a derivation. The first part of the dissertation deals with the derivation of dynamical large deviation principles for kinetic theories starting from the particle dynamics; and the second part is concerned with the derivation of fluctuating hydrodynamics starting from kinetic large deviation principles.

The first chapter of the first part (chapter 3) serves as a general introduction to large deviation theory and how it relates to kinetic theory. It also includes generic methods to obtain kinetic large deviation principle, as well as the derivation of large deviation principles for N diffusions coupled in a mean-field way, and N independent particles submitted to a jump (Run-And-Tumble) process. These are not new results, but they are used throughout the manuscript and serve as pedagogical examples in this chapter. In chapter 4, we obtain the dynamical large deviation principle extending the Balescu-Guernsey-Lenard equation, which is the kinetic equation describing the large N behavior of a Hamiltonian system of particles coupled via a long-range potential. This is the first new result of this dissertation. The next chapter (5) focuses on the derivation of the dynamical large deviation principle associated with the Landau kinetic equation. It is obtained as an approximation of the Balescu-Guernsey-Lenard result, when the interaction potential is a Coulomb potential and the scales investigated much smaller than the Debye length. The large deviation result for the Landau equation is also linked to the results about the large deviations for the Boltzmann equation within the grazing collision limit. This result is also an original one, and is notably connected with recent results on the gradient-flow structure of the Landau equation [65, 66]. Alongside already established results about large deviations for the Boltzmann equation, those two large deviations results for the Balescu-Guernsey-Lenard and the Landau equations complete the picture of the large deviations for classical kinetic theories.

The second part of the dissertation begins with chapter 6 that introduces the tools used in the following chapters to bridge from kinetic large deviation principles to fluctuating

hydrodynamics. This is done by investigating the derivation of the fluctuating diffusion equation for N independent particles diffusing via a jump (Run-And-Tumble) process. The derivation of this equation is not new, but it serves a pedagogical goal, and it allows to introduce the key conceptual tools used in the second part: the Chapman-Enskog expansion, the contraction principle of the kinetic large deviation principle toward the hydrodynamic large deviation principle, and the "Gaussianization" of the large deviation principle within the hydrodynamic limit. We apply this program in chapter 7 to the microscopical derivation of the fluctuating compressible and incompressible Navier-Stokes equations, with the large deviations for the Boltzmann equation as a starting point. A notable side result of this chapter, is the obtaining of gradient-flow structures, as a consequence of the large deviations principles, for the incompressible (respectively compressible) Navier-Stokes equations, illustrating the geometry of the dissipation of the kinetic energy (resp. the negative of the entropy) in these equations. In chapter 8, we derive a kinetic large deviation principle and the ensuing fluctuating hydrodynamics for an active particle gas (similar to the Vicsek model) in the dilute limit. This work is also original and is one of the first[6] to propose a microscopical derivation of the noise term in a fluctuating hydrodynamics description of an active system. Another interesting technical point of this chapter is the derivation of fluid equations for a particle system that lacks conservation laws, using the notion of Generalized Collision Invariant first introduced by Degond [87]. In chapter 9, we assess the robustness of the derivation of fluctuating hydrodynamics from kinetic large deviation principle in the specific case where the hydrodynamical limit is a hyperbolic conservation law. Such PDEs are known to exhibit non-unique solutions with steep gradients, and we explain, with the example of a 1D Run-And-Tumble process that the asymptotic expansions we used to obtain fluctuating hydrodynamics might be wrong to quantify the probability of certain non-smooth weak solutions hydrodynamic profiles. In particular, there is no reason for the Jensen-Varadhan functional (derived in [133, 205] for the Totally Asymmetric Exclusion Process) that quantifies the probability of non-entropic shocks to hold in general.

[6] Alongside [29]. To our knowledge, it is the first work that derives the noise term for a particle model based on binary interactions.

2. Introduction en français

Cette thèse traite de l'étude de la limite hydrodynamique de systèmes de particules dans le cadre de la théorie des grandes déviations. L'objectif principal est d'étudier la dérivation d'équations fluides décrivant la matière comme un continuum à l'échelle macroscopique, à partir de la dynamique microscopique discrète des particules. Plus particulièrement, ce manuscrit s'intéresse à l'étude des fluctuations dans la limite hydrodynamique, par exemple à la quantification de la précision de la description d'un système de particules comme un continuum et la prise en compte d'effet de nombre de particules fini dans la description du fluide. Bien qu'historiquement, les techniques de mécanique statistique présentées dans ce manuscrit aient été développées pour faire le lien entre la description moléculaire des gaz et leur description fluide [157, 158, 69, 14], elles sont applicables à un large éventail de systèmes. Par exemple, elles peuvent être utilisées pour étudier les grands conglomérats d'étoiles [41, 124, 68], la synchronisation dans l'activation des neurones [193], ainsi que le mouvement collectif de nuées d'oiseaux ou de colonies de bactéries [40, 12, 23]. Ainsi, les termes "particule" et "dynamique microscopique" ne se réfèrent pas nécessairement à des objets physiquement petits mais plutôt aux entités fondamentales d'un système composé d'un grand nombre d'entre elles. Dans la suite, nous commençons par introduire les concepts de dynamique microscopique des particules, de théorie cinétique et d'équations hydrodynamiques, ainsi que les liens entre ces différents niveaux de description.

2.1. Equations du mouvement pour les particules et équations hydrodynamiques

Une façon de décrire l'évolution d'un système de particules classique est la donnée d'équations du mouvement pour la vitesse et la position de chacune des particules. Dans cette thèse, nous considérons les équations du mouvement pour les particules comme le point de départ, qu'elles soient une conséquence des lois de Newton ou qu'elles soient postulées phénoménologiquement. Nous appelons $\{\mathbf{r}_n(t), \mathbf{v}_n(t)\}_{1\leq n\leq N}$ les positions et les vitesses des N particules à un instant donné $t \in [0, T]$. Généralement, $\mathbf{r}_n \in \mathbb{R}^3$ ou $\mathbb{T}^3$, ce qui signifie que les particules évoluent dans un espace continu de dimension 3, qui peut être infini ou périodique. Ces équations peuvent être des équations différentielles ordinaires (EDO) ou des équations différentielles stochastiques (EDS). Par exemple, dans le cas d'une dynamique Hamiltonienne, avec un Hamiltonien

$$\mathcal{H} = \frac{1}{2}m\sum_{n=1}^{N}\mathbf{v}^2 + \frac{1}{2}\sum_{p\neq n} W\left(\mathbf{r}_n - \mathbf{r}_p\right),$$

les équations du mouvement sont des EDO :

$$\begin{cases} \dfrac{\mathrm{d}\mathbf{r}_n}{\mathrm{d}t} & = \mathbf{v}_n, \\ m\dfrac{\mathrm{d}\mathbf{v}_n}{\mathrm{d}t} & = -\displaystyle\sum_{p\neq n} \nabla W\left(\mathbf{r}_n - \mathbf{r}_p\right), \end{cases} \tag{2.1}$$

où W est le potentiel d'interaction par paire, prescrivant l'interaction d'une particule avec une autre, et m est la masse d'une particule. Les équations (2.1) ne sont rien d'autre qu'une reformulation de la seconde loi de Newton. En principe, il est possible de prédire les trajectoires des particules à partir des conditions initiales des équations (2.1), par intégration numérique par exemple. Cependant, cette approche présente deux limites inhérentes. Premièrement, une prédiction précise des trajectoires ne peut être obtenue qu'avec une connaissance infiniment précise des données initiales, en particulier si le système est sensible aux conditions initiales, c'est-à-dire si le système est chaotique. Deuxièmement, si N le nombre de particules est grand, le temps nécessaire pour intégrer numériquement (2.1) est au moins[1] proportionnel à N. Par exemple, si nous voulions modéliser l'écoulement de l'air autour de l'aile d'un avion, il serait inenvisageable d'intégrer (1.1) pour chaque molécule de diazote ou de dioxygène entourant l'avion, en supposant que nous sachions comment elles interagissent individuellement. Au XIXe siècle, malgré le scepticisme généralisé quant à l'existence des atomes et des molécules, de grandes avancées ont été réalisées dans le domaine de la dynamique des fluides. Il est évident qu'à cette époque, les équations du mouvement des molécules n'étaient jamais utilisées pour décrire la dynamique des fluides. Les ingénieurs et les physiciens utilisaient plutôt des équations fluides (ou hydrodynamiques). Les équations de Navier-Stokes pour un fluide incompressible sont probablement les équations fluides les plus utilisées en physique et en ingénierie :

$$\begin{cases} \partial_t \mathbf{u} + \mathbf{u}\cdot\nabla\mathbf{u} + \nabla\left(\frac{P}{\rho_0}\right) = \nu\Delta\mathbf{u}, \\ \nabla\cdot\mathbf{u} = 0. \end{cases} \tag{2.2}$$

Il s'agit d'un ensemble d'équations différentielles partielles (EDP) qui décrivent l'évolution temporelle du champ de vitesse $\mathbf{u}\left(\mathbf{r},t\right)$ et du champ de pression $P\left(\mathbf{r},t\right)$ d'un fluide incompressible et visqueux, caractérisé par sa viscosité ν et sa masse volumique ρ_0. Bien que les questions mathématiques concernant l'existence et la régularité des solutions des équations de Navier-Stokes restent ouvertes [149, 62, 143, 188], leur simulation numérique directe (DNS) a permis des avancées dans un certain nombre d'applications telles que l'aérodynamique et les prévisions météorologiques [185, 174, 6].

[1] Si W est un potentiel à longue portée, c'est-à-dire que chaque particule interagit avec toutes les autres, le temps de calcul pourrait être proportionnel à $N\log N$ ou N^2 selon l'algorithme utilisé [129].

2.2. Intérêts et importance d'une approche statistique de l'hydrodynamique

Par définition, le champ de vitesse dans les équations de Navier-Stokes (2.2) est défini en tout point de l'espace et décrit la matière comme un continuum. Une façon courante de comprendre l'origine de ces équations (2.2) est de le considérer comme les équations de conservation de la quantité de mouvement pour le fluide. Plus précisément, les équations hydrodynamiques peuvent être obtenues comme une conséquence de la deuxième loi de Newton appliquée à un volume de contrôle du fluide : "une région de l'espace à travers laquelle le fluide s'écoule" comme expliqué dans [211], de taille commodément choisie pour obtenir un résultat simple. Un volume de contrôle est un objet abstrait qui ne peut être ni observé ni défini avec précision. Pour de nombreuses applications, y compris éducatives, cette justification des équations de Navier-Stokes est utile. Du point de vue du physicien statisticien, il est cependant intrigant d'essayer d'expliquer comment les équations de Navier-Stokes peuvent être reliées aux équations de Newton (2.1) qui régissent le comportement du fluide à l'échelle moléculaire. "Relier la vision atomistique aux lois du mouvement du continuum" est une question intégrée au sixième problème de Hilbert [81, 212], qui énonce certains objectifs de l'axiomatisation de la physique, tels que la définition claire des processus asymptotiques qui conduisent aux descriptions de la matière de l'échelle atomique à l'échelle macroscopique.

La compréhension de la dérivation microscopique des équations hydrodynamiques n'a pas seulement un objectif axiomatique. Elle permet également de mieux maitriser le domaine de validité de la description hydrodynamique. A partir de combien de particules est-il raisonnable de décrire un système de particule discret comme un fluide continu ? Comment pouvons-nous quantifier la précision de cette approximation ? Pourquoi l'évolution macroscopique du système prédite par les équations hydrodynamiques est-elle irréversible alors que sa dynamique microscopique ne l'est pas ? Il s'agit de questions clés qui nécessitent non seulement une compréhension précise de la dérivation des équations hydrodynamiques, mais qui impliquent également le besoin de nouveaux outils pour quantifier leur précision. Comme c'est souvent le cas en physique statistique, le point clé est que lorsque le nombre de particules composant le système est important, nous pouvons les traiter de manière statistique, plutôt que de façon déterministe en prédisant le comportement de chaque particule individuellement. En ce sens, les équations hydrodynamiques peuvent être considérées comme une Loi des Grands Nombres (LGN) ; lorsqu'il y a beaucoup de particules, il suffit de décrire leur comportement moyen, par exemple, leur vitesse moyenne en un certain point de l'espace, qui est donnée par la valeur du champ de vitesse en ce point. Toutefois, cette approche ne permet pas de quantifier les écarts éventuels d'une réalisation du système par rapport à son comportement moyen. Bien que rares, de tels écarts peuvent avoir des effets radicaux sur le système (en déclenchant une transition de phase, par exemple). L'outil probabiliste approprié pour l'étude de ces événements rares est la théorie des grandes déviations. Elle est largement utilisée dans ce manuscrit, non seulement pour dériver les équations hydrodynamiques depuis la dynamique des particules, mais aussi pour quantifier la probabilité que le com-

portement macroscopique du système de particules s'écarte de la trajectoire d'évolution moyenne prédite par l'hydrodynamique. Pour mieux comprendre où la LGN entre en jeu dans la dérivation de l'hydrodynamique et comment prendre en compte les fluctuations dans la limite hydrodynamique, nous introduisons de manière heuristique la notion de limite hydrodynamique dans la section suivante.

2.3. Des particules à l'hydrodynamique : une dérivation qui implique deux limites

Essayons d'abord d'imaginer comment une description en termes de trajectoires $\{\mathbf{r}_n(t), \mathbf{v}_n(t)\}$ peut être liée à une description en terme de champ de vitesse $\mathbf{u}(\mathbf{r}, t)$. Naïvement, nous pouvons essayer de calculer le champ de vitesse en un certain point de l'espace $\mathbf{u}(\mathbf{r}, t)$ en calculant une moyenne locale des particules de vitesse situées à proximité :

$$\mathbf{u}(\mathbf{r}, t) \approx \frac{1}{|B(\mathbf{r}, l)|} \sum_{\mathbf{r}_n \in B(\mathbf{r}, l)} \mathbf{v}_n(t), \tag{2.3}$$

où $B(\mathbf{r}, l)$ est une boule de centre $\mathbf{r}$ et de rayon l, et $|B(\mathbf{r}, l)|$ est le nombre de particules dans une telle boule. Puisque nous connaissons les équations (2.1) régissant l'évolution temporelle de $\mathbf{v}_n$ et $\mathbf{r}_n$, nous pouvons en théorie calculer l'évolution temporelle du champ de vitesse $\mathbf{u}$. Cependant, l'estimation du champ de vitesse par la formule empirique (2.3) pose deux problèmes.

1. Pour que l'équation (2.3) ait un sens, nous devons nous assurer que dans toute boule de rayon l du système, nous pouvons trouver au moins une particule. Puisque le champ de vitesse est calculé comme une moyenne locale, nous devons également nous assurer qu'il n'y a pas qu'une seule particule dans cette boule, mais qu'il y en a beaucoup. Si $\rho_0 = N/L^3$ est la densité moyenne du système, et L la taille du système, cette exigence peut être traduite mathématiquement par $\rho_0 l^3 \gg 1$. Cette hypothèse est en quelque sorte une hypothèse de type LGN : lorsque $\rho_0 l^3 \gg 1$, la moyenne empirique calculée dans (2.3) est proche de la moyenne statistique.

2. Cependant, le rayon de la boule l ne peut pas être trop grand. Si l a le même ordre de grandeur que la taille du système L, alors $\mathbf{u}(\mathbf{r}, t)$ aurait globalement la même valeur en tout point $\mathbf{r}$ du système, et correspondrait à la vitesse moyenne globale de toutes les particules du système, plutôt qu'à un champ de vitesse. Une façon de s'assurer que le champ de vitesse construit à partir de (2.3) ne souffre pas de ce problème est de choisir un rayon l beaucoup plus petit que la taille du système : $l \ll L$. Ceci est nécessaire mais pas suffisant en fonction de la nature du système de particules.

Ces deux écueils potentiels révèlent que la dérivation des équations hydrodynamiques à partir des équations du mouvement des particules implique deux limites. Comme on peut aisément le deviner, la première limite est liée à la LGN et est une limite de type "grand

N”, appelée *limite cinétique*. De manière moins évidente, pour que les équations hydrodynamiques aient un sens, le système doit également présenter une grande séparation d’échelles entre l’échelle microscopique de la dynamique des particules et l’échelle à laquelle nous observons le système macroscopique. Cette limite de séparation des grandes échelles est appelée *limite hydrodynamique*.

2.4. La théorie cinétique : la limite “grand N”

Une première étape vers la dérivation de l’hydrodynamique à partir de la dynamique des particules consiste à obtenir une description cinétique. L’idée principale de la théorie cinétique est, dans l’esprit d’une LGN, que lorsque le nombre de particules N est grand, au lieu de décrire les trajectoires $\{\mathbf{r}_n(t), \mathbf{v}_n(t)\}_{1\leq n\leq N}^{0\leq t\leq T}$ de chaque particule, il suffit de décrire les statistiques de leurs positions et de leurs vitesses. Pour ce faire, on introduit la fonction de distribution f. La fonction de distribution f est une fonction qui dépend de la vitesse et de la variable de position, ainsi que du temps. Son interprétation physique est la suivante :

$$f(\mathbf{r}, \mathbf{v}, t)\, \mathrm{d}\mathbf{r}\mathrm{d}\mathbf{v}$$

est le nombre moyen de particules qui ont une position $\mathbf{r}$ à $\mathrm{d}\mathbf{r}$ près, une vitesse $\mathbf{v}$ à $\mathrm{d}\mathbf{v}$ près, à un certain instant t. L’objectif de la théorie cinétique est d’établir une EDP qui régit l’évolution temporelle de la fonction de distribution. Une telle EDP est appelée équation cinétique. Pour une dynamique telle que (2.1), l’équation cinétique s’écrit généralement comme suit :

$$\partial_t f + \underbrace{\mathbf{v}\cdot\nabla f}_{\text{terme de transport}} = \underbrace{Q(f)}_{\text{terme de collision}}, \tag{2.4}$$

où le terme de transport rend compte du transport des particules dû à leurs propres vitesses, et le terme de collision[2] rend compte de manière générique de l’effet des interactions sur la distribution des vitesses. Une façon courante d’obtenir une équation d’évolution pour la fonction de distribution f est de partir du théorème de Liouville, qui stipule que la fonction de distribution conjointe des N particules $f_{\text{N part}}(\mathbf{r}_1, \mathbf{v}_1, \cdots, \mathbf{r}_N, \mathbf{v}_N, t)$ est conservée par la dynamique Hamiltonienne (2.1). Ensuite, par intégration successive de l’équation de Liouville, on peut exprimer l’évolution temporelle de la fonction de distribution f en fonction de la distribution conjointe à deux particules dans l’espace des phases $f_2(\mathbf{r}_1, \mathbf{v}_1, \mathbf{r}_2, \mathbf{v}_2, t)$. Cette méthode est connue sous le nom de hiérarchie BBGKY. Une façon de clore cette hiérarchie est de supposer qu’à l’ordre dominant, $f_2(\mathbf{r}_1, \mathbf{v}_1, \mathbf{r}_2, \mathbf{v}_2, t) \approx f(\mathbf{r}_1, \mathbf{v}_1, t)\, f(\mathbf{r}_2, \mathbf{v}_2, t)$. C’est exactement le cas lorsqu’il n’y a pas d’interaction entre les N particules et qu’elles ne sont pas initialement corrélées. Dans le

[2] La terminologie “terme de collision” est historique et se réfère au terme d’interaction de l’équation de Boltzmann qui rend compte de l’effet des collisions élastiques entre les particules sur la fonction de distribution. Nous utilisons toujours le terme “collisions” même si l’interaction entre les particules n’est pas collisionnelle.

cas contraire, la précision de cette approximation n'est pas seulement liée au nombre de particules dans le système, mais aussi à l'intensité de leurs interactions. Il y a principalement deux scénarios où l'on peut justifier cette approximation, du moins du point de vue de la physique théorique. Premièrement, lorsque les interactions entre les particules sont suffisamment rares pour que l'on puisse les considérer comme statistiquement indépendantes. C'est le cas pour le gaz dilué, c'est-à-dire lorsque le potentiel d'interaction W dans (2.1) est à courte portée, qui est décrit au niveau cinétique par l'équation de Boltzmann, à savoir (2.4) où le terme de collision est défini par

$$Q(f)(\mathbf{r},\mathbf{v}) = \iiint \mathrm{d}\mathbf{v}_2 \mathrm{d}\mathbf{v}_1' \mathrm{d}\mathbf{v}_2' \, w(\mathbf{v}_1', \mathbf{v}_2'; \mathbf{v}, \mathbf{v}_2) \, \left[f(\mathbf{r},\mathbf{v}_1') f(\mathbf{r},\mathbf{v}_2') - f(\mathbf{r},\mathbf{v}) f(\mathbf{r},\mathbf{v}_2) \right]. \tag{2.5}$$

Une autre situation importante est celle où toutes les particules interagissent entre elles, mais avec un potentiel d'interaction faible. Cela correspond au cas où W est à longue portée mais proportionnel à $1/N$, de sorte que la somme des forces exercées sur une particule est toujours d'ordre un. Dans ce cas, lorsque le système est spatialement homogène, il peut être décrit par l'équation cinétique de Balescu-Guernsey-Lenard

$$\partial_t f = \frac{\partial}{\partial \mathbf{v}} \cdot \left(\int \mathrm{d}\mathbf{v}_2 \, \mathbf{B}\left[f\right](\mathbf{v},\mathbf{v}_2) \cdot \left(-\frac{\partial f}{\partial \mathbf{v}_2} f(\mathbf{v}) + f(\mathbf{v}_2) \frac{\partial f}{\partial \mathbf{v}} \right) \right), \tag{2.6}$$

with

$$\mathbf{B}\left[f\right](\mathbf{v}_1,\mathbf{v}_2) = \frac{\pi}{L^3} \int_{-\infty}^{+\infty} \mathrm{d}\omega \sum_{\mathbf{k}\in(2\pi/L)\mathbb{Z}^3} \frac{\hat{W}(\mathbf{k})^2 \, \mathbf{k}\otimes\mathbf{k}}{\left|\varepsilon[f](\mathbf{k},\omega)\right|^2} \delta\left(\omega - \mathbf{k}.\mathbf{v}_1\right) \delta\left(\omega - \mathbf{k}.\mathbf{v}_2\right), \tag{2.7}$$

où cette fois f ne dépend que de la variable vitesse en raison de l'homogénéité spatiale, $\hat{W}$ est la transformée de Fourier du potentiel, et ε est la fonction diélectrique, qui dépend de façon non linéaire de f et sera introduite en détail dans le chapitre 4.

Le gaz dilué, décrit par l'équation de Boltzmann, et les systèmes de particules avec des interactions à longue portée, décrits par l'équation de Balescu-Guernsey-Lenard, seront discutés en détail tout au long de cette thèse, car ils constituent des exemples paradigmatiques de théories cinétiques. Le régime asymptotique spécifique dans lequel elles sont valides sera clarifié plus loin dans le manuscrit, mais toutes deux requièrent que le nombre de particules dans le système aille à l'infini. Dans les deux cas, la fonction de distribution f est obtenue comme une LGN pour la mesure empirique

$$f_N(\mathbf{r},\mathbf{v},t) = \frac{1}{N} \sum_{n=1}^{N} \delta\left(\mathbf{r} - \mathbf{r}_n(t)\right) \delta\left(\mathbf{v} - \mathbf{v}_n(t)\right),$$

une distribution sur l'espace μ (l'espace de phase à une particule) qui dépend des trajectoires exactes des N particules, et qui permet de passer de la description particulaires à la description cinétique dans la limite des grands N.

L'intérêt d'étudier de telles théories cinétiques est double. Premièrement, les équations cinétiques telles que les équations de Boltzmann et de Balescu-Guernsey-Lenard donnent

des informations physiques sur le système qui ne découlent pas de façon immédiate des équations de mouvement. Un exemple frappant est que ces deux équations décrivent la relaxation vers l'équilibre, c'est-à-dire que la distribution des vitesses relaxe vers une distribution normale, communément appelée distribution de Maxwell-Boltzmann. Plus intéressant encore, l'équation de Boltzmann est également la première étape dans la dérivation des équations hydrodynamiques telles que les équations de Navier-Stokes à partir de la dynamique moléculaire.

2.5. Des équations cinétiques aux équations hydrodynamiques

Une fois que nous avons établi une équation cinétique décrivant l'évolution temporelle de la fonction de distribution f dans un régime asymptotique lié à une limite de grand N, il est possible d'étudier l'évolution temporelle des champs hydrodynamiques. Ces champs sont généralement liés aux moments de la fonction de distribution par rapport à la variable de vitesse. Par exemple, les moments d'ordre zéro, un et deux

$$\rho\left(\mathbf{r},t\right)=\int\mathrm{d}\mathbf{v}\,f\left(\mathbf{r},\mathbf{v},t\right),$$

$$\rho\mathbf{u}\left(\mathbf{r},t\right)=\int\mathrm{d}\mathbf{v}\,\mathbf{v}f\left(\mathbf{r},\mathbf{v},t\right),$$

$$\rho e\left(\mathbf{r},t\right)=\int\mathrm{d}\mathbf{v}\,\frac{v^2}{2}f\left(\mathbf{r},\mathbf{v},t\right),$$

peuvent être interprétés comme le nombre moyen de particules ρ, la vitesse moyenne $\mathbf{u}$, et l'énergie cinétique moyenne e en un point donné de l'espace $\mathbf{r}$ et du temps t. En général, il n'est pas possible d'obtenir des équations d'évolution des champs hydrodynamiques par simple intégration de l'équation cinétique sur la variable de vitesse. Sans autre hypothèse, l'évolution des champs hydrodynamiques dépend de l'ensemble de la fonction de distribution et pas seulement des autres champs hydrodynamiques. Ce problème peut être surmonté par une étude précise des lois de conservation associées à la dynamique des particules et de leur relation avec les équilibres locaux de l'équation cinétique, c'est-à-dire les fonctions de distribution qui annulent l'opérateur de collision $Q\left(f\right)=0$. En supposant que l'équation cinétique relaxe vers ses équilibres locaux sur des échelles de temps beaucoup plus courtes que l'échelle de temps d'observation macroscopique, il est possible d'obtenir des équations fermées sur les champs hydrodynamiques. Pour l'équation de Boltzmann par exemple, une façon de réaliser ce programme est de chercher des solutions à l'équation de Boltzmann comme un développement de Chapman-Enskog au voisinage d'un équilibre local de l'équation de Boltzmann (une distribution de Maxwell-Boltzmann). Cette procédure est asymptotique et est associée à un petit paramètre : le nombre de Knudsen, c'est-à-dire le rapport entre les échelles microscopique et macroscopique (temps ou longueur) du système. Selon le scaling choisi

entre les échelles de temps et de longueur du système, il est possible de dériver les équations d'Euler et de Navier-Stokes compressibles ou incompressibles dans la limite de petit Knudsen à partir de l'équation de Boltzmann.

2.6. Fluctuations dans les limites cinétiques et hydrodynamiques

Les équations fluides dérivées en suivant les étapes détaillées précédemment sont valables dans la limite d'un nombre de particules infini. Par conséquent, elles ne peuvent pas décrire les effets de "N fini". Par exemple, en effectuant une simulation de dynamique moléculaire à l'aide des équations du mouvement (2.1) et en reconstruisant numériquement le champ de vitesse empirique (2.3), nous pouvons observer que l'évolution résultante du champ de vitesse est bruitée. Plus précisément, le champ de vitesse empirique devrait ressembler à la solution des équations hydrodynamiques déterministes (avec les conditions initiales appropriées) auxquelles se superposent de petites fluctuations, visiblement aléatoires. A mesure que le nombre de particules augmente, l'amplitude de ces fluctuations décroît. Ceci est analogue au fait que si nous échantillonnons N réalisations de variables aléatoires identiquement, indépendamment et normalement distribuée et représentons l'échantillonnage dans un histogramme, l'histogramme apparaît plus lisse et plus proche de la distribution normale au fur et à mesure que le nombre de réalisations augmente. À partir de cette observation, il a été postulé que dans un régime de grand N, il est raisonnable de supposer que l'évolution des champs hydrodynamiques empiriques peut être considérée comme l'addition de celle d'un champ déterministe dérivé de la LGN, et d'un bruit aléatoire qui devient plus petit à mesure que N augmente. C'est par exemple ce que prédit le système de Navier-Stokes incompressible fluctuant (également connu sous le nom de système de Landau-Lifshitz-Navier-Stokes) dérivé pour la première fois dans [147, 113, 42, 137] :

$$\begin{cases} \partial_t \mathbf{u} + \mathbf{u} \cdot \nabla \mathbf{u} + \nabla \left(\frac{P}{\rho_0} \right) = \nu \Delta \mathbf{u} + \nabla \cdot \mathbf{J}, \\ \nabla \cdot \mathbf{u} = 0. \end{cases} \tag{2.8}$$

où $\mathbf{J}$ est un tenseur aléatoire de statistique Gaussienne dont les composantes J_{ij} satisfont

$$\mathbb{E}\left(J_{ij}\left(\mathbf{r},t\right) J_{kl}\left(\mathbf{r}',t'\right)\right) = \frac{2\nu k_B T_0}{\rho_0} \left(\delta_{ik}\delta_{jl} + \delta_{il}\delta_{jk} - \frac{2}{3}\delta_{ij}\delta_{kl} \right) \delta(t-t')\delta(\mathbf{r}-\mathbf{r}'), \tag{2.9}$$

où T_0 est la température du fluide, ρ_0 sa masse volumique, et k_B la constante de Boltzmann. À partir de la variance du terme de bruit (2.9), nous constatons que dans la limite d'un grand nombre de particules N, le terme de bruit disparaît et nous retrouvons l'équation de Navier-Stokes incompressible en tant que LGN. [3] Même si le système de Landau-Lifshitz-Navier-Stokes est largement utilisé dans sa forme non linéaire (2.8), la plupart

[3] Il convient de noter que l'interprétation des équations de Navier-Stokes en tant que loi des grands nombres doit être traitée avec prudence. Par exemple, la dynamique d'un scalaire passif advecté par

des travaux consacrés à sa dérivation se limitent au cas linéarisé [147, 113, 42, 137]. Ces dérivations reposent soit sur l'ajout d'un terme de bruit aux équations de Navier-Stokes linéarisées sur la base de considérations thermodynamiques, soit sur l'utilisation du formalisme de Mori-Zwanzig [161, 42, 128]. Ce formalisme permet d'ajouter un terme de bruit à l'équation cinétique de Boltzmann linéarisée, dont la valeur moyenne et la structure de corrélation sont basées sur des relations de fluctuation-dissipation. Une dérivation à partir des "premiers principes" des équations de Navier-Stokes fluctuantes non linéaires est proposée dans [100], sur la base de [214] qui dérive une équation de Fokker-Planck fonctionnelle généralisée pour les champs hydrodynamiques. L'affirmation de "premier principe" dans cette dérivation se réfère au point de départ de [214] qui est une équation de Liouville pour des champs hydrodynamiques "microscopiques" coarse-grainés dont la relation avec la dynamique réelle des particules n'est pas explicite. Dans la littérature mathématique, la caractérisation des fluctuations au-delà des équations de Navier-Stokes a notamment été discutée par Quastel et Yau. Dans [182], ils établissent un résultat de grandes déviations pour les équations de Navier-Stokes incompressibles à partir de la dynamique stochastique simplifiée d'un gaz sur réseau, dans la perspective d'établir des résultats rigoureux sur la dérivation microscopique des équations de Navier-Stokes sans hypothèse sur la régularité de ses solutions.

La cohérence des équations de Navier-Stokes fluctuantes avec les approches de dynamique moléculaire a été évaluée numériquement et confirmée [118, 119, 153]. Il convient de noter que toutes les dérivations des équations de Navier-Stokes fluctuantes supposent l'expression du terme de bruit au niveau cinétique ou hydrodynamique à partir des relations de fluctuation-dissipation plutôt que de le dériver depuis la dynamique microscopique. Notamment, leur point de départ est l'équation de Boltzmann déterministe, qui, d'une certaine manière, suppose déjà une limite de N infini. De plus, leur validité est limitée aux cas où le système microscopique sous-jacent a une dynamique réversible dans le temps, permettant l'utilisation de théorèmes de fluctuation-dissipation. Cette hypothèse est valable pour la dynamique des gaz dilués, mais ne permet pas de décrire des systèmes plus génériques et hors d'équilibre. Une autre question découlant de ces dérivations provient de leur point de départ : une équation de Boltzmann fluctuante avec un terme de bruit Gaussien. Etant donné la dynamique du système de particules sous-jacent, il n'y a aucune raison pour que ce bruit soit Gaussien, et a priori, aucune raison non plus pour que le terme de bruit dans l'hydrodynamique fluctuante soit Gaussien.

Dans cette thèse, nous adoptons une approche différente pour dériver l'hydrodynamique fluctuante, en ayant la dynamique microscopique des particules comme point de départ. Comme expliqué précédemment, les effets de N fini disparaissent dans l'équation cinétique grâce à une approximation de type LGN. Par conséquent, nous visons à affiner les asymptotiques de grand N à ce niveau pour garder une trace des fluctua-

les équations de Navier-Stokes incompressibles et soumis à des fluctuations thermiques semble rester stochastique même dans la limite de diffusion et du bruit thermique allant vers zéro[103, 28]. Ce phénomène est essentiellement lié à la rugosité engendrée par le terme d'advection et est appelé *stochasticité spontanée*. Dans ce manuscrit, la dénomination "loi des grands nombres" vient du fait que nous dérivons l'équation des fluides de l'équation cinétique qui est de fait une loi des grands nombres pour la mesure empirique.

tions dans la limite hydrodynamique. Plutôt que de décrire simplement l'évolution de la moyenne de la mesure empirique, à savoir la fonction de distribution au niveau cinétique, nous introduisons des principes de grandes déviations pour quantifier la probabilité de grandes déviations de la mesure empirique dans la limite de grand N. Dans certains cas, ces fluctuations peuvent être représentées par une équation cinétique fluctuante avec un petit terme de bruit qui décrit les effets de N fini. Nous considérons ensuite la limite hydrodynamique pour dériver des équations hydrodynamiques fluctuantes, telles que 2.8. La théorie des grandes déviations a été largement utilisée pour décrire les fluctuations dans les champs macroscopiques des systèmes de particules. Un des xemples les plus célèbres est la théorie des fluctuations macroscopiques (Macroscopic Fluctuation Theory, MFT) qui décrit les fluctuations du champ de densité au-delà de sa dynamique diffusive [32] pour un large éventail de systèmes de particules, tels que les processus d'exclusion simples. Pour ces systèmes, il n'y a pas de notion de vitesse (les particules sautent d'un nœud à un voisin à des taux fixes), il n'y a pas de théorie cinétique et le chemin pour obtenir l'hydrodynamique fluctuante est légèrement différent. Ici, nous rappelons les principaux travaux qui se sont précisément concentrés sur l'établissement de principes de grandes déviations pour les théories cinétiques qui décrivent des systèmes de particules dont la dynamique est donnée par des équations différentielles sur leurs positions et leurs vitesses, comme dans (2.1). La littérature à ce sujet comprend des travaux qui ont formellement compris les grandes déviations pour l'équation de Boltzmann [50], mathématiquement pour des modèles-jouets de type Boltzmann [184, 126, 18] ; récemment des résultats rigoureux de grandes déviations ont été établis à partir de la dynamique du gaz de sphères durs pour des temps courts [46, 45]. Des résultats de type théorème central limite pour l'équation de Boltzmann ont déjà été établis et coïncident avec ceux des grandes déviations pour décrire les petites fluctuations autour de l'équilibre [191, 192]. Pour les particules interagissant faiblement (à travers une interaction de type champ moyen), nous nous référons au travail pionnier de Dawson et Gartner [82], qui établit un résultat de grandes déviations pour la mesure empirique de N particules Browniennes couplées par une interaction de type champ moyen. Ce résultat a été réinterprété comme une équation cinétique fluctuante connue sous le nom d'équation de Dean-Kawasaki par les physiciens [86, 136].

2.7. Quelques applications des équations hydrodynamiques fluctuantes

Avant de se lancer dans les grandes lignes de cette thèse, nous discutons dans ce paragraphe de certaines des motivations qui nous poussent à étudier les fluctuations dans les limites hydrodynamiques et cinétiques. Jusqu'à présent, nous nous sommes principalement concentrés sur les motivations théoriques. Ces motivations théoriques sont détaillées dans le chapitre 3. En résumé, construire une approche statistique des trajectoires plutôt que des configurations statiques (d'équilibre) à travers les grandes déviations pour la théorie cinétique, permet une généralisation naturelle aux systèmes hors

d'équilibre. Ici, nous nous concentrons sur quelques applications possibles de l'hydrodynamique fluctuante. D'une manière générale, les fluctuations de N fini, ou les fluctuations thermiques comme on les appelle dans la littérature historique, deviennent importantes lorsque la nature moléculaire de la matière ne peut pas être ignorée. C'est le cas lorsqu'on étudie un fluide à des échelles micro ou nanométriques [43], avec des interactions de surface, et lorsque des processus biologiques [165, 178, 91] ou chimiques sont impliqués. En conséquence, le développement de schémas numériques pour simuler l'hydrodynamique fluctuante comme le système de Landau-Lifshitz-Navier-Stokes (LLNS) 2.8 a permis des avancées majeures dans ces domaines [9, 39, 96]. Notamment, des fluctuations géantes de concentration ont été prédites par l'hydrodynamique fluctuante via le système de LLNS dans [170][4], lors du mélange diffusif de l'eau et du glycérol, ce qui avait déjà été observé dans des simulations de dynamique moléculaire [95] et expérimentalement [204, 80, 203]. Un autre domaine d'application des équations de Navier-Stokes fluctuantes est l'étude de la turbulence. Comme le suggèrent les travaux fondateurs de Betchov [35, 36, 37], les fluctuations thermiques semblent modifier le spectre de la cascade d'énergie cinétique en turbulence. Ces effets ont été étudiés numériquement [117] et analytiquement [102, 13, 19] à partir de la description hydrodynamique fluctuante.

Tous ces travaux partent des équations de Navier-Stokes fluctuantes, pour lesquelles les termes de bruit ont déjà été caractérisés à partir de considérations thermodynamiques. Lorsque le terme de bruit ne peut pas être supposé à partir de la thermodynamique d'équilibre, la dérivation microscopique de l'hydrodynamique fluctuante devient cruciale. Un exemple important est celui de la matière active. Les systèmes actifs sont composés d'unités capables d'extraire de l'énergie non thermique de leur environnement et de la dissiper pour se propulser. Les bactéries ou les mammifères sont des exemples de tels unités. La modélisation d'un tel système commence généralement par une dynamique des particules qui rompt explicitement le bilan détaillé, comme dans le cas paradigmatique du modèle de Vicsek [209]. Les descriptions hydrodynamiques fluctuantes de ces systèmes sont cruciales, étant donné que dans les applications biologiques, le nombre de particules reste relativement faible. En l'absence d'argument thermodynamique, le terme de bruit dans une telle description est généralement ajouté de façon ad hoc [199, 200, 198].

2.8. Contenu du manuscrit

Ce manuscrit traite de la dérivation des équations hydrodynamiques fluctuantes à partir de la dynamique microscopique des particules. Son organisation suit naturellement les deux étapes d'une telle dérivation. La première partie du manuscrit traite de la dérivation des principes de grandes déviations dynamiques pour les théories cinétiques à partir de la dynamique des particules ; et la deuxième partie concerne la dérivation de

[4] En étudiant le mélange de deux liquides en l'absence de gravité (avec des techniques de microgravité par exemple), on sait que le spectre de l'intensité des fluctuations de concentration est proportionnel à k^{-4} avec le nombre d'ondes k [85] ce qui donne des fluctuations macroscopiques propagatives d'origine thermique à de petits nombres d'ondes.

l'hydrodynamique fluctuante à partir des principes de grandes déviations cinétiques.

Le premier chapitre de la première partie (chapitre 3) sert d'introduction générale à la théorie des grands déviations et son lien avec la théorie cinétique. Il comprend également des méthodes génériques pour obtenir des principes de grandes déviations cinétiques, ainsi que la dérivation de principes de grandes déviations pour N diffusions couplées en champ moyen, et N particules indépendantes soumises à un processus de saut (Run-And-Tumble). Ces résultats ne sont pas nouveaux, mais ils sont utilisés tout au long du manuscrit et servent d'exemples pédagogiques dans ce chapitre. Dans le chapitre 4, nous obtenons le principe de grandes déviations dynamique étendant l'équation de Balescu-Guernsey-Lenard, qui est l'équation cinétique décrivant le comportement à grand N d'un système Hamiltonien de N particules couplées par l'intermédiaire d'un potentiel à longue portée. Il s'agit du premier résultat original de cette thèse. Le chapitre suivant (5) se concentre sur la dérivation du principe de grandes déviations dynamique associé à l'équation cinétique de Landau. Il est obtenu comme une approximation du résultat de celui associé à l'équation de Balescu-Guernsey-Lenard, lorsque le potentiel d'interaction est un potentiel de Coulomb et que les échelles étudiées sont beaucoup plus petites que la longueur de Debye. Le résultat de grandes déviations pour l'équation de Landau est également lié aux résultats concernant les grandes déviations pour l'équation de Boltzmann dans la limite des collisions rasantes. Ce résultat est également original et est notamment lié à des résultats récents sur la structure de flot-gradient de l'équation de Landau [65, 66]. En plus des résultats déjà établis sur les grandes déviations pour l'équation de Boltzmann, ces deux résultats sur les grandes déviations pour les équations de Balescu-Guernsey-Lenard et de Landau complètent le triptyque des grandes déviations pour les théories cinétiques classiques.

La deuxième partie de la thèse commence par le chapitre 6 qui introduit les outils utilisés dans les chapitres suivants pour passer des principes de grandes déviations cinétiques à l'hydrodynamique fluctuante. Pour ce faire, on étudie la dérivation de l'équation de diffusion fluctuante pour N particules indépendantes diffusant via un processus de saut (Run-And-Tumble). La dérivation de cette équation n'est pas nouvelle, mais elle sert un objectif pédagogique et permet d'introduire les outils conceptuels clés utilisés dans la deuxième partie : le développement de Chapman-Enskog, le principe de contraction du principe de grandes déviations cinétique vers le principe de grandes déviations hydrodynamique, et la "Gaussianisationé du principe de grande déviation dans la limite hydrodynamique. Nous appliquons ce programme dans le chapitre 7 à la dérivation microscopique des équations de Navier-Stokes compressibles et incompressibles fluctuantes, avec le principe de grandes déviations pour l'équation de Boltzmann comme point de départ. Un résultat secondaire notable de ce chapitre est l'obtention de structures de flot-gradient, comme conséquence des principes de grandes déviations, pour les équations de Navier-Stokes incompressibles (respectivement compressibles), illustrant la géométrie de la dissipation de l'énergie cinétique (respectivement de la néguentropie) dans ces équations. Dans le chapitre 8, nous dérivons un principe de grandes déviations cinétique et l'hydrodynamique fluctuante qui en découle pour un gaz de particules actives (similaire au modèle de Vicsek) dans la limite diluée. Un point technique intéressant de ce chapitre est la dérivation des équations hydrodynamiques pour un système de particules

manquant de lois de conservation, en utilisant la notion d'invariant de collision généralisé introduite par Degond [87]. Dans le chapitre 9, nous évaluons la robustesse de la dérivation de l'hydrodynamique fluctuante à partir des principes des grandes déviations cinétiques dans le cas spécifique où la limite hydrodynamique est une loi de conservation hyperbolique. De telles EDP sont connues pour présenter des solutions non uniques avec des gradients abrupts, et nous expliquons, avec l'exemple d'un modèle-jouet en une dimension, que les développement asymptotiques que nous avons utilisées pour obtenir l'hydrodynamique fluctuante à partir de la dynamique des particules pourraient être erronées pour quantifier la probabilité de certains profils hydrodynamiques non lisses. En particulier, nous expliquons qu'il n'y a aucune raison pour que la fonctionnelle de Jensen-Varadhan (dérivée dans [133, 205] pour le processus d'exclusion totalement asymétrique, ASEP) qui quantifie la probabilité de chocs non-entropiques soit valable en général.

Part I.

Dynamical large deviations for kinetic theories

3. Introduction to the dynamical large deviations for kinetic theories

In this chapter, we introduce some concepts of large deviation theory. We also explain how they can be useful to comprehend kinetic theory. We illustrate the link between dynamical large deviation theories in two toy models. Some of the sections are adapted from [106, 105]. All the examples and properties discussed in this chapter are used throughout the manuscript.

3.1. Beyond equilibrium statistics and relaxation to equilibrium: dynamical fluctuations

In the field of statistical physics, the literature that describes the static fluctuations of a system around equilibrium and its relaxation to equilibrium is very rich. For instance, working in the appropriate thermodynamic ensemble, we can express the probability of observing a given state of a system as a function of the corresponding thermodynamic potential. Beyond equilibrium, classical kinetic theories describe the relaxation to equilibrium in some asymptotic regimes. For instance the Boltzmann equation describes the relaxation to equilibrium of a dilute gas in the Boltzmann-Grad limit, and the Balescu-Guernsey-Lenard equation in the opposite limit of particles with long range interactions, for instance plasma in the weak coupling limit or self-gravitating systems. The Landau equation is either an approximation of the Balescu-Guernsey-Lenard equation that describes the relaxation of plasma at a scale much smaller than the Debye length, or an approximation of the Boltzmann equation in the grazing collision limit. All those classical kinetic equations describe the relaxation of the empirical measure

$$f_N(\mathbf{r}, \mathbf{v}, t) \equiv \frac{1}{N} \sum_{n=1}^{N} \delta(\mathbf{v} - \mathbf{v}_n(t)) \delta\left(\mathbf{r} - \mathbf{r}_n(t)\right),$$

where δ are Dirac delta functions, t is time, $(\mathbf{r}_n(t), \mathbf{v}_n(t))_{1 \leq n \leq N}$ are the N particle positions and velocities. The six-dimensional space of one-particle position-velocity, with points $(\mathbf{r}, \mathbf{v})$, is called the μ-space. f_N is a distribution over the μ-space that evolves with time.

The probability $\mathbb{P}_{\text{eq}}\left(f_N = f^0\right)$ to observe f_N close to a given distribution f_0 of the μ-space, at some fixed arbitrary time, in the microcanonical ensemble, satisfies

$$\mathbb{P}_{\text{eq}}\left(f_N = f^0\right) \propto \mathrm{e}^{N\frac{\mathcal{S}[f^0]}{k_B}}. \tag{3.1}$$

This is the classical Einstein formula relating the specific entropy $\mathcal{S}[f^0]$ of the macrostate f^0 with its equilibrium probability. k_B is the Boltzmann constant. This can be seen as a definition of the Boltzmann entropy $\mathcal{S}[f^0]$ of the macrostate f^0. For a dilute gas, because the particles are independent at leading order, for systems with long range interactions, because the two-body interactions are weak, it is known that $\mathcal{S}$ is the negative of the Boltzmann $\mathcal{H}$ function ($\mathcal{S}[f^0] = -k_B \int \mathbf{drdv}\, f^0 \log f^0$) if the macrostate f^0satisfies the conservation laws (mass, momentum and energy), and $\mathcal{S}\left[f^0\right] = -\infty$ otherwise.

However all those classical works and results in equilibrium statistical mechanics and kinetic theory do not describe the probability of paths that may lead to any macrostate f^0. More generally, the macroscopic or mesoscopic stochastic process for f_N is not described by classical theories, and dynamical description is restricted to relaxation to equilibrium. In principle, very rarely, the microscopic dynamics can lead the distribution function to follow other paths than the relaxation paths described by the kinetic equation. What is the probability of such rare excursions? How do these probabilities depend on the paths? Those are key questions. Answering them is the starting point for solving many other non-equilibrium problems, as explained in section 3.5. Moreover, if the microscopic dynamics is time-reversible (in the sense of dynamical systems), for instance if the microscopic dynamics is Hamiltonian, then we expect the stochastic process for f_N to be also time-reversible (in the sense of stochastic processes). It is a fundamental question to describe this stochastic process for the empirical measure f_N.

More precisely we need to estimate the probability $\mathbb{P}\left(\{f_N(t)\}_{0\leq t\leq T} = \{f(t)\}_{0\leq t\leq T}\right)$ to observe the evolution of $\{f_N(t)\}$ to be in a neighborhood of any prescribed path $\{f(t)\}$, for times $0 \leq t \leq T$, in some asymptotic limit when the kinetic description is valid, with the prescription that $f_N(t=0)$ is in the neighborhood of $f(t=0)$. The mathematical and theoretical formalism adapted to this problem is large deviation theory.

3.2. Short introduction to large deviation theory

Large deviation theory is the branch of probability theory that formalizes the study of extreme events in random systems in some asymptotic regime. In section 3.2.1, we introduce the large deviation principle for the sum of N i.i.d. random variables, also recalling results about the law of large numbers and the central limit theorem: the two other asymptotic frameworks of probability theory. In section 3.2.2, we introduce the Freidlin-Wentzell theory that allows to establish large deviation results for dynamical systems subjected to small random perturbations, and to bridge from SDEs with Gaussian noise to large deviation principles. In section 3.2.3, we discuss the contraction principle in large deviation theory. For a mathematical introduction to large deviation theory

and a rigorous definition of the large deviation principle, we refer to [206, 89]. For the discussion of some physical applications, we refer to [17, 201, 202].

3.2.1. Sum of N independent random variables

We start by discussing the paradigmatic example of the sum of N independent random variables and its associated limiting theorems. We consider N i.i.d. random variables $\{X_i\}_{1\leq i\leq N}$ taking values in $\mathbb{R}$. We define the cumulant generating function for $k \in \mathbb{R}$ as following

$$\lambda(k) = \log \mathbb{E}\left(\exp\left(kX_1\right)\right).$$

We define the empirical average $S_N = \frac{1}{N}\sum_{i=1}^{N} X_i$ of these random variables. The first limiting theorem about the large N asymptotics of S_N is the Law of Large Numbers (LLN). The only required assumption is that the X_i have a finite average: $\mathbb{E}(X_1) = \mu$ and it states that the empirical average converges almost surely toward the average of the X_i:

$$\lim_{N\to+\infty} S_N = \mu.$$

To study small fluctuations of the empirical average around its expected value, the correct tool is the Central Limit Theorem (CLT). If in addition to having a finite average, the random variables have a finite variance σ^2, then their empirical average converges in distribution as N goes to infinity toward a normal distribution with the following scaling

$$\sqrt{N}\left(S_N - \mu\right) \sim \mathcal{N}\left(0, \sigma^2\right).$$

Finally, if all the cumulants of the random variables are finite, or equivalently there is an interval J such that $0 \in \mathring{J}$ and for all k in J, $\lambda(k)$ is finite, we can assess the probability of rare realization of the empirical average. The result is a Large Deviation Principle (LDP), i.e. a logarithmic equivalence describing the large N asymptotics of $\mathbb{P}(S_N = s)$ when $s \neq \mu$ and is known as the Cramér theorem [79]. It reads

$$\mathbb{P}(S_N = s) \underset{N\to+\infty}{\asymp} \mathrm{e}^{-NI(s)},$$

where the symbol $\underset{N\to+\infty}{\asymp}$ roughly means a logarithmic equivalence ($a_N \underset{N\uparrow\infty}{\asymp} \exp(Na) \iff \lim_{N\uparrow\infty} N^{-1}\log a_N = a$), $1/N$ is called the large deviation rate and I is the large deviation function. I is given by Legendre-Fenchel transform of the cumulant generating function:

$$I(s) = \sup_{k\in J}\left\{ks - \lambda(k)\right\}.$$

Typically, the large deviation rate function is convex as the Legendre-Fenchel transform of a convex function.

There is a heuristic way to understand how the assumption on the cumulant generating function enables to compute the probability of any realization for the empirical average. This is because when all the cumulants are finite, the possible amplitudes of every realization of X_i are highly constrained as their probability density function cannot have large tails. As a result, the most probable way to achieve a large deviation of the empirical average is by having realizations of X_i that contribute equally to this deviation. Conversely, it is highly unlikely to achieve a large deviation of the empirical average driven by a very large deviation of only one or a few realizations of X_i due to the constraints on the cumulants. In other words, of all the ways to obtain an unlikely event, the least improbable way is overwhelmingly more likely than the others.

3.2.2. Freidlin-Wentzell theory and the SDE-LDP (in)equivalence

Freidlin-Wentzell theory deals with establishing LDPs for the evolution paths of dynamical systems subjected to small random perturbations [115]. In this section, we give an informal account of the Freidlin-Wentzell theorem, allowing to estimate the probability that the trajectory of a Ito diffusion deviates from its mean path. Let us consider a positive number ϵ and a family of stochastic processes$\{X_{\epsilon,t}\}_{0\leq t\leq T}$ taking values in $\mathbb{R}^n$ evolving according to the following Ito SDE

$$\mathrm{d}X_{\epsilon,t} = b\left(X_{\epsilon,t}\right)\mathrm{d}t + \sqrt{2\epsilon}\sigma\left(X_{\epsilon,t}\right)\mathrm{d}W_t, \tag{3.2}$$

where $\sigma : \mathbb{R}^n \to \mathbb{R}^{n\times m}$, $b : \mathbb{R}^n \to \mathbb{R}^n$ and W_t is a m-dimensional Wiener process with uncorrelated components. The LLN guarantees that when ϵ goes to zero, if at initial time we have

$$\lim_{\epsilon\to 0} X_{\epsilon,0} = x_0,$$

then for all $t \in [0,T]$, we have

$$\lim_{\epsilon\to 0} X_{\epsilon,t} = \bar{x}\left(t\right),$$

where

$$\frac{\mathrm{d}\bar{x}}{\mathrm{d}t} = b(\bar{x}), \quad \text{and} \quad \bar{x}\left(t=0\right) = x_0. \tag{3.3}$$

In other words, as ϵ goes to zero, the evolution paths of $X_{\epsilon,t}$ concentrate close to its mean path, whose trajectory is given by the zero-noise equation (3.3). The terminology "law of large numbers" may seem inappropriate since we are investigating a small noise limit rather than a large N limit. It can be understood when discretizing the evolution equation (3.2). In this case, the evolution of $X_{\epsilon,t}$ is the result of the sum of a large number of small amplitude, random and independent moves, whose average effect is zero. In this case, the “large numbers” terminology refers to the large number of random increments driving the evolution of the stochastic process.

To assess the probability of any other evolution path, one has to turn to large deviation theory. The Freidlin-Wentzell theorem establishes the following large deviation estimate for the probability of any evolution path of (3.2):

$$\mathbb{P}\left(\{X_{\epsilon,t\epsilon}(t)\}_{0\leq t\leq T}=\{x(t)\}_{0\leq t\leq T}\right)\underset{\epsilon\to 0}{\asymp}\mathrm{e}^{-\frac{1}{\epsilon}I_T[x]}, \tag{3.4}$$

where

$$I_T\left[x\right]=\int_0^T \mathrm{d}t\,\frac{1}{4}\left(\dot{x}-b(x)\right)^\top a^{-1}\left(x\right)\left(\dot{x}-b(x)\right), \tag{3.5}$$

where the dot denotes a time derivative, and $a\left(x\right)=\sigma\left(x\right)\sigma\left(x\right)^\top$. This result is extensively used throughout the manuscript, and we assume it is still valid when the stochastic dynamics takes value on functional spaces. In particular, the LDP (3.4) implies the LLN. As ϵ goes to zero, the probability of all the evolution paths becomes exponentially small except for the one that satisfies $I_T\left[\bar{x}\right]=0$. This path, called the relaxation path, is nothing else than the solution of (3.3).

It is customary to formulate the large deviation rate function with a Hamiltonian formalism. Introducing the Hamiltonian

$$H\left(x,p\right)=\sup_{\dot{x}}\left\{\dot{x}\cdot p-\frac{1}{4}\left(\dot{x}-b(x)\right)^\top a^{-1}\left(x\right)\left(\dot{x}-b(x)\right)\right\}=p^\top a\left(x\right)p+b\left(x\right)\cdot p,$$

which is still a convex function, one can rewrite the rate function without the need to inverse a (which can be a non invertible operator in higher dimension)

$$I_T\left[x\right]=\int_0^T \mathrm{d}t\,\sup_p\left\{\dot{x}\cdot p-H\left(x,p\right)\right\}.$$

We say that the LDP is Gaussian when the Hamiltonian is quadratic in its conjugate momentum p. A general result is that every SDE with a Gaussian noise is associated with a Gaussian LDP. An important remark is that this is not a one-to-one correspondence.

A counterexample can be obtained by adding a deterministic term of order $\sqrt{\epsilon}$ to (3.2)

$$\mathrm{d}X_{\epsilon,t}=\left[b\left(X_{\epsilon,t}\right)+\sqrt{\epsilon}c\left(X_{\epsilon,t}\right)\right]\mathrm{d}t+\sqrt{2\epsilon}\sigma\left(X_{\epsilon,t}\right)\mathrm{d}W_t. \tag{3.6}$$

One can show that (3.6) satisfies the LDP (3.4) with the rate function (3.5)[1], even if typical evolution paths of (3.6) differ from the one of (3.2). This remark highlights two key points when hopping from SDEs with Gaussian noises to Gaussian LDPs:

1. There is no one-to-one relationship between SDEs with Gaussian noise, and Gaussian LDPs. In particular, two different SDEs can satisfy the same LDP.

[1]Tools to prove such a result are introduced in section 3.6 of this chapter.

2. The LDP does not include all the information about the central limit theorem. For instance, from the LDP, we cannot quantify small fluctuations around the mean evolution path as finely as with the CLT. We would typically miss deterministic terms of order $\sqrt{\epsilon}$. However, if we look at a rare realization of (3.6) that deviates largely from the mean path (3.3), the SDE without deterministic terms of order $\sqrt{\epsilon}$ is still relevant. Indeed, in those cases, the deviations created by the noise are of order 1 with respect to ϵ and the deterministic term of order $\sqrt{\epsilon}$ becomes negligible.

Throughout the manuscript, we switch casually from Gaussian LDP to S(P)DEs with Gaussian noise. However, each S(P)DE will have to be understood from the large deviation perspective, in the sense that it is a way to represent the Gaussian LDP. It is also important to stress that the associated S(P)DE, even if not equivalent to a CLT, is still relevant to investigate rare realizations of the noise yielding large deviations from the mean path.

3.2.3. The contraction principle

Let us assume we know the rate function $I(x)$ describing the large deviations of a certain random variable X_ϵ in the small ϵ regime

$$\mathbb{P}\left(X_\epsilon = x\right) \underset{\epsilon\to 0}{\asymp} \mathrm{e}^{-\frac{1}{\epsilon}I(x)}. \tag{3.7}$$

If $Y_\epsilon = f\left(X_\epsilon\right)$ is another random variable that can be expressed as a smooth function of X_ϵ, it also satisfies a LDP, with speed ϵ and rate function

$$J\left(y\right) = \inf_x \left\{I\left(x\right), \;\; y = f(x)\right\}.$$

This result is called a contraction principle [89]. It is also another instance of the principle stating that "an unlikely event is overwhelmingly likely to be realized in the least unlikely way". The contraction principle is fundamental as it allows to turn several large deviation problems into optimization ones. We use it extensively in the manuscript to obtain large deviations for hydrodynamic fields starting from kinetic LDPs.

3.3. Large deviation for kinetic theories: a natural framework for the statistical mechanics of trajectories

A kinetic theory describes the LLN for the μ-space empirical measure of a particle system. Generally, we will work with a rescaled empirical measure

$$f_\epsilon(\mathbf{r},\mathbf{v},t) = \epsilon \sum_{n=1}^{N} \delta(\mathbf{v}-\mathbf{v}_n(t))\delta\left(\mathbf{r}-\mathbf{r}_n(t)\right),$$

where ϵ is a small parameter associated to the kinetic limit. ϵ could be $1/N$, but it depends on the physical system under consideration.

Assuming that the empirical measure concentrates close to a given distribution at an initial time:

$$\lim_{\epsilon \to 0} f_\epsilon(t=0) = f_0, \tag{3.8}$$

the kinetic theory would be the following LLN

$$\lim_{\epsilon \to 0} \{f_\epsilon(\mathbf{r}, \mathbf{v}, t)\}_{0 \leq t \leq T} = \{f(\mathbf{r}, \mathbf{v}, t)\}_{0 \leq t \leq T},$$

where f is a distribution on the μ-space, the phase space of a single particle, that solves a certain PDE

$$\partial_t f = \text{Kin}[f] \quad \text{with} \quad f(t=0) = f_0,$$

called the kinetic equation, and where Kin is a (integro-)differential operator depending on the particle dynamics of the system. To quantify large deviations of the empirical measure rather than its average behavior, we need to estimate the asymptotics of the logarithm of its own probability distribution

$$\log \mathbb{P}\left(\{f_\epsilon(t)\}_{0 \leq t \leq T} = \{f(t)\}_{0 \leq t \leq T}\right).$$

In other words, we need to prove the following LDP

$$\mathbb{P}\left(\{f_\epsilon(t)\}_{0 \leq t \leq T} = \{f(t)\}_{0 \leq t \leq T}\right) \underset{\epsilon \to 0}{\asymp} \mathrm{e}^{-\frac{1}{\epsilon} \int_0^T \mathrm{d}t \, \mathrm{Sup}_p \left\{ \int \dot{f} p \, \mathrm{d}\mathbf{r}\mathrm{d}\mathbf{v} - H[f,p] \right\}}, \tag{3.9}$$

where $\dot{f}$ is the time derivative of f, p is a function over the μ-space and is called the conjugated momentum of $\dot{f}$, the Hamiltonian H is a functional of f and p that characterizes the dynamical fluctuations. We note that H is not the Hamiltonian of the microscopic dynamics but H rather defines a statistical field theory that quantifies the probabilities of paths of the empirical measure. H is associated with a Lagrangian $L\left[f, \dot{f}\right] = \mathrm{Sup}_p \left\{ \int \dot{f} p \, \mathrm{d}\mathbf{r}\mathrm{d}\mathbf{v} - H[f,p] \right\}$ and an action $\int_0^T \mathrm{d}t \, L\left(f, \dot{f}\right)$. An important question at this stage is how to define the expectation and the probability in those equations when the microscopic dynamics is chaotic but deterministic. For such systems, the randomness comes from the initial conditions. We then define the probability with respect to an ensemble of initial conditions for the positions and velocities $(\mathbf{r}_n(0), \mathbf{v}_n(0))$ distributed according to a measure $f_N^0(\mathbf{r}_1, \mathbf{v}_1, \cdots, \mathbf{r}_n, \mathbf{v}_n) \prod_{n=1}^N \mathrm{d}\mathbf{r}_n \mathrm{d}\mathbf{v}_n$. The requirement (3.8) can then be satisfied by taking the tensor product measure $f_N^0 = f_0^{\otimes N}$, but this not necessarily the case.

3.4. Expected properties of a dynamical large deviation principle for a kinetic theory

In this section, we describe the expected properties of any such large deviation principle for the kinetic theory of the empirical measure. A more detailed account of a similar discussion can be found in [50].

Most probable evolution. We consider the properties of a stochastic process whose rare fluctuations are described, at the level of large deviations, by the action

$$\mathcal{A}[f] = \int_0^T \mathrm{d}t\, L\left[f, \dot{f}\right] = \int_0^T \mathrm{d}t\, \sup_p \left[\int p\dot{f} - H[f,p]\right]. \tag{3.10}$$

The kinetic equation is expected to be the most probable evolution corresponding to the action (3.10), and with initial condition $f_r(t=0) = f_0$. It is also called a ***relaxation path issued from*** f_0. It solves $\frac{\partial f_r}{\partial t} = R[f_r]$, with initial condition $f_r(t=0) = f_0$, where $R[f] = \arg\inf_{\dot{f}} L\left[f, \dot{f}\right]$. Then one easily proves that

$$\dot{f} = \frac{\delta H}{\delta p}[f, p=0], \tag{3.11}$$

is the kinetic equation.

Quasipotential and macrostate entropy. We assume that the stochastic process f_ϵ has a stationary distribution $\mathbb{P}_s$ following the LDP

$$\mathbb{P}_s(f) \equiv \mathbb{E}\left[\delta\left(f_\epsilon - f\right)\right] \underset{\epsilon\downarrow 0}{\asymp} \exp\left(-\frac{U[f]}{\epsilon}\right), \tag{3.12}$$

where U is called the ***quasipotential***. In order to simplify the following discussion, we also assume that the relaxation equation has a single fixed point f_0 and that any solution to the relaxation equation converges to f_0 . Then the quasipotential satisfies

$$U[f] = \inf_{\left\{\{g(t)\}_{-\infty\le t\le 0} \middle| g(-\infty)=f_0 \text{ and } g(0)=f\right\}} \int_{-\infty}^0 \mathrm{d}t\, L[g, \dot{g}]. \tag{3.13}$$

The minimizer of this variational problem, that is the most probable path starting from f_0 and ending at f, is denoted $f_i(t,f)$ and is called the ***fluctuation path ending at*** f**.**

For many kinetic theories, we expect from equilibrium statistical mechanics that the quasipotential $U[f]$ is the opposite of the entropy $S[f] = -k_B \int \mathbf{dvdr}\, f \log f$ constrained by the conserved quantities (for instance mass, momentum and energy here)

$$U[f] = \begin{cases} -S[f]/k_B + S_m(E)/k_B & \text{if } \int \mathbf{drdv}\, f = 1, \quad \int \mathbf{drdv}\, \mathbf{v} f = 0, \text{ and } \int \mathbf{drdv}\, \frac{\mathbf{v}^2}{2} f = E \\ -\infty \text{ otherwise.} \end{cases},$$

where

$$S_m(E) = \sup_f \left\{ S[f] \middle| \int \mathbf{drdv}\, f = 1, \quad \int \mathbf{drdv}\, \mathbf{v} f = 0, \text{ and } \int \mathbf{drdv}\, \frac{\mathbf{v}^2}{2} f = E \right\}$$

is the equilibrium entropy.

We have the following properties which are direct consequences of the definitions of H and L, and whose proofs are classical and given for example in sections 7.2 to 7.4 of [50]:

1. H is a convex function of the variable p and $H\left[f, p=0\right]=0$.

2. The quasipotential solves the stationary **Hamilton–Jacobi equation**

$$H\left[f, \frac{\delta U}{\delta f}\right]=0. \tag{3.14}$$

3. **The fluctuation paths** solve

$$\dot{f}=F\left[f\right]\equiv\frac{\delta H}{\delta p}\left[f, \frac{\delta U}{\delta f}\right].$$

4. As H is convex, the quasipotential decreases along the relaxation paths

$$\frac{\mathrm{d}U}{\mathrm{d}t}\left[f_r\right]=H[f_r,0]-H\left[f_r, \frac{\delta U}{\delta f}\left[f_r\right]\right]+\int \mathbf{drdv}\,\frac{\delta H}{\delta p}\left[f_r,0\right]\frac{\delta U}{\delta f}\left[f_r\right]\leq 0. \tag{3.15}$$

   For kinetic theories, because the quasipotential is the negative of the entropy whenever the conservation laws are verified, we can immediately conclude that the entropy will increase along the solution of the kinetic equation.

5. As H is convex, the quasipotential increases along the fluctuation paths

$$\frac{\mathrm{d}U}{\mathrm{d}t}\left[f_i\right]=H[f_i,0]-H\left[f_i, \frac{\delta U}{\delta f}\left[f_i\right]\right]+\int \mathbf{drdv}\,\frac{\delta H}{\delta p}\left[f_i, \frac{\delta U}{\delta f}\left[f_i\right]\right]\frac{\delta U}{\delta f}\left[f_i\right]\geq 0 \tag{3.16}$$

   For kinetic theories, because the quasipotential is the negative of the entropy whenever the conservation laws are verified, we can immediately conclude that the entropy will decrease along the fluctuation paths.

6. ***Generalized detailed balance***. Let I be an involution that characterizes time-reversal symmetry (for instance the map that corresponds to velocity or momentum inversion in many systems). We assume that I is self adjoint for the L^2 scalar product, that is $\int \mathbf{drdv}\, I\left[f\right]p=\int \mathbf{drdv}\, f I\left[p\right]$. For any systems for which the microscopic dynamics is time reversible, we can infer that the stochastic process of the empirical measure has to be time-reversal symmetric, that reads

$$\mathbb{P}_T\left(f_\epsilon(T)=f_2\,|f_\epsilon(0)=f_1\right)\mathbb{P}_s\left(f_\epsilon=f_1\right)=\mathbb{P}_T\left(f_\epsilon(T)=I\left[f_2\right]|f_\epsilon(0)=I\left[f_2\right]\right)\mathbb{P}_s\left(f_\epsilon=I\left[f_2\right]\right), \tag{3.17}$$

   where $\mathbb{P}_s$ is the stationary distribution given by (3.12), and $\mathbb{P}_T$ is the transition probability obtained by minimizing the large deviation action constraining on the initial and final point

$$\mathbb{P}_T\left(f_\epsilon(T)=f_2\,|f_\epsilon(0)=f_1\right)\underset{\epsilon\downarrow 0}{\asymp}\exp\left(-\frac{1}{\epsilon}\inf_{f(0)=f_1,f(T)=f_2}\int_0^T \mathrm{d}t\,\sup_p\left[\int p\dot{f}-H\left[f,p\right]\right]\right).$$

(3.18)

The generalized detailed balance condition (3.17), and the one for the quasipotential U: $U[f] = U[I[f]]$, yields at the level of the large deviation Hamiltonian the following symmetry

$$H[I[f], -I[p]] = H\left[f, p + \frac{\delta U}{\delta f}\right]. \tag{3.19}$$

7. If the generalized detailed balance conditions is verified, then U satisfies the stationary Hamilton-Jacobi equation (3.14). Indeed, with $p = 0$, (3.19) reads $H\left[f, \frac{\delta U}{\delta f}\right] = H[I[f], 0]$. Then, using the definition of the Hamiltonian and the fact that $\inf_{\dot{f}} L\left[f, \dot{f}\right] = 0$, we obtain the stationary Hamilton-Jacobi equation

$$H\left[f, \frac{\delta U}{\delta f}\right] = H[I[f], 0] = \sup_{\dot{f}} \left\{-L\left[I[f], \dot{f}\right]\right\} = 0.$$

8. If the generalized detailed balance condition is verified, and if U is the quasipotential, then for a path $\{f(t)\}_{0\le t\le T}$ and its time reversed one $\{I[f(T-t)]\}_{0\le t\le T}$ we have the symmetry for the path probability

$$\mathbb{P}\left[\{f_\epsilon(t)\}_{0\le t\le T} = \{f(t)\}_{0\le t\le T}\right] \mathrm{e}^{-\frac{U[f(t=0)])}{\epsilon}} = \mathbb{P}\left[\{f_\epsilon(t)\}_{0\le t\le T} = \{I[f(T-t)]\}_{0\le t\le T}\right] \mathrm{e}^{-\frac{U[I[f(t=T)]]}{\epsilon}}. \tag{3.20}$$

9. ***Conserved quantities.*** At the level of the large deviations, the condition for $C[f]$ to be a conserved quantity is either

$$\text{for any } f \text{ and } \dot{f},\ \ L\left[f, \dot{f}\right] = +\infty \text{ if } \int \mathbf{dr}\mathbf{dv}\, \frac{\partial f}{\partial t}\frac{\delta C}{\delta f} \neq 0,$$

or

$$\text{for any } f \text{ and } p,\ \ \int \mathbf{dr}\mathbf{dv}\, \frac{\delta H}{\delta p}[f, p]\frac{\delta C}{\delta f} = 0. \tag{3.21}$$

Kinetic theories can conserve mass, momentum and energy but not necessarily. Sometimes there is an infinite number of conserved quantities (for instance the Vlasov equation), for instance, when dealing with integrable systems. Understanding macroscopic fluctuations arising in coarse-grained descriptions of such systems is a hot topic [84, 151].

10. ***A sufficient condition for U to be the quasipotential.*** If U solves the Hamilton–Jacobi equation, if U has a single minimum f_0 with $U[f_0] = 0$, and if for any f the solution of the reverse fluctuation path dynamics $\frac{\partial g}{\partial t} = -F[g] = -\frac{\delta H}{\delta p}\left[g, \frac{\delta U}{\delta g}\right]$ with $g(0) = f$ converges to f_0 for large times, then U is the quasipotential.

3.5. Some motivations to study large deviations for kinetic theories

In this section, we discuss the interest of uncovering such statistical field theories to describe extended physical systems, by exhibiting some results we can extract from the existence and the computation of the LDP (3.9).

Irreversibility paradox. Let us consider an equilibrium situation where the equations of motion at the microscopic scale are time-reversible. The kinetic theory breaks this time-symmetry, because it describes the relaxation to equilibrium of the system in a time-arrowed way. This is what is known as the irreversibility paradox. How an irreversible macroscopic evolution can emerge from a time-reversible microscopic dynamics? The large deviation structure gives a clear answer to this question, and erases this seemingly paradox.

First, the LDP contains the information about the kinetic theory. As explained in 2. of section 3.4, the most probable evolution path $\{f_c\}_{0\leq t\leq T}$ for the empirical measure is given by the so-called relaxation path and satisfies

$$\frac{\partial f_c}{\partial t} = \frac{\delta H}{\delta p}\left[f_c, p=0\right].$$

This equation is the kinetic theory and describes the relaxation to equilibrium of the system. The LDP (3.9) also describes the probability of any evolution path for the empirical measure other than the solution of the kinetic theory. At the large deviation level any evolution path is possible for the empirical measure, but as ϵ goes to zero, only the most probable one will be observable with an overwhelming probability. This most probable evolution path breaks the time-reversibility symmetry. However, the large deviation Hamiltonian still keeps track of the time-reversibility of the microscopic dynamics by exhibiting symmetry properties (see 7. in section 3.4).

Quasipotential and out-of-equilibrium generalization of thermodynamic potential. It is also possible to extract from a LDP the information about the stationary state of the system, whether it is an equilibrium state or a non-equilibrium steady state. Assuming the LDP (3.9) holds, if we know that our system reaches a stationary state, described by f_s, its stationary probability density function in μ-space, we can compute a large deviation estimate of the stationary probability $P_{s,\epsilon}$ to observe any other state f. In this case, the large deviation rate function is nothing else than the quasipotential U_{f_s}

$$P_{s,\epsilon}\left[f\right] \underset{\epsilon\downarrow 0}{\asymp} \exp\left(-\frac{U_{f_s}\left[f\right]}{\epsilon}\right).$$

In an equilibrium context, the quasipotential U coincides with the thermodynamical potential. However, the quasipotential does not require thermodynamic equilibrium to be defined. When we study a system that does not relax to equilibrium, but for an instance to a non-equilibrium steady state, the quasipotential generalizes the notion of thermodynamical potential.

Bistability and Eyring–Kramers formula. One of the main motivation to compute large deviations for kinetic theory, is the study of systems exhibiting multistability, especially in a out of equilibrium context.

Let us take the example of the study of transitions between two attractors in a bistable system submitted. In classical statistical mechanics, there is a well known relation, called the Eyring–Kramers formula, that links the transition rate between two stable attractors for a bistable system, to the height of the potential barrier between these two attractors [8, 142, 104]. It is not possible to make use of such a formula in an out-of-equilibrium context where there is no obvious way to define this potential. However, the large deviation structure and the quasipotential allow to generalize the Eyring–Kramers formula.

Let us assume that the probability density f in μ-space of the system exhibits two attractors, meaning that the kinetic theory has two stationary solutions. For instance, such bistability is possible in system with long-range interactions [167]. Finite-number of particles induced fluctuations can trigger transitions between two stable states f_A and f_B that are not described by the kinetic theory. Other detailed accounts of non-equilibrium situations exhibiting metastability can be found in [26, 25, 8, 123].

If out-of-equilibrium, the classical Eyring–Kramers formula cannot give information about the transition rate of the system between this two attractors either. This is where the large deviation structure is useful. It is possible to establish a similar formula from the Freidlin-Wentzell theory [115] by defining the height of the potential barrier with respect to the large deviation quasipotential. Assuming the existence of a quasipotential from a LDP (3.13), the mean transition time $\tau_{A\to B}$ from attractor f_A to attractor f_B follows a LDP

$$\mathbb{E}\left(\tau_{A\to B}\right) \underset{\epsilon\downarrow 0}{\asymp} \exp\left(\frac{U_{f_A}\left[f_*\right]}{\epsilon}\right), \tag{3.22}$$

where f_* is the saddle-point between the two attractors. This formula is very useful when studying bistability and possible transition between stable attractors. A recent work [54] managed to extend this LDP by computing the preexponential factor in (3.22), in relation with the geometry of the quasipotential, and the most probable path taken by the system during the transition. Such a path is called an instanton and can be obtained by solving a variational problem on the large deviation action:

$$\underset{f \text{ s.t. } f(0)=f_A \text{ and } f(T)=f_B}{\operatorname{arginf}} \int_0^T \mathrm{d}t \sup_p \left\{ \int \dot{f} p \, \mathbf{dr}\mathbf{dv} - H[f,p] \right\}.$$

Within the large deviations framework, the notion of quasipotential allows to generalize a lot of other results from classical equilibrium statistical mechanics to out of equilibrium situations, such as the Gallavotti-Cohen fluctuation theorem [148], in relation with formula (3.20) from section 3.4. The computation of LDPs to extend kinetic theories is a truly fundamental question. It provides a natural generalization of classical statistical mechanics concepts to non-equilibrium situations. It does so by studying trajectory statistics instead of stationary configuration statistics. Therefore, we should

emphasize that this manuscript focuses specifically on dynamical large deviations principles, i.e. we try to compute the probability of evolution paths of the empirical measure rather than its stationary statistics.

Gradient-flow structure. It is customary and classical to observe that many dynamical models related to kinetic theories and mesoscopic systems in interaction with thermal baths have a gradient-transverse structure

$$\frac{\partial f}{\partial t} = -\mathrm{Grad}_f \mathfrak{H}\left[f\right] - \mathcal{T}\left[f\right], \tag{3.23}$$

where $\mathfrak{H}$ might be the free energy or the negative of the entropy, where for any f $(\mathrm{Grad}_f \mathfrak{H}, \mathcal{G}) = 0$. Grad_f is the gradient with respect to a f-dependent norm $(p, C\left[f\right] p)$, where C is a quadratic form: $\mathrm{Grad}_f \mathfrak{H}\left[f\right] = C\left[f\right] \frac{\delta \mathfrak{H}}{\delta f}$. $\mathcal{T}$ is often associated to the microscopic reversible dynamics or the free transport.

For example, for the Fourier law $\partial_t \rho = D\Delta_{\mathbf{r}} \rho$, has this structure [171, 210], where $\mathfrak{H} = \int \mathrm{d}\mathbf{r}\, \rho \log \rho$ is the negative of the relative entropy, the metric used to compute the gradient is the Wasserstein distance with $C\left[f\right](\mathbf{r}, \mathbf{r}') = D\Delta_{\mathbf{r}} \left(\rho(\mathbf{r}) \delta\left(\mathbf{r} - \mathbf{r}'\right)\right)$, and $\mathcal{T} = 0$. Another classical example is the McKean-Vlasov equation [171, 210].

Even if this gradient-transverse structure is customarily observed, it is not always easy to determine the quadratic form C. Moreover a general explanation of the source of this structure is of interest. In [160], a close relation between the large deviations of the empirical measure of particle system with detailed balance, and the gradient-transverse flow structure of the partial differential equations that describe kinetic theories is established. Whenever the detailed balance condition (3.19) is satisfied at the large deviations level, and whenever the large deviation Hamiltonian is quadratic in p, $\mathfrak{H}$ is the quasipotential, and the metric used to compute the gradient in (3.23) is given by the quadratic part of the large deviation Hamiltonian.

The gradient-flow structure of a PDE (3.23) can then be used as an analytical tool to study existence and behavior of the PDE's solutions [5, 134, 171], or as a practical tool to implement numerical schemes for its simulation [131].

This list of motivations and applications is far from being exhaustive, but it aims to show why uncovering such statistical field theories is important.

3.6. A few ways to compute the large deviation Hamiltonian

In this section, we present two important frameworks that allow to compute dynamical large deviations: on one hand, large deviations due to N independent small increments leading to an effect of order 1, and on the other hand, large deviations for slow-fast systems.

The results are given in the case where the stochastic processes take value in finite dimensional space. In order to obtain formal results on the empirical measure of physical particle systems, we will assume that they hold more generally.

3.6.1. Large deviation rate functions from the infinitesimal generator of a continuous time Markov process

When the evolution of a stochastic process is the consequence of the effect of a large number of small amplitude and statistically independent moves, in the limit of a large number of moves, a LLN naturally follows. For continuous time Markov processes, for instance diffusions with small noises as in section 3.2.2, or more generally locally infinitely divisible processes[2], a general framework can be developed in order to estimate the probability of large deviations. In this section, taken from [50, 106] and initially inspired by [109, 115], we present this framework briefly and the main result: the formula (3.25) for computing the large deviation Hamiltonian in this case.

We consider $\{X_\epsilon(t)\}_{0\leq t\leq T}$, where for any t, $X_\epsilon(t) \in \Omega$, a family of continuous time Markov processes parametrized by a real number ϵ. We denote G_ϵ the infinitesimal generator of the process X_ϵ. G_ϵ acts on the space of test functions $\phi : \Omega \to \mathbb{R}$. It is defined by

$$G_\epsilon[\phi](x) = \lim_{t\downarrow 0} \frac{\mathbb{E}_x[\phi(X_\epsilon(t))] - \phi(x)}{t}, \tag{3.24}$$

where $\mathbb{E}_x$ is the average over the stochastic process $\{X_\epsilon(t)\}_{0\leq t\leq T}$ conditioned on the initial condition $X_\epsilon(t=0) = x$. We assume that for all $p \in \Omega$ the limit

$$H[x,p] = \lim_{\epsilon\downarrow 0} \epsilon G_\epsilon\left[\mathrm{e}^{\frac{1}{\epsilon}\langle p,\cdot\rangle}\right](x)\,\mathrm{e}^{-\frac{1}{\epsilon}\langle p,x\rangle} \tag{3.25}$$

exists. Then the family X_ϵ satisfies a LDP with rate ϵ and rate function

$$L[x,\dot{x}] = \sup_p \{\langle p,\dot{x}\rangle - H[x,p]\}. \tag{3.26}$$

This means that the probability that the path $\{X_\epsilon(t)\}_{0\leq t<T}$ be in a neighborhood of $\{x(t)\}_{0\leq t<T}$, with the prescription that $X_\epsilon(t=0)$ is in the neighborhood of $x(t=0)$, satisfies

$$\mathbb{P}\left(\{X_\epsilon(t)\}_{0\leq t<T} = \{x(t)\}_{0\leq t<T}\right) \underset{\epsilon\downarrow 0}{\asymp} \exp\left(-\frac{\int_0^T \mathrm{d}t\, L[x,\dot{x}]}{\epsilon}\right). \tag{3.27}$$

This result is proven for specific cases (diffusions, locally infinitely divisible processes) in the Theorem 2.1, page 127, of the third edition of Freidlin-Wentzell textbook [115]. A general heuristic derivation is given in section 7.1.2 of [50]. The main idea of this derivation is to decompose the path $X_\epsilon(t)$ into subpath using the Markov property. Then, applying a Gartner-Ellis type formula to the Newton ratio $(X_\epsilon(t) - x)/t$ for small t and reconstructing the path $X_\epsilon(t)$ with a path integral yields the LDP (3.27).

[2] An infinitely divisible process is a process whose probability distribution can be seen as the one of a sum of an arbitrary number of independent and identically distributed random variables. A Lévy process is an example of an infinitely divisible process.

In formula (3.25) the infinitesimal generator is tested through the function $x \mapsto \mathrm{e}^{\frac{1}{\epsilon}\langle p,x\rangle}$. In the small ϵ limit, this tests changes of the observable which are of order of ϵ. The ϵ prefactor in the right hand side of equation (3.25) means that the overall effect of these small changes of order ϵ is expected to be of order $1/\epsilon$. H in formula (3.25) thus accounts for the effects of a large number (of order $1/\epsilon$) of small amplitude statistically independent moves (each one of order ϵ).

3.6.2. Large deviation for slow-fast systems

Another classical framework for large deviations are large deviations for the effective dynamics of the slow variable in a slow-fast dynamics (time averaging of the fast degrees of freedom). This classical framework is discussed in the case of stochastic processes in [208, 115]. When the slow dynamics is deterministic similar results have been proven for instance by Kifer [141].

We consider the slow-fast dynamics

$$\left\{\begin{array}{rcl} \frac{\mathrm{d}X_\epsilon}{\mathrm{d}\tau} & = & \alpha(X_\epsilon, Y_\epsilon) \\ \mathrm{d}Y_\epsilon & = & \frac{1}{\epsilon}\beta(X_\epsilon, Y_\epsilon)\mathrm{d}\tau + \frac{1}{\sqrt{\epsilon}}\gamma(X_\epsilon, Y_\epsilon)\mathrm{d}W_\tau \end{array}\right. , \tag{3.28}$$

where X_ϵ is the slow variable, Y_ϵ the fast variable, W a Wiener process, and ϵ quantifies the time scale separation. We assume that the dynamics for Y_ϵ is mixing over timescales of order ϵ, i.e. on these timescales the process for Y_ϵ looses the memory of its initial condition. The following discussion would apply for other classes of dynamics for Y_ϵ, beyond diffusions, with little modifications, for instance for chaotic deterministic systems with mixing hypothesis.

We are interested in the slow dynamics for X_ϵ. Then for generic hypotheses, with the prescription that $X_\epsilon(\tau = 0)$ is in the neighborhood of $x(\tau = 0)$, we have the LDP

$$\mathbb{P}\left(X_\epsilon = x\right) \underset{\epsilon\to 0}{\asymp} \mathrm{e}^{-\frac{1}{\epsilon}\int_0^T \mathrm{Sup}_p\{\dot{x}.p - H(x,p)\}\mathrm{d}\tau} \tag{3.29}$$

$$\text{with} \quad H(x,p) = \lim_{T\to\infty} \frac{1}{T} \log \mathbb{E}_x \left\{ \exp\left[p \cdot \int_0^T \alpha(x, Y_x(t))\mathrm{d}t \right] \right\}, \tag{3.30}$$

where p is conjugated to $\dot{x}$, the average $\mathbb{E}_x$ is an average over the Y_x process with frozen x (the solution of $\frac{\mathrm{d}Y_x}{\mathrm{d}t} = \beta\left(x, Y_x\right) + \gamma\left(x, Y_x\right)\frac{\mathrm{d}W}{\mathrm{d}t}$).

This classical result is proven in the case of stochastic processes in [208, 115]. A simple heuristic account for any Markov dynamics is given in [51]. The result (3.28-3.30) is heuristically understood as $L(x,\dot{x}) = \sup_p\left\{\dot{x}.p - H(x,p)\right\}$ appears as a large-time large deviations result, of the Freidlin-Wentzell type, for the Newton increment of the slow variable

$$\frac{X_\epsilon(\tau + \Delta\tau) - x}{\Delta\tau} = \frac{1}{\Delta\tau}\int_0^{\Delta\tau} \alpha\left(X_\epsilon(u), Y_\epsilon\left(u\right)\right)\,\mathrm{d}u \simeq \frac{\epsilon}{\Delta\tau}\int_0^{\frac{\Delta\tau}{\epsilon}} \alpha\left(x, Y_x\left(t\right)\right)\,\mathrm{d}t.$$

Then formula (3.30), with $L(x,\dot{x}) = \mathrm{Sup}_p \{\dot{x}.p - H(x,p)\}$, appears as a Gärtner–Ellis formula for the large time large deviations

$$\mathbb{E}_x \left[\delta \left(\frac{X_\epsilon(\tau + \Delta\tau) - x}{\Delta\tau} - \dot{x} \right) \right] \underset{\epsilon \to 0}{\asymp} \mathrm{e}^{-\frac{L(x,\dot{x})\Delta\tau}{\epsilon}}.$$

This last formula is the temporal increment of formula (3.30).

[51] discusses also at length the case when the fast variable is an Ornstein-Uhlenbeck and the coupling with the slow variable is through a quadratic form. In this specific case the Hamiltonian can be computed by solving a matrix Riccati equation.

We will use formula (3.28-3.30) in chapter 4 to investigate large deviations associated with the kinetic theory of particles with long-range interactions.

3.7. Derivation of the kinetic large deviation principle for two toy-models

In this section, we derive dynamical LDPs for the empirical measure of two families of microscopic dynamics. First, we describe the large deviations of the empirical measure of N diffusions in section 3.7.1. In section 3.7.2 we describe the large deviations of the empirical measure of N particles undergoing a run-and-tumble dynamics, which corresponds to a jump process for the particles dynamics. The derivation of the large deviation Hamiltonians for these two toy models encapsulates the main ideas needed to understand large deviations of the empirical measure of more realistic particle models, which we will address in the remainder of the manuscript.

3.7.1. Large deviations for the empirical measure of N diffusion processes

In section 3.7.1.1 we derive the large deviation rate function for the empirical measure defined as $f_N(\mathbf{v},t) = \frac{1}{N}\sum_{n=1}^{N} \delta\left(\mathbf{r}_n(t) - \mathbf{r}\right) \delta\left(\mathbf{v}_n(t) - \mathbf{v}\right)$ of N independent particles, where each $(\mathbf{r}_n(t), \mathbf{v}_n(t))$ is governed by a Markov dynamics with infinitesimal generator G.

In section 3.7.1.2 we apply this to the case when the N independent Markov dynamics are Ito diffusions of inertial particles

$$\begin{cases} \dot{\mathbf{r}}_n & = \mathbf{v}_n \\ \mathrm{d}\mathbf{v}_n & = \left[\mathbf{b}\left(\mathbf{v}_n\right) + \frac{\partial}{\partial \mathbf{v}}.\mathbf{D}\left(\mathbf{v}_n\right)\right] \mathrm{d}t + \sqrt{2}\sigma\left(\mathbf{v}_n\right) \mathrm{d}W_{n,t}, \end{cases} \tag{3.31}$$

where we defined $\mathbf{D}$ the diffusion tensor as $\mathbf{D} = \sigma\sigma^\top$ and $(W_{n,t})_{1\leq n\leq N}$ are independent Wiener processes. In section 3.7.1.3 when the particles are not independent anymore but are coupled in a mean field way, as in (4.17). For each of these cases we prove that with the prescription that $f_N(t=0)$ is in the neighborhood of $f(t=0)$

$$\mathbf{P}\left(\{f_N(t)\}_{0\leq t\leq T} = \{f(t)\}_{0\leq t\leq T}\right) \underset{N\to\infty}{\asymp} \mathrm{e}^{-N\mathrm{Sup}_p \int_0^T \left\{\int \mathrm{d}\mathbf{v}\, \dot{f} p - H[f,p]\right\}}, \tag{3.32}$$

where the corresponding H are given by formula (3.35), (3.38) and (3.44), respectively. The Hamiltonian associated with the diffusions of the velocities in (3.31) is a well-known result. The method we present in this section allows to easily extend them to the kinetic case (when there the velocity of a particle actually affects its position) by computing the terms of the Hamiltonian associated with the transport.

3.7.1.1. Large deviations for the empirical measure of N independent Markov processes

We consider N continuous time independent Markov processes $\{\mathbf{r}_n(t), \mathbf{v}_n(t)\}_{t\in[0,T],1\leq n\leq N}$, where each $(\mathbf{r}_n(t), \mathbf{v}_n(t))$ is governed by a Markov dynamics with infinitesimal generator G. G acts on functions $\phi : \mathbb{R}^3 \times \mathbb{R}^3 \to \mathbb{R}$ and is defined by

$$G[\phi](\mathbf{r},\mathbf{v}) = \lim_{t\to 0} \frac{\mathbb{E}_{\mathbf{r},\mathbf{v}}\left[\phi\left(\mathbf{r}_1(t), \mathbf{v}_1(t)\right)\right] - \phi(\mathbf{r},\mathbf{v})}{t}. \tag{3.33}$$

Then, with the prescription that $f_N(t=0)$ is in the neighborhood of $f(t=0)$, the empirical measure f_N satisfies a LDP

$$\mathbf{P}(f_N = f) \underset{N\to\infty}{\asymp} \mathrm{e}^{-N\mathrm{Sup}_p \int_0^T \left\{\int \mathbf{drdv}\, \dot{f}p - H[f,p]\right\}} \tag{3.34}$$

where

$$H[f,p] = \int \mathbf{drdv}\, f(\mathbf{r},\mathbf{v}) G\left[\mathrm{e}^{p(\cdot,\cdot)}\right](\mathbf{r},\mathbf{v})\mathrm{e}^{-p(\mathbf{r},\mathbf{v})}, \tag{3.35}$$

in this expression, the variable p is the conjugate momentum to $\dot{f}$, and it is a scalar function of the position and the velocity $\mathbf{r},\mathbf{v}$. We abusively use the notation $G\left[\mathrm{e}^{p(\cdot,\cdot)}\right](\mathbf{r},\mathbf{v})$ to note $G[\phi](\mathbf{r},\mathbf{v})$ where $\phi : (\mathbf{r},\mathbf{v}) \mapsto \mathrm{e}^{p(\mathbf{r},\mathbf{v})}$.

Formal proof. The empirical measure f_N is also itself a continuous time Markov process. We denote G_f its infinitesimal generator, defined by

$$G_{f_N}[\psi](f) = \lim_{t\to 0} \frac{\mathbb{E}_f\left[\psi\left(f_N(t)\right)\right] - \psi(f)}{t},.$$

where ψ is a functional. Then, from the result explained in section 3.6.1, we know that if the limit

$$H[f,p] = \lim_{N\to\infty} \frac{1}{N} \mathrm{e}^{-N\int \mathbf{drdv}\, pf} G_{f_N}\left[\mathrm{e}^{N\int \mathbf{drdv}\, p\times\cdot}\right](f),$$

exists (see (3.25)), then we have the LDP (3.34). Using the definition of the empirical measure

$$\exp\left(N\int \mathbf{drdv}\, pf_N\right) = \exp\left(\sum_{n=1}^{N} p\left(\mathbf{r}_n(t), \mathbf{v}_n(t)\right)\right),$$

we find

$$\begin{aligned} G_{f_N}\left[\mathrm{e}^{N\int \mathbf{drdv}\, p\times\cdot}\right](f) &= \lim_{t\to 0}\left(\mathbb{E}_f\left[\mathrm{e}^{N\int \mathbf{drdv}\, pf_N}\right]-\mathrm{e}^{N\int \mathbf{drdv}\, pf}\right)/t, \\ &= \lim_{t\to 0}\left(\mathbb{E}_f\left[\mathrm{e}^{\sum_{n=1}^N p(\mathbf{r}_n(t),\mathbf{v}_n(t))}\right]-\mathrm{e}^{\sum_{n=1}^N p(\mathbf{r}_n(0),\mathbf{v}_n(0))}\right)/t. \end{aligned} \tag{3.36}$$

Then, using that the particles are independent

$$H[f,p]=\lim_{N\to\infty}\lim_{t\to 0}\frac{1}{Nt}\left(\prod_{n=1}^N \mathbb{E}\left(\mathrm{e}^{\Delta p(\mathbf{r}_n(t),\mathbf{v}_n(t))}\right)-1\right),$$

where $\mathbb{E}\left(\mathrm{e}^{\Delta p(\mathbf{r}_n(t),\mathbf{v}_n(t))}\right)=\mathbb{E}\left(\mathrm{e}^{p(\mathbf{r}_n(t),\mathbf{v}_n(t))}\right)\mathrm{e}^{-p(\mathbf{r}_n(0),\mathbf{v}_n(0))}$. Furthermore, using the definition of the infinitesimal generator of the process for a single particle (3.33), we have

$$\mathbb{E}\left(\mathrm{e}^{\Delta p(\mathbf{r}_n(t),\mathbf{v}_n(t))}\right)=1+tG\left[\mathrm{e}^{p(\cdot,\cdot)}\right](\mathbf{r}_n(0),\mathbf{v}_n(0))\,\mathrm{e}^{-p(\mathbf{r}_n(0),\mathbf{v}_n(0))}+o(t)\quad(t\to 0).$$

To the same precision we can compute the product for $1\leq n\leq N$

$$\prod_{n=1}^N \mathbb{E}\left(\mathrm{e}^{\Delta p(\mathbf{r}_n(t),\mathbf{v}_n(t))}\right)-1=t\sum_{n=1}^N G\left[\mathrm{e}^{p(\cdot,\cdot)}\right](\mathbf{r}_n(0),\mathbf{v}_n(0))\,\mathrm{e}^{-p(\mathbf{r}_n(0),\mathbf{v}_n(0))}+o(t)\quad(t\to 0).$$

From this expansion, it is possible to compute the limit as t goes to 0

$$\lim_{t\to 0}\frac{1}{Nt}\left(\prod_{n=1}^N \mathbb{E}\left(\mathrm{e}^{\Delta p(\mathbf{r}_n(t),\mathbf{v}_n(t))}\right)-1\right)=\sum_{n=1}^N G\left[\mathrm{e}^{p(\cdot,\cdot)}\right](\mathbf{r}_n(0),\mathbf{v}_n(0))\,\mathrm{e}^{-p(\mathbf{r}_n(0),\mathbf{v}_n(0))}.$$

It is important to note that the order of the limits $N\to\infty$ and $t\to 0$ is crucial. From there, we have

$$\begin{aligned} H[f,p] &= \lim_{N\to\infty}\frac{1}{N}\sum_{n=1}^N G\left[\mathrm{e}^{p(\cdot,\cdot)}\right](\mathbf{r}_n(0),\mathbf{v}_n(0))\,\mathrm{e}^{-p(\mathbf{r}_n(0),\mathbf{v}_n(0))}, \\ &= \lim_{N\to\infty}\int \mathbf{drdv}\, f_N(\mathbf{r},\mathbf{v})\,G\left[\mathrm{e}^{p(\cdot,\cdot)}\right](\mathbf{r},\mathbf{v})\,\mathrm{e}^{-p(\mathbf{r},\mathbf{v})}. \end{aligned}$$

Recalling the prescription that the f_N concentrate close to f, we obtain

$$H[f,p]=\int \mathbf{drdv}\, f(\mathbf{r},\mathbf{v})G\left[\mathrm{e}^{p(\cdot,\cdot)}\right](\mathbf{r},\mathbf{v})\mathrm{e}^{-p(\mathbf{r},\mathbf{v})}.$$

We remark that the Hamiltonian (3.35) is in general not quadratic in p, reflecting the fact that the large deviations are not Gaussian, although they arise from the sum of N independent contributions.

3.7.1.2. Large deviations for the empirical measure of N independent diffusions

From equation (3.35), it is straightforward to compute the Hamiltonian that describes the large deviations for the empirical measure of N inertial particles with independent diffusions.

Let us consider the dynamics N particles with positions and velocities $\{\mathbf{r}_n, \mathbf{v}_n\}_{1\leq n\leq N}$ whose velocities are diffusing following a Ito diffusion dynamics:

$$\begin{cases} \dot{\mathbf{r}}_n & = \mathbf{v}_n \\ \mathrm{d}\mathbf{v}_n & = \left[\mathbf{b}\left(\mathbf{v}_n\right) + \frac{\partial}{\partial \mathbf{v}} \cdot \mathbf{D}\left(\mathbf{v}_n\right)\right] \mathrm{d}t + \sqrt{2}\sigma\left(\mathbf{v}_n\right) \mathrm{d}W_{n,t}, \end{cases} \tag{3.37}$$

where $(W_{n,t})_{1\leq n\leq N}$ are independent Wiener processes. This dynamics is a Klein–Kramers dynamics without external potential [142], i.e. an underdamped Langevin dynamics. We call f the probability density function of $(\mathbf{r}_n, \mathbf{v}_n)$ for some n. It does not depend on n as we consider N non-interacting particles, we can write the Fokker-Planck equation associated with the diffusion of a particle

$$\frac{\partial f}{\partial t} + \mathbf{v} \cdot \frac{\partial f}{\partial \mathbf{r}} = \frac{\partial}{\partial \mathbf{v}} \cdot \left\{ -f\mathbf{b} + \mathbf{D}\frac{\partial f}{\partial \mathbf{v}} \right\}.$$

This equation describe the average behavior of the empirical measure

$$f_N(\mathbf{v}, t) = \frac{1}{N} \sum_{n=1}^{N} \delta\left(\mathbf{r}_n(t) - \mathbf{r}\right) \delta\left(\mathbf{v}_n(t) - \mathbf{v}\right).$$

We want to compute $H[f, p]$ the Hamiltonian associated with the LDP for the empirical measure

$$\mathbf{P}(f_N = f) \underset{N\to\infty}{\asymp} \mathrm{e}^{-N \mathrm{Sup}_p \int_0^T \left\{ \int \mathrm{d}\mathbf{r}\mathrm{d}\mathbf{v}\, \dot{f} p - H[f,p] \right\}}$$

We showed in section 3.7.1.1 that in the case where the N particles are independent, H is given by

$$H[f, p] = \int \mathrm{d}\mathbf{r}\mathrm{d}\mathbf{v}\, f(\mathbf{r}, \mathbf{v}) G\left[\mathrm{e}^{p(\cdot,\cdot)}\right](\mathbf{r}, \mathbf{v}) \mathrm{e}^{-p(\mathbf{r},\mathbf{v})},$$

where G is the infinitesimal generator of the stochastic process described by the trajectory of one particle $(\mathbf{r}_1, \mathbf{v}_1)$. It is a classical result in stochastic analysis that the infinitesimal generator G of the diffusion stochastic process (3.37) is

$$G = \mathbf{v} \cdot \frac{\partial}{\partial \mathbf{r}} + \mathbf{b} \cdot \frac{\partial}{\partial \mathbf{v}} + \frac{\partial}{\partial \mathbf{v}} \cdot \left(\mathbf{D} \cdot \frac{\partial}{\partial \mathbf{v}} \right),$$

the adjoint of the Fokker-Planck operator [120]. This leads to the Hamiltonian associated with the empirical measure of N particles undergoing independent Klein-Kramers dynamics

$$H\left[f,p\right]=\int \mathbf{dr}\mathbf{dv}\, f\left\{\mathbf{v}\cdot\frac{\partial p}{\partial \mathbf{r}}+\mathbf{b}\cdot\frac{\partial p}{\partial \mathbf{v}}+\frac{\partial}{\partial \mathbf{v}}\cdot\left(\mathbf{D}\cdot\frac{\partial p}{\partial \mathbf{v}}\right)+\mathbf{D}:\frac{\partial p}{\partial \mathbf{v}}\frac{\partial p}{\partial \mathbf{v}}\right\}, \tag{3.38}$$

where the symbol ":" means the contraction of two second order symmetric tensors: $\mathbf{M}:\mathbf{N}=\mathrm{Tr}\left(\mathbf{MN}\right)=\sum_{ij}M_{ij}N_{ij}$.

We remark that the Hamiltonian (3.35) is quadratic in p. As discussed in section 3.2.2, this means that the large deviations are Gaussian. This reflects the fact that the large deviations arise from the sum of N independent Gaussian increments. Because of this property, we can also recover from the Hamiltonian an equivalent stochastic differential equation for the empirical measure f_N that involves a Gaussian noise. More precisely, a quadratic Hamiltonian

$$H\left[f,p\right]=\int \mathbf{dr}\mathbf{dv}\, A[f]\left(\mathbf{r},\mathbf{v}\right)p\left(\mathbf{r},\mathbf{v}\right)+\iint \mathbf{dr}\mathbf{dr}'\mathbf{dv}\mathbf{dv}'p\left(\mathbf{r},\mathbf{v}\right)C\left[f\right]\left(\mathbf{r},\mathbf{r}',\mathbf{v},\mathbf{v}'\right)p\left(\mathbf{r}',\mathbf{v}'\right) \tag{3.39}$$

is the Hamiltonian that describes the dynamical large deviations of the stochastic differential equation

$$\frac{\partial f_N}{\partial t}=A\left[f_N\right]\left(\mathbf{r},\mathbf{v}\right)+\sqrt{\frac{2}{N}}\eta\left(\mathbf{r},\mathbf{v},t\right) \tag{3.40}$$

with

$$\mathbb{E}\left(\eta\left(\mathbf{r},\mathbf{v},t\right)\eta\left(\mathbf{r}',\mathbf{v}',t'\right)\right)=C\left[h_N\right]\left(\mathbf{r},\mathbf{r}',\mathbf{v},\mathbf{v}'\right)\delta\left(t-t'\right). \tag{3.41}$$

Using partial integration, we can identify $A[f]$ and $C\left[f\right]$ for the Hamiltonian (3.38). The associated stochastic differential equation for the empirical measure is

$$\frac{\partial f_N}{\partial t}+\mathbf{v}\cdot\frac{\partial f_N}{\partial \mathbf{r}}=\frac{\partial}{\partial \mathbf{v}}\cdot\left\{-f_N\mathbf{b}+\mathbf{D}\cdot\frac{\partial f_N}{\partial \mathbf{v}}\right\}+\sqrt{\frac{2}{N}}\eta\left(\mathbf{r},\mathbf{v},t\right) \tag{3.42}$$

with,

$$\mathbb{E}\left(\eta\left(\mathbf{r},\mathbf{v},t\right)\eta\left(\mathbf{r}',\mathbf{v}',t'\right)\right)=\frac{\partial^2}{\partial \mathbf{v}\partial \mathbf{v}'}:\left(f_N(\mathbf{v})\delta\left(\mathbf{v}-\mathbf{v}'\right)\mathbf{D}\right)\delta\left(\mathbf{r}-\mathbf{r}'\right)\delta\left(t-t'\right).$$

It should be noted that the mathematical meaning of equation (3.42) is not clear and in this manuscript it should be considered as a notation referring to the underlying LDP. Recalling that $\mathbf{D}=\sigma\sigma^{\top}$, we can rewrite equation (3.42) as a conservative equation

$$\frac{\partial f_N}{\partial t}+\mathbf{v}\cdot\frac{\partial f_N}{\partial \mathbf{r}}=\frac{\partial}{\partial \mathbf{v}}\cdot\left\{-f_N\mathbf{b}+\mathbf{D}\cdot\frac{\partial f_N}{\partial \mathbf{v}}+\sqrt{\frac{2}{N}f_N}\sigma\xi\left(\mathbf{r},\mathbf{v},t\right)\right\},$$

with ξ a tridimensional Gaussian noise that satisfies

$$\mathbb{E}\left(\xi^i\left(\mathbf{r},\mathbf{v},t\right)\xi^j\left(\mathbf{r}',\mathbf{v}',t'\right)\right)=\delta^{ij}\delta\left(\mathbf{r}-\mathbf{r}'\right)\delta\left(\mathbf{v}-\mathbf{v}'\right)\delta\left(t-t'\right).$$

3.7.1.3. Large deviations for N diffusions with mean field coupling

In the previous section, we have derived the large deviation Hamiltonian for the empirical measure of N independent inertial particles driven by the diffusion (3.37). We now consider the case when the drift and diffusion coefficients depend on the empirical measure itself:

$$\begin{cases} \frac{\mathrm{d}\mathbf{r}_n}{\mathrm{d}t} & = \mathbf{v}_n \\ \mathrm{d}\mathbf{v}_n & = \left[\mathbf{b}\left[f_N\right](\mathbf{v}_n) + \frac{\partial}{\partial \mathbf{v}} \cdot \mathbf{D}\left[f_N\right](\mathbf{v}_n)\right] \mathrm{d}t + \sqrt{2}\sigma\left[f_N\right](\mathbf{v}_n)\, \mathrm{d}W_{n,t}, \end{cases} \tag{3.43}$$

with $f_N(\mathbf{v},t) = \frac{1}{N}\sum_{n=1}^{N} \delta\left(\mathbf{r}_n(t) - \mathbf{r}\right)\delta\left(\mathbf{v}_n(t) - \mathbf{v}\right)$. We denote $\mathbf{D}\left[f_N\right] = \sigma\left[f_N\right]\sigma\left[f_N\right]^{\top}$. For this case, the particles are no more statistically independent. However, for such a mean field coupling, it is possible to adapt the derivation that leads to the Hamiltonian (3.35) in section 3.7.1.1 to this specific case[3]. We find that the Hamiltonian that describes the large deviation of the empirical measure is

$$H_{MF}\left[f,p\right] = H_T\left[f,p\right] + H_{MF,h}\left[f,p\right],$$

where

$$H_T\left[f,p\right] = \int \mathbf{dr}\mathbf{dv}\, f\mathbf{v}\cdot\frac{\partial p}{\partial \mathbf{r}},$$

and

$$H_{MF,h}\left[f,p\right] = \int \mathbf{dr}\mathbf{dv}\, f\left\{\mathbf{b}\left[f\right].\frac{\partial p}{\partial \mathbf{v}} + \frac{\partial}{\partial \mathbf{v}}\left(\mathbf{D}\left[f\right]\frac{\partial p}{\partial \mathbf{v}}\right) + \mathbf{D}\left[f\right] : \frac{\partial p}{\partial \mathbf{v}}\frac{\partial p}{\partial \mathbf{v}}\right\}. \tag{3.44}$$

The subscript T denotes the transport part of the Hamiltonian and MF,h denotes that this is the Hamiltonian for a mean field dynamics without spatial structure[4]. We note that this Hamiltonian is the same as (3.38), but with drift and diffusion constant that depend of f. The corresponding stochastic dynamics is

$$\frac{\partial f_N}{\partial t} + \mathbf{v}\cdot\frac{\partial f_N}{\partial \mathbf{r}} = \frac{\partial}{\partial \mathbf{v}}\cdot\left\{-f_N\mathbf{b}\left[f_N\right] + \mathbf{D}\left[f_N\right]\cdot\frac{\partial f_N}{\partial \mathbf{v}} + \sqrt{\frac{2}{N}f_N}\sigma\left[f_N\right]\xi\left(\mathbf{r},\mathbf{v},t\right)\right\}, \tag{3.45}$$

with ξ a tridimensional Gaussian noise that satisfies

$$\mathbb{E}\left(\xi^i\left(\mathbf{r},\mathbf{v},t\right)\xi^j\left(\mathbf{r}',\mathbf{v}',t'\right)\right) = \delta^{ij}\delta\left(\mathbf{r}-\mathbf{r}'\right)\delta\left(\mathbf{v}-\mathbf{v}'\right)\delta\left(t-t'\right).$$

[3] The key point is that in (3.36), at fixed empirical measure $f_N(t) = f$, the particles $\left(\mathbf{r}_n\left(t+\delta t\right), \mathbf{v}_n\left(t+\delta t\right)\right)_{1\leq n\leq N}$ are independent for small δt.

[4] This means $H_{MF,h}$ would be the large deviation Hamiltonian for the velocity empirical measure $\frac{1}{N}\sum\delta\left(\mathbf{v}-\mathbf{v}_n\left(t\right)\right)$ whose dynamics is given by the second equations of (3.43) and the position variable plays no role.

Remark: link with the Dean–Kawasaki equation and possible misinterpretations. If we start from the dynamics

$$\mathrm{d}\mathbf{r}_n = \left[\mathbf{b}\left[f_N\right]\left(\mathbf{r}_n\right) + \frac{\partial}{\partial \mathbf{v}} \cdot \mathbf{D}\left[f_N\right]\left(\mathbf{r}_n\right)\right] \mathrm{d}t + \sqrt{2}\sigma\left[f_N\right]\left(\mathbf{r}_n\right) \mathrm{d}W_{n,t}, \tag{3.46}$$

i.e. the dynamics of N diffusions with a mean-field coupling for the position variable, where the velocity does not play a role anymore, we can obtain a large deviation result for the empirical density $\rho_N = N^{-1} \sum \delta\left(\mathbf{r} - \mathbf{r}_n\left(t\right)\right)$ and derive an equation analogue to (3.45). The result is nothing else than the Dean–Kawasaki equation [86, 136, 82] for the empirical density $\rho_N = N^{-1} \sum \delta\left(\mathbf{r} - \mathbf{r}_n\left(t\right)\right)$

$$\frac{\partial \rho_N}{\partial t} = \nabla \cdot \left\{-\rho_N \mathbf{b}\left[\rho_N\right] + \mathbf{D}\left[\rho_N\right] \cdot \nabla \rho_N + \sqrt{\frac{\rho_N}{N}} \sigma\left[\rho_N\right] \xi\left(\mathbf{r}, t\right)\right\}. \tag{3.47}$$

We stress that in (3.47), ρ_N is an empirical density $N^{-1} \sum \delta\left(\mathbf{r} - \mathbf{r}_n\left(t\right)\right)$ rather than a smooth density field. Hence, it is not obvious how to make sense of the SPDE (3.47) mathematically. In most cases, the only meaning that can be given to (3.47) is a reformulation of the equations of motion (3.46)[5]. However, recent works [76, 77] seem to indicate that a regularized version of (3.47) could have solutions that describe the law of fluctuations for the particle system in the large N limit. The arguments of [76, 77] does not seem to apply in the case the dynamics is not the one of N diffusions weakly coupled in a mean-field way. Our only claim here is that the large deviations behavior of the solutions of (3.47) is the same as the one of the empirical density of N diffusions coupled in a mean field way. In other words, we consider the SPDE a symbolic way to rephrase the underlying Gaussian LDP.

Relaxation paths and most probable evolution. Using the equation for relaxation paths (equation (3.11) in section 3.4) we check that the most probable evolution path for the empirical measure is the nonlinear Fokker–Planck equation

$$\frac{\partial f}{\partial t} = \frac{\delta H_{MF}}{\delta p}[f, p = 0] = -\mathbf{v} \cdot \frac{\partial f}{\partial \mathbf{r}} + \frac{\partial}{\partial \mathbf{v}} \cdot \left\{-f \mathbf{b}\left[f\right] + \mathbf{D}\left[f\right] \cdot \frac{\partial f}{\partial \mathbf{v}}\right\}. \tag{3.48}$$

Relative entropy and quasipotential. In section 3.6.1 we define the quasipotential for the empirical measure f_N. It is defined as $\mathbb{P}\left(f_N = f\right) \underset{N \to \infty}{\asymp} \mathrm{e}^{-NU[f]}$. As the N particles are coupled only in a mean field way, in view of Sanov's theorem adapted for this case [186], it is natural to conjecture that the quasipotential for the dynamics of the empirical measure is $U\left[f\right] = -\mathcal{S}_{\mathrm{rel}}\left[f\right]$ where $\mathcal{S}_{\mathrm{rel}}$ is the relative entropy

$$\mathcal{S}_{\mathrm{rel}}\left[f\right] = -\int \mathrm{d}\mathbf{r}\mathrm{d}\mathbf{v}\, f \log\left(f / f_{\mathrm{eq}}\right),$$

[5] This is how (3.47) is derived in [86]. The author obtains the equation on the empirical density by applying Ito's lemma and rewriting the noise term thanks to a large N simplification that they call "thermal averaging".

where f_{eq} is the stationary solution of the Fokker–Planck equation (3.48). A necessary condition for $\mathcal{S}_{\text{rel}}$ to be the quasipotential is the stationary Hamilton--Jacobi equation

$$H_{MF}\left[f, -\delta\mathcal{S}_{\text{rel}}/\delta f\right] = 0. \tag{3.49}$$

We check in the appendix A.1 that this stationary Hamilton–Jacobi equation is indeed verified when $\mathbf{b}\left[f\right] = \mathbf{b}$ and $\mathbf{D}\left[f\right] = \mathbf{D}$ do not depend on f, i.e. when the N diffusions are independent from each other. However, we also check that this is no more the case in general if $\mathbf{b}\left[f\right]$ and $\mathbf{D}\left[f\right]$ actually depend on f. As noted in appendix A.1, a notable case where (3.49) holds with $\mathbf{b}\left[f\right]$ and $\mathbf{D}\left[f\right]$ depending non-trivially on f, is when $\mathbf{b}\left[f\right]$ and $\mathbf{D}\left[f\right]$ are chosen to mimic the Balescu-Guernsey-Lenard equation at the kinetic level.

3.7.2. Large deviations for the empirical measure of N particles submitted to Run-and-Tumble dynamics

In this section, we now examine the case of the large deviation for the empirical measure of N particles undergoing a stochastic jump process rather than a diffusion. More precisely, we derive a LDP that describes the probability for an evolution path of the rescaled empirical measure $f_\epsilon(\mathbf{r},\theta,t) = \epsilon\sum_n \delta\left(\mathbf{r}_n - \mathbf{r}\right)\delta\left(\theta_n - \theta\right)$ of N non-interacting particles undergoing a Run-and-Tumble dynamics to be close to the evolution path of a prescribed smooth distribution f. The LDP reads

$$\mathbb{P}\left[\left\{f_\epsilon(t)\right\}_{0\leq t<T} = \left\{f(t)\right\}_{0\leq t<T}\right] \underset{\epsilon\downarrow 0}{\asymp} \exp\left(-\frac{1}{\epsilon}\int_0^T \mathrm{d}t\, \sup_p\left(\int \mathbf{dr}\mathrm{d}\theta\, p\dot{f} - H_{RT}\left[f,p\right]\right)\right), \tag{3.50}$$

where ϵ is the small kinetic parameter, related to $1/N$ and to be determined, $p(\mathbf{r},\theta)$ is the momentum conjugated to $\dot{f}$, and H_{RT} is the large deviation Hamiltonian, a functional of both f and p. In section 3.7.2.1, we introduce the Run-and-Tumble particle dynamics. In section 3.7.2.2, we explain how to compute H_{RT} in the case of Run-and-Tumble particles.

3.7.2.1. Particle dynamics and kinetic description.

We consider N non-interacting particles in a two-dimensional periodic box of size L traveling at a constant speed v_0. Since the modulus of their velocity is fixed, the velocity of the n-th particle is noted θ_n and is an angle that we call its orientation. A particle changes its orientation from θ to θ' with a rate λ following a distribution P_t on $[-\pi,\pi)$ which is even. Such a dynamics is called a Run-and-Tumble dynamics because a particle alternates between "running" (ballistic motion at fixed velocity) and "tumbling" events that instantly change its velocity. Figure 3.1 illustrates this dynamics for a single particle.

At the kinetic level the distribution function $f(\mathbf{r},\theta,t)$ of the position and orientation of the N particles satisfies

$$\partial_t f + v_0\mathbf{e}_\theta\cdot\nabla f = -\lambda f + \lambda\int \mathrm{d}\theta'\, P_t\left(\theta'-\theta\right) f\left(\theta'\right),$$

Figure 3.1.: A particle with orientation θ travels balistically with a velocity $\mathbf{v} = v_0\mathbf{e}_\theta = v_0\,(\cos\theta, \sin\theta)$. It undergoes a tumbling event at a rate λ. As the particle tumbles, its orientation is updated to $\theta' = \theta + \theta_{\text{jump}}$ where θ_{jump} is drawn in $[-\pi, \pi)$ according to the distribution P_t.

where $\int \mathbf{dr}d\theta\, f = 1$. This kinetic equation is heuristically obtained by only considering the average effect of tumbling events on the distribution function. We define the mean free path, i.e. the average distance traveled by a particle between two tumbling events, $\ell = v_0/\lambda$ and we rescale space and time $\mathbf{r}' = \mathbf{r}/\ell, t' = tv_0/\ell$. Dropping the primes, it yields

$$\partial_t f + \mathbf{e}_\theta \cdot \nabla f = -f + \int \mathrm{d}\theta'\, P_t\,(\theta' - \theta)\, f\,(\theta')\,. \tag{3.51}$$

We consider the rescaled empirical measure

$$f_\epsilon(\mathbf{r}, \theta, t) = \epsilon \sum_n \delta\,(\mathbf{r}_n - \mathbf{r})\,\delta\,(\theta_n - \theta)\,,$$

with $\epsilon = L^2/\,(N\ell^2)$ being the inverse of the number of particles in a box of the size of the mean free path. Equation (3.51) can be seen as a LLN for the empirical measure f_ϵ: in the limit as ϵ goes to zero, the random object f_ϵ concentrates on the distribution function f which is a solution of (3.51). This equation tells us about the average effect of tumbling events on the distribution function. For the kinetic equation to makes sense as a LLN for the empirical measure, there must be many particles in the typical evolution length for the distribution function, which here is the mean free path ℓ. That is why we choose ϵ to be the small kinetic parameter rather than $1/N$.

3.7.2.2. Large deviations for the empirical measure

We now assess the probability of any evolution path for the empirical measure. Since we are interested in the dynamics of the empirical measure of N independent Markov processes, it is possible to use the result (3.35) from section 3.7.1.1 to derive the large deviation Hamiltonian. However for the sake of pedagogy, we will start again from the result (3.25) of section 3.6.1. To do so, we have to compute the infinitesimal generator of the Markov process describing the evolution of the empirical measure f_N. Then, from the infinitesimal generator G_f, the large deviation Hamiltonian is deduced through the

following formula

$$H_{RT}[f,p] = \lim_{\epsilon \downarrow 0} \epsilon G_{f_\epsilon} \left[\mathrm{e}^{\frac{1}{\epsilon}\int \mathbf{dr}\mathrm{d}\theta\, p \times \cdot} \right](f)\, \mathrm{e}^{-\frac{1}{\epsilon}\int \mathbf{dr}\mathrm{d}\theta\, pf}, \tag{3.52}$$

where the definition of the infinitesimal generator is

$$G_{f_\epsilon}[\phi](f) = \lim_{t \to 0} \frac{\mathbb{E}_f\left[\phi\left[f_\epsilon(t)\right]\right] - \phi[f]}{t}, \tag{3.53}$$

where ϕ is a test functional of the empirical measure. In (3.53), $\mathbb{E}_f$ denotes an expectation over the stochastic process f_ϵ conditioned by $f_\epsilon(t=0) = f$. The generator can be split into two terms

$$G_{f_\epsilon} = G_{f,\mathcal{T}} + G_{f,\mathrm{tumb}},$$

where $G_{f,\mathcal{T}}$ is due to free transport, and $G_{f,\mathrm{tumb}}$ to tumbling events. A Taylor expansion of $\phi\left[f_\epsilon(t)\right]$ at small times allows to compute the transport part of the generator

$$G_{f,\mathcal{T}}[\phi](f) = -\int \mathbf{dr}\mathrm{d}\theta\, \mathbf{e}_\theta \cdot \nabla f \frac{\delta \phi}{\delta f(\mathbf{r},\theta)}. \tag{3.54}$$

To compute $G_{f,\mathrm{tumb}}$, we need to evaluate the effect of tumbling events on the empirical measure. If f is the empirical measure, the rate of tumbling events that change the orientation of a particle from θ_1 to θ_1' in the volume element $\mathbf{dr}_1$ centered at point $\mathbf{r}_1$ is:

$$\frac{1}{\epsilon} f(\mathbf{r}_1,\theta_1,t) P_t(\theta_1 - \theta_1')\, \mathrm{d}\theta_1 \mathrm{d}\theta_1' \mathbf{dr}_1. \tag{3.55}$$

Each tumbling event of this type changes the empirical measure from $f(\mathbf{r},\theta)$ to $f(\mathbf{r},\theta) - \epsilon\delta(\mathbf{r}-\mathbf{r}_1)\,\delta(\theta-\theta_1) + \epsilon\delta(\mathbf{r}-\mathbf{r}_1)\,\delta(\theta-\theta_1')$. Therefore, from (3.53) and (3.55), we deduce the part of the infinitesimal generator due to tumbling events

$$G_{f,\mathrm{tumb}}[\phi](f) = \frac{1}{\epsilon}\int \mathbf{dr}\mathrm{d}\theta_1 \mathrm{d}\theta_1'\; f(\mathbf{r},\theta_1,t) P_t(\theta_1-\theta_1')\left(\phi[\tilde{f}] - \phi[f]\right), \tag{3.56}$$

where $\tilde{f}(\mathbf{r}_0,\theta,t) = f(\mathbf{r}_0,\theta,t) + \epsilon\delta(\mathbf{r}_0-\mathbf{r})\left(-\delta(\theta-\theta_1) + \delta(\theta-\theta_1')\right)$. We can then apply (3.52) to deduce the large deviation Hamiltonian

$$H_{RT}[f,p] = H_{\mathcal{T}}[f,p] + H_{\mathrm{tumb}}[f,p], \tag{3.57}$$

where

$$H_{\mathcal{T}}[f,p] = -\int \mathbf{dr}\mathrm{d}\theta\, p(\mathbf{r},\theta,t)\mathbf{e}_\theta \cdot \nabla f(\mathbf{r},\theta,t), \tag{3.58}$$

$$H_{\mathrm{tumb}}[f,p] = \int \mathbf{dr}\mathrm{d}\theta_1 \mathrm{d}\theta_1'\, f(\mathbf{r},\theta_1,t) P_t(\theta_1-\theta_1')\left\{ e^{-p(\mathbf{r},\theta_1,t)+p(\mathbf{r},\theta_1',t)} - 1 \right\}. \tag{3.59}$$

The most probable evolution for the empirical measure is the one that maximizes the right hand side of the LDP (3.50). This maximization condition is simply the Hamilton

equation associated with the large deviation Hamiltonian (3.57), which gives: $\partial_t f = \frac{\delta H_{RT}}{\delta p}[f, p=0]$ or, explicitly, equation (3.51).

Tumbling events conserve locally the number of particles $N[f] = \int \mathbf{dr}d\theta\, f$. According to the property 10. of section 3.4, this is checked at the level of large deviations as the following property holds

$$\int \mathbf{dr}d\theta \frac{\delta H_{RT}}{\delta p(\mathbf{r},\theta)} \frac{\delta N}{\delta f} = 0.$$

The large deviation Hamiltonian H_{RT} is non-quadratic in the conjugated momentum p. This means that, if we wanted to write a stochastic partial differential equation for the empirical measure, it would contain non-Gaussian noise. This is typical when the particle dynamics is a jump process rather than a diffusion process.

3.7.2.3. Quasipotential and time-reversibility

In the absence of interactions, the quasipotential is given by Sanov's theorem; the probability for the empirical measure to be close to a certain distribution f is given by the number of phase-space configurations that are compatible with this distribution f:

$$\mathbb{P}_S(f_\epsilon = f) \underset{\epsilon \downarrow 0}{\asymp} \exp\left(\frac{1}{\epsilon}\mathcal{S}[f]\right), \tag{3.60}$$

where $\mathcal{S}[f] = -\int \mathbf{dr}d\theta\, f \log f$ is the entropy. According to property 11. of section 3.4, a necessary condition for the compatibility of (3.60) and the LDP (3.50) is provided by the Hamilton–Jacobi equation:

$$H_{RT}\left[f, -\frac{\delta \mathcal{S}}{\delta f}\right] = 0 \tag{3.61}$$

which can be explicitly checked to hold. This fact is related to the presence of the generalized time-reversal symmetry $\theta \to \theta + \pi, t \to -t$. We note that this symmetry holds as a consequence of the one of the tumbling probability $P_t(\theta) = P_t(-\theta)$. Defining $I[f](\mathbf{r},\theta,t) = f(\mathbf{r},\theta+\pi,-t)$, this symmetry translates into the following identity for the large deviation Hamiltonian:

$$H_{RT}\big[I[f], -I[p]\big] = H_{RT}\left[f, p - \frac{\delta \mathcal{S}}{\delta f}\right], \tag{3.62}$$

as predicted by the property 7. of section 3.4.

4. Dynamical large deviations for the kinetic theory of long-range interacting particles: beyond the Balescu-Guernse-Lenard equation

In this chapter we derive the main result of the first part of the manuscript: the derivation of a large deviation principle for the empirical measure of N particles submitted to a Hamiltonian dynamics, coupled through a long-range interaction potential. This chapter is mainly an adaptation of [107]. The specific case of the one-component plasma, i.e. when the interaction potential is the Coulomb one is discussed in the next chapter.

4.1. Introduction: particles with long-range interaction, kinetic theory, and large deviations

We consider the Hamiltonian dynamics of particles that interact through a mean-field potential. The dynamics reads

$$\begin{cases} \dfrac{\mathrm{d}\mathbf{r}_n}{\mathrm{d}t} &= \mathbf{v}_n \\ \dfrac{\mathrm{d}\mathbf{v}_n}{\mathrm{d}t} &= -\dfrac{1}{N}\displaystyle\sum_{m\neq n} \frac{\mathrm{d}}{\mathrm{d}\mathbf{r}_n} W\left(\mathbf{r}_n - \mathbf{r}_m\right) \end{cases} \tag{4.1}$$

where $\{\mathbf{r}_n\}_{1\leq n\leq N}$ are the positions and $\{\mathbf{v}_n\}_{1\leq n\leq N}$ the velocities. This set-up is relevant for plasmas in the weak coupling regime [169], self-gravitating systems [172, 73], and many particle systems with long range interactions [52]. It also shares many theoretical analogies with two-dimensional and geostrophic turbulence, through the point vortex model [72, 139]. The kinetic theory of systems with mean-field potentials (or long range interactions) is a classical piece of theoretical physics. The relaxation to equilibrium of the empirical measure[1]

$$g_N(\mathbf{r},\mathbf{v},t) = \frac{1}{N}\sum_{n=1}^{N} \delta(\mathbf{r}-\mathbf{r}_n(t))\delta(\mathbf{v}-\mathbf{v}_n(t)),$$

[1] In this chapter and the next one, the empirical measure is noted g_N instead of f_N, because the letter f will be used to denote the velocity distribution, as customary in plasma phyiscs.

is described by the Balescu-Guernsey-Lenard kinetic equation in the limit of a large number of particles. This result has been formally derived by Balescu, Guernsey and Lenard [10, 11]. In the context of plasma physics where we consider N charged particles submitted to Coulomb interactions, we refer to Nicholson [169] for a derivation using the BBGKY hierarchy, or to Lifshitz and Pitaevskii [150] who follow the Klimontovich approach.

In this chapter we extend this classical kinetic theory by describing the statistics of the large deviations for time dependent trajectories (paths) of the empirical measure. For simplicity, we restrict our analysis to paths of the empirical measure which remain close to homogeneous distributions[2]. We consider the projection of the empirical measure on homogeneous distributions: $f_N(\mathbf{v},t) = N^{-1}L^{-3}\int \mathrm{d}\mathbf{r}\, g_N(\mathbf{r},\mathbf{v},t) = N^{-1}L^{-3}\sum_{n=1}^{N}\delta(\mathbf{v}-\mathbf{v}_n(t))$, where L^3 is the volume of the system. The natural evolution of f_N occurs on time scales of order N (except in dimension $d=1$ [213]). After time rescaling $\tau = t/N$, we study the probability of $f_N^s(\mathbf{v},\tau) = f_N(\mathbf{v},N\tau)$ (by abuse of notation and for convenience, we still denote $f_N^s = f_N$). We justify that the probability that a path $\{f_N(\tau)\}_{0\leq\tau\leq T}$ remains in the neighborhood of a prescribed path $\{f(\tau)\}_{0\leq t\leq T}$ satisfies the large deviation principle

$$\mathbb{P}\left(\{f_N(\tau)\}_{0\leq\tau\leq T} = \{f(\tau)\}_{0\leq\tau\leq T}\right) \underset{N\to\infty}{\asymp} \mathrm{e}^{-NL^3\int_0^T \mathrm{d}\tau\, \mathrm{Sup}_p\left\{\int \mathrm{d}\mathbf{v}\, \dot{f}p - H_{\mathrm{BGL}}[f,p]\right\}}\mathrm{e}^{-NI_0\left[f^0\right]}, \quad (4.2)$$

where $\dot{f}$ is the time derivative of f, p is a function over the velocity space and is the conjugated momentum to $\dot{f}$, the Hamiltonian H_{BGL} is a functional of f and p that characterizes the dynamical fluctuations, I_0 is a large deviation rate function for the initial conditions[3] of f_N. We note that H_{BGL} is not the Hamiltonian of the microscopic dynamics.

The main result of this chapter is the first computation of an explicit expression for H_{BGL} and the study of its symmetry properties. The explicit expression for H_{BGL} is

$$H_{\mathrm{BGL}}[f,p] = -\frac{1}{4\pi L^3}\sum_{\mathbf{k}}\int \mathrm{d}\omega\, \log\left\{1-\mathcal{J}[f,p](\mathbf{k},\omega)\right\}, \quad (4.3)$$

with

$$\mathcal{J}[f,p](\mathbf{k},\omega) = 4\pi\int \mathrm{d}\mathbf{v}_1\mathrm{d}\mathbf{v}_2\, \frac{\partial p}{\partial \mathbf{v}_1}\cdot\mathbf{A}[f](\mathbf{k},\omega,\mathbf{v}_1,\mathbf{v}_2)\cdot\left\{\frac{\partial f}{\partial \mathbf{v}_2}f(\mathbf{v}_1) - f(\mathbf{v}_2)\frac{\partial f}{\partial \mathbf{v}_1}\right\}$$
$$+ 4\pi\int \mathrm{d}\mathbf{v}_1\mathrm{d}\mathbf{v}_2\left\{\frac{\partial p}{\partial \mathbf{v}_1}\frac{\partial p}{\partial \mathbf{v}_1} - \frac{\partial p}{\partial \mathbf{v}_1}\frac{\partial p}{\partial \mathbf{v}_2}\right\} : \mathbf{A}[f](\mathbf{k},\omega,\mathbf{v}_1,\mathbf{v}_2)\, f(\mathbf{v}_1)f(\mathbf{v}_2), \quad (4.4)$$

where the $\mathbf{A}(\mathbf{k},\omega,\mathbf{v}_1,\mathbf{v}_2)$ is a symmetric tensor which can be expressed through the Fourier transform of the interaction potential and the dielectric function.

[2] We discuss the generalization to inhomogeneous systems in section 5.7.

[3] The prescription of the rate function for the initial condition is not necessary but aims at recalling that the probability considered here are with respect to the measure on the ensemble of initial conditions of the particles' positions and velocities.

Equations (4.3-4.4) clearly show that the Hamiltonian is not quadratic in the conjugated momentum p. This shows that the fluctuations that lead to large deviations are not locally Gaussian, by contrast with many other cases, for instance when diffusive limits are involved as in the case of macroscopic fluctuation theory [32], or for plasma fluctuations at scales much smaller than the Debye length [106] (that are discussed in the next chapter). It is striking that it is possible to get explicit formulas (4.3-4.4) for the large deviation Hamiltonian, for which cumulants of all order are relevant and non trivial. The four key theoretical ideas and technical tools we use are: making the connection with large deviation theory for slow-fast systems and identifying the statistics of the fast motion, expressing the Hamiltonian as a functional determinant on a space of functions that depend both on time and velocity, using the Szegö–Widom theorem to reduce this functional determinant to a simpler one on a space of functions that depend on velocity only, and finally computing explicitly those determinants on the space of functions that depend on velocity only.

The key point of this work is to establish large deviation principles for particle systems with Hamiltonian dynamics. At first sight it might seem surprising to obtain a stochastic process for an effective kinetic description, starting from a deterministic dynamics. However it is well known that, after taking the limit with an infinite time scale separation between the slow and fast degrees of freedom, the effective dynamics of a slow-fast dynamical system, with chaotic fast degrees of freedom, is stochastic. At the level of large deviations, for deterministic dynamical systems, mathematicians have proven theorems that establish large deviation principles for the effective stochastic process of the slow variable, from natural hypotheses [140, 141]. This behavior can also be illustrated numerically, for instance coupling a slow dynamics with a fast chaotic Lorenz model dynamics [159]. This work, also reported in [106, 107] along with [45, 50, 46] establish the first large deviation principles, in kinetic theory that do not start from stochastic dynamics, like for instance in macroscopic fluctuation theory [32]. While in [45, 46] the result is proven for dilute gases in the Boltzmann–Grad limit for times of order of the collision time, our derivations are not mathematical proofs. All the steps of our derivation are however exact computations, once natural hypothesis are made, in the spirit of the most precise classical works by theoretical physicists in kinetic theory, and the result is expected to be valid for times much larger that the kinetic times.

Our large deviation principle for paths immediately implies a gradient flow structure for the Balescu-Guernsey-Lenard operator, adapting to this specific case the general connection between path large deviation and gradient flows first discussed in [160] and simply explained in section 5 of [50] or section 3.5 of this manuscript. As far as we know, no gradient flow structure was known before for the Balescu-Guernsey-Lenard operator.

The subject of plasma fluctuations is a classical one, see for instance §51 of [150], or chapter 11 of [4], among hundreds of other publications. For instance, the space-time two-point correlations for the fluctuations of the distribution function and potential of a plasma with a non-equilibrium distribution function which is stable for Vlasov dynamics, for times much smaller than the evolution time of the distribution function itself, can be computed either from a Klimontovich approach [150], a truncation of the BBGKY hierarchy [169], or using equipartition of local van Kampen modes [163]. One may wonder

how the present work connects to those classical results. First, as will be clear in section 4.4.2, our derivation starts from the classical formulas for the local in time fluctuations of non-equilibrium stable distributions. Then our approach is fully consistent with the classical results of fluctuations in plasma. However, we address a question of a nature that has never been considered so far: the probability that those local fluctuations lead to a large deviation in the long term evolution of the distribution function. Our main result, the large deviation Hamiltonian that describes the long term path probability for the distribution function, is thus entirely new, as far as we know. It is fully compatible with the classical theories of local fluctuations in plasmas.

In parallel to our results, many mathematical results have been obtained for the kinetic theory of plasma and systems with long range interactions. The derivation of the Vlasov equation from the N particle dynamics had been first proved by Neunzert [168], Braun and Hepp [58] and Dobrushin [94], for interactions through a smooth potential. This question is still under study for interaction potentials with singularities, for instance with the Coulomb interaction (see for instance [125]). Kiessling's review [138] provides a recent report on the mathematical justification of the Vlasov equation from the microscopic dynamics of interacting particles. The stability of stationary states of the Vlasov equation, for describing the dynamics of the empirical measure over time scales that diverge with N, but which are much smaller than the kinetic time, has been proven in [63]. The description of Gaussian fluctuations of the potential, for dynamics close to the Vlasov equilibrium, has been established by Braun and Hepp for smooth interaction potentials, or in the book [192]. More recent works [144, 145, 146, 175, 207, 97] discuss the Gaussian process of the fluctuations of the potential close to a Vlasov solution. A recent proof has been proposed for the the validity of the Balescu-Guernsey-Lenard equation up to time scales of order N^r with $r < 1$ [98].

In section 4.2 we define the Hamiltonian dynamics, as well as the classical kinetic equation that describes the relaxation to equilibrium. In section 4.5, we establish a large deviation principle for the empirical measure using the slow-fast decomposition of the quasilinear dynamics. In section 4.5, we provide an explicit computation of the large deviation Hamiltonian. In section 4.6, we check that this Hamiltonian is fully compatible with the conservation laws of the system, as well as its time-reversal symmetry, and that it is consistent with statistics in the microcanonical ensemble. The main steps of the derivation are summed up in figure 4.1.

4.2. Dynamics of particles with long range interactions

In this section we set up the definitions, and present classical results about the kinetic theory of the dynamics of N particles with long range interactions, in the limit of large N. In section 4.2.1, we define the Hamiltonian dynamics. In section 4.2.2, we introduce the Vlasov equation that describes the evolution of the empirical measure on timescales

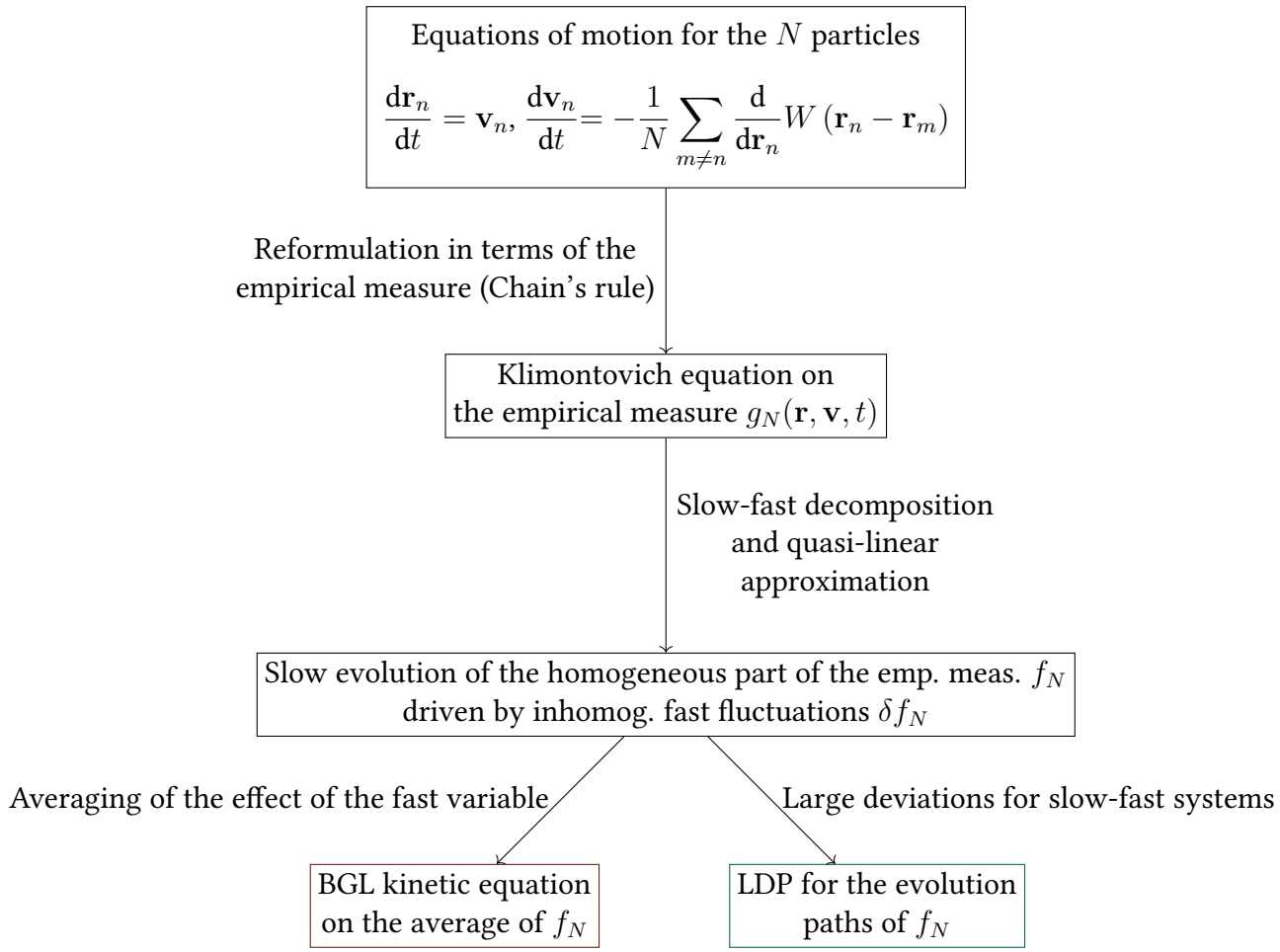


Figure 4.1.: Derivation scheme of the Balescu-Guernsey-Lenard kinetic equation and its associated LDP for the homogeneous part of the empirical measure

of order one. In section 4.2.3, we introduce the Balescu-Guernsey-Lenard equation that describes the long time relaxation of the empirical measure, from Vlasov stationary solutions to the Maxwell-Boltzmann equilibrium distribution, and some of its important physical properties.

4.2.1. Hamiltonian dynamics of N particles with long range interactions

We consider N particles with positions $\{\mathbf{r}_n\}_{1\leq n\leq N}$ and velocities $\{\mathbf{v}_n\}_{1\leq n\leq N}$ governed by a Hamiltonian dynamics

$$\begin{cases} \dfrac{\mathrm{d}\mathbf{r}_n}{\mathrm{d}t} &= \mathbf{v}_n \\ \dfrac{\mathrm{d}\mathbf{v}_n}{\mathrm{d}t} &= -\dfrac{1}{N}\displaystyle\sum_{m\neq n} \frac{\mathrm{d}}{\mathrm{d}\mathbf{r}_n} W\left(\mathbf{r}_n - \mathbf{r}_m\right) \end{cases} \tag{4.5}$$

where the interaction potential $W(\mathbf{r})$ is an even function of $\mathbf{r}$. In the following, we consider that $\mathbf{r}_n$ belongs to a 3-dimensional torus of size L^3, and $\mathbf{v}_n \in \mathbb{R}^3$. We stress that our results are actually valid for any space dimension $d > 1$. We assume that the potential W is a long range potential: the decay of W is slow enough, so that the interaction is dominated by the collective effects of the N particles rather than by local effects. In an infinite space this condition would be met if the potential decays asymptotically like a power law $1/r^d$ or more slowly. This condition is met in many physical systems, for instance self-gravitating systems or weak interacting plasma (with a large plasma parameter). For any finite L, the condition that the potential decays more slowly than $1/r^d$ is a sufficient condition for the potential to be long range.

We call $\mu-$space the $(\mathbf{r}, \mathbf{v})$ space. The $\mu-$space is of dimension 6. Let us define g_N the $\mu-$space empirical measure for the positions and velocities of the N particles

$$g_N(\mathbf{r}, \mathbf{v}, t) = \frac{1}{N}\sum_{n=1}^{N} \delta(\mathbf{r} - \mathbf{r}_n(t))\delta(\mathbf{v} - \mathbf{v}_n(t)).$$

In the following, we will study the stochastic process of the asymptotic dynamics of g_N, as the number of particles N goes to infinity.

4.2.2. The Vlasov equation

From equation (4.5), one immediately obtains the Klimontovich equation

$$\frac{\partial g_N}{\partial t} + \mathbf{v}\cdot\frac{\partial g_N}{\partial \mathbf{r}} - \frac{\partial V\left[g_N\right]}{\partial \mathbf{r}}\cdot\frac{\partial g_N}{\partial \mathbf{v}} = 0, \tag{4.6}$$

where $V[g_N](\mathbf{r}, t) = \int \mathrm{d}\mathbf{v}'\mathrm{d}\mathbf{r}' W(\mathbf{r}-\mathbf{r}')g_N(\mathbf{r}', \mathbf{v}', t)$. This is an exact equation for the evolution of g_N, if W is regular enough. For the Coulomb interaction, the formal equation (4.6) has to be interpreted carefully. In the following, we do not discuss the divergences that might occur related to small scale interactions. At a mathematic level, this would be equivalent to considering a potential which is regularized at small scales, and smooth. The Klimontovich equation (4.6) contains all the information about the trajectories of

the N particles. We would like to build a kinetic theory, that describes the stochastic process for g_N at a mesoscopic level.

An important first result is that the sequence $\{g_N\}$ obeys a law of large numbers when $N \to +\infty$. More precisely, if we assume that there is a set of initial conditions $\{g_N^0\}$ such that $\lim_{N\to+\infty} g_N^0(\mathbf{r},\mathbf{v}) = g^0(\mathbf{r},\mathbf{v})$, then over a finite time interval $t \in [0,T]$, $\lim_{N\to+\infty} g_N(\mathbf{r},\mathbf{v},t) = g(\mathbf{r},\mathbf{v},t)$ where g solves the Vlasov equation

$$\frac{\partial g}{\partial t} + \mathbf{v}\cdot\frac{\partial g}{\partial \mathbf{r}} - \frac{\partial V[g]}{\partial \mathbf{r}}\cdot\frac{\partial g}{\partial \mathbf{v}} = 0 \text{ with } g(\mathbf{r},\mathbf{v},t=0) = g^0(\mathbf{r},\mathbf{v}). \tag{4.7}$$

While the solution of the Klimontonvich equation is a distribution that carries the whole information about the positions and velocities of all the particles, the Vlasov equation describes the evolution of a continuous mesoscopic density for the same dynamics. As the Klimontovich and the Vlasov equations are formally the same, this law of large numbers is actually a stability result for the Vlasov equation in a space of distributions. Such a result has first been proven for smooth potentials by Braun and Hepp [58] , Neunzert [168] and Dobrushin [94].

The Vlasov equation has infinitely many Casimir conserved quantities[4]. As a consequence, it has an infinite number of stable stationary states [213]. Any homogeneous distribution $g(\mathbf{r},\mathbf{v}) = f(\mathbf{v})$ is a stationary solution of the Vlasov equation. In the following, we will consider dynamics close to any homogeneous f which is a linearly stable stationary solution of the Vlasov equation. This linear stability can be assessed by studying the dielectric susceptibility $\varepsilon[f](\mathbf{k},\omega)$ [169, 150], defined by

$$\varepsilon[f](\mathbf{k},\omega) = 1 - \hat{W}(\mathbf{k})\int \mathrm{d}\mathbf{v}\frac{\mathbf{k}.\frac{\partial f}{\partial \mathbf{v}}}{\mathbf{k}.\mathbf{v}-\omega-i\eta}, \tag{4.8}$$

where $\hat{W}(\mathbf{k})$ is the $\mathbf{k}$-th Fourier component of the interaction potential: $\hat{W}(\mathbf{k}) = \int \mathrm{d}\mathbf{r}\,\exp(-i\mathbf{k}.\mathbf{r})\,W(\mathbf{r})$. Equation (4.8) and every other equations involving $\pm i\eta$ have to be understood as the limit as η goes to zero with η positive. The dielectric susceptibility function ε plays the role of a dispersion relation in the linearized dynamics, and a solution f is stable if $\varepsilon[f]$ has no zeros except for ω on the real line. We note that $\varepsilon[f](-\mathbf{k},-\omega) = \varepsilon^*[f](\mathbf{k},\omega)$. Another important property of the dielectric susceptibility is $\varepsilon[I[f]](\mathbf{k},-\omega) = \varepsilon^*[f](\mathbf{k},\omega)$, where $I[f(\mathbf{v})] = f(-\mathbf{v})$. This last property, associated to the time-reversal symmetry of the Hamiltonian dynamics, will be used in section 4.6.2. In this section we have discussed the linear stability of stationary solutions of the Vlasov equation while [213] defines different notions of stability.

From the point of view of dynamical systems, those homogeneous solutions might be attractors of the Vlasov equation, with some sort of asymptotic stability. At a linear level, this convergence for some of the observables, for instance the potential, is called Landau damping [169, 150]. Such a stability might also be true for the full dynamics. Indeed some non-linear Landau damping results have recently been proven [164].

[4] We say that $C[g](t) = \int \mathrm{d}\mathbf{r}\mathrm{d}\mathbf{v}\, c[g(\mathbf{r},\mathbf{v},t)]$ is a Casimir conserved quantity for the Vlasov equation if $\mathrm{d}C[g]/\mathrm{d}t = 0$, when g evolves according to the Vlasov equation.

In the following we will study the dynamics of g_N, when its initial condition is close to a homogeneous stable state $f(\mathbf{v})$. On time scales of order one, the distribution is stable and remains close to f according to the Vlasov equation. However a slow evolution occurs on a timescale τ of order N, in spaces of dimension $d > 1$. For this reason, such f are called quasi-stationary states [213]. In the following section, we explain that this slow evolution is described by the Balescu-Guernsey-Lenard equation for most initial conditions.

As a conclusion, the Balescu-Guernsey-Lenard equation appears as a mesoscopic description of the solution of the Klimontovich equation, for homogeneous solutions, which is valid up to time scales of order N, while the Vlasov equation is valid only up to time scales of order one. The Balescu-Guernsey-Lenard equation is a crucial correction to the Vlasov equation close to homogeneous solutions. Indeed homogeneous solution have no evolution through the Vlasov equation as they are stationary, while they have an evolution of order one over times scales of order N through the Balescu-Guernsey-Lenard equation.

4.2.3. The Balescu-Guernsey-Lenard equation

With the rescaling of time $\tau = t/N$, we expect a law of large numbers in the sense that "for almost all initial conditions" the empirical measure g_N converges to f, with f that evolves according to the Balescu-Guernsey-Lenard equation

$$\frac{\partial f}{\partial \tau} = \frac{\partial}{\partial \mathbf{v}}. \int \mathrm{d}\mathbf{v}_2 \, \mathbf{B}\left[f\right](\mathbf{v}, \mathbf{v}_2) \left(-\frac{\partial f}{\partial \mathbf{v}_2} f(\mathbf{v}) + f(\mathbf{v}_2) \frac{\partial f}{\partial \mathbf{v}} \right), \tag{4.9}$$

with

$$\mathbf{B}\left[f\right](\mathbf{v}_1, \mathbf{v}_2) = \frac{\pi}{L^3} \int_{-\infty}^{+\infty} \mathrm{d}\omega \sum_{\mathbf{k} \in (2\pi/L)\mathbb{Z}^3} \frac{\hat{W}\left(\mathbf{k}\right)^2 \mathbf{k}\mathbf{k}}{\left|\varepsilon[f]\left(\mathbf{k}, \omega\right)\right|^2} \delta\left(\omega - \mathbf{k}.\mathbf{v}_1\right) \delta\left(\omega - \mathbf{k}.\mathbf{v}_2\right), \tag{4.10}$$

where $\mathbf{k}\mathbf{k}$ denotes the tensor product $\mathbf{k} \otimes \mathbf{k}$. The tensor $\mathbf{B}$ is called the collision kernel of the Balescu-Guernsey-Lenard equation (by analogy with the Boltzmann equation).

A recent proof has been proposed for the the validity of the Balescu-Guernsey-Lenard equation up to time scales t of order N^r with $r < 1$ [98]. We know no mathematical proof of such a result for time scales t of order N (τ of order one). In the theoretical physics literature, this equation is derived as an exact consequence of the dynamics once natural hypotheses are made. Two classes of derivations are known, either the BBGKY hierarchy detailed in [169] or the Klimontovich approach presented for instance in [150]. The Klimontovich derivation is the more straightforward from a technical point of view. We now recall the main steps of the Klimontovich derivation, that will be useful later.

In the following we will consider statistical averages over measures of initial conditions for the N particle initial conditions $\{\mathbf{r}_n^0, \mathbf{v}_n^0\}$. We denote $\mathbb{E}_S$ the average with

respect to this measure of initial conditions. As an example the measure of initial conditions could be the product measure $\prod_{n=1}^{N} g^0\left(\mathbf{r}_n^0, \mathbf{v}_n^0\right) \mathrm{d}\mathbf{r}_n \mathrm{d}\mathbf{v}_n$. But we might consider other measures of initial conditions. We assume that for the statistical ensemble of initial conditions, the law of large numbers $\lim_{N\to\infty} g_N^0\left(\mathbf{r}, \mathbf{v}\right) = g^0\left(\mathbf{r}, \mathbf{v}\right)$ is valid at the initial time. This is true for instance for the product measure. In the following, for simplicity, we restrict the discussion to cases when the initial conditions are statistically homogenous: $g^0\left(\mathbf{r}, \mathbf{v}\right) = P^0(\mathbf{v})$. In the following, we define f as the statistical average of g_N over the initial conditions $f(\mathbf{v}, t) = \mathbb{E}_S\left(g_N(\mathbf{r}, \mathbf{v}, t)\right)$.

We define the fluctuations δg_N by $g_N(\mathbf{r}, \mathbf{v}, t) = f(\mathbf{v}) + \delta g_N/\sqrt{N}$. The scaling $1/\sqrt{N}$ is natural when we see the Vlasov equation (4.7) as a law of large numbers for the empirical measure. For the potential we obtain $V\left[g_N\right] = V\left[\delta g_N\right]/\sqrt{N}$, as f is homogeneous. If we introduce this decomposition in the Klimontovich equation (4.6), we obtain

$$\frac{\partial f}{\partial t} = \frac{1}{N}\mathbb{E}_S\left(\frac{\partial V\left[\delta g_N\right]}{\partial \mathbf{r}} \cdot \frac{\partial \delta g_N}{\partial \mathbf{v}}\right), \tag{4.11}$$

$$\frac{\partial \delta g_N}{\partial t} + \mathbf{v} \cdot \frac{\partial \delta g_N}{\partial \mathbf{r}} - \frac{\partial V\left[\delta g_N\right]}{\partial \mathbf{r}} \cdot \frac{\partial f}{\partial \mathbf{v}} = \frac{1}{\sqrt{N}}\left[\frac{\partial V\left[\delta g_N\right]}{\partial \mathbf{r}} \cdot \frac{\partial \delta g_N}{\partial \mathbf{v}} - \mathbb{E}_S\left(\frac{\partial V\left[\delta g_N\right]}{\partial \mathbf{r}} \cdot \frac{\partial \delta g_N}{\partial \mathbf{v}}\right)\right]. \tag{4.12}$$

In the first equation, the right hand side of the equation $\frac{1}{N}\mathbb{E}_S\left(\frac{\partial V[\delta g_N]}{\partial \mathbf{r}} \cdot \frac{\partial \delta g_N}{\partial \mathbf{v}}\right)$ is called the averaged non linear term and is responsible for the long term evolution of the distribution f. The right hand side of the second equation $\frac{1}{\sqrt{N}}\left[\frac{\partial V[\delta g_N]}{\partial \mathbf{r}} \cdot \frac{\partial \delta g_N}{\partial \mathbf{v}} - \mathbb{E}_S\left(\frac{\partial V[\delta g_N]}{\partial \mathbf{r}} \cdot \frac{\partial \delta g_N}{\partial \mathbf{v}}\right)\right]$ describes the fluctuations of the non-linear term. For stable distributions f, and on timescales much smaller than $\sqrt{N}$, we can neglect this term, following Klimontovich and classical textbooks [150]. Please see [63] for a mathematical proof of a sufficient condition of stability on time scales of order N^α, for some $\alpha < 1$. Neglecting the terms much smaller than $\sqrt{N}$ closes the hierarchy of the correlation functions. The Bogoliubov approximation then amounts to using the time scale separation between the evolution of f and δg_N. Then for fixed f, the equation for δg_N (4.12) is linear when f is fixed. One computes the correlation function $\mathbb{E}_S\left(\frac{\partial V[\delta g_N]}{\partial \mathbf{r}} \cdot \frac{\partial \delta g_N}{\partial \mathbf{v}}\right)$ resulting from (4.12) with fixed f, and argues that this two point correlation function converges to a stationary quantity on time scales much smaller than $\sqrt{N}$. Using this quasi-stationary correlation function $\mathbb{E}_S\left(\frac{\partial V[\delta g_N]}{\partial \mathbf{r}} \cdot \frac{\partial \delta g_N}{\partial \mathbf{v}}\right)$, one can compute the right hand side of (4.11) as a function of f.

After time rescaling $\tau = t/N$, we define $g_N^s\left(\mathbf{r}, \mathbf{v}, \tau\right) = g_N\left(\mathbf{r}, \mathbf{v}, N\tau\right)$. By abuse of notation and for convenience, we still denote $g_N^s(\tau) = g_N(\tau)$. The closed equation for $g_N(\tau)$, which is obtained from (4.11) is the Balescu-Guernsey-Lenard equation (4.9). We do not reproduce these lengthy and classical computations that can be found in plasma physics textbooks, for instance in Chapter 51 of [150]. A natural conjecture is that we have a law of large numbers $\lim_{N\to\infty} g_N\left(\mathbf{r}, \mathbf{v}, \tau\right) = f(\mathbf{v}, \tau)$, where f solves the Balescu-Guernsey-Lenard equation (4.9), and valid for any finite time τ.

Symmetries and conservation properties. The Balescu-Guernsey-Lenard equation (4.9) has several important physical properties:

1. It conserves the mass $M[f]$, momentum $\mathbf{P}[f]$ and total kinetic energy $E[f]$ defined by

$$M[f] = \int \mathrm{d}\mathbf{v}\, f(\mathbf{v}), \quad \mathbf{P}[f] = \int \mathrm{d}\mathbf{v}\, \mathbf{v} f(\mathbf{v}) \quad \text{and} \quad E[f] = \int \mathrm{d}\mathbf{v}\, \frac{\mathbf{v}^2}{2} f(\mathbf{v}). \tag{4.13}$$

2. It increases monotonically the entropy $S[f]$ defined by

$$S[f] = -k_B \int \mathrm{d}\mathbf{v}\, f(\mathbf{v}) \log f(\mathbf{v}), \tag{4.14}$$

   where k_B is the Boltzmann constant.

3. It converges towards the Boltzmann distribution for the corresponding energy

$$f_B(\mathbf{v}) = \frac{\beta^{3/2}}{(2\pi)^{3/2}} \exp\left(-\beta \frac{\mathbf{v}^2}{2}\right).$$

4.2.4. The Balescu-Guernsey-Lenard equation as a non-linear Fokker-Planck equations

It is possible to consider the Balescu-Guernsey-Lenard as a non-linear Fokker-Planck equation. Indeed, introducing the drift and the diffusion terms

$$\begin{cases} \mathbf{b}[f](\mathbf{v}) &= \int \mathrm{d}\mathbf{v}_2 \mathbf{B}[f](\mathbf{v}, \mathbf{v}_2) \frac{\partial f}{\partial \mathbf{v}_2} \\ \mathbf{D}[f](\mathbf{v}) &= \int \mathrm{d}\mathbf{v}_2 \mathbf{B}[f](\mathbf{v}, \mathbf{v}_2) f(\mathbf{v}_2), \end{cases} \tag{4.15}$$

the Balescu-Guernsey-Lenard equation writes

$$\frac{\partial f}{\partial t} = \frac{\partial}{\partial \mathbf{v}} \left\{ -f \mathbf{b}[f] + \mathbf{D}[f] \frac{\partial f}{\partial \mathbf{v}} \right\}. \tag{4.16}$$

This is the functional form of a Fokker-Planck equation, but by contrast with the linear Fokker-Planck equation with constant drift and diffusion coefficient, the drift and diffusion coefficients depend on f.

As noticed in section 3.7.1.3, this equation could be obtained from the dynamics of N particles governed by the Ito diffusion

$$\mathrm{d}\mathbf{v}_n = \mathbf{b}[f_N](\mathbf{v}_n)\, \mathrm{d}t + \frac{\partial}{\partial \mathbf{v}} . \mathbf{D}[f_N](\mathbf{v}_n)\, \mathrm{d}t + \sqrt{2}\sigma[f_N](\mathbf{v}_n)\, \mathrm{d}W_{n,t}, \tag{4.17}$$

with

$$f_N(\mathbf{v},t) = \frac{1}{NL^3}\sum_{n=1}^{N}\delta\left(\mathbf{v}_n(t)-\mathbf{v}\right), \tag{4.18}$$

where σ is such that $\mathbf{D}[f_N](\mathbf{v}_n) = \sigma[f_N](\mathbf{v}_n)\,\sigma[f_N](\mathbf{v}_n)^\top$, and $W_{n,t}$ are Wiener processes that satisfy $\mathbb{E}\left(\mathrm{d}W_{m,t}\mathrm{d}W_{n,t'}\right) = \delta_{m,n}\delta\left(t'-t\right)\mathrm{d}t$. In this equation, the drift and diffusion coefficients $\mathbf{b}[f_N]$ and $\mathbf{D}[f_N]$ and the matrix σ depend on a mean field way on the empirical measure f_N.

The law of large numbers for the empirical measure f_N for these N particles with mean field coupling insures that $\lim_{N\to\infty} f_N = f$ where f satisfies the Balescu-Guernsey-Lenard equation (4.16). From this remark, a natural question is whether the dynamical large deviations for the empirical measure f_N in (4.17-4.18) are the same as the dynamical large deviations of N particles undergoing the Hamiltonian dynamics (4.5) (the large deviation of the Balescu-Guernsey-Lenard equation). We discuss this hypothesis in the following section.

4.3. Large deviations for N diffusions with mean field coupling

The aim of this section is to address the following question: are the dynamical large deviations for the empirical measure f_N in (4.17) the same as the dynamical large deviations of N particles with mean field interactions (the large deviations for the Balescu-Guernsey-Lenard equation)?

In section 3.7.1.3 of chapter 3 we discussed the large deviations associated with N particles diffusing in velocity space with mean-field coupled drift and diffusion parameters. We proved that with the prescription that $f_N(t=0)$ is in the neighborhood of $f(t=0)$

$$\mathbb{P}\left(\{f_N(t)\}_{0\le t\le T} = \{f(t)\}_{0\le t\le T}\right) \underset{N\to\infty}{\asymp} \mathrm{e}^{-NL^3 \mathrm{Sup}_p \int_0^T \left\{\int \mathrm{d}\mathbf{v}\, \dot{f}p - H_{MF,h}[f,p]\right\}}, \tag{4.19}$$

where

$$H_{MF,h}[f,p] = \int \mathrm{d}\mathbf{v}\, f\left\{\mathbf{b}[f].\frac{\partial p}{\partial \mathbf{v}} + \frac{\partial}{\partial \mathbf{v}}\left(\mathbf{D}[f]\frac{\partial p}{\partial \mathbf{v}}\right) + \mathbf{D}[f] : \frac{\partial p}{\partial \mathbf{v}}\frac{\partial p}{\partial \mathbf{v}}\right\}. \tag{4.20}$$

More precisely, the result stated above is an instance of the discussion of section 3.7.1.3 in the special case where there is no spatial dynamics nor dependence on the position of the distribution function. The velocity empirical measure (4.18) is renormalized by the volume of the system because it is interpreted as distribution on the μ-space of a homogeneous system rather than a velocity distribution.

Even though the most probable evolution path of the empirical measure associated with the Hamiltonian (4.20) is the Balescu-Guernsey-Lenard equation (see paragraph 3.7.1.3), it cannot describe the large deviations for the empirical measure of particles undergoing the Hamiltonian dynamics (4.5). First, the Hamiltonian (4.20) is not consistent

with the conservation of momentum and energy expected for the dynamics (4.5). From 10. in section 3.4, we know that if $C[f]$ is a conserved quantity of the dynamics, the following symmetry of the large deviation Hamiltonian should hold

$$\int \mathrm{d}\mathbf{v}\, \frac{\delta C}{\delta f} \frac{\delta H_{MF,h}}{\delta p} = 0.$$

From there, we note that momentum $\mathbf{P}[f] = \int \mathrm{d}\mathbf{v}\, \mathbf{v} f(\mathbf{v})$ and kinetic energy $E[f] = \int \mathrm{d}\mathbf{v}\, \frac{\mathbf{v}^2}{2} f(\mathbf{v})$ conservations are not consistent with the Hamiltonian (4.20). This means that evolution paths of the empirical measure that do not conserve total momentum and kinetic energy could have non-zero probability from the large deviation principle (4.19). As a consequence it cannot be a good large deviation description of the Hamiltonian dynamics (4.5). Of course, this is not surprising since the stochastic dynamics (4.17) from which we derive the Hamiltonian (4.20) does not conserve momentum or energy.

4.4. Derivation of the large deviation principle from the quasi-linear dynamics

In this section, we derive a large deviation principle for the empirical measure of N particles with long range interactions, directly from the dynamics (4.5).

In section 4.4.1, we introduce the quasi-linear dynamics of the empirical measure of N long range interacting particles, for which the law of large numbers is the Balescu-Guernsey-Lenard kinetic theory. In section 4.4.1, we explain that this quasi-linear dynamics for the empirical measure can be seen as a slow-fast system, for which we can define the path large deviation functional for the slow variable. In section 4.4.2, we characterize the stochastic process for the quasi-linear dynamics of the fluctuations of the empirical measure as a stationary Gaussian process.

4.4.1. The Klimontovich approach, quasilinear and slow-fast dynamics

We begin by equations which are similar to (4.11-4.12), but by contrast to the discussion of the previous section, we will not compute just the average for the effect of fluctuations on the evolution of f_N, but all the cumulants after time averaging.

We consider the empirical measure

$$g_N(\mathbf{r}, \mathbf{v}, t) = \frac{1}{N} \sum_{n=1}^{N} \delta(\mathbf{v} - \mathbf{v}_n(t)) \delta(\mathbf{r} - \mathbf{r}_n(t)),$$

of N particles which interact through a long range pair potential according to the dynamics (4.5). From these equations of motion, we can deduce the Klimontovich equation

$$\frac{\partial g_N}{\partial t} + \mathbf{v} \cdot \frac{\partial g_N}{\partial \mathbf{r}} - \frac{\partial V[g_N]}{\partial \mathbf{r}} \cdot \frac{\partial g_N}{\partial \mathbf{v}} = 0. \tag{4.21}$$

We consider the decomposition

$$g_N(\mathbf{r},\mathbf{v},t) = f_N(\mathbf{v}) + \frac{1}{\sqrt{N}}\delta g_N(\mathbf{r},\mathbf{v},t),$$

where $f_N(\mathbf{v},t) = \frac{1}{L^3}\int \mathrm{d}\mathbf{r}\, g_N(\mathbf{r},\mathbf{v},t)$ is the projection of g_N on homogeneous distributions (distributions that depend on velocity only) and δg_N describes the inhomogeneous fluctuations of the empirical measure g_N. Alternatively, we can understand f_N as the empirical measure of the N particles in the velocity space:

$$f_N(\mathbf{r},\mathbf{v},t) = \frac{1}{NL^3}\sum_{n=1}^{N}\delta(\mathbf{v}-\mathbf{v}_n(t)).$$

From the Klimontovich equation (4.21), we straightforwardly write

$$\frac{\partial f_N}{\partial t} = \frac{1}{NL^3}\int \mathrm{d}\mathbf{r}\left(\frac{\partial V[\delta g_N]}{\partial \mathbf{r}}.\frac{\partial \delta g_N}{\partial \mathbf{v}}\right), \tag{4.22}$$

$$\frac{\partial \delta g_N}{\partial t} = -\mathbf{v}.\frac{\partial \delta g_N}{\partial \mathbf{r}} + \frac{\partial V[\delta g_N]}{\partial \mathbf{r}}.\frac{\partial f_N}{\partial \mathbf{v}} \tag{4.23}$$

$$+\frac{1}{\sqrt{N}}\left[\frac{\partial V[\delta g_N]}{\partial \mathbf{r}}.\frac{\partial \delta g_N}{\partial \mathbf{v}} - \frac{1}{L^3}\int \mathrm{d}\mathbf{r}\left(\frac{\partial V[\delta g_N]}{\partial \mathbf{r}}.\frac{\partial \delta g_N}{\partial \mathbf{v}}\right)\right]. \tag{4.24}$$

Just like in the section 4.2.2, we will consider statistical averages over a probability measure for the initial conditions $\{\mathbf{r}_n^0,\mathbf{v}_n^0\}$ of the N particles. As the microscopic dynamics is deterministic, the only source of randomness is the ensemble of initial conditions. We assume that this ensemble of initial conditions is sampled from a spatially homogeneous measure and that the set of corresponding g_N is concentrated close to homogeneous distributions in the $(\mathbf{r},\mathbf{v})$ space. Moreover we assume that the large deviation principle

$$\mathbb{P}\left(f_N(t=0)=f^0\right) \underset{N\to\infty}{\asymp} \mathrm{e}^{-NI_0[f^0]}, \tag{4.25}$$

holds, where I_0 is a large deviation rate function for $f_N(\tau=0)$ the initial conditions of f_N. As an example, the measure of initial conditions $\{\mathbf{r}_n^0,\mathbf{v}_n^0\}$ could be the homogeneous product measure $\prod_{n=1}^{N} P^0(\mathbf{v}_n^0)\,\mathrm{d}\mathbf{v}_n\mathrm{d}\mathbf{r}_n/L^3$, with $\int \mathrm{d}\mathbf{v}P^0(\mathbf{v}) = 1$. Then I_0 would then be the Kullback–Leibler divergence of f^0 with respect to P^0. But we might consider other ensembles of initial conditions.

We now assume the validity of the quasi-linear approximation[5], which amounts to neglecting terms of order $N^{-1/2}$ in the evolution equation for δg_N. We also change the timescale $\tau = t/N$ and obtain the quasilinear dynamics

$$\frac{\partial f_N}{\partial \tau} = \frac{1}{L^3}\int \mathrm{d}\mathbf{r}\left(\frac{\partial V[\delta g_N]}{\partial \mathbf{r}}.\frac{\partial \delta g_N}{\partial \mathbf{v}}\right), \tag{4.26}$$

$$\frac{\partial \delta g_N}{\partial \tau} = N\left\{-\mathbf{v}.\frac{\partial \delta g_N}{\partial \mathbf{r}} + \frac{\partial V[\delta g_N]}{\partial \mathbf{r}}.\frac{\partial f_N}{\partial \mathbf{v}}\right\}. \tag{4.27}$$

[5]It is still an open question to justify the validity of this approximation at the level of the large deviations.

When N goes to infinity, we observe that the equation for δg_N is a fast process, with timescales for τ of order $1/N$, while the equation for f_N is a slow one with timescales for τ of order 1. For such slow-fast dynamics, it is natural to consider f_N fixed (frozen) in equation (4.27) on time scales for τ of order $1/N$. For fixed f_N the dynamics for δg_N is linear and can be solved. Computing then the average of the term $\int \mathrm{d}\mathbf{r}\, \frac{\partial V[\delta g_N]}{\partial \mathbf{r}}.\frac{\partial \delta g_N}{\partial \mathbf{v}}$, for the asymptotic process for δg_N for fixed f_N leads to the Guernsey–Lenard–Balescu equation, as explained in section 4.2.3. Those computation can be found in classical textbooks [150].

In the following we want to go beyond these classical computations, by estimating not just the average of the right hand side in (4.22), $\int \mathrm{d}\mathbf{r}\, \frac{\partial V[\delta g_N]}{\partial \mathbf{r}}.\frac{\partial \delta g_N}{\partial \mathbf{v}}$, but all the cumulants of the time averages $\int_0^{\Delta T} \int \mathrm{d}\mathbf{r}\, \frac{\partial V[\delta g_N]}{\partial \mathbf{r}}.\frac{\partial \delta g_N}{\partial \mathbf{v}}$ in order to describe the large deviations for the process f_N. For slow-fast dynamics, the theory for the large deviations of the effective evolution of the slow variable is a classical one both in theoretical physics (see for instance [51]) and mathematics. In the mathematics literature, it is for instance treated for diffusions [115, 208], or chaotic deterministic systems [140, 141]. The result for the path large deviations for the slow dynamics is explained in section 3.6.2 (see equations (3.28-3.30)). After rescaling time $\tau = t/N$, we then have

$$\mathbf{P}\left(\{f_N(\mathbf{v},\tau)\}_{0\leq\tau\leq T} = \{f(\mathbf{v},\tau)\}_{0\leq\tau\leq T}\right) \underset{N\to\infty}{\asymp} \mathrm{e}^{-NL^3 \mathrm{Sup}_p \int_0^T \mathrm{d}\tau \left\{\int \mathrm{d}\mathbf{v}\, \dot{f}p - H_{\mathrm{BGL}}[f,p]\right\}} \mathrm{e}^{-NI_0[f_0]}, \tag{4.28}$$

where I_0 is a large deviation rate function for the initial conditions of f_N, see equation (4.25), and with

$$H_{\mathrm{BGL}}[f,p] = \lim_{T\to\infty} \frac{1}{TL^3} \log \mathbb{E}_f \left[\exp\left(\int_0^T \mathrm{d}t \int \mathrm{d}\mathbf{v}\, p(\mathbf{v}) \int \mathrm{d}\mathbf{r}' \frac{\partial V[\delta g_N]}{\partial \mathbf{r}'}.\frac{\partial \delta g_N}{\partial \mathbf{v}}\right)\right] \tag{4.29}$$

and where $\mathbb{E}_f$ denotes the expectation on the process for δg_N, evolving according to

$$\frac{\partial \delta g_N}{\partial t} = -\mathbf{v}.\frac{\partial \delta g_N}{\partial \mathbf{r}} + \frac{\partial V[\delta g_N]}{\partial \mathbf{r}}.\frac{\partial f}{\partial \mathbf{v}}. \tag{4.30}$$

In this equation, $f_N = f$ is fixed and time independent. We note that the classical mathematical results to justify (4.29) would require to prove mixing properties for the fast process, and stability of the invariant measure, that nobody has proven yet for (4.30).

We note that to obtain equation (4.29) from equation (3.30), we have considered f_N as a function of the μ-space. Then the conjugated momentum $p(\mathbf{r},\mathbf{v})$ should also be a function of the μ-space and the scalar product be the one of the μ-space. However, recognizing that for homogeneous f, p should also be homogeneous ($p(\mathbf{r},\mathbf{v}) = p(\mathbf{v})$), and performing trivial integration over $\mathbf{r}$ leads to (4.29). The L^3 factor in the large deviation principle (4.28) also comes from a trivial integration over $\mathbf{r}$ of $\dot{f}p$. In the definition of H, in (4.29) we have divided the scaled cumulant generating function by L^3 for convenience, such that the action in (4.28) appears as a natural action for homogeneous distributions.

The goal of the following sections and the contribution of this work is to obtain an explicit expression for (4.29).

4.4.2. The quasi-stationary Gaussian process for δg_N

In order to compute (4.29), we need to estimate averages over the stochastic process which corresponds to generic sets of initial condition for δg_N, and where δg_N satisfies equation (4.30). We first note that for fixed f, equation (4.30) is linear. If the set of initial conditions for $\delta g_N(t=0)$ is a Gaussian random variable, then the stochastic process $\{\delta g_N(t)\}_{t\geq 0}$ will be a Gaussian process. Several mathematical works [144, 145, 146, 175, 207, 97] discuss some properties of the Gaussian process of the fluctuations close to a Vlasov solution. For instance [146] proves that, when starting from sets of Gaussian initial conditions of the form of relevant central limit theorems, at long times, the stochastic process converges to a statistically *stationary* Gaussian process. The fact that for generic sets of initial conditions, the stochastic process of the fluctuations δg_N converges to a stochastically stationary process, which is independent of the initial conditions, has long been understood by physicists. This is for instance explained in §51 of [150], where the asymptotic stationary process is precisely characterized. This striking convergence result, despite the lack of dissipation in the equation for δg_N, is related to the Landau damping and the fact that we deal with particle systems. The work [49] derives another characterization of this stationary process, based on an integral equation, and illustrates numerically the convergence. In the following we will thus consider averages in equation (4.29) as averages over this stationary Gaussian process. Such stationary averages are denoted $\mathbb{E}_S$.

We do not reproduce the classical and lengthy computations of the correlation functions of this stationary process, but just report the formulas which can be found for instance in §51 of [150]. The potential autocorrelation function is homogeneous because of the space translation symmetry. Then

$$\mathbb{E}_S\left(V\left[\delta g_N\right](\mathbf{r}_1,t_1)\,V\left[\delta g_N\right](\mathbf{r}_2,t_2)\right)=\mathcal{C}_{VV}\left(\mathbf{r}_1-\mathbf{r}_2,t_1-t_2\right),$$

We define $\tilde{\varphi}$ the space-time Fourier transform of a function φ as

$$\tilde{\varphi}\left(\mathbf{k},\omega\right)=\int_{[0,L]^3}\mathrm{d}\mathbf{r}\int_{-\infty}^{\infty}\mathrm{d}t\,\mathrm{e}^{-i(\mathbf{k}.\mathbf{r}-\omega t)}\varphi\left(\mathbf{r},t\right), \tag{4.31}$$

following the same convention as in [150]. According to equation (51.20), §51 of [150], with the identification $V=e\phi$ and $\hat{W}(k)=4\pi e^2/k^2$, the space-time Fourier transform of the autocorrelation function of the potential then reads

$$\widetilde{\mathcal{C}_{VV}}\left(\mathbf{k},\omega\right)=2\pi\left[\int\mathrm{d}\mathbf{v}'\,f\left(\mathbf{v}'\right)\delta\left(\omega-\mathbf{k}.\mathbf{v}'\right)\right]\frac{\hat{W}(\mathbf{k})^2}{\left|\varepsilon\left[f\right](\mathbf{k},\omega)\right|^2}. \tag{4.32}$$

Similarly the time stationary correlation function between the potential and distribution fluctuation is space-time homogeneous

$$\mathbb{E}_S\left(V\left[\delta g_N\right](\mathbf{r}_1,t_1)\,\delta g_N\left(\mathbf{r}_2,\mathbf{v},t_2\right)\right)=\mathcal{C}_{VG}\left(\mathbf{r}_1-\mathbf{r}_2,t_1-t_2,\mathbf{v}\right).$$

According to equation (51.21) of [150], its space-time Fourier transform reads

$$\widetilde{\mathcal{C}_{VG}}\left(\mathbf{k},\omega,\mathbf{v}\right)=-\frac{\mathbf{k}}{\omega-\mathbf{k}.\mathbf{v}-i\eta}.\frac{\partial f}{\partial\mathbf{v}}\left(\mathbf{v}\right)\widetilde{\mathcal{C}_{VV}}\left(\mathbf{k},\omega\right)+2\pi\frac{\hat{W}\left(\mathbf{k}\right)}{\varepsilon\left[f\right](\mathbf{k},\omega)}f\left(\mathbf{v}\right)\delta\left(\omega-\mathbf{k}.\mathbf{v}\right).$$

(4.33)

We also define the autocorrelation function of the distribution fluctuations

$$\mathbb{E}_S\left(\delta g_N\left(\mathbf{r}_1,\mathbf{v}_1,t_1\right)\delta g_N\left(\mathbf{r}_2,\mathbf{v}_2,t_2\right)\right)=\mathcal{C}_{GG}\left(\mathbf{r}_1-\mathbf{r}_2,t_1-t_2,\mathbf{v}_1,\mathbf{v}_2\right).$$

According to equation (51.23) of [150], its space-time Fourier transform reads

$$\begin{aligned}\widetilde{\mathcal{C}_{GG}}\left(\mathbf{k},\omega,\mathbf{v}_1,\mathbf{v}_2\right) &= 2\pi\delta\left(\mathbf{v}_1-\mathbf{v}_2\right)f\left(\mathbf{v}_1\right)\delta\left(\omega-\mathbf{k}.\mathbf{v}_1\right) \\ &+ \frac{\widetilde{\mathcal{C}_{VV}}\left(\mathbf{k},\omega\right)}{\left(\omega-\mathbf{k}.\mathbf{v}_1+i\eta\right)\left(\omega-\mathbf{k}.\mathbf{v}_2-i\eta\right)}\mathbf{k}.\frac{\partial f}{\partial\mathbf{v}}\left(\mathbf{v}_1\right)\mathbf{k}.\frac{\partial f}{\partial\mathbf{v}}\left(\mathbf{v}_2\right) \\ &- 2\pi\hat{W}(\mathbf{k})\mathbf{k}.\frac{\partial f}{\partial\mathbf{v}}\left(\mathbf{v}_1\right)\frac{f(\mathbf{v}_2)\delta\left(\omega-\mathbf{k}.\mathbf{v}_2\right)}{\varepsilon\left(\mathbf{k},\omega\right)\left(\omega-\mathbf{k}.\mathbf{v}_1+i\eta\right)} \\ &- 2\pi\hat{W}(\mathbf{k})\mathbf{k}.\frac{\partial f}{\partial\mathbf{v}}\left(\mathbf{v}_2\right)\frac{f(\mathbf{v}_1)\delta\left(\omega-\mathbf{k}.\mathbf{v}_1\right)}{\varepsilon^*\left(\mathbf{k},\omega\right)\left(\omega-\mathbf{k}.\mathbf{v}_2-i\eta\right)}.\end{aligned} \tag{4.34}$$

We note that the order in the correlation functions for V and g_N matters. We have

$$\mathbb{E}_S\left(\delta g_N\left(\mathbf{r}_1,\mathbf{v},t_1\right)V\left[\delta g_N\right]\left(\mathbf{r}_2,t_2\right)\right)=\mathcal{C}_{GV}\left(\mathbf{r}_1-\mathbf{r}_2,t_1-t_2,\mathbf{v}\right),$$

with

$$\widetilde{\mathcal{C}_{VG}}\left(\mathbf{k},\omega,\mathbf{v}\right)=\widetilde{\mathcal{C}_{GV}}\left(-\mathbf{k},-\omega,\mathbf{v}\right)=\widetilde{\mathcal{C}_{GV}}^*\left(\mathbf{k},\omega,\mathbf{v}\right).$$

We also note the symmetry property for $\widetilde{\mathcal{C}_{GG}}$: $\widetilde{\mathcal{C}_{GG}}\left(\mathbf{k},\omega,\mathbf{v}_1,\mathbf{v}_2\right)=\widetilde{\mathcal{C}_{GG}}\left(-\mathbf{k},-\omega,\mathbf{v}_2,\mathbf{v}_1\right)$. It is a consequence of the symmetry $\mathcal{C}_{GG}\left(\mathbf{r},t,\mathbf{v}_1,\mathbf{v}_2\right)=\mathcal{C}_{GG}\left(-\mathbf{r},-t,\mathbf{v}_2,\mathbf{v}_1\right)$. Moreover, since C_{GG} is real, we have $\widetilde{\mathcal{C}_{GG}}\left(-\mathbf{k},-\omega,\mathbf{v}_2,\mathbf{v}_1\right)=\widetilde{\mathcal{C}_{GG}}^*\left(\mathbf{k},\omega,\mathbf{v}_2,\mathbf{v}_1\right)$. We thus have the symmetry

$$\widetilde{\mathcal{C}_{GG}}\left(\mathbf{k},\omega,\mathbf{v}_1,\mathbf{v}_2\right)=\widetilde{\mathcal{C}_{GG}}^*\left(\mathbf{k},\omega,\mathbf{v}_2,\mathbf{v}_1\right). \tag{4.35}$$

We note that as a mere consequence of the definition of $V\left[\delta g_N\right]$, we have the following relations between the two-point correlation functions

$$\widetilde{\mathcal{C}_{VG}}\left(\mathbf{k},\omega,\mathbf{v}_1\right)=\hat{W}(\mathbf{k})\int\mathrm{d}\mathbf{v}_2\,\widetilde{\mathcal{C}_{GG}}\left(\mathbf{k},\omega,\mathbf{v}_1,\mathbf{v}_2\right), \tag{4.36}$$

$$\widetilde{\mathcal{C}_{VV}}\left(\mathbf{k},\omega\right)=\left(\hat{W}(\mathbf{k})\right)^2\int\mathrm{d}\mathbf{v}_1\mathrm{d}\mathbf{v}_2\,\widetilde{\mathcal{C}_{GG}}\left(\mathbf{k},\omega,\mathbf{v}_1,\mathbf{v}_2\right). \tag{4.37}$$

4.5. Computation of the large deviation Hamiltonian

In this section, we obtain an explicit formula for the large deviation functional of the empirical measure of N particles with long range interactions, starting from equation (4.29). We noticed in section 4.4.2 that the fluctuations of the homogeneous part empirical measure are described by the average of a quadratic form over a Gaussian stationary process. In section 4.5.1, we explain how this makes the computation of the Hamiltonian (4.29) equivalent to the computation of a functional determinant. In section 4.5.3, this functional determinant is explicitly computed, using the Szegö–Widom theorem and an explicit computation of determinants in the space of observables over velocity distributions.

4.5.1. The large deviation Hamiltonian as a functional Gaussian integral

Within the quasi-linear approximation, the fluctuations of the empirical measure δg_N follow a stationary Gaussian process over functions of the μ-space. The goal of this subsection is to show that the computation of the large deviation Hamiltonian is equivalent to the computation of a Gaussian functional integral of the fluctuations of the empirical measure δg_N.

We consider $\mathcal{H}_{\mathbf{v}}$, the Hilbert space of complex functions over the velocity space, with $\langle .,. \rangle$, the Hermitian product: $\langle a, b \rangle = \int \mathrm{d}\mathbf{v}\, a^* (\mathbf{v})\, b (\mathbf{v})$. We can conveniently express the argument of the exponential in the formula (4.29) for the large deviation Hamiltonian using a spatial Fourier decomposition of the fluctuations of the empirical measure $\delta \hat{g} (\mathbf{k}, \mathbf{v}, t) = \int_{[0,L]^3} \mathrm{d}\mathbf{r}\, \mathrm{e}^{-i\mathbf{k}.\mathbf{r}} \delta g_N (\mathbf{r}, \mathbf{v}, t)$. Using this Fourier decomposition, the definition of the potential $V [\delta g_N]$ and partial integration with respect to the velocity integral, we obtain

$$\int \mathrm{d}\mathbf{v}\, p (\mathbf{v}) \int \mathrm{d}\mathbf{r}' \frac{\partial V [\delta g_N]}{\partial \mathbf{r}'} . \frac{\partial \delta g_N}{\partial \mathbf{v}} = \frac{1}{2} \sum_{\mathbf{k} \in (2\pi/L)\mathbb{Z}^3} \langle \delta \hat{g}_N (\mathbf{k}, \cdot, t)\, , \mathbf{M} (\mathbf{k}) [\delta \hat{g}_N (\mathbf{k}, \cdot, t)] \rangle, \tag{4.38}$$

where we define the Hermitian operator $\mathbf{M} (\mathbf{k})$ acting on $\varphi \in \mathcal{H}_{\mathbf{v}}$ as

$$\mathbf{M} (\mathbf{k}) [\varphi] (\mathbf{v}_1) = \int \mathrm{d}\mathbf{v}_2\, M (\mathbf{k}; \mathbf{v}_1, \mathbf{v}_2)\, \varphi (\mathbf{v}_2)\, , \tag{4.39}$$

with the kernel M defined by

$$M (\mathbf{k}; \mathbf{v}_1, \mathbf{v}_2) = \frac{i}{L^6} \hat{W} (\mathbf{k})\, \mathbf{k} . \left\{ - \frac{\partial p}{\partial \mathbf{v}} (\mathbf{v}_1) + \frac{\partial p}{\partial \mathbf{v}} (\mathbf{v}_2) \right\} . \tag{4.40}$$

There is a factor $1/2$ on the r.h.s. of (4.38) because we chose to symmetrize the expression, such that $M (\mathbf{k}; \mathbf{v}_1, \mathbf{v}_2) = M (\mathbf{k}; \mathbf{v}_2, \mathbf{v}_1)^*$. $\mathbf{M} (\mathbf{k})$ is then an Hermitian operator.

The goal of the following of this subsection is to express the sum on the r.h.s. of (4.38) as a sum of independent terms to make the computation of (4.29) easier. Since for every $\mathbf{k} \in (2\pi/L)\, \mathbb{Z}^3$, $\mathbf{M} (\mathbf{k})$ is an Hermitian operator, $\mathbf{M} (\mathbf{k})^* = \mathbf{M} (-\mathbf{k})$, and

$$\delta \hat{g}_N^* (\mathbf{k}, \cdot, t) = \delta \hat{g}_N (-\mathbf{k}, \cdot, t)\, ,$$

we have the following relation

$$\langle \delta \hat{g}_N (\mathbf{k}, \cdot, t)\, , \mathbf{M} (\mathbf{k}) [\delta \hat{g}_N (\mathbf{k}, \cdot, t)] \rangle = \langle \delta \hat{g}_N (-\mathbf{k}, \cdot, t)\, , \mathbf{M} (-\mathbf{k}) [\delta \hat{g}_N (-\mathbf{k}, \cdot, t)] \rangle. \tag{4.41}$$

This implies that on the r.h.s. of (4.38), the contribution of an index $\mathbf{k} \in (2\pi/L)\, \mathbb{Z}^3$ will be equal to the contribution of its negative $-\mathbf{k}$.

Because the stochastic process $\delta g_N (\mathbf{r}, \cdot, t)$, for the fluctuations of the distribution function is spatially homogeneous, the stochastic process $\delta \hat{g}_N (\mathbf{k}, \cdot, t)$ is statistically mutually

independent with every other $\delta\hat{g}_N(\mathbf{k}',\cdot,t)$ as long as $\mathbf{k}' \neq -\mathbf{k}$. Because $\delta\hat{g}_N(\mathbf{k},\cdot,t)$ is not statistically independent from $\delta\hat{g}_N(-\mathbf{k},\cdot,t)$, it is useful to treat them together. We define $\mathbb{Z}^3_\pm = \mathbb{Z}^3/Z_2$ the quotient of group $\mathbb{Z}^3$ with Z_2, the cyclic group of order 2. In other words, $\mathbb{Z}^3_\pm$ is the set of triplets of integers where we identify a triplet $(a,b,c) \in \mathbb{Z}^3$ with its negative $(-a,-b,-c)$. Then, using (4.41), the sum over $\mathbf{k} \in (2\pi/L)\,\mathbb{Z}^3$ can be rewritten as

$$\frac{1}{2}\sum_{\mathbf{k}\in(2\pi/L)\mathbb{Z}^3} \langle \delta\hat{g}_N(\mathbf{k},\cdot,t)\,, \mathbf{M}(\mathbf{k})\,[\delta\hat{g}_N(\mathbf{k},\cdot,t)]\rangle = \sum_{\mathbf{k}\in(2\pi/L)\mathbb{Z}^3_\pm} \langle \delta\hat{g}_N(\mathbf{k},\cdot,t)\,, \mathbf{M}(\mathbf{k})\,[\delta\hat{g}_N(\mathbf{k},\cdot,t)]\rangle\,. \tag{4.42}$$

As a consequence, the r.h.s of (4.42) is a sum of statistically independent terms. We can then use the fact that the expected value of a product of independent random variables is the product of their expected values, as well as equations (4.38) and (4.42) to obtain

$$\mathbb{E}\left[\exp\left(\int_0^T \mathrm{d}t \int \mathrm{d}\mathbf{v}\, p(\mathbf{v}) \int \mathrm{d}\mathbf{r}' \frac{\partial V[\delta g_N]}{\partial \mathbf{r}'}.\frac{\partial \delta g_N}{\partial \mathbf{v}}\right)\right] = \prod_{\mathbf{k}\in(2\pi/L)\mathbb{Z}^3_\pm} \mathbb{E}\left[\exp\left(\int_0^T \mathrm{d}t\, \langle \delta\hat{g}_N(\mathbf{k},\cdot,t)\,, \mathbf{M}(\mathbf{k})\,[\delta\hat{g}_N(\mathbf{k},\cdot,t)]\rangle\right)\right]. \tag{4.43}$$

We can then go back to (4.29) using (4.41) and (4.43) to express the large deviation Hamiltonian as a sum over the wavevectors

$$H_{\mathrm{BGL}}[f,p] = \sum_{\mathbf{k}\in(2\pi/L)\mathbb{Z}^3} \hat{H}[f,p](\mathbf{k})\,, \tag{4.44}$$

where

$$\hat{H}[f,p](\mathbf{k}) = \lim_{T\to\infty} \frac{1}{2TL^3} \log \mathbb{E}\left[\exp\left(\int_0^T \mathrm{d}t\ \langle \delta\hat{g}_N(\mathbf{k},\cdot,t)\,, \mathbf{M}(\mathbf{k})\,[\delta\hat{g}_N(\mathbf{k},\cdot,t)]\rangle\right)\right]. \tag{4.45}$$

4.5.2. The Szegö–Widom theorem

The computation of (4.44-4.45) requires to estimate large time large deviations of a quadratic functional of a Gaussian stochastic process. More precisely, the Gaussian process involved in (4.45) is the stochastic process of the $\mathbf{k}$-th Fourier mode of the fluctuations of the empirical measure $\delta\hat{g}_N(\mathbf{k},\cdot,t)$, and the quadratic functional is defined by the Hermitian operator $\mathbf{M}(\mathbf{k})$ (4.39). Since $\delta\hat{g}_N(\mathbf{k},\cdot,t)$ is a Gaussian process, it is possible to compute (4.45) via functional determinants. Thanks to the Szegö–Widom theorem, it is possible to evaluate the asymptotics of this Fredholm determinant in terms of much simpler determinants of an operator on $\mathcal{H}_\mathbf{v}$. This program was first implemented in [57], with a nice application to a model inspired by 2D and geophysical turbulence. Here is a simple statement of this theorem in a case where the Hilbert space has a finite dimension.

We first define integral operators on $L^2\left([0,T],\mathbb{C}^n\right)$. We considers maps $\varphi:[0,T]\to\mathbb{C}^n$ and $K:\mathbb{R}\to\mathcal{M}_n\left(\mathbb{C}\right)$, where $\mathcal{M}_n\left(\mathbb{C}\right)$ is the set of $n\times n$ complex matrices. We define the integral operator $\mathbf{K}_T$ by

$$\mathbf{K}_T\varphi\left(t\right)=\int_0^T K\left(t-s\right)\varphi\left(s\right)\mathrm{d}s, \tag{4.46}$$

$\mathbf{K}_T$ is a linear operator of $L^2\left([0,T],\mathbb{C}^n\right)$. K is called the kernel of the operator $\mathbf{K}_T$.

The Szegö–Widom theorem allows to compute large T asymptotics of the logarithm of the Fredholm determinant of the integral operator $\mathrm{Id}+\mathbf{K}_T$. The result is

$$\log\det_{[0,T]}\left(\mathrm{Id}+\mathbf{K}_T\right)\underset{T\to\infty}{\sim}\frac{T}{2\pi}\int\mathrm{d}\omega\,\log\det\left(I_n+\int_{\mathbb{R}}\mathrm{e}^{i\omega t}K\left(t\right)\mathrm{d}t\right), \tag{4.47}$$

where I_n is the $n\times n$ identity matrix. Whereas the determinant on the l.h.s. of this expression, denoted by the subscript $[0,T]$ is a Fredholm determinant, the determinant on the r.h.s. is a matrix determinant which can be more easily computed. Further details about this theorem and its possible applications can be found in [57].

4.5.3. Application of the Szegö-Widom theorem

In appendix A.2 we explain the details of this program for Gaussian processes with complex variables. The result (A.5) of the appendix A.2, adapted to the case where the Hilbert space is $\mathcal{H}_{\mathbf{v}}$, reads

$$\log\mathbb{E}\left[\exp\left(\int_0^T\mathrm{d}t\left\langle\delta\hat{g}_N\left(\mathbf{k},\cdot,t\right),\mathbf{M}\left(\mathbf{k}\right)\left[\delta\hat{g}_N\left(\mathbf{k},\cdot,t\right)\right]\right\rangle\right)\right]\underset{T\to\infty}{\sim}-\frac{T}{2\pi}\int\mathrm{d}\omega\,\log\det_{\mathcal{H}_{\mathbf{v}}}\left(u_{\mathbf{k},\omega}\right), \tag{4.48}$$

where, for any $\mathbf{k}$ and ω, and $\varphi\in\mathcal{H}_{\mathbf{v}}$, $u_{\mathbf{k},\omega}\left[\varphi\right]$ is defined by

$$u_{\mathbf{k},\omega}\left[\varphi\right]\left(\mathbf{v}_1\right)\;=\;\varphi\left(\mathbf{v}_1\right)+\int\mathrm{d}\mathbf{v}_2\mathrm{d}\mathbf{v}_3\,M\left(\mathbf{k};\mathbf{v}_1,\mathbf{v}_2\right)\widetilde{\mathcal{C}_{GG}}\left(\mathbf{k},\omega,\mathbf{v}_2,\mathbf{v}_3\right)\varphi\left(\mathbf{v}_3\right).$$

$u_{\mathbf{k},\omega}$ is a linear operator of $\mathcal{H}_{\mathbf{v}}$. The subscript $\mathcal{H}_{\mathbf{v}}$ in (4.48) indicates that the determinant is a determinant of an operator over $\mathcal{H}_{\mathbf{v}}$. Then, combining equations (4.45) and (4.48) yields

$$\hat{H}\left[f,p\right]\left(\mathbf{k}\right)=-\frac{1}{4\pi L^3}\int\mathrm{d}\omega\,\log\det_{\mathcal{H}_{\mathbf{v}}}\left(u_{\mathbf{k},\omega}\right). \tag{4.49}$$

Our next task to obtain an explicit formula for $\hat{H}\left[f,p\right]\left(\mathbf{k}\right)$ and thus for the full large deviation Hamiltonian H (4.44) is to compute $\det_{\mathcal{H}_{\mathbf{v}}}\left(u_{\mathbf{k},\omega}\right)$. This determinant can be easily

computed once we realize that the range of $u_{\mathbf{k},\omega} - \mathrm{Id}$ is two-dimensional. The explicit computation is performed in appendix A.3. The result reads

$$\det_{\mathcal{H}_{\mathbf{v}}} \left(u_{\mathbf{k},\omega}\right) = 1 - \mathcal{J}\left[f,p\right]\left(\mathbf{k},\omega\right), \tag{4.50}$$

with

$$\begin{aligned}\mathcal{J}\left[f,p\right]\left(\mathbf{k},\omega\right) = -2\int \mathrm{d}\mathbf{v}_1\, \mathbf{k}.\frac{\partial p}{\partial \mathbf{v}_1}\Im\left(\widetilde{\mathcal{C}_{VG}}\left(\mathbf{k},\omega,\mathbf{v}_1\right)\right) \\ - \int \mathrm{d}\mathbf{v}_1\mathrm{d}\mathbf{v}_2\, \mathbf{k}.\frac{\partial p}{\partial \mathbf{v}_1}\mathbf{k}.\frac{\partial p}{\partial \mathbf{v}_2}\left\{\widetilde{\mathcal{C}_{VG}}\left(\mathbf{k},\omega,\mathbf{v}_1\right)\widetilde{\mathcal{C}_{VG}}\left(\mathbf{k},\omega,\mathbf{v}_2\right)^* \right. \\ \left. - \widetilde{\mathcal{C}_{VV}}\left(\mathbf{k},\omega\right)\widetilde{\mathcal{C}_{GG}}\left(\mathbf{k},\omega,\mathbf{v}_1,\mathbf{v}_2\right)\right\}.\end{aligned} \tag{4.51}$$

Using the expressions of the two-point correlation functions (4.32-4.34), we obtain that

$$\mathcal{J}\left[f,p\right] = \mathcal{L}\left[f,p\right] + Q\left[f,p,p\right], \tag{4.52}$$

where $\mathcal{L}$ depends linearly on p and Q depends on p as a quadratic form. We have

$$\mathcal{L}\left[f,p\right]\left(\mathbf{k},\omega\right) = 4\pi\int \mathrm{d}\mathbf{v}_1\mathrm{d}\mathbf{v}_2\, \mathbf{A}\left[f\right]\left(\mathbf{k},\omega,\mathbf{v}_1,\mathbf{v}_2\right) : \frac{\partial p}{\partial \mathbf{v}_1}\left\{\frac{\partial f}{\partial \mathbf{v}_2}f(\mathbf{v}_1) - f(\mathbf{v}_2)\frac{\partial f}{\partial \mathbf{v}_1}\right\} \tag{4.53}$$

and

$$\begin{aligned}Q\left[f,p,q\right]\left(\mathbf{k},\omega\right) = 2\pi\int \mathrm{d}\mathbf{v}_1\mathrm{d}\mathbf{v}_2\, \mathbf{A}\left[f\right]\left(\mathbf{k},\omega,\mathbf{v}_1,\mathbf{v}_2\right) : \left\{\frac{\partial p}{\partial \mathbf{v}_1}\frac{\partial q}{\partial \mathbf{v}_1}\right. \\ \left. + \frac{\partial p}{\partial \mathbf{v}_2}\frac{\partial q}{\partial \mathbf{v}_2} - \frac{\partial p}{\partial \mathbf{v}_1}\frac{\partial q}{\partial \mathbf{v}_2} - \frac{\partial p}{\partial \mathbf{v}_2}\frac{\partial q}{\partial \mathbf{v}_1}\right\} f(\mathbf{v}_1)f(\mathbf{v}_2),\end{aligned} \tag{4.54}$$

with

$$\mathbf{A}\left[f\right]\left(\mathbf{k},\omega,\mathbf{v}_1,\mathbf{v}_2\right) = \pi\frac{\mathbf{k}\mathbf{k}\hat{W}(\mathbf{k})^2}{\left|\varepsilon\left[f\right]\left(\mathbf{k},\omega\right)\right|^2}\delta\left(\omega - \mathbf{k}.\mathbf{v}_1\right)\delta\left(\omega - \mathbf{k}.\mathbf{v}_2\right). \tag{4.55}$$

We note that the tensor $\mathbf{A}$ is related to the tensor $\mathbf{B}$ of the Balescu-Guernsey-Lenard equation (4.9):

$$\mathbf{B}\left[f\right]\left(\mathbf{v}_1,\mathbf{v}_2\right) = \frac{1}{L^3}\sum_{\mathbf{k}}\int \mathrm{d}\omega\, \mathbf{A}\left[f\right]\left(\mathbf{k},\omega,\mathbf{v}_1,\mathbf{v}_2\right),$$

and that it shares all of its properties: it is symmetric as a tensor, it is symmetric in its velocities argument

$$\mathbf{A}\left(\mathbf{k},\omega,\mathbf{v}_1,\mathbf{v}_2\right) = \mathbf{A}\left(\mathbf{k},\omega,\mathbf{v}_1,\mathbf{v}_2\right)$$

(momentum conservation), and we have

$$\mathbf{A}\left(\mathbf{k},\omega,\mathbf{v}_1,\mathbf{v}_2\right).\left(\mathbf{v}_1-\mathbf{v}_2\right)=0$$

(energy conservation). These properties are related to the conservation laws of the physical system, as we will see in section 4.6.1. Using $\varepsilon\left[f\right]\left(-\mathbf{k},-\omega\right)=\varepsilon^*\left[f\right]\left(\mathbf{k},\omega\right)$, we also have

$$\mathbf{A}\left[f\right]\left(\mathbf{k},\omega,\mathbf{v}_1,\mathbf{v}_2\right)=\mathbf{A}\left[f\right]\left(-\mathbf{k},-\omega,\mathbf{v}_1,\mathbf{v}_2\right).$$

$\mathbf{A}$ also has a symmetry property related to the time reversal symmetry. Recalling that $I\left[f\right]\left(\mathbf{v}\right)=f\left(-\mathbf{v}\right)$ is the velocity inversion involution, we recall that $\varepsilon\left[I\left[f\right]\right]\left(\mathbf{k},-\omega\right)=\varepsilon^*\left[f\right]\left(\mathbf{k},\omega\right)$ and as a consequence

$$\mathbf{A}\left[I\left[f\right]\right]\left(\mathbf{k},-\omega,-\mathbf{v}_1,-\mathbf{v}_2\right)=\mathbf{A}\left[f\right]\left(\mathbf{k},\omega,\mathbf{v}_1,\mathbf{v}_2\right).$$

We will discuss more deeply this property in section 4.6.2.

Using equations (4.44), (4.49) and (4.50) we obtain an explicit formula for the large deviation Hamiltonian

$$H_{\mathrm{BGL}}\left[f,p\right]=-\frac{1}{4\pi L^3}\sum_{\mathbf{k}}\int\mathrm{d}\omega\,\log\left\{1-\mathcal{J}\left[f,p\right]\left(\mathbf{k},\omega\right)\right\},\tag{4.56}$$

where $\mathcal{J}\left[f,p\right]\left(\mathbf{k},\omega\right)$ is defined in equations (4.52-4.54).

As a conclusion, in this section, we have established the path large deviation principle

$$\mathbb{P}\left(\left\{f_N(\tau)\right\}_{0\leq\tau\leq T}=\left\{f(\tau)\right\}_{0\leq\tau\leq T}\right)\underset{N\to\infty}{\asymp}\mathrm{e}^{-NL^3\int_0^T\mathrm{d}\tau\,\mathrm{Sup}_p\left\{\int\mathrm{d}\mathbf{v}\,\dot{f}p-H_{\mathrm{BGL}}[f,p]\right\}}\mathrm{e}^{-NI_0[f(\tau=0)]},\tag{4.57}$$

where H is given by (4.56) and where $\tau=t/N$.

Density-current formulation of the large deviation principle. We define the current as

$$\mathbf{j}_N\left(\mathbf{v},t\right)=-\frac{1}{NL^3}\int\mathrm{d}\mathbf{r}\,\left(\frac{\partial V\left[\delta g_N\right]}{\partial\mathbf{r}}\delta g_N\right).$$

In appendix A.4, we prove that the large deviation principle (4.57) is equivalent to a empirical measure-current formulation:

$$\mathbb{P}\left(\left\{f_N(\tau),\mathbf{j}_N\left(\tau\right)\right\}_{0\leq t\leq T}=\left\{f(\tau),\mathbf{j}\left(\tau\right)\right\}_{0\leq t\leq T}\right)\underset{N\to\infty}{\asymp}\mathrm{e}^{-N\mathcal{A}[f,\mathbf{j}]}\mathrm{e}^{-NI_0[f(\tau=0)]},\tag{4.58}$$

where $\mathbf{j}_N\left(\tau\right)$ should be interpreted as a time-averaged current after time rescaling, with

$$\mathcal{A}\left[f,\mathbf{j}\right]=\begin{cases}L^3\int_0^T\mathrm{d}\tau\,\tilde{L}\left[f,\mathbf{j}\right] & \text{if }\ \dot{f}+\frac{\partial}{\partial\mathbf{v}}\cdot\mathbf{j}=0,\\ +\infty & \text{otherwise.}\end{cases}$$

and where $\tilde{L}\left[f,\mathbf{j}\right]=\underset{\mathbf{E}}{\mathrm{Sup}}\left\{\int\mathrm{d}\mathbf{v}\,\mathbf{j}\cdot\mathbf{E}-\tilde{H}[f,\mathbf{E}]\right\}$, and $\tilde{H}$ is defined by $H_{\mathrm{BGL}}\left[f,p\right]=\tilde{H}\left[f,\partial p/\partial\mathbf{v}\right]$.

4.6. Properties of the large deviation Hamiltonian

In this section we check that the large deviation Hamiltonian (4.56) satisfies all the expected symmetry properties. In section 4.6.1, we check that the Hamiltonian (4.56) is consistent with the mass, momentum and energy conservation laws. In section 4.6.2, we show that the Hamiltonian (4.56) has a time-reversal symmetry, and has the negative of the entropy, with conservation law constraints and up to constants, as a quasipotential.

4.6.1. Conservation laws

As stated in section 3.4, any conservation law is equivalent to a symmetry property of the large deviation Hamiltonian. More precisely, we know that a functional $C[f]$ is a conserved quantity of the large deviation principle (4.28) if and only if for any f and p

$$\int \mathrm{d}\mathbf{v}\, \frac{\delta H_{\mathrm{BGL}}}{\delta p\left(\mathbf{v}\right)} \frac{\delta C}{\delta f\left(\mathbf{v}\right)} = 0, \tag{4.59}$$

or equivalently, if for any f, p and $\alpha \in \mathbb{R}$:

$$H_{\mathrm{BGL}}[f,p] = H_{\mathrm{BGL}}\left[f, p + \alpha \frac{\delta C}{\delta f}\right]. \tag{4.60}$$

We will need the expression of the functional derivative of the Hamiltonian H_{BGL} with respect to its conjugate momentum p throughout this section. It reads

$$\frac{\delta H_{\mathrm{BGL}}}{\delta p\left(\mathbf{v}\right)}[f,p] = \frac{1}{4\pi L^3} \sum_{\mathbf{k}} \int \mathrm{d}\omega\, \frac{\frac{\delta \mathcal{J}}{\delta p(\mathbf{v})}[f,p]\left(\mathbf{k},\omega\right)}{1 - \mathcal{J}\left[f,p\right]\left(\mathbf{k},\omega\right)}, \tag{4.61}$$

with

$$\begin{aligned} &\frac{\delta \mathcal{J}}{\delta p\left(\mathbf{v}\right)}[f,p]\left(\mathbf{k},\omega\right) = \\ &-4\pi \int \mathrm{d}\mathbf{v}_2\, \frac{\partial}{\partial \mathbf{v}} \left\{ \mathbf{A}\left(\mathbf{k},\omega,\mathbf{v},\mathbf{v}_2\right) \left[\frac{\partial f}{\partial \mathbf{v}_2} f(\mathbf{v}) - \frac{\partial f}{\partial \mathbf{v}} f(\mathbf{v}_2) + 2 f(\mathbf{v}) f(\mathbf{v}_2) \left(\frac{\partial p}{\partial \mathbf{v}} - \frac{\partial p}{\partial \mathbf{v}_2} \right) \right] \right\}. \end{aligned} \tag{4.62}$$

Mass conservation. The conservation of the total mass $M\left[f\right] = \int \mathrm{d}\mathbf{v}\, f$ is immediately visible from equation (4.60) as H only depends on the derivative of the conjugated momentum p.

Momentum conservation. We define the total momentum $\mathbf{P}\left[f\right] = \int \mathrm{d}\mathbf{v}\, \mathbf{v} f$. It follows that $\frac{\delta \mathbf{P}}{\delta f(\mathbf{v})} = \mathbf{v}$. Using equation (4.62) and partial integration, the relation

$$\int \mathrm{d}\mathbf{v}_1 \frac{\delta \mathcal{J}}{\delta p\left(\mathbf{v}_1\right)}[f,p]\left(\mathbf{k},\omega\right) \frac{\delta \mathbf{P}}{\delta f\left(\mathbf{v}_1\right)} = 0$$

is a direct consequence of the symmetry $\mathbf{A}(\mathbf{k},\omega,\mathbf{v}_1,\mathbf{v}_2) = \mathbf{A}(\mathbf{k},\omega,\mathbf{v}_2,\mathbf{v}_1)$. Then, using the relation (4.61) between the functional derivatives of $\mathcal{J}$ and H_{BGL}, we obtain

$$\int \mathrm{d}\mathbf{v}_1 \frac{\delta H_{\mathrm{BGL}}}{\delta p(\mathbf{v}_1)}[f,p](\mathbf{k},\omega)\frac{\delta \mathbf{P}}{\delta f(\mathbf{v}_1)} = 0.$$

We have thus checked that the large deviation principle conserves momentum.

The conservation of mass and momentum should have been expected as momentum and mass conservations were already granted from the expression of the Hamiltonian (4.29), as a direct consequence of mass and momentum conservations for f_N that can be deduced from either equation (4.22) or equation (4.26) .

Energy conservation. We define the total kinetic energy $E[f] = \int \mathrm{d}\mathbf{v}\, \frac{\mathbf{v}^2}{2} f$. It follows that $\frac{\delta E}{\delta f(\mathbf{v})} = \mathbf{v}^2/2$. Using equation (4.62) and partial integration, one can check that the relation

$$\int \mathrm{d}\mathbf{v}_1 \frac{\delta \mathcal{J}}{\delta p(\mathbf{v}_1)}[f,p](\mathbf{k},\omega)\frac{\delta E}{\delta f(\mathbf{v}_1)} = 0$$

is a direct consequence of the following symmetries of the tensor:

$$\mathbf{A}(\mathbf{k},\omega,\mathbf{v}_1,\mathbf{v}_2).(\mathbf{v}_1-\mathbf{v}_2) = 0,$$

and

$$\mathbf{A}(\mathbf{k},\omega,\mathbf{v}_1,\mathbf{v}_2) = \mathbf{A}(\mathbf{k},\omega,\mathbf{v}_2,\mathbf{v}_1).$$

Then, using the relation (4.61) between the functional derivatives of $\mathcal{J}$ and H, we obtain

$$\int \mathrm{d}\mathbf{v}_1 \frac{\delta H_{\mathrm{BGL}}}{\delta p(\mathbf{v}_1)}(\mathbf{k},\omega)\frac{\delta E}{\delta f(\mathbf{v}_1)} = 0.$$

From the result (4.59) we deduce that the large deviation principle conserves the kinetic energy.

The conservation of the kinetic energy is not a trivial consequence of equation (4.22) or equation (4.26). Indeed, from equation (4.22) or equation (4.26), at any time some energy can be exchanged between the kinetic part $\int \mathrm{d}\mathbf{v}\, \frac{\mathbf{v}^2}{2} f_N$ and the potential part related to δg_N. However $\int_0^T \mathrm{d}t \int \mathrm{d}\mathbf{v}\, \frac{\mathbf{v}^2}{2}\frac{\partial f_N}{\partial t}$ is equal to the negative of the variations of the potential energy. Then, over any time T, these variations should remain bounded, for the system to stay close to the set of homogenous solutions. As a consequence, in accordance with our hypothesis of spatial homogeneity, $\lim_{T\to\infty}\frac{1}{T}\int_0^T \mathrm{d}t \int \mathrm{d}\mathbf{v}\, \frac{\mathbf{v}^2}{2}\frac{\partial f_N}{\partial t} = 0$. This is the reason why we should have expected the conservation of kinetic energy by the large deviation principle. The conservation of kinetic energy by the large deviation principle, which is a conservation for the slow effective dynamics for the empirical measure, should thus be interpreted as a conservation for time averages for the fast process. If the system became inhomogeneous, this conservation could be broken.

4.6.2. Time-reversal symmetry, quasipotential, and entropy

For the Hamiltonian dynamics (4.5), we consider the microcanonical measure with fixed energy E and momentum fixed and equal to zero, and denote $\mathbb{E}_m$ averages with respect to the microcanonical measure. We expect the stationary probability to observe $f_N = f$, to satisfy a large deviation principle

$$\mathbb{P}_s\left[f_N = f\right] \underset{N\to\infty}{\asymp} \exp\left\{-NU\left[f\right]\right\}, \tag{4.63}$$

where this large deviation principle defines the quasipotential U.

From classical equilibrium statistical mechanics considerations, for this system with long range interactions, it is easy to justify that the quasipotential is

$$U\left[f\right] = \begin{cases} -\frac{S[f]}{k_B} + \frac{S_m(E)}{k_B} & \text{if } \int \mathrm{d}\mathbf{v}\, f = 1, \ \int \mathrm{d}\mathbf{v}\, \mathbf{v} f = 0, \text{ and } \int \mathrm{d}\mathbf{v}\, \frac{\mathbf{v}^2}{2} f = E; \\ +\infty & \text{otherwise,} \end{cases} \tag{4.64}$$

where

$$S\left[f\right] = -k_B \int \mathrm{d}\mathbf{v}\, f \log f$$

is the entropy of the macrostate f and

$$S_m(E) = -k_B \inf_f \left\{ \int f \log f \,\middle|\, \int \mathrm{d}\mathbf{v}\, f = 1, \ \int \mathrm{d}\mathbf{v}\, \mathbf{v} f = 0, \text{ and } \int \mathrm{d}\mathbf{v}\, \frac{\mathbf{v}^2}{2} f = E \right\}.$$

is the equilibrium entropy. We have $S_m(E) = k_B\left[3\log(E)/2 + 3\log(4\pi)/2 + 3/2\right]$.

It is also classically known that the Hamiltonian dynamics (4.5) is time-reversible: the dynamics is symmetric by the change of variable $(t, \mathbf{r}_n, \mathbf{v}_n) \to (-t, \mathbf{r}_n, -\mathbf{v}_n)$. This is equivalent to say that if $\{\mathbf{r}_n(t), \mathbf{v}_n(t)\}_{t\in[0,T]}$ is a solution of the Hamiltonian dynamics, then $\{\mathbf{r}_n(T-t), -\mathbf{v}_n(T-t)\}_{t\in[0,T]}$ is also a solution. In order to take into account the change of sign for the velocity, we define the linear operator on the set of function of the velocity $I\left[f\right](\mathbf{v}) = f\left(-\mathbf{v}\right)$. We note that I is an involution: $I^2 = \mathrm{Id}$. From the time reversal symmetry for the Hamiltonian dynamical system, it is straightforward to conclude that the stochastic process for the empirical measure f_N should verify a generalized detailed balance symmetry. This symmetry writes

$$\mathbb{P}_T\left(f_N(T) = f_2 \,|f_N(0) = f_1\right) \mathbb{P}_m\left(f_N = f_1\right) = \mathbb{P}_T\left(f_N(T) = I\left[f_2\right] |f_N(0) = I\left[f_2\right]\right) \mathbb{P}_m\left(f_N = I\left[f_2\right]\right), \tag{4.65}$$

where $\mathbb{P}_m$ is the stationary measure with respect to the microcanonical measure, $\mathbb{P}_T$ are the transition probabilities for the microcanonical measure. The term "generalized" means that the symmetry holds using the involution I. As discussed in section 3.4, the

detailed balance condition (4.65) implies a detailed balance symmetry at the level of the Hamiltonian: for any f and p,

$$H_{\mathrm{BGL}}\left[I\left[f\right], -I\left[p\right]\right] = H_{\mathrm{BGL}}\left[f, p + \frac{\delta U}{\delta f}\right]. \tag{4.66}$$

From the relation (4.64) between the quasipotential U and the entropy S, using the conservation law symmetries of the large deviation Hamiltonian (4.60) we can conclude that the generalized detailed balance symmetry (4.66) is equivalent to the symmetry: for any f and p,

$$H_{\mathrm{BGL}}\left[I\left[f\right], -I\left[p\right]\right] = H_{\mathrm{BGL}}\left[f, p - \frac{1}{k_B}\frac{\delta S}{\delta f}\right]. \tag{4.67}$$

One may directly check this symmetry, from (4.56), using the time reversal symmetry for A:

$$\mathbf{A}\left[I\left[f\right]\right](\mathbf{k}, -\omega, -\mathbf{v}_1, -\mathbf{v}_2) = \mathbf{A}\left[f\right](\mathbf{k}, \omega, \mathbf{v}_1, \mathbf{v}_2).$$

It is however simpler to first note that for spatially homogeneous systems, which is the case in this paper, one has the further symmetry :

$$H_{\mathrm{BGL}}\left[I\left[f\right], I\left[p\right]\right] = H_{\mathrm{BGL}}\left[f, p\right].$$

This symmetry can be checked starting from (4.56) and (4.52), using

$$\mathbf{A}\left[I\left[f\right]\right](\mathbf{k}, -\omega, -\mathbf{v}_1, -\mathbf{v}_2) = \mathbf{A}\left[f\right](\mathbf{k}, \omega, \mathbf{v}_1, \mathbf{v}_2),$$

to conclude that

$$\mathcal{J}\left[I\left[f\right], I\left[p\right]\right](\mathbf{k}, \omega) = \mathcal{J}\left[f, p\right](\mathbf{k}, -\omega).$$

With this remark, we can conclude that the generalized detailed balance condition is equivalent to: for any f and p,

$$H_{\mathrm{BGL}}\left[f, -p\right] = H_{\mathrm{BGL}}\left[f, p - \frac{1}{k_B}\frac{\delta S}{\delta f}\right]. \tag{4.68}$$

This last condition is a detailed balance condition at the level of large deviations. In order to check directly (4.68), one can start from (4.56) and (4.52), and see that this follows from $\mathcal{J}\left[f, p - k_B^{-1}\delta S/\delta f\right] - \mathcal{J}\left[f, -p\right] = 0$. One can see that this last equality is equivalent to the relation: for any f and p, $\mathcal{L}\left[f, p\right] = Q\left[f, p, k_B^{-1}\delta S/\delta f\right]$, using (4.52) and that $\mathcal{L}$ is linear and $\mathcal{Q}$ quadratic with respect to p. Using (4.53) and (4.54) and $\partial/\partial\mathbf{v}(\delta S/\delta f)/k_B = 1/f\partial f/\partial\mathbf{v}$, this is easily verified using $\mathbf{A}\left[f\right](\mathbf{k}, \omega, \mathbf{v}_1, \mathbf{v}_2) = \mathbf{A}\left[f\right](\mathbf{k}, \omega, \mathbf{v}_2, \mathbf{v}_1)$.

As a final remark, we note that the quasipotential and the entropy are solutions to the stationary Hamilton-Jacobi equation

$$H_{\mathrm{BGL}}\left[f, \frac{\delta U}{\delta f}\right] = H_{\mathrm{BGL}}\left[f, -\frac{1}{k_B}\frac{\delta S}{\delta f}\right] = 0.$$

Those are direct consequences of any of the detailed balance symmetries: (4.68), (4.66) or (4.67).

In this section we have explained that U (4.64) is the quasipotential. We have argued that the large deviation Hamiltonian satisfies the generalized detailed balance symmetry (4.67) as a consequence of the microscopic time reversibility, and checked directly this relation from the explicit Hamiltonian equations. We have moreover justified that that the large deviation Hamiltonian satisfies the detailed balance symmetry (4.68). This proves that U satisfies the stationary Hamilton-Jacobi equation.

4.7. Perspectives

The main result of this chapter is the derivation of a large deviation principle (4.2), for the velocity empirical measure, for the Hamiltonian dynamics of N particles which interact through a pairwise long-range interaction potential. We have obtained an explicit formula for the large deviation Hamiltonian (4.3-4.4) and we have checked all its conservation and symmetry properties. This result opens many mathematical and theoretical questions, as well as interesting applications.

This large deviation result relies on natural assumptions. Some of these assumptions are also required to establish the Balescu-Guernsey-Lenard kinetic equation, but the hypotheses made to obtain the large deviation principle seem stronger. The first assumption is the validity of the quasilinear approximation: we neglected non linear terms of order $1/\sqrt{N}$ in the equation for the fluctuations of the empirical measure. This amounts to neglecting possible effects of large deviations of the fluctuations, and describing the fluctuation process at a Gaussian level only. The second assumption is the convergence of the process of fluctuations to a stationary Gaussian process and more specifically the convergence of the large time asymptotics for the large deviation estimates over this process. A proof would also require the study of the mixing properties for this Gaussian process. The mixing properties are critical to justify the Markov behavior described by the slow-fast large deviation principle. While the proofs of these assumptions are beyond the scope of this paper, they open very interesting questions for both theoretical physicists and mathematicians.

Systems with long range interactions are important for many phenomena. However, more elaborate models than the one we used in this paper could be more appropriate to describe physical situations where rare event are important for applications. Of special interest would be the dynamics of N point-vortices for two-dimensional hydrodynamics. Another generalization should also consider dynamics of particles driven by stochastic forces, which generically lead to irreversible stochastic processes. For those systems, explicit results for the large deviation theory would be extremely useful for explaining non-equilibrium phase transitions in two dimensional [56] and geostrophic turbulence [55], or in systems with long range interactions [167, 166]. Finally, another direction that could be taken is the extension of this work to 1D system. For 1D system with long range interactions, the Balescu-Guernsey-Lenard operator vanishes and the relaxation

to equilibrium of the distribution function is driven by $1/N^2$ effects (3-body correlation effects)[112, 111]; the large deviation theory extending the kinetic theory has yet to be established.

5. Dynamical large deviations for the kinetic theory of plasmas: beyond the Landau equation

In this chapter, we derive a large deviation principle for the empirical measure of N same-charge particles within the Landau approximation when the interaction potential is a repulsive Coulomb one. The kinetic equation associated with the dynamics of such a system is the Landau equation. The Landau equation can be obtained from the Balescu-Guernsey-Lenard equation ignoring collective effects. Interestingly, the Landau equation can also be connected to the Boltzmann equation in the grazing collision limit. In this chapter, we derive the large deviation principle associated with the Landau equation using two methods. First, by using already existing work on the large deviations associated with the Boltzmann equation [50]. Then, we show that the same result can be recovered from the large deviations associated with the Balescu-Guernsey-Lenard equation, describing the dynamics of particles coupled with a generic long-range potential, in the so-called Landau approximation.

This chapter is an adaption of the following articles: [106, 108, 107].

5.1. The dynamics of the Coulomb plasma

Let us consider of a Coulomb plasma of N particles with positions $\{\mathbf{r}_n\}_{1\leq n\leq N}$ and velocities $\{\mathbf{v}_n\}_{1\leq n\leq N}$, and with equal charge e and mass m. The dynamics is a Hamiltonian one with

$$\begin{cases} \dfrac{\mathrm{d}\mathbf{r}_n}{\mathrm{d}t} &= \mathbf{v}_n \\ \dfrac{\mathrm{d}\mathbf{v}_n}{\mathrm{d}t} &= -\dfrac{e^2}{4\pi\epsilon_0 m}\displaystyle\sum_{m\neq n}\frac{\mathrm{d}}{\mathrm{d}\mathbf{r}_n}W\left(\mathbf{r}_n-\mathbf{r}_m\right) \end{cases} \tag{5.1}$$

where ϵ_0 is the vacuum permittivity and W is the Coulomb potential. In both a finite box and an infinite space, W can be defined through its Fourier transform

$$\hat{W}\left(\mathbf{k}\right) = \int \mathrm{d}\mathbf{r}\, \mathrm{e}^{-i\mathbf{k}.\mathbf{r}} W\left(\mathbf{r}\right),$$

with

$$\hat{W}\left(\mathbf{k}\right) = \frac{1}{k^2},$$

and where $k = |\mathbf{k}|$ (this definition is equivalent to $-\Delta W = \delta(\mathbf{r})$). We define the Debye length $\lambda_D = \left(\frac{\epsilon_0 k_B T L^3}{e^2 N}\right)^{1/2}$, where k_B is the Boltzmann constant and T the temperature. This length is the typical length beyond which Coulomb interaction are screened [169]. We also define the plasma electron frequency $\omega_{pe} = \left(\frac{e^2 N}{\epsilon_0 m L^3}\right)^{1/2}$, which is the pulsation of the Langmuir waves in a plasma [169], and the thermal velocity $v_T = \lambda_D \omega_{pe} = \sqrt{k_B T/m}$. Then, if we use the dimensionless variables

$$\tilde{\mathbf{r}} = \mathbf{r}/\lambda_D, \quad \tilde{\mathbf{v}} = \mathbf{v}/v_T \quad \text{and} \quad \tilde{t} = \omega_{pe} t,$$

the dimensionless dynamical equations (5.1) read

$$\begin{cases} \dfrac{\mathrm{d}\tilde{\mathbf{r}}_n}{\mathrm{d}\tilde{t}} &= \tilde{\mathbf{v}}_n \\ \dfrac{\mathrm{d}\tilde{\mathbf{v}}_n}{\mathrm{d}\tilde{t}} &= -\dfrac{1}{\Lambda} \displaystyle\sum_{m \neq n} \frac{\mathrm{d}}{\mathrm{d}\tilde{\mathbf{r}}_n} \tilde{W}\left(\tilde{\mathbf{r}}_n - \tilde{\mathbf{r}}_m\right) \end{cases} \tag{5.2}$$

where $\Lambda \equiv N\left(\lambda_D/L\right)^3$ is the so-called plasma parameter. Λ is the number of particles in a box of size of the Debye length. In this new system of units, called plasma units, $\tilde{\mathbf{r}}_n$ belongs to the 3-dimensional torus $(L/\lambda_D)\,\mathbb{T}^3$. The dimensionless Coulomb potential $\tilde{W}$ is defined by

$$\hat{W}\left(\tilde{\mathbf{k}}\right) = \int \mathrm{d}\tilde{\mathbf{r}}\, \mathrm{e}^{-i\tilde{\mathbf{k}}.\tilde{\mathbf{r}}} \tilde{W}\left(\tilde{\mathbf{r}}\right),$$

with $\hat{W}\left(\tilde{\mathbf{k}}\right) = \frac{1}{\tilde{k}^2}$. For simplicity, in the following we omit the tildes when referring to the dimensionless variables. We will work in dimensionless variables, and give the main results in both dimensionless and physical variables.

We note that (5.2) is a specific instance of the generic dynamics of particles with long-range interaction (4.5), with the specificity that the force is renormalized by the plasma parameter rather than the number of particles.

We call $\mu-$space the $(\mathbf{r}, \mathbf{v})$ space. The $\mu-$space is of dimension 6. Let us define g_Λ the $\mu-$space rescaled empirical distribution function for the positions and velocities of the N particles rescaled by the plasma parameter

$$g_\Lambda(\mathbf{r}, \mathbf{v}, t) = \frac{1}{\Lambda} \sum_{n=1}^{N} \delta(\mathbf{r} - \mathbf{r}_n(t)) \delta(\mathbf{v} - \mathbf{v}_n(t)). \tag{5.3}$$

In the following we will consider the large plasma parameter limit, $\Lambda \to \infty$. Considering that Λ is the number of particles in a box of size of the Debye length, and that in our non-dimensional units the Debye length is fixed, the scaling $1/\Lambda$ in front of the empirical density (5.3) is natural.

If the box size L is larger than the Debye length λ_D, the interactions are screened beyond the Debye length and the effective interaction length scale is λ_D. Otherwise, if the size of the box is smaller than the Debye length, then the interactions are not screened in the box and they take place on a length scale L. We call $\ell = \min\{\lambda_D, L\}$ the effective interaction length scale.

In the following, we study the asymptotic dynamics of g_Λ as the number of particles in a box of the size of the effective interaction length scale, e.g. $N\ell^3/L^3$ goes to infinity. If $L > \lambda_D$, this asymptotic regime is the limit of a large plasma parameter Λ; if $L < \lambda_D$, it is the limit of a large number of particles N. In this paper, we present detailed results for the case $L > \lambda_D$, and we briefly discuss the slight modifications relevant for the case $L < \lambda_D$ in section 5.5.

5.2. Kinetic description of the Coulomb plasma within the Landau approximation

Although mathematically more intricate as some of the integrals involved may diverge, the large Λ asymptotic dynamics of g_Λ is formally the same as the large N asymptotics of g_N for a generic long-range interaction potential. In particular, after time rescaling, $\tau = t/\Lambda$, assuming a set of initial conditions that $\lim_{\Lambda\uparrow\infty} g_\Lambda(\mathbf{r}, \mathbf{v}, t = 0) = f_0(\mathbf{v})$ where f_0 is a stable stationary solution of the Vlasov equation (4.7), we have that $\lim_{\Lambda\uparrow\infty} g_\Lambda(\mathbf{r}, \mathbf{v}, t) = f(\mathbf{v}, t)$ where f solves the Balescu-Guernsey-Lenard equation (4.9).

Neglecting the collective effects in the Balescu-Guernsey-Lenard equation, i.e., setting the dielectric function (4.8) to 1, we obtain the Landau equation

$$\frac{\partial f}{\partial \tau} = \frac{\partial}{\partial \mathbf{v}}. \int \mathrm{d}\mathbf{v}_2\, \mathbf{B}(\mathbf{v}, \mathbf{v}_2) \left(-\frac{\partial f}{\partial \mathbf{v}_2} f(\mathbf{v}) + f(\mathbf{v}_2) \frac{\partial f}{\partial \mathbf{v}} \right), \tag{5.4}$$

where $\mathbf{B}$ for the Landau equation is given by the same expression as the one for $\mathbf{B}$ in equation (4.10), but with $\varepsilon(\mathbf{k}, \omega) = 1$:

$$\mathbf{B}(\mathbf{v}_1, \mathbf{v}_2) = \pi \left(\frac{\lambda_D}{L} \right)^3 \int_{-\infty}^{+\infty} \mathrm{d}\omega \sum_{\mathbf{k} \in 2\pi(\lambda_D/L)\mathbb{Z}^{*3}} \hat{W}(\mathbf{k})^2\, \mathbf{k}\mathbf{k}\delta(\omega - \mathbf{k}.\mathbf{v}_1)\, \delta(\omega - \mathbf{k}.\mathbf{v}_2), \tag{5.5}$$

where the interaction potential is the Coulomb potential: $\hat{W}(\mathbf{k}) = k^{-2}$. The Landau approximation of the Balescu-Guernsey-Lenard equation is valid to describe plasma at scales which are much smaller than the Debye length λ_D (associated with large wavenumbers compared to $1/\lambda_D$), or globally when the effect of those scales dominate the collision kernel $\mathbf{B}$. Within this approximation, we can assume that $\varepsilon(\mathbf{k}, \omega) = 1$ which means that the dielectric susceptibility does not depend on the distribution f anymore. This approximation is relevant for many applications in plasma physics [169].

All the properties of the Balescu-Guernsey-Lenard equation discussed in section 4.2.3 still hold for the Landau equation. The Landau equation conserves total mass, momentum and kinetic energy associated with the distribution function. It increases monotonically the entropy (4.14); and its stationary solutions are the Boltzmann distriutions.

5.3. Large deviations associated with the Landau kinetic theory from the Boltzmann kinetic theory

The Landau equation has been presented in section 5.2 as an approximation of the Balescu-Guernsey-Lenard equation. However it also has a strong link with the Boltzmann equation that describes a dilute gas of particles in the Boltzmann-Grad limit. One can look for instance in [150] for a first account of this connection. Moreover, the large deviation Hamiltonian for the Boltzmann equation has already been obtained, for toy models which are analogue to the dilute gas dynamics [184] or for the dilute gas dynamics [45, 50]. The aim of this section is to derive the large deviation Hamiltonian associated with the Landau equation from the large deviation Hamiltonian associated with the Boltzmann equation.

In section 5.3.1, we introduce the notations for the Boltzmann equation and the large deviation Hamiltonian for a dilute gas in the Boltzmann–Grad limit. In section 5.3.2, following [150], we derive the Landau equation from the Boltzmann equation using the grazing collision limit. Using the same limit but for the large deviation Hamiltonian, rather than for the kinetic equation, we derive the large deviation Hamiltonian for the Landau equation (5.20) in section 5.3.3. In section 5.3.4, we show that this Hamiltonian satisfies all the expected symmetries and conservation properties. In section 5.3.5, we derive the gradient flow structure of the Landau equation associated with this Hamiltonian.

5.3.1. The Boltzmann equation for a dilute gas

We consider the dynamics of a dilute gas composed of atoms or molecules. We neglect any internal degrees of freedom. We assume that the N particles evolve through a Hamiltonian dynamics with short range two body interactions, for instance hard sphere collisions.

Let us first define the collision kernel and the collision cross-section. We consider a thread of particles with velocities $\mathbf{v}_1$ that meets a thread of particles with velocities $\mathbf{v}_2$. We assume that particles of each velocity type are distributed according to a homogeneous Poisson point process with densities $\varrho(\mathbf{v}_1)\mathrm{d}\mathbf{v}_1$ and $\varrho(\mathbf{v}_2)\mathrm{d}\mathbf{v}_2$, respectively. These particle distributions will give rise to collisions where $(\mathbf{v}_1, \mathbf{v}_2)$ particle pairs undergo a random change towards pairs of the type $(\mathbf{v}_1', \mathbf{v}_2')$, up to $(\mathrm{d}\mathbf{v}_1', \mathrm{d}\mathbf{v}_2')$. This occurs at a rate per unit of time and unit of volume which is proportional to the $\mathbf{v}_1$ incident particle number $\varrho(\mathbf{v}_1)\mathrm{d}\mathbf{v}_1$, the $\mathbf{v}_2$ incident particle number $\varrho(\mathbf{v}_2)\mathrm{d}\mathbf{v}_2$, $\mathrm{d}\mathbf{v}_1'$, and $\mathrm{d}\mathbf{v}_2'$. The

proportionality coefficient is called the collision kernel and is denoted

$$w_0\left(\mathbf{v}_1', \mathbf{v}_2'; \mathbf{v}_1, \mathbf{v}_2\right)/2. \tag{5.6}$$

The local conservation of momentum and energy implies that

$$w_0(\mathbf{v}_1', \mathbf{v}_2'; \mathbf{v}_1, \mathbf{v}_2) = \sigma_0(\mathbf{v}_1', \mathbf{v}_2'; \mathbf{v}_1, \mathbf{v}_2)\delta\left(\mathbf{v}_1 + \mathbf{v}_2 - \mathbf{v}_1' - \mathbf{v}_2'\right)\delta\left(\mathbf{v}_1^2 + \mathbf{v}_2^2 - \mathbf{v'}_1^2 - \mathbf{v'}_2^2\right), \tag{5.7}$$

where σ_0 is the diffusion cross-section. σ_0 is of the order of a^2 where a is a typical atom size. We detail the different symmetry properties of the collision kernel in appendix A.6.

Several length scales are important to describe a dilute gas: a typical atom size a, that we will defined more precisely below in relation with the diffusion cross-section, a typical interparticle distance $1/\rho^{1/3}$ where ρ is the averaged gas density, the mean free path which is the averaged length a particle travels between two collisions, and a typical box size L. The mean free path is given by $l = c/a^2\rho$, where c is a non-dimensional number that depends on the collision kernel. The gas is said dilute if we have the following relation between those scales

$$a \ll \frac{1}{\rho^{1/3}} \ll l.$$

A limit in which those inequalities are satisfied is called a Boltzmann–Grad limit. We consider the 4 physically independent parameters a, L, N and the inverse temperature β ($\rho = N/L^3$). From those four, we can choose two independent non-dimensional parameters. In the following we choose N and the Knudsen number $\alpha = l/L$ as those two independent parameters. The inverse of the number of particles in a volume of the size l is then $\epsilon = 1/l^3\rho = a^2/l^2 = a^6\rho^2$ and is another non-dimensional parameter.

We will use the large deviation result in the limit $N \to \infty$ with fixed Knudsen number α [1]. In this limit, from $l = c/a^2\rho$ we see that $a^2 = c/\alpha N$. As the diffusion cross-section σ_0 is of the order of a^2, in the limit $N \to \infty$, it is thus natural to consider the rescaled cross-section $\sigma = N\sigma_0$. Moreover, in the following it will be convenient to consider momentum exchange. We thus use the following definition of w

$$w\left(\mathbf{v}_1 + \frac{1}{2}\mathbf{q}, \mathbf{v}_2 - \frac{1}{2}\mathbf{q}; \mathbf{q}\right) = \gamma N w_0(\mathbf{v}_1 + \mathbf{q}, \mathbf{v}_2 - \mathbf{q}; \mathbf{v}_1, \mathbf{v}_2), \tag{5.8}$$

where $\mathbf{q}$ is the momentum transfer between the incident particles with momenta $(\mathbf{v}_1, \mathbf{v}_2)$ and the scattered particles with momenta $(\mathbf{v}_1 + \mathbf{q}, \mathbf{v}_2 - \mathbf{q})$. Writing the collision kernel this way automatically takes into account momentum conservation during the collision process. In this reasoning, the coefficient γ is any non-dimensional coefficient which is held fixed in the limit $N \to \infty$. In the following sections, for the specific case of the Coulomb interaction, we will consider

$$\gamma = \left(\frac{\lambda_D}{L}\right)^3,$$

[1] In the second part of the manuscript, we study the limit $\alpha \to 0$ which is the hydrodnamical limit for the dilute gas.

where λ_D is the Debye length and L the size of the box.

We define a rescaled empirical density

$$g_\gamma(\mathbf{r},\mathbf{v},t) = (\gamma N)^{-1} \sum_{n=1}^{N} \delta(\mathbf{v}-\mathbf{v}_n(t))\delta(\mathbf{r}-\mathbf{r}_n(t)). \tag{5.9}$$

We note that with $\gamma = (\lambda_D/L)^3$, g_γ coincides with $g_\Lambda(\mathbf{r},\mathbf{v},t) = \Lambda^{-1}\sum_{n=1}^{N}\delta(\mathbf{v}-\mathbf{v}_n(t))\delta(\mathbf{r}-\mathbf{r}_n(t))$ (see (5.3), page 88). When these N particles undergo a dilute gas dynamics, the empirical density g_γ has a law of a large numbers. More precisely, if we assume that for a set of initial conditions, an initial law of large numbers holds: $\lim_{N\to\infty} g_\gamma(\mathbf{r},\mathbf{v},0) = g^0(\mathbf{r},\mathbf{v})$, then we have at a time t the law of large numbers $\lim_{N\to\infty} g_\gamma(\mathbf{r},\mathbf{v},t) = g(\mathbf{r},\mathbf{v},t)$, where g is a solution of the Boltzmann equation.

$$\frac{\partial g}{\partial t} + \mathbf{v}.\frac{\partial g}{\partial \mathbf{r}} = \int \mathrm{d}\mathbf{v}_2\mathrm{d}\mathbf{q}\, w\left(\mathbf{v}+\frac{1}{2}\mathbf{q},\mathbf{v}_2-\frac{1}{2}\mathbf{q};\mathbf{q}\right)\left[g(\mathbf{v}+\mathbf{q},\mathbf{r})\,g(\mathbf{v}_2-\mathbf{q},\mathbf{r}) - g(\mathbf{v},\mathbf{r})\,g(\mathbf{v}_2,\mathbf{r})\right], \tag{5.10}$$

with initial condition $g(\mathbf{r},\mathbf{v},0) = g^0(\mathbf{r},\mathbf{v})$. We refer to classical textbooks in kinetic theories, for instance [150], or [50] for a detailed presentation of an heuristic derivation of the Boltzmann equation.

In [50], a large deviation principle for the empirical density is derived (equations (1) to (3) in [50]). This large deviation is derived in the limit $\epsilon = 1/N\alpha^3 \to 0$. In this chapter, we will consider the limit $\gamma N \to \infty$, with fixed Knudsen number and fixed γ. In this limit, we have $\epsilon = 1/N\alpha^3 \to 0$. Then the large deviation result justified in [50] can be directly used in this paper. After adapting equations (1) to (3) in [50] to the notations (5.8) and (5.9), with the prescription that $g_\gamma(t=0)$ is in the neighborhood of $g(t=0)$, we have

$$\mathbf{P}\left(\{g_\gamma(\mathbf{r},\mathbf{v},t)\}_{0\le t\le T} = \{g(\mathbf{r},\mathbf{v},t)\}_{0\le t\le T}\right) \underset{N\to\infty}{\asymp} \mathrm{e}^{-\gamma N\int_0^T \mathrm{Sup}_p\left\{\int \mathrm{d}\mathbf{r}\mathrm{d}\mathbf{v}\,\dot{g}p - H_B[g,p]\right\}}, \tag{5.11}$$

where

$$H_B[g,p] = H_C[g,p] + H_T[g,p], \tag{5.12}$$

and with the collision Hamiltonian

$$H_C[g,p] = \frac{1}{2}\int \mathrm{d}\mathbf{v}_1\mathrm{d}\mathbf{v}_2\mathrm{d}\mathbf{q}\mathrm{d}\mathbf{r}\, w\left(\mathbf{v}_1+\frac{1}{2}\mathbf{q},\mathbf{v}_2-\frac{1}{2}\mathbf{q};\mathbf{q}\right) \times g(\mathbf{r},\mathbf{v_1})g(\mathbf{r},\mathbf{v}_2)\left\{\mathrm{e}^{[-p(\mathbf{r},\mathbf{v}_1)-p(\mathbf{r},\mathbf{v}_2)+p(\mathbf{r},\mathbf{v}_1+\mathbf{q})+p(\mathbf{r},\mathbf{v}_2-\mathbf{q})]}-1\right\}, \tag{5.13}$$

and the free transport Hamiltonian

$$H_T[g,p] = -\int \mathrm{d}\mathbf{r}\mathrm{d}\mathbf{v}\, p(\mathbf{r},\mathbf{v})\mathbf{v}.\frac{\partial g}{\partial \mathbf{r}}(\mathbf{r},\mathbf{v}). \tag{5.14}$$

The steps used to compute the Boltzmann large deviation Hamiltonian (5.12) are very close to the one presented in section 3.7.2 for the derivation of the large deviation principle associated with the dynamics of N particles undergoing a Run-and-Tumble dynamics. Both Hamiltonian are the ones of jump processes of the empirical measure, explaining the exponential dependence in the conjugate momentum p. For the Boltzmann dilute gas, the particles are interacting, in the sense that the jump rate of the empirical measure depends on the empirical measure quadratically as it stems from a binary collision process. This is why at variance with the tumbling Hamiltonian (3.59), the collision Hamiltonian (5.13) is quadratic in g.

5.3.2. From the Boltzmann to the Landau equations

In the case of long-range interactions between particles, e.g. Coulomb type interactions, the two-particle collisions are dominated by small-angle scattering events. This allows some simplification. The related limit is called the **grazing collision limit**. In this section we justify that in the grazing collision limit and for a homogeneous gas, from the Boltzmann equation one obtains the Landau equation

$$\frac{\partial f}{\partial t} = \frac{1}{\Lambda}\frac{\partial}{\partial \mathbf{v}} \int \mathrm{d}\mathbf{v}_2 \, \mathbf{B}(\mathbf{v}, \mathbf{v}_2) \left(-\frac{\partial f}{\partial \mathbf{v}_2} f(\mathbf{v}) + \frac{\partial f}{\partial \mathbf{v}} f(\mathbf{v}_2) \right), \tag{5.15}$$

where the tensor $\mathbf{B}$ is defined by (5.5), page 89. In equation (5.4) of section (5.2), we expressed this equation with the time variable $\tau = t/\Lambda$ rescaled by the plasma parameter. This is why there is no factor Λ^{-1} in the right hand side of equation (5.4).

The following derivation of the Landau equation from the Boltzmann equation is strongly inspired by the paragraph §42 of [150]. However, here we present a slightly different derivation. First, we consider homogenous solutions of the Boltzmann equation $g(\mathbf{r}, \mathbf{v}, t) = f(\mathbf{v}, t)$ that do not depend on the position variable. The homogeneous Boltzmann equation reads

$$\frac{\partial f}{\partial t} = \underbrace{\int \mathrm{d}\mathbf{v}_2 \mathrm{d}\mathbf{q} \, w\left(\mathbf{v} + \frac{1}{2}\mathbf{q}, \mathbf{v}_2 - \frac{1}{2}\mathbf{q}; \mathbf{q}\right) [f(\mathbf{v}+\mathbf{q}) f(\mathbf{v}_2 - \mathbf{q}) - f(\mathbf{v}) f(\mathbf{v}_2)]}_{I(\mathbf{v})}. \tag{5.16}$$

From there, we will work in the grazing collision limit, meaning that we will only take into account collisions that imply small transfer of momentum. More precisely, we consider only collisions with $|\mathbf{q}| \ll |\mathbf{v}|, |\mathbf{v}_2|$. This approximation is relevant and often used in plasma physics, where Coulomb interactions tend to make collisions with small scattering angles more numerous and more influential than the other ones, see the first chapter of [169] for quantitative arguments. In order to understand at which precision we shall use this approximation, let us first give the relation between $\mathbf{B}$ and the collision kernel:

$$\mathbf{B}(\mathbf{v}_1, \mathbf{v}_2) = \frac{1}{2}\Lambda \int \mathrm{d}\mathbf{q} \, w(\mathbf{v}_1, \mathbf{v}_2; \mathbf{q}) \mathbf{q} \otimes \mathbf{q}, \tag{5.17}$$

where $\mathbf{q}_1 \otimes \mathbf{q}_2$ is the tensor product of the two vectors $\mathbf{q}_1$ and $\mathbf{q}_2$ (a tensor of rank 2). In appendix A.5, we prove that for Coulomb interaction the two expressions for $\mathbf{B}$, (5.17) and (5.5) are equal. In the following, we will omit the tensor product symbol, and a product of vector without a dot should be understood as a tensor product: $\mathbf{q}_1\mathbf{q}_2 \equiv \mathbf{q}_1 \otimes \mathbf{q}_2$. In the case of the Landau equation, the tensor $\mathbf{B}$ is well known and has a list of properties related to the geometry and the physics of the collisions (conservation laws and symmetry properties). For our study, we will retain that $\mathbf{B}$ is a symmetric tensor, that $\mathbf{B}$ is symmetric with respect to the exchange of its two arguments: $\mathbf{B}(\mathbf{v}_1, \mathbf{v}_2) = \mathbf{B}(\mathbf{v}_2, \mathbf{v}_1)$, and that $\mathbf{B}(\mathbf{v}_1, \mathbf{v}_2).(\mathbf{v}_1 - \mathbf{v}_2) = \overrightarrow{0}$, we prove these properties in appendix A.6.2. We will make a link between those properties and the symmetries of the Landau equation (5.15) in section 5.3.4.2.

In appendix A.7.1, we develop I in the Boltzmann equation (5.16) at order 2 in $\mathbf{q}$ and we obtain the Landau equation (5.15). We have thus justified the Landau equation as an approximation of the Boltzmann equation in the grazing collision limit.

5.3.3. Deriving Landau's large deviation principle from Boltzmann's large deviation principle

In this section we derive the Hamiltonian for the path large deviations of the Landau equation from the Hamiltonian for the path large deviations of the Boltzmann equation, using the grazing collision limit.

We start from the large deviation principle discussed in section (5.3.1). Adapting the discussion of section (5.3.1), with

$$g_\Lambda(\mathbf{r}, \mathbf{v}, t) = \Lambda^{-1} \sum_{n=1}^{N} \delta(\mathbf{v} - \mathbf{v}_n(t)) \delta(\mathbf{r} - \mathbf{r}_n(t)),$$

and with $\gamma = (\lambda_D/L)^3$, with the prescription that $g_\Lambda(\tau = 0)$ is in the neighborhood of $g(\tau = 0)$, we have

$$\mathbf{P}\left(\{g_\Lambda(\mathbf{r}, \mathbf{v}, \tau)\}_{0 \le \tau \le T} = \{g(\mathbf{r}, \mathbf{v}, \tau)\}_{0 \le \tau \le T}\right) \underset{\Lambda \to \infty}{\asymp} \mathrm{e}^{-\Lambda \int_0^T \mathrm{Sup}_p \left\{ \int \mathrm{d}\mathbf{r}\mathrm{d}\mathbf{v}\, \dot{g} p - \Lambda H_B[g,p] \right\} \mathrm{d}\tau},$$

where H_B is given by (5.12) and where we used the rescaled time variable $\tau = t/\Lambda$ by the plasma parameter Λ in the large deviation action.

In the following we will be interested in the case of homogeneous distributions, i.e. distributions that only depend on the velocity variable, denoted by the letter f: $g(\mathbf{r}, \mathbf{v}, \tau) = f(\mathbf{v}, \tau)$. Then the large deviation principle reads

$$\mathbf{P}(g_\Lambda = f) \underset{N \to \infty}{\asymp} \mathrm{e}^{-\Lambda \int_0^T \mathrm{Sup}_p \left\{ \int \mathrm{d}\mathbf{r}\mathrm{d}\mathbf{v}\, \dot{f} p - H[f,p] \right\} \mathrm{d}\tau}, \tag{5.18}$$

with the prescription that $g_\Lambda(\tau = 0)$ is in the neighborhood of $f(\tau = 0)$, and with

$$H[f,p] = \frac{\Lambda}{2} \int \mathrm{d}\mathbf{r}\mathrm{d}\mathbf{v}_1\mathrm{d}\mathbf{v}_2\mathrm{d}\mathbf{q}\, w\left(\mathbf{v}_1 + \frac{1}{2}\mathbf{q}, \mathbf{v}_2 - \frac{1}{2}\mathbf{q}; \mathbf{q}\right) \times f(\mathbf{v}_1) f(\mathbf{v}_2) \left\{ \mathrm{e}^{[-p(\mathbf{v}_1) - p(\mathbf{v}_2) + p(\mathbf{v}_1 + \mathbf{q}) + p(\mathbf{v}_2 - \mathbf{q})]} - 1 \right\}. \tag{5.19}$$

The idea to obtain the large deviation Hamiltonian for the Landau equation, is to use the same hypothesis of grazing collisions used in section (5.3.2). As in section (5.3.2), we will make a Taylor expansion in $\mathbf{q}$ at order 2. Rather than doing this expansion for the Boltzmann equation, we do it in the large deviation Hamiltonian (5.19). The full computation is detailed in appendix A.7.2, and we find that the large deviation Hamiltonian $H_{\text{Landau}}[f,p]$ for the Landau equation is

$$H_{\text{Landau}}[f,p] = H_{MF,h}[f,p] + H_I[f,p], \tag{5.20}$$

with

$$H_{MF,h}[f,p] = \int \mathbf{dr}\mathbf{dv}_1 f \left\{ \mathbf{b}[f] . \frac{\partial p}{\partial \mathbf{v}_1} + \frac{\partial}{\partial \mathbf{v}_1} \left(\mathbf{D}[f] \frac{\partial p}{\partial \mathbf{v}_1} \right) + \mathbf{D}[f] : \frac{\partial p}{\partial \mathbf{v}_1} \frac{\partial p}{\partial \mathbf{v}_1} \right\},$$

and

$$H_I[f,p] = -\int \mathbf{dr}\mathbf{dv}_1\mathbf{dv}_2 f(\mathbf{v}_1) f(\mathbf{v}_2) \frac{\partial p}{\partial \mathbf{v}_1} \frac{\partial p}{\partial \mathbf{v}_2} : \mathbf{B}(\mathbf{v}_1, \mathbf{v}_2),$$

where $\mathbf{b}[f]$ and $\mathbf{D}[f]$ are defined in equation (4.15), and in which we recognize that $H_{MF,h}$ is the mean field Hamiltonian (3.44) and a new additional term H_I.

We have thus justified a large deviation principle for the rescaled empirical density g_Λ in the limit of a large plasma parameter Λ. It reads

$$\mathbf{P}\left(\{g_\Lambda(\mathbf{r},\mathbf{v},\tau)\}_{0\le\tau\le T} = \{f(\mathbf{v},\tau)\}_{0\le\tau\le T} \right) \underset{\Lambda\to\infty}{\asymp} \mathbf{e}^{-\Lambda \text{Sup}_p \int_0^T \mathrm{d}\tau \left\{ \int \mathbf{dr}\mathbf{dv}\, \dot{f} p - H_{\text{Landau}}[f,p] \right\}}, \tag{5.21}$$

with the prescription that $g_\Lambda(\tau = 0)$ is in the neighborhood of $f(\tau = 0)$, and where H_{Landau} is defined in (5.20).

We note that this Hamiltonian is quadratic in its conjugate momentum p. Then, in the grazing collision limit, the large deviations are Gaussian. This is a consequence of neglecting the collisions that involve large changes of velocity for the particles. This constrains the fluctuations of the empirical density g_Λ in a reduced range where they can be considered as Gaussian fluctuations. As mentioned in section 3.7.1.3, a quadratic large deviation Hamiltonian can be associated with a stochastic differential equation involving a Gaussian noise. In this case,

$$\frac{\partial g_\Lambda}{\partial \tau} = \frac{\partial}{\partial \mathbf{v}} \cdot \left\{ -g_\Lambda \mathbf{b} + \mathbf{D} \frac{\partial g_\Lambda}{\partial \mathbf{v}} \right\} + \sqrt{\frac{2}{\Lambda}} \eta(\mathbf{v},\tau), \tag{5.22}$$

with

$$\mathbb{E}\left(\eta(\mathbf{r},\mathbf{v},\tau)\, \eta(\mathbf{r}',\mathbf{v}',\tau') \right) = \frac{\partial^2}{\partial \mathbf{v} \partial \mathbf{v}'} : \left(g_\Lambda(\mathbf{v}) \delta(\mathbf{v}-\mathbf{v}') \mathbf{D} - g_\Lambda(\mathbf{v}) g_\Lambda(\mathbf{v}') \mathbf{B}(\mathbf{v},\mathbf{v}') \right) \delta(\mathbf{r}-\mathbf{r}') \delta(\tau-\tau').$$

The Gaussian fluctuations have a non-trivial correlation structure.

5.3.4. Verification of the expected properties of the Hamiltonian

Let us check all the expected properties for the Hamiltonian (5.20).

5.3.4.1. Most probable evolution

First, we should verify that the most probable evolution associated with this Hamiltonian is the Landau equation, i.e. that

$$\frac{\partial f}{\partial \tau} = \frac{\delta H_{\text{Landau}}}{\delta p}[f, p=0] = \frac{\partial}{\partial \mathbf{v_1}} \left\{ -f\mathbf{b}\left[f\right] + \mathbf{D}\left[f\right] \frac{\partial f}{\partial \mathbf{v}_1} \right\}. \tag{5.23}$$

We start by computing the functional derivative of H_{Landau} term by term

$$\frac{\delta H_{MF,h}}{\delta p}[f, p=0] = \frac{\partial}{\partial \mathbf{v}_1} \left\{ -f\mathbf{b}\left[f\right] + \mathbf{D}\left[f\right] \frac{\partial f}{\partial \mathbf{v}_1} \right\}$$

and

$$\frac{\delta H_I}{\delta p}[f,p] = -2\frac{\partial}{\partial \mathbf{v}_1} \left\{ \int \mathrm{d}\mathbf{v}_2\, f(\mathbf{v}_1) f(\mathbf{v}_2) \mathbf{B}(\mathbf{v}_1, \mathbf{v}_2) \frac{\partial p}{\partial \mathbf{v}_2} \right\},$$

in particular, $\frac{\delta H_I}{\delta p}[f, p=0] = 0$. Thus, property (5.23) is verified. It is important to notice that, since we rescaled the time variable $\tau = t/\Lambda$ by the plasma parameter, there is no factor Λ^{-1} in the right hand side of (5.23).

5.3.4.2. Conservation laws

From the result (3.21) of section 3.4, we know that a functional $C[f]$ is a conserved quantity if and only if $\int \mathrm{d}\mathbf{r}\mathrm{d}\mathbf{v} \frac{\delta H_{\text{Landau}}}{\delta p} \frac{\delta C}{\delta f} = 0$ or equivalently, if for any f, p and α: $H_{\text{Landau}}[f,p] = H_{\text{Landau}}[f, p + \alpha \frac{\delta C}{\delta f}]$.

Mass conservation. It is easily checked that the mass $M[f]$ defined as $M[f] = \int \mathrm{d}\mathbf{v} f$ is conserved. Indeed, $\frac{\delta M}{\delta f} = 1$ and $H_{\text{Landau}}\left[f, p+\alpha\right] = H_{\text{Landau}}\left[f,p\right]$ as H does not depend explicitly on p but only on its derivatives.

Momentum conservation. Let us check the conservation of $\mathbf{P}$ the momentum defined as $\mathbf{P}[f] = \int \mathrm{d}\mathbf{v}\mathbf{v} f$. First, we notice that $\frac{\delta \mathbf{P}}{\delta f} = \mathbf{v}$. The functional derivative of H is

$$\frac{\delta H_{\text{Landau}}}{\delta p} = \int \mathrm{d}\mathbf{v}_2 \frac{\partial}{\partial \mathbf{v}} \left\{ -\mathbf{B}(\mathbf{v}, \mathbf{v}_2) \left[\frac{\partial f}{\partial \mathbf{v}_2} f(\mathbf{v}) - \frac{\partial f}{\partial \mathbf{v}} f(\mathbf{v}_2) + 2 f(\mathbf{v}) f(\mathbf{v}_2) \left(\frac{\partial p}{\partial \mathbf{v}} - \frac{\partial p}{\partial \mathbf{v}_2} \right) \right] \right\}.$$

Hence, integrating by parts we have

$$\int \mathrm{d}\mathbf{r}\mathrm{d}\mathbf{v}\, \frac{\delta H_{\text{Landau}}}{\delta p} \frac{\delta \mathbf{P}}{\delta f} = \int \mathrm{d}\mathbf{r}\mathrm{d}\mathbf{v}\mathrm{d}\mathbf{v}_2\, \mathbf{B}(\mathbf{v}, \mathbf{v}_2) \left[\frac{\partial f}{\partial \mathbf{v}_2} f(\mathbf{v}) - \frac{\partial f}{\partial \mathbf{v}} f(\mathbf{v}_2) + 2 f(\mathbf{v}) f(\mathbf{v}_2) \left(\frac{\partial p}{\partial \mathbf{v}} - \frac{\partial p}{\partial \mathbf{v}_2} \right) \right].$$

Then, using the fact that $\mathbf{B}(\mathbf{v}, \mathbf{v}_2) = \mathbf{B}(\mathbf{v}_2, \mathbf{v})$, we find

$$\int \mathbf{dr}\mathbf{dv} \, \frac{\delta H_{\text{Landau}}}{\delta p} \frac{\delta \mathbf{P}}{\delta f} = 0.$$

This means that the total momentum $\mathbf{P}$ is conserved by the dynamics. During this calculation, it is interesting to notice that both linear term in p and the quadratic term in p of H_{Landau} preserve the momentum independently. This means that both the deterministic part of H_{Landau} and the noise part of H_{Landau} preserve the momentum independently. More precisely, the last term that came up with our approach, which did not appear when investigating the large deviations for N diffusions coupled in a mean-field way in section 4.3, compensates the contribution of the last term of H_{MF}. Another interesting property, is that a necessary condition for the deterministic part of the Hamiltonian to conserve the momentum is the following relation between the deterministic drift $\mathbf{b}$ and the deterministic diffusion coefficient $\mathbf{D}$: $\int \mathrm{d}\mathbf{v} \, f(\mathbf{v}) \left\{ \mathbf{b}[f] + \frac{\partial}{\partial \mathbf{v}} \cdot \mathbf{D}[f] \right\} = 0$.

Energy conservation. Now we should check that the total kinetic energy E is conserved, with $E[f] = \frac{1}{2} \int \mathrm{d}\mathbf{v} \, \mathbf{v}^2 f$. Here, $\frac{\delta E}{\delta f} = \frac{1}{2}\mathbf{v}^2$. Using an integration by part we can write

$$\int \mathrm{d}\mathbf{v} \, \frac{\delta H_{\text{Landau}}}{\delta p} \frac{\delta E}{\delta f} = \int \mathrm{d}\mathbf{v}\mathrm{d}\mathbf{v}_2 \, \mathbf{B}(\mathbf{v}, \mathbf{v}_2) \left\{ \left(\frac{\partial f}{\partial \mathbf{v}_2} f(\mathbf{v}) - \frac{\partial f}{\partial \mathbf{v}} f(\mathbf{v}_2) \right) . \mathbf{v} \right.$$
$$\left. + 2 \left(f(\mathbf{v}) f(\mathbf{v}_2) \left(\frac{\partial p}{\partial \mathbf{v}} - \frac{\partial p}{\partial \mathbf{v}_2} \right) \right) . \mathbf{v} \right\},$$

and because $\mathbf{B}(\mathbf{v}, \mathbf{v}_2) = \mathbf{B}(\mathbf{v}_2, \mathbf{v})$, we have

$$\int \mathrm{d}\mathbf{v} \, \frac{\delta H_{\text{Landau}}}{\delta p} \frac{\delta E}{\delta f} = \int \mathrm{d}\mathbf{v}\mathrm{d}\mathbf{v}_2 \left\{ \frac{\partial f}{\partial \mathbf{v}_2} f(\mathbf{v}) + 2 f(\mathbf{v}) f(\mathbf{v}_2) \frac{\partial p}{\partial \mathbf{v}} \right\} \mathbf{B}(\mathbf{v}, \mathbf{v}_2).(\mathbf{v} - \mathbf{v_2}).$$

We have seen in appendix (A.6.2), that $\mathbf{B}(\mathbf{v}, \mathbf{v}_2).(\mathbf{v} - \mathbf{v}_2) = \overrightarrow{0}$, as a consequence of energy conservation in each collision. Then the integrand of the last formula is zero and we find that the total kinetic energy is conserved. Here too, both the deterministic part and the noise part of H preserve energy independently.

5.3.4.3. Entropy, quasipotential and time reversal symmetry

Entropy and quasipotential. We define $S[f]$ the entropy functional:

$$S[f] = -k_B \int \mathrm{d}\mathbf{v} f \log f \tag{5.24}$$

Using results from section 3.4, we are going to check that $-S$ is a quasipotential as long as the conservation laws of mass, momentum and energy hold. Here, we only check the necessary condition which is that $-S$ satisfies the Hamilton-Jacobi equation, more

precisely that: $H_{\text{Landau}}\left[f, -\frac{\delta S}{\delta f}\right] = 0$. Given the definition of S, $\frac{\delta S}{\delta f} = -\log f + c$ where c is a constant which, because of the mass conservation, has no effect and we have

$$H_{\text{Landau}}\left[f, -\frac{\delta S}{\delta f}\right] = \int \mathbf{dr}\mathbf{dv}\mathbf{dv}_2 \left(f(\mathbf{v}) f(\mathbf{v}_2) \frac{\partial^2 \mathbf{B}}{\partial \mathbf{v} \partial \mathbf{v}_2} - \frac{\partial f}{\partial \mathbf{v}} \frac{\partial f}{\partial \mathbf{v}_2} \mathbf{B} \right).$$

Integrating by parts twice the second term, we find out that the integrand is zero and that $-S$ satisfies the Hamilton-Jacobi equation: $H\left[f, -\frac{\delta S}{\delta f}\right] = 0$.

Time reversal symmetry. We define the time reversal operator I by $I[f](\mathbf{v}) = f(-\mathbf{v})$. One can easily check that $H_{\text{Landau}}\left[I[f], -I[p]\right] = H_{\text{Landau}}\left[f, p - \frac{\delta S}{\delta f}\right]$. The computation is very close to the one above, that was performed to prove that the entropy is the negative of the quasipotential up to conservation laws. We stated in section 3.4 that $H_{\text{Landau}}\left[I[f], -I[p]\right] = H_{\text{Landau}}\left[f, p - \frac{\delta S}{\delta f}\right]$ implies a time reversal symmetry of the path $\{f(t)\}_{0 \leq t \leq T}$ at the level of large deviations. The fluctuation paths are thus the time reversed of the relaxation paths. Moreover, from results (3.16) and (3.15) of section 3.4, we deduce that entropy increases along the relaxation paths. Thanks to the time reversal symmetry of the large deviation structure, we can also conclude that the entropy decreases along the fluctuation paths.

As a conclusion, we have derived the Hamiltonian for the Landau equation and we have checked all its expected properties.

5.3.5. The gradient flow structure of the Landau equation derived from the large deviation Hamiltonian

In section 3.5 and in section 5 of [50], we explain simply, following [160], that there is a close relation between large deviations associated with a kinetic equation and its gradient-transverse structure.

If we apply this general result to the Landau equation, using the large deviation principle that we just derived (5.20-5.21), we can conclude that the Landau equation has a gradient flow structure

$$\frac{\partial f}{\partial t} = -\text{Grad}_f \mathcal{U}\left[f\right]$$

(in this case $\mathcal{G} = 0$ for homogeneous distribution). More precisely, the Landau equation reads

$$\frac{\partial f}{\partial t} = \int \mathbf{dv}' \, C\left[f\right](\mathbf{v}, \mathbf{v}') \, \frac{\delta S}{\delta f}(\mathbf{v}') \tag{5.25}$$

where $S\left[f\right] = -\int \mathbf{dv} f \log f$ is the Boltzmann entropy functional (the negative of the quasipotential), and $C\left[f\right]$ is the quadratic part of the Hamiltonian (5.20) and reads

$$C\left[f\right](\mathbf{v}, \mathbf{v}') = \frac{\partial^2}{\partial \mathbf{v} \partial \mathbf{v}'} : \left(f(\mathbf{v}) \delta\left(\mathbf{v} - \mathbf{v}'\right) \mathbf{D}\left[f\right](\mathbf{v}) - f(\mathbf{v}) f(\mathbf{v}') \mathbf{B}\left[f\right](\mathbf{v}, \mathbf{v}') \right). \tag{5.26}$$

As discussed in section 3.5, for independent particles, for instance independent Brownian motion leading to the Fourier law, the gradient is computed with respect to the Wasserstein distance. For particles with mean field interactions, for instance leading to the McKean–Vlasov equation, the relevant metric is still the Wasserstein one. More generally for particles with mean field interaction with a diffusion coefficient that might be non-uniform and f dependent, as described in section 3.7.1.3, from the quadratic part of the Hamiltonian one finds $C[f](\mathbf{v},\mathbf{v}') = \frac{\partial^2}{\partial\mathbf{v}\partial\mathbf{v}'} : (f(\mathbf{v})\delta(\mathbf{v}-\mathbf{v}')\mathbf{D}[f](\mathbf{v}))$. This metric is still a kind of deformed Wasserstein one, that involves a f dependent diffusion coefficient. However for plasma in the weak coupling limit, and the Landau equation, one can see from equation (5.26) that the metric is no more simply related to the Wasserstein distance. One see in equation (5.26), that to the Wasserstein like term linear in f associated to independent motion of particles, one has to add a quadratic term in f related to the weak two-body interactions. This metric has also been recognized as the appropriate one to describe the Landau equation in [65, 66].

5.4. From the Balescu-Guernsey-Lenard large deviation Hamiltonian to the Landau Hamiltonian

In the previous chapter, we derived a large deviation principle for the empirical measure of N particles with generic long range interactions, directly from the dynamics (4.5). All the computations on the dynamics of the empirical measure, especially its slow-fast structure, still hold in the specific case where the interaction potential is the Coulomb potential and the time-scale separation parameter is the plasma parameter Λ rather than the number of particles N. In particular, the Hamiltonian (4.56) is still valid to describe the large deviations of the empirical measure of N particles coupled with a Coulomb potential. With the appropriate scaling of space and time introduced in section 4.2, and the prescription that the sequence $\{f_\Lambda(\mathbf{v},0)\}_\Lambda$ concentrates close to $f(\mathbf{v},0)$, the large deviation principle (4.2) can be recast into

$$\mathbf{P}\left(\{f_\Lambda(\mathbf{v},\tau)\}_{0\leq\tau\leq T} = \{f(\mathbf{v},\tau)\}_{0\leq\tau\leq T}\right) \underset{\Lambda\to\infty}{\asymp} \mathrm{e}^{-\Lambda \mathrm{Sup}_p \int_0^T \mathrm{d}\tau\left\{\int \mathbf{dr}\mathbf{dv}\, \dot{f}p - H^s_{\mathrm{BGL}}[f,p]\right\}}, \quad (5.27)$$

where

$$f_\Lambda(\mathbf{v},\tau) = \frac{1}{\Lambda}\left(\frac{\lambda_D}{L}\right)^3 \sum_{n=1}^{n} \delta(\mathbf{v}-\mathbf{v}_n(\tau)),$$

and

$$H^s_{\mathrm{BGL}}[f,p] = -\frac{1}{4\pi L^3} \sum_{\mathbf{k}\in 2\pi(\lambda_D/L)\mathbb{Z}^3} \int \mathbf{dr}\mathrm{d}\omega\, \log\{1-\mathcal{J}[f,p](\mathbf{k},\omega)\}, \quad (5.28)$$

where $\mathcal{J}$ is still defined by (4.52)[2].

[2]We note that $H^s_{\mathrm{BGL}} = \int \mathbf{dr}\, H_{\mathrm{BGL}}$. All the integrations on the spatial variable $\mathbf{r}$ in (5.27-5.28) are trivial and yield a global $(L/\lambda_D)^3$ if performed. We chose not to perform them for the sake of generality and to compare the result with the one derived from the Boltzmann Hamiltonian (5.18).

As explained in section 5.2, it is possible to derive the Landau equation from the Balescu-Guernsey-Lenard equation within the Landau approximation: i.e. when the effects of scales much smaller than the Debye length dominate. Hence, we expect to recover the Landau large deviation Hamiltonian (5.20) from the Hamiltonian (5.28) within the same Landau approximation.

As noted in section 5.3.3, the Hamiltonian for the Landau equation is quadratic in its conjugate momentum p, whereas the one for the Balescu-Guernsey-Lenard equation (5.28) is not. However, we can expand the logarithm in (5.28) using

$$\log\left(1-x\right) = -\sum_{n=1}^{+\infty} \frac{x^n}{n}.$$

As shown in appendix A.8, within the Landau approximation $k\lambda_D \gg 1$, only the the two first terms of the logarithm series expansion are relevant for the large deviation Hamiltonian (5.28) and we recover the Landau large deviation Hamiltonian (5.20) derived from the Boltzmann Hamiltonian. We then have

$$H^s_{\mathrm{BGL}}\left[f,p\right] \underset{k\lambda_D\gg 1}{\simeq} H_{\mathrm{Landau}}\left[f,p\right],$$

where the symbol $\underset{k\lambda_D\gg 1}{\simeq}$ means that the two sides are asymptotically equivalent as all the wavevectors' magnitudes satisfy $k\lambda_D \gg 1$.

Although this Hamiltonian is exactly the one we derived in section 5.3 from the large deviation Hamiltonian associated with the Boltzmann equation, the large deviation principle (5.27) is slightly different from (5.21). Indeed, the large deviation principle (5.21) describes large deviations of the empirical density g_Λ, whereas the large deviation principle (5.27) only describes the large deviations for f_Λ which is the projection of g_Λ over homogeneous distributions. However, it is possible to obtain (5.27) from (5.21) through the use of the contraction principle. In large deviation theory, the contraction principle states that if we know a large deviation principle for a random variable X with a large deviation function $I\left(x\right)$ it is possible to obtain a large deviation principle for any function $\varphi\left(X\right)$ of this random variable and the associated large deviation function is $I_\varphi\left(y\right) = \inf_{\varphi(x)=y} I\left(x\right)$. The two results are thus fully consistent.

5.5. Large deviations for the Landau equation when $L < \lambda_D$

Whenever the size of the domain is smaller than the Debye length, the relevant large deviation parameter is the number of particles in a box of the size of the effective interaction length scale $\ell = L$; i.e. the relevant large deviation parameter is N. We can then study the asymptotics of the empirical density g_Λ and its homogeneous projection as N goes to infinity. Because $\Lambda = \left(\lambda_D/L\right)^3 N$, when $L < \lambda_D$ the large N limit implies the large Λ limit, which is responsible for the kinetic behavior of the empirical density. In

order to make explicit that N is the natural large deviation rate, we perform the trivial integral on the positions in the large deviation principle (5.27). It is then possible to rephrase the large deviation principle (5.27) as following

$$\mathbf{P}(f_\Lambda = f) \underset{N\to\infty}{\asymp} \mathrm{e}^{-N\mathrm{Sup}_p \int_0^T \left\{\int \mathrm{d}\mathbf{v}\, \dot{f} p - H_{\text{Landau},h}[f,p]\right\}}, \tag{5.29}$$

with the prescription that $f_\Lambda(\tau = 0)$ is in the neighborhood of $f(\tau = 0)$, and by defining $H_{\text{Landau},h}$ as the large deviation Hamiltonian divided by the volume of the domain, such that

$$H_{\text{Landau}} = \int \mathbf{dr} H_{\text{Landau},h} = \left(\frac{L}{\lambda_D}\right)^3 H_{\text{Landau},h},$$

and

$$H_{\text{Landau},h}[f,p] = \int \mathrm{d}\mathbf{v}_1 f \left\{ \mathbf{b}[f] . \frac{\partial p}{\partial \mathbf{v}_1} + \frac{\partial}{\partial \mathbf{v}_1} . \left(\mathbf{D}[f] \frac{\partial p}{\partial \mathbf{v}_1}\right) + \mathbf{D}[f] : \frac{\partial p}{\partial \mathbf{v}_1}\frac{\partial p}{\partial \mathbf{v}_1} \right\} - \int \mathrm{d}\mathbf{v}_1 \mathrm{d}\mathbf{v}_2 f(\mathbf{v}_1) f(\mathbf{v}_2) \frac{\partial p}{\partial \mathbf{v}_1}\frac{\partial p}{\partial \mathbf{v}_2} : \mathbf{B}(\mathbf{v}_1, \mathbf{v}_2).$$

Using this same relation between N and Λ, we already have remarked that

$$f_\Lambda(\mathbf{v}, t) = \frac{1}{\Lambda}\left(\frac{\lambda_D}{L}\right)^3 \sum_{n=1}^N \delta(\mathbf{v} - \mathbf{v}_n(t)) = \frac{1}{N}\sum_{n=1}^N \delta(\mathbf{v} - \mathbf{v}_n(t)) = h_N(\mathbf{v}, t),$$

where h_N is the velocity empirical density rescaled by the number of particles. Then, we have the following large deviation principle for h_N

$$\mathbf{P}(h_N = f) \underset{N\to\infty}{\asymp} \mathrm{e}^{-N\mathrm{Sup}_p \int_0^T \left\{\int \mathrm{d}\mathbf{v}\, \dot{f} p - H_{\text{Landau},h}[f,p]\right\}},$$

with the prescription that $h_N(\tau = 0)$ is in the neighborhood of $f(\tau = 0)$.

If in addition to $L < \lambda_D$ we have $L \ll \lambda_D$, then, because the wavevectors $\mathbf{k}$ are elements of $2\pi(\lambda_D/L)\mathbb{Z}^3$ we have for all scales $k \gg 1$. This amounts at saying that the Landau approximation holds at all scales and that the large deviations described by (5.27) are Gaussian regardless of the scale of the fluctuations.

5.6. Large deviations for the Landau equation expressed in physical variables

In section 5.3.3, we established a large deviation principle (equations (5.20)-(5.21)) that describes the large deviations of the probability of homogeneous evolution paths for the empirical density $g_\Lambda(\mathbf{r}, \mathbf{v}, t) = \Lambda^{-1}\sum_{n=1}^N \delta(\mathbf{v} - \mathbf{v}_n(t))\delta(\mathbf{r} - \mathbf{r}_n(t))$. As discussed in section 5.4, this result is consistent with the large deviation principle for the projection of the empirical density on homogeneous paths $f_\Lambda(\mathbf{v}, t) = \Lambda^{-1}(\lambda_D/L)^3 \sum_{n=1}^N \delta(\mathbf{v} - \mathbf{v}_n(t))$.

So far, we expressed those results in a set of non-dimensional variables adapted to Coulomb plasmas.

We can express this large deviation result in physical variables, with the change of variables

$$\mathbf{v}_\varphi = v_T \mathbf{v}, \mathbf{k}_\varphi = \mathbf{k}/\lambda_D, t_\varphi = \Lambda\tau/\omega_{pe},$$

where v_T the thermal velocity, λ_D the Debye length, and ω_{pe} the plasma electron frequency are defined in section 5.1., and we denoted dimensional variables expressed in physical units with a subscript φ.

In the following we omit the subscript φ. The result is a large deviation principle for the empirical density in physical units

$$g_\Lambda(\mathbf{r}, \mathbf{v}, t) = \frac{1}{\Lambda} \sum_{n=1}^{N} \delta(\mathbf{v} - \mathbf{v}_n(t)) \delta(\mathbf{r} - \mathbf{r}_n(t))$$

which reads

$$\mathbf{P}\left(\{g_\Lambda\}_{0\leq t\leq T} = \{f\}_{0\leq t\leq T}\right) \underset{\Lambda\to\infty}{\asymp} \mathbf{e}^{-\Lambda \mathrm{Sup}_p \int_0^T \mathrm{d}t \left\{\int \mathbf{dr dv} \dot{f} p - H_{\mathrm{Landau}}[f,p]\right\}},$$

with the prescription that $g_\Lambda(t=0)$ is in the neighborhood of $f(t=0)$, and where

$$H_{\mathrm{Landau}}[f,p] = \int \mathbf{dr dv}_1 f \left\{ \mathbf{b}[f] . \frac{\partial p}{\partial \mathbf{v}_1} + \frac{\partial}{\partial \mathbf{v}_1} . \left(\mathbf{D}[f] \frac{\partial p}{\partial \mathbf{v}_1} \right) + \mathbf{D}[f] : \frac{\partial p}{\partial \mathbf{v}_1} \frac{\partial p}{\partial \mathbf{v}_1} \right\} - \int \mathbf{dr dv}_1 \mathbf{dv}_2 f(\mathbf{v}_1) f(\mathbf{v}_2) \frac{\partial p}{\partial \mathbf{v}_1} \frac{\partial p}{\partial \mathbf{v}_2} : \mathbf{B}(\mathbf{v}_1, \mathbf{v}_2) .$$

with

$$\begin{cases} \mathbf{b}[f](\mathbf{v}) & = \int \mathbf{dv}_2 \mathbf{B}(\mathbf{v}, \mathbf{v}_2) \frac{\partial f}{\partial \mathbf{v}_2} \\ \mathbf{D}[f](\mathbf{v}) & = \int \mathbf{dv}_2 \mathbf{B}(\mathbf{v}, \mathbf{v}_2) f(\mathbf{v}_2), \end{cases} \tag{5.30}$$

and

$$\mathbf{B}(\mathbf{v}_1, \mathbf{v}_2) = \frac{\Lambda q^4}{m^2 \epsilon_0^2} \frac{\pi}{L^3} \sum_{\mathbf{k} \in (2\pi/L)\mathbb{Z}^{*3}} \left(\hat{W}(\mathbf{k}) \right)^2 \mathbf{k}\mathbf{k} \delta(\mathbf{k}.\mathbf{v}_2 - \mathbf{k}.\mathbf{v}_1) . \tag{5.31}$$

And the associated Landau equation reads

$$\frac{\partial f}{\partial t} = \frac{\partial}{\partial \mathbf{v}} . \int \mathbf{dv}_2 \, \mathbf{B}(\mathbf{v}_1, \mathbf{v}_2) \left(-\frac{\partial f}{\partial \mathbf{v}_2} f(\mathbf{v}) + f(\mathbf{v}_2) \frac{\partial f}{\partial \mathbf{v}} \right) . \tag{5.32}$$

This differs slightly with the Landau equation one can find in the plasma literature [189, 150, 169] by a factor Λ in the tensor $\mathbf{B}$ (5.31). Typically, in those references, the Landau equation is an evolution equation for the average of the non-rescaled empirical density. Here, we rescaled the empirical density by the plasma parameter Λ. In order to recover the Landau equation of [189, 150, 169], one should replace f in equation (5.32) by f_0/Λ. The resulting evolution equation for f_0 would be the usual Landau equation, where $f_0 = \mathbb{E}(\Lambda g_\Lambda)$ is the distribution function typically used in plasma textbooks

5.7. Inhomogeneous systems: astrophysics, plasma physics

All the large deviation principles and kinetic equations described in this chapter and the previous one only apply to the study of spatially **homogeneous** systems with long-range interactions. From a technical point of view, this is very convenient since the kinetic description reduces to the evolution of the velocity distribution $f(\mathbf{v})$ of the particles, instead of the evolution of the μ-space distribution $g(\mathbf{r}, \mathbf{v})$. However, inhomogeneity is ubiquitous in systems with long-range interactions. For instance, if we consider an attractive gravitational potential instead of a repulsive electrostatic one, particles tend to cluster, favoring inhomogeneous configurations of the system [41]. Spatial inhomogeneities can also emerge in purely repulsive plasmas [64, 197]. It is then a crucial question to study these systems for various astrophysics and plasma physics applications. This is an exciting application, that would open the way to the study of the rare destabilization of globular clusters or galaxies, or the formation of inhomogeneous structures of smaller scales in self gravitating systems

However, when the interaction potential has sufficient symmetries taking advantage of the structure of Hamiltonian systems, a well chosen change of coordinates makes the problem easier. Instead of describing the position and velocity $(\mathbf{r}_i, \mathbf{v}_i)$ of each particles, we turn to angle-action coordinates $(\boldsymbol{\theta}_i, \mathbf{J}_i)$ [121, 48, 41]. As a consequence, at the kinetic level, the distribution $g(\boldsymbol{\theta}, \mathbf{J})$ of the particles over the one particle angle-action phase space $(\boldsymbol{\theta}, \mathbf{J})$ only depends on the action coordinate and reduces to $f(\mathbf{J})$ and its time-evolution can be described with Landau and Balescu-Guernsey-Lenard type kinetic equations [74, 127]. The homogeneous case is retrieved when the angles are the positions of the particles $\boldsymbol{\theta}_i = \mathbf{r}_i$ and their actions are their velocities $\mathbf{J}_i = \mathbf{v}_i$.

With Jean-Baptiste Fouvry, we developed the large deviation theory associated with the inhomogeneous Landau equation that describes the kinetic behavior of particle systems with long-range interactions neglecting collective effect [108]. The extension to the study of large deviations associated with the inhomogeneous Balescu-Guernsey-Lenard equation is still an open question. The main technical obstacle to the extension of the computations of chapter 4 is that in the inhomogeneous case, the correlation structure of the fluctuations of the empirical measure described in section 4.4.2 is more intricate, as the Fourier modes are not delta-correlated.

5.8. Perspectives and conclusions of the first part

The main result of this chapter is the derivation of a large deviation principle (5.21) for the empirical measure of N particles coupled via a Coulomb repulsive potential. We have obtained an explicit formula for the large deviation Hamiltonian (5.12-5.14) and we have checked all its symmetry properties. This result has been obtained both from the large deviations associated with the Boltzmann equation; and from the Hamiltonian associated with the Balescu–Guerseny–Lenard obtained in chapter 4 within the Landau approximation.

Another important result of this chapter is the derivation of a gradient-flow structure for the Landau equation, giving a new insight on the geometry of the entropy creation associated with the Landau equation.

In this first part of the manuscript, we introduced and motivated dynamical large deviations for kinetic theories. First, we presented well-known results about large deviations of the empirical measure of N independent particles undergoing various stochastic dynamics. More interestingly, the two main results of the first part are the derivation of large deviation principles for the empirical measure of N particles undergoing a Hamiltonian dynamics and coupled by a long-range potential in the general case, and within the Landau approximation when the potential is a Coulomb one. Alongside previous results about the large deviation associated with the dilute gas and the Boltzmann equation [45, 46, 50], these results complete the picture of dynamical large deviations associated with classical kinetic theories: the Boltzmann equation, the Landau equation, and the Balescu-Guernsey-Lenard equation.

A natural follow-up question is to study how fluctuations at the level of the kinetic theory can be transferred to macroscopic fluctuations. For instance, it is known that one can obtain the Navier–Stokes equations describing the macroscopic behavior of fluids from the Boltzmann equation through a Chapman–Enskog expansion. In the next part of the manuscript, we will study how to carry fluctuations at the kinetic level through hydrodynamical limits.

Part II.

Large deviations in the hydrodynamical limit

6. From the kinetic to the hydrodynamic scales: a large deviation perspective

The second part of this manuscript is devoted to the derivation of fluctuating hydrodynamics from kinetic LDPs. First, we have to briefly recall the main tools to bridge from kinetic to hydrodynamic equations. Kinetic equations generally describe the evolution of the distribution function $f(\mathbf{r}, \mathbf{v}, t)$ that gives the information about the average number of particles having a velocity $\mathbf{v}$, a position $\mathbf{r}$ at a time t. The hydrodynamic equations only describe the evolution of the first moments with respect to the velocity variable of the distribution function. For example, the zero order moment corresponds to the density field $\int \mathrm{d}\mathbf{v}\, f(\mathbf{r}, \mathbf{v}, t)$, the first order moment to the velocity field $\int \mathrm{d}\mathbf{v}\, \mathbf{v} f(\mathbf{r}, \mathbf{v}, t)$, and the second order moment to the kinetic energy field $\int \mathrm{d}\mathbf{v}\, v^2 f(\mathbf{r}, \mathbf{v}, t)/2$. As explained in the introduction, without further assumptions, it is in general impossible to obtain closed equations for those hydrodynamic fields from the kinetic equation. One way to overcome this problem is to use the Chapman-Enskog method, which in a regime of large separation of time and space scales allows to obtain closed equations for the hydrodynamic fields.

The Chapman–Enskog method [69] was originally developed to derive the Navier-Stokes equations starting from the Boltzmann equation – the kinetic equation associated with the dynamics of a dilute gas. This procedure is an asymptotic one and relies on a perturbative analysis of the solutions of the Boltzmann equation. In addition to the hydrodynamical limit which leads to the Navier-Stokes equations, the Chapman-Enskog method can be applied to obtain various fluid descriptions such as magnetohydrodynamics or relativistic fluid equations, starting from the associated kinetic theories [130, 183]. Perhaps one of the greatest achievements of the Chapman-Enskog method is the computation of transport and diffusion coefficients from the microscopic parameters of the particle model. For the Navier-Stokes equation, the Chapman-Enskog method gives microscopic expressions for the viscosity and the thermal diffusivity, agreeing with experimental results for dilute gases [69]. However, there are still some open questions regarding the mathematical understanding of such asymptotic expansions, and for certain type of particle dynamics, the Chapman-Enskog expansion is known to diverge [122, 61, 187].

In this manuscript, we adopt a more general approach to the hydrodynamical limits of kinetic equations. We are interested in the derivation of fluctuating hydrodynamics, rather than deterministic fluid equations, that also quantify finite number of particles

fluctuations. Fluctuating hydrodynamics can be expressed as Stochastic PDEs (SPDEs), PDEs with a noise term, that characterize the effective evolution of continuum macroscopic fields with a noise term sourced by finite N fluctuations, or alternately as a LDP for the empirical hydrodynamic fields, that directly allows to quantify the probability of any evolution path for the empirical hydrodynamic fields in the large N limit.

To do so, instead of taking the kinetic equation as a starting point, we study the hydrodynamical limit of the kinetic LDP in order to keep track of the finite N fluctuations in the hydrodynamical limit. This can be done by a formal Chapman–Enskog expansion of the fluctuating kinetic equation, which is the SPDE for the empirical measure that is associated with the kinetic LDP. In this case, the computations are very close to the ones that lead to the classic deterministic fluid equation, with a supplementary term sourced by a noise term. However, the mathematical meaning of such SPDEs is still unclear, and the SPDE formulation only allows a complete characterization of the noise term when the kinetic LDP is Gaussian. Although the computations are formally equivalent, in this manuscript, when possible we also explain how to obtain fluctuating hydrodynamics as LDPs for the empirical hydrodynamic fields, starting from the kinetic LDP and working at the level of the large deviation functionals, in the spirit of [16]. This is also a first step toward a rigorous derivation of such results.

In this introductory chapter, we take the example of the derivation of the fluctuating hydrodynamics of N particles independently diffusing according to a Run-and-Tumble process in 2D. We apply the program explained in the previous paragraph to this system. The outline of this chapter is summed up in figure 6.1. In section 6.1, we recall the kinetic description of the N independent Run-and-Tumbling particles model, that we use to introduce the derivation of fluctuating hydrodynamics. In section 6.2, we introduce the different rescalings of space and time that can be used to obtain hydrodynamic equations when there is a large separation between the microscopic and macroscopic scales of the system. In section 6.3, we explain how to identify the hydrodynamic fields of the model, and their relationship with the local equilibria of the kinetic equation and its conserved quantities. In section 6.4, we use a Chapman-Enskog expansion to obtain the deterministic evolution equation for the hydrodynamic field. In section 6.5, we extend this computation, starting from the noisy fluctuating kinetic equation describing finite N fluctuations derived from the kinetic LDP, to obtain fluctuating hydrodynamics describing the finite N fluctuations of the empirical hydrodynamic field. In section 6.6, instead of working with SPDEs, we obtain fluctuating hydrodynamics by studying the convergence of the kinetic LDP that describes fluctuations of the empirical measure toward the hydrodynamic LDP for the empirical hydrodynamic field.

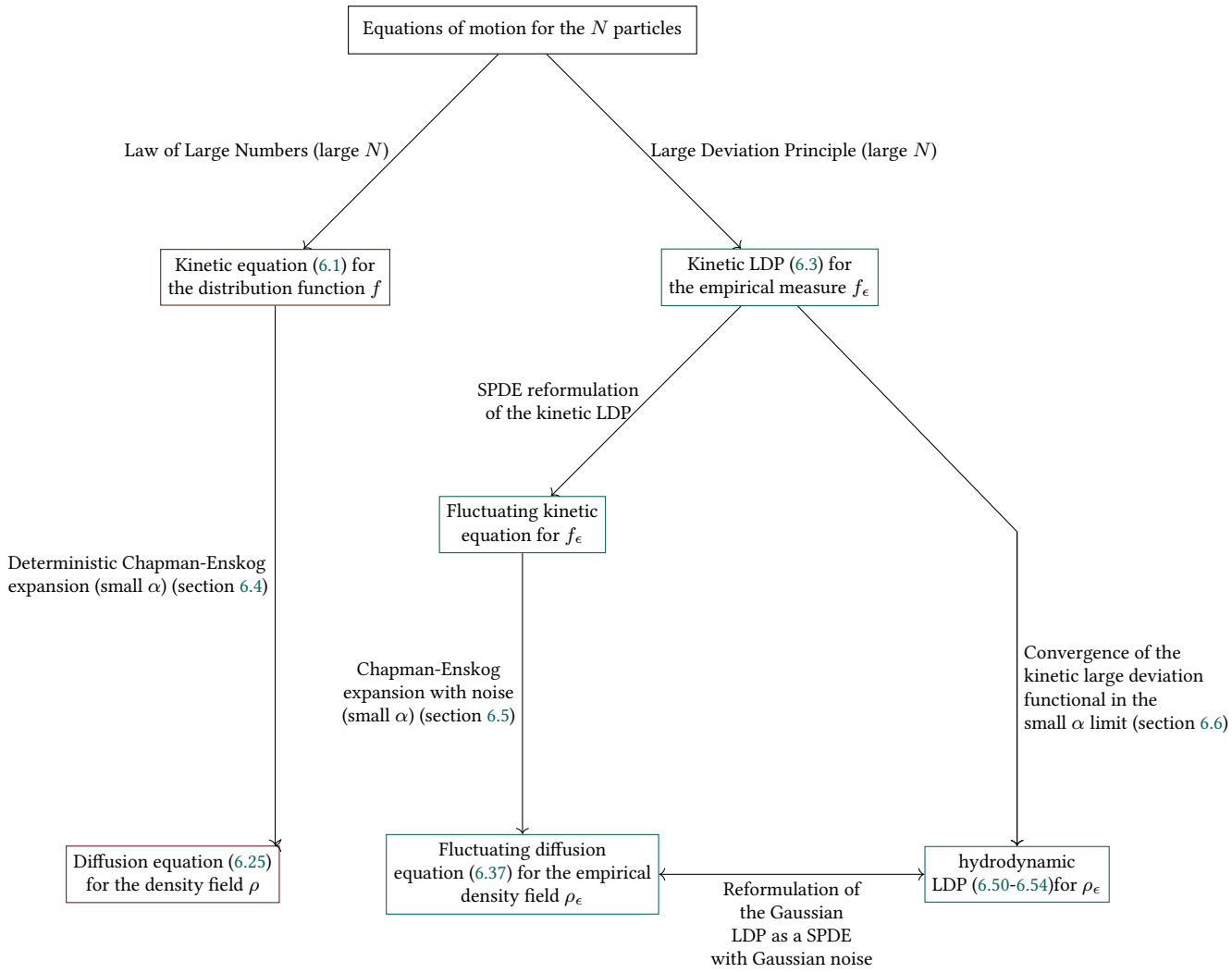


Figure 6.1.: Outline of the chapter. Starting from the kinetic description of the particle model recalled in section 6.1, we derive its fluid description. If we take the kinetic equation (the LLN for the empirical measure) as a starting point, we obtain in the small Knudsen number (α) limit the deterministic hydrodynamic equation (section 6.4). Starting from the kinetic LDP, we can either derive fluctuating hydrodynamics working from a SPDE formulation of the kinetic LDP in the small Knudsen number (section 6.5), or we can directly derive a hydrodynamic LDP describing the fluctuations of the empirical hydrodynamic field (section 6.6).

6.1. The example of the fluctuating diffusion equation for N independent Run-and-Tumbling particles

In this section, we will take as an illustrative example a system of N independent particles undergoing a Run-and-Tumble dynamics described in section 3.7.2.1. We recall the main results of section 3.7.2.1. The rescaled empirical measure of the position and

orientation (velocity) of the particles

$$f_\epsilon(\mathbf{r},\theta,t) = \epsilon \sum_{n=1}^{N} \delta(\mathbf{r} - \mathbf{r}_n(t))\,\delta(\theta - \theta_n(t)),$$

where $\epsilon = L^2/(N\ell^2)$ is the inverse of the number of particles in a box of the size of the mean free path, admits a law of large numbers. With the prescription that

$$\lim_{\epsilon\to 0} f_\epsilon(\mathbf{r},\theta,0) = f_0(\mathbf{r},\theta),$$

then

$$\lim_{\epsilon\to 0} f_\epsilon(\mathbf{r},\theta,t) = f(\mathbf{r},\theta,t),$$

where f is a solution of the kinetic equation

$$\partial_t f + \mathbf{e}_\theta \cdot \nabla f = L[f] \quad \text{and} \quad f(\mathbf{r},\theta,0) = f_0(\mathbf{r},\theta), \tag{6.1}$$

where $\mathbf{e}_\theta = (\cos\theta, \sin\theta)$, P is the tumbling reorientation distribution probability and

$$L[f] = -f + \int \mathrm{d}\theta'\, P(\theta' - \theta)\, f(\theta'). \tag{6.2}$$

We also established the following LDP for the empirical measure

$$\mathbb{P}\left(\{f_\epsilon(t)\}_{0\le t<T} = \{f(t)\}_{0\le t<T}\right) \underset{\epsilon\downarrow 0}{\asymp} \exp\left(-\frac{1}{\epsilon} I_T[f]\right), \tag{6.3}$$

where

$$I_T[f] = \int_0^T \mathrm{d}t \sup_p \left(\int \mathbf{r}\mathrm{d}\theta\, p\,(\partial_t f - \mathbf{e}_\theta \cdot \nabla f) - H_{\text{tumb}}[f,p]\right), \tag{6.4}$$

and

$$H_{\text{tumb}}[f,p] = \int \mathbf{r}\mathrm{d}\theta\mathrm{d}\theta'\, f(\mathbf{r},\theta,t) P(\theta - \theta') \left\{e^{-p(\mathbf{r},\theta,t)+p(\mathbf{r},\theta',t)} - 1\right\}. \tag{6.5}$$

We noticed that the large deviation Hamiltonian is non quadratic, making the large deviations non Gaussian, as usual for jump processes. Given the isotropic, diffusive nature of the particle dynamics[1], it does not come as a surprise that the density field ρ of N non-interacting Run-and-Tumbling particles[2] evolves according to a diffusion equation [23, 195]

$$\partial_t \rho = D\Delta\rho,$$

[1] This is an important precision. If the tumbling probability distribution is biased toward a certain direction, the resulting hydrodynamic equation would be a transport equation. Another interesting case is if the bias is small (with respect to the Knudsen number), in this case, we obtain a transport-diffusion equation as the hydrodynamical limit.

[2] Since the particles are independent, the density field can also be understood as the spatial probability distribution of a single particle.

where D is a diffusion coefficient. Recalling arguments from Dean and Kawasaki [86, 136, 82], one could further conjecture that the empirical density

$$\rho_\epsilon(\mathbf{r},t) = \epsilon \sum_{n=1}^{N} \delta(\mathbf{r} - \mathbf{r}_n(t))$$

obeys the Dean-Kawasaki equation

$$\partial_t \rho_\epsilon = D\Delta\rho_\epsilon + \nabla \cdot \left(\sqrt{2\gamma\epsilon D\rho_\epsilon}\boldsymbol{\zeta}\right) \tag{6.6}$$

where $\boldsymbol{\xi}$ is a tridimensional Gaussian noise with correlation matrix

$$\mathbb{E}(\boldsymbol{\zeta}(\mathbf{r},t) \otimes \boldsymbol{\zeta}(\mathbf{r}',t')) = \mathrm{Id}\delta(\mathbf{r}-\mathbf{r}')\delta(t-t'),$$

and γ is a number to be determined depending on the parameters of the model. As previously stated, the meaning of the SPDE (6.6) is not obvious (see [76, 77]), and in this manuscript we consider it as a rewriting of the Gaussian LDP for the empirical density

$$\mathbb{P}\left(\{\rho_\epsilon(t)\}_{0\le t\le T} = \{\rho(t)\}_{0\le t\le T}\right) \underset{\epsilon\downarrow 0}{\asymp} \mathrm{e}^{-\frac{1}{\epsilon\gamma} I_{\text{hydro}}[\rho]}, \tag{6.7}$$

where

$$I_{\text{hydro}}[\rho] = \int_0^T \mathrm{d}t \sup_{p_\rho} \left\{ \int \mathbf{dr}\, p_\rho \partial_t \rho - H_{\text{hydro}}[\rho, p_\rho] \right\}, \tag{6.8}$$

with

$$H_{\text{hydro}}[\rho, p_\rho] = D \int \mathbf{dr}\ \left(p_\rho \Delta\rho + \rho |\nabla p_\rho|^2\right), \tag{6.9}$$

In this section, we introduce several ways to retrieve the fluctuating hydrodynamics equation (6.6) starting from the kinetic LDP (6.3). We also explain in which asymptotic regime the fluctuating hydrodynamics is relevant. An important point is that in (6.6), the noise term is Gaussian, whereas the large deviations of the probability distribution for the evolution paths of the empirical measure is clearly non Gaussian according to the LDP (6.3). In section 6.6, we explain how non Gaussian fluctuations at the kinetic level can lead to Gaussian fluctuating hydrodynamics.

6.2. Hydrodynamic scaling

As explained in section 2.1 of the introduction, to obtain hydrodynamics equation from the particle dynamics, not only we have to consider large N asymptotics, but the microscopic and macroscopic scales must be well-separated. Quantitatively, we introduce the Knudsen number α

$$\alpha = \frac{\text{Microscopic length}}{\text{Macroscopic length}} = \frac{\ell}{L},$$

where $\ell = v_0\lambda$ is the mean free path of a particle, i.e. the average distance spanned by a particle between two tumbling events, and L is the size of the system. For a system of interacting particles, ℓ would be the average distance traveled by a particle between two interactions. We expect that a hydrodynamic description of the system should be accurate in the regime of small Knudsen numbers. Then, hydrodynamic fields, such as the density field should evolve on time and length scales much larger than the typical kinetic time (the typical evolution time of the distribution function, here this is the inverse of the tumbling rate λ^{-1}). The first step to derive hydrodynamics is thus to rescale time and space in line with the hydrodynamics scales. The precise rescaling we choose depends on whether we expect the dynamics of the hydrodynamic fields to be a diffusive one, or a wave propagation one [135, 196]. A parabolic choice of scaling is made by rescaling space and time as following:

$$\tilde{\mathbf{r}} = \alpha\mathbf{r}, \quad \tilde{t} = \alpha^2 t, \tag{6.10}$$

and is suited to describe the dynamics of quantities that have a diffusive dynamics. The terminology "parabolic" refers to the parabolic nature of the PDE that would describe the evolution of the hydrodynamic fields. The Fourier heat law and the incompressible Navier-Stokes equations are instances of such PDEs.

We can also choose a hyperbolic rescaling:

$$\tilde{\mathbf{r}} = \alpha\mathbf{r}, \quad \tilde{t} = \alpha t, \tag{6.11}$$

that is suited to describe transport phenomena and wave propagation. This is typically the rescaling that leads to transport and conservation laws PDEs, e.g. the compressible Euler equations, that are hyperbolic PDEs.

To describe the hydrodynamical limit of N Run-and-Tumbling particles, we expect a diffusion equation, we then turn to a parabolic rescaling. With the new choice of space and time units (6.10) and dropping the tildes for convenience, the kinetic equation (6.1) reads

$$\alpha^2 \partial_t f^\alpha + \alpha \mathbf{e}_\theta \cdot \nabla f^\alpha = L\left[f^\alpha\right], \tag{6.12}$$

where the distribution function now depends on α, as reminded by the superscript.

6.3. Conservation laws, hydrodynamic modes, and local equilibria of the kinetic equation

This manuscript has not yet addressed the issue of the identification of the hydrodynamic modes: the macroscopic fields that exhibit non-trivial dynamics on time scales of order $1/\alpha$ as α goes to zero. In general, each quantity that is conserved by the particle dynamics, and thus the kinetic equation, will be associated with a hydrodynamic mode. The underlying key point is that hydrodynamic modes are linked to the elements of the kernel of the adjoint of the collision operator. We illustrate this in the specific case of the dynamics of the Run-and-Tumbling particles.

If we start from (6.12), in the small α limit we note that solutions quickly relax toward local equilibria f_{eq} that cancel the r.h.s. of the kinetic equation:

$$L\left[f_{\text{eq}}\right] = 0.$$

The characterization of such local equilibria is related to the conservation laws and the hydrodynamic modes of the system. For the collision operator $L[f]$ (6.2), the local equilibria are the distribution functions that are uniform in angle, and depend only on the position. Thus, they are indexed by a density field $\rho(\mathbf{r}, t)$ that fully characterizes a local equilibrium:

$$f_{\text{eq}}(\mathbf{r}, \theta, t) = \frac{1}{2\pi}\rho(\mathbf{r}, t).$$

This density field is the only hydrodynamic mode for N independent Run-and-Tumbling particles. We note that the fact that any distribution that does not depend on the orientation is a local equilibrium can be rewritten $\ker L = \text{span}\{\mathbf{1}\}$, where $\mathbf{1} : \theta \mapsto 1$ is a function that does not depend on the orientation variable. Since L is self-adjoint[3] with respect to the scalar product

$$\langle a, b\rangle = \int \mathrm{d}\theta\, a(\theta) b(\theta), \tag{6.13}$$

we also have $\ker L^\dagger = \text{span}\{\mathbf{1}\}$, where $L^\dagger$ is the adjoint of L. In other words, we have

$$\int \mathrm{d}\theta\, L[g](\theta) = 0 \tag{6.14}$$

for every distribution g. From the particle point of view, this is a consequence of the conservation of the number of particles, or at the kinetic level of the total mass $M[f] = \int \mathrm{d}\mathbf{r}\mathrm{d}\theta\, f$ of the system. However, hydrodynamic modes do not have to be associated with a conservation law, they can also be associated with spontaneous symmetry breaking (e.g. Goldstone modes), or be the slow mode associated with the critical slowing down for a system that exhibits a bifurcation [31]. For instance, in chapter 8 we generalize the notion of collision invariant (element of the kernel of the adjoint collision operator) based on [87] to obtain a fluid equation on the velocity for a particle dynamics that does not conserve momentum.

6.4. From the kinetic equation to hydrodynamics

In this section, we explain how to derive a deterministic evolution equation for the hydrodynamic mode starting from the kinetic equation in the small Knudsen number limit. The starting point is to build a Chapman-Enskog expansion. In other words, we look for

[3] The collision operator is not necessarily self-adjoint. This actually depends on the dynamics under consideration.

a solution of the kinetic equation (6.12) close to a local equilibrium, indexed by the density field ρ:

$$f^\alpha(\mathbf{r},\theta,t) = \frac{1}{2\pi}\rho(\mathbf{r},t) + \alpha g_1(\mathbf{r},\theta,t) + \alpha^2 g_2(\mathbf{r},\theta,t) + \mathcal{O}\left(\alpha^3\right), \tag{6.15}$$

where $\int \mathrm{d}\theta\, g_i(\mathbf{r},\theta,t) = 0$ for $i \in \{1,2\}$ so that the hydrodynamic content of f^α is described by ρ. Introducing (6.15) in the kinetic equation after the parabolic rescaling (6.12) yields[4]

$$\frac{\alpha^2}{2\pi}\partial_t\rho + \frac{\alpha}{2\pi}\mathbf{e}_\theta\cdot\nabla\rho + \alpha^2\mathbf{e}_\theta\cdot\nabla(g_1) = \alpha L[g_1] + \alpha^2 L[g_2] + \mathcal{O}\left(\alpha^3\right). \tag{6.16}$$

The objective of this computation is to get a closed equation on the density field ρ. At leading order in α, (6.16) yields

$$\frac{1}{2\pi}\mathbf{e}_\theta\cdot\nabla\rho = L[g_1]. \tag{6.17}$$

The collision operator L satisfies a Fredholm alternative [114], which means that the equation $L[a] = b$ has a solution if $b \in (\ker L)^\perp$ (i.e. $\int \mathrm{d}\theta\, b = 0$), and this solution is unique if $a \in (\ker L)^\perp$ (i.e. $\int \mathrm{d}\theta\, a = 0$). Since $\int \mathrm{d}\theta\, \mathbf{e}_\theta = 0$ and $\int \mathrm{d}\theta\, g_1 = 0$, we can fully determine g_1 by inverting L. Once we know g_1, we use the conservation of the total mass at the kinetic level, or equivalently the relation (6.14) to obtain an equation for the time evolution of the density. More precisely, the integration of (6.16) over the orientation variable θ yields[5]

$$\partial_t\rho + \int \mathrm{d}\theta\, \mathbf{e}_\theta\cdot\nabla(g_1) = \mathcal{O}(\alpha), \tag{6.18}$$

where g_1 can be computed from (6.17). Given the definition of the collision operator L, we can take advantage of working in the Fourier space introducing the definition of the k-th Fourier mode for $k \in \mathbb{Z}$

$$\hat{f}_k = \int \mathrm{d}\theta\, \mathrm{e}^{-ik\theta} f(\theta), \tag{6.19}$$

and the inversion formula

$$f(\theta) = \frac{1}{2\pi}\sum_k \mathrm{e}^{ik\theta}\hat{f}_k.$$

Using that L is diagonal on the basis $\left\{\theta \mapsto \mathrm{e}^{ik\theta}\right\}_{k\in\mathbb{Z}}$:

$$\widehat{(L[f])}_k = \hat{f}_k\left(\hat{P}_k - 1\right), \tag{6.20}$$

[4] Because we deal with a system of independent particles, the collision operator L is linear. In general, in the Chapman-Enskog expansion, L would be replaced by the linearization of the collision operator close the local equilibrium around which we look for solutions of the kinetic equation.

[5] Conveniently, g_2 does not appear in this equation as a consequence of the mass-preserving property of the kinetic equation, or more weakly, because $\mathbf{1} \in \ker L^\dagger$.

we can compute its inverse when it exists:

$$L^{-1}[g](\theta) = \frac{1}{2\pi}\sum_k \mathrm{e}^{ik\theta}\frac{\hat{g}_k}{\hat{P}_k - 1}, \tag{6.21}$$

i.e. when $\int \mathrm{d}\theta\, g = 0$, or equivalently when $g \in (\ker L)^\perp$. Hence, it is possible to invert (6.17) to obtain

$$g_1 = \frac{1}{2\pi}\frac{\mathbf{e}_\theta \cdot \nabla\rho}{\hat{P}_1 - 1}. \tag{6.22}$$

Introducing (6.22) in (6.18) yields an equation on ρ that does not depend on g_1 anymore:

$$\partial_t\rho + \frac{1}{2\pi}\int \mathrm{d}\theta\, \mathbf{e}_\theta \cdot \nabla\left(\frac{\mathbf{e}_\theta \cdot \nabla\rho}{\hat{P}_1 - 1}\right) = \mathcal{O}(\alpha). \tag{6.23}$$

Using $\int \mathrm{d}\theta\, \mathbf{e}_\theta \otimes \mathbf{e}_\theta = \pi\mathrm{Id}$, where Id is the 2×2 identity matrix, and introducing the diffusion coefficient

$$D = \frac{1}{2\left(1 - \hat{P}_1\right)}, \tag{6.24}$$

we can recast (6.23) into

$$\partial_t\rho = D\Delta\rho + \mathcal{O}(\alpha), \tag{6.25}$$

which is the expected hydrodynamic equation for the density field ρ when we drop higher order terms in α. One of the success of the Chapman-Enskog expansion is that we obtain an explicit relationship between the microscopical parameter of the model (here $\hat{P}_1$ the first Fourier mode of the tumbling probability distribution) and the macroscopic diffusion coefficient D. As expected, the diffusion coefficient (6.24) is positive ($\hat{P}_1 < 1$ by triangle inequality) and diverges if the tumbling probability distribution is a Dirac delta distribution $P(\theta) = \delta(\theta)$, which corresponds to an absence of tumbling event. All these computations were made in the specific case where $P(\theta) = P(-\theta)$. They can be extended to the case where this symmetry does not hold, by replacing every occurrence of $\hat{P}_1$ by its real part $\Re\hat{P}_1$.

6.5. Toward fluctuating hydrodynamics: the SPDE approach

In the previous section, we explained how to derive the deterministic hydrodynamic equation starting from the kinetic equation in the small Knudsen number limit. A common way to quantify dynamical fluctuations of the hydrodynamic field is to write fluctuating hydrodynamics as a SPDE for the hydrodynamic fields, where the noise terms models finite N fluctuations of those fields. In this section, starting from a fluctuating kinetic

equation (a SPDE for the μ-space empirical measure), we obtain a SPDE describing the evolution and the fluctuations of the empirical density slightly adapting the Chapman-Enskog expansion presented above. The fluctuating kinetic equation is obtained as the Gaussian SPDE associated with the kinetic LDP where we assumed the Hamiltonian to be quadratic.

6.5.1. From the kinetic LDP to the fluctuating kinetic equation

The first step is to establish the fluctuating kinetic equation, i.e. the SPDE modeling the evolution of the empirical measure of the N particles. As explained in equations (3.39-3.41) of chapter 3, we can associate a LDP with a quadratic Hamiltonian, to a S(P)DE with Gaussian noise whose small noise large deviations are described by the aforementioned LDP. However, here the Hamiltonian (6.5) is non quadratic. In this section, we truncate the Hamiltonian H_{tumb} to its quadratic part

$$H^{(2)}[f,p] = \frac{1}{2}\int \mathrm{d}\mathbf{r}\mathrm{d}\theta\mathrm{d}\theta'\, f(\mathbf{r},\theta,t)P_t(\theta-\theta')\left(-p(\mathbf{r},\theta,t)+p(\mathbf{r},\theta',t)\right)^2. \tag{6.26}$$

In section 6.6, we justify this approximation for this specific model by studying the convergence of the kinetic large deviation functional in the small Knudsen number regime.

Applying result (3.39-3.41) from section 3.7.1, we can write the following SPDE for the empirical measure

$$\partial_t f_\epsilon + \mathbf{e}_\theta\cdot\nabla f_\epsilon = L[f_\epsilon] + \sqrt{\epsilon}\eta[f_N](\mathbf{r},\theta,t), \tag{6.27}$$

where η is a Gaussian noise characterized by its covariance operator

$$\mathbb{E}\left(\eta[f_\epsilon](\mathbf{r},\theta,t)\,\eta[f_\epsilon](\mathbf{r}',\theta',t')\right) = \delta(t-t')\,\delta(\mathbf{r}-\mathbf{r}')\,Q_{f_\epsilon}, \tag{6.28}$$

where $Q_f[\varphi] = \frac{\delta H^{(2)}}{\delta p}[f,\varphi]$. The covariance (6.28) has to be understood as an operator through its action on test functions φ, ψ:

$$\begin{aligned}\int \mathrm{d}\mathbf{r}\mathrm{d}\mathbf{r}'\mathrm{d}\theta\mathrm{d}\theta'\,\varphi(\mathbf{r},\theta,t)\,\psi(\mathbf{r}',\theta',t')\,\mathbb{E}\left(\eta[f_\epsilon](\mathbf{r},\theta,t)\,\eta[f_\epsilon](\mathbf{r}',\theta',t')\right)\\ = \delta(t-t')\int \mathrm{d}\mathbf{r}\mathrm{d}\theta\,\varphi(\mathbf{r},\theta,t)\,Q_{f_\epsilon}[\psi](\mathbf{r},\theta,t).\end{aligned} \tag{6.29}$$

As we explained in chapter 3, the small-noise SPDE to LDP correspondence is not a one-to-one correspondence. Then, the fluctuating kinetic equation (6.27) is only one equation among many others whose small noise large deviations are described by the large deviation Hamiltonian (6.26).

6.5.2. Chapman-Enskog expansion with noise

The next step is to establish a SPDE ruling the evolution of the empirical density ρ_ϵ in the small Knudsen number regime. As previously, we proceed to a parabolic rescaling

(6.10) with respect to the Knudsen number and we keep the same notation (we omit the tildes) for the sake of readability. The resulting fluctuating kinetic equation reads

$$\alpha^2 \partial_t f_\epsilon^\alpha + \alpha \mathbf{e}_\theta \cdot \nabla f_\epsilon^\alpha = L\left[f_\epsilon^\alpha\right] + \sqrt{\alpha^4 \epsilon}\eta\left[f_\epsilon^\alpha\right](\mathbf{r}, \theta, t)\,. \tag{6.30}$$

The α dependency of the noise term within the parabolic rescaling is obtained by dimensional analysis (as its covariance should be proportional to the square of the inverse of a distance, and to the inverse of a time). Let us look for a solution to the fluctuating kinetic equation as a Chapman-Enskog expansion

$$f_\epsilon^\alpha(\mathbf{r}, \theta, t) = \frac{1}{2\pi}\rho_\epsilon(\mathbf{r}, t) + \alpha g_1(\mathbf{r}, \theta, t) + \alpha^2 g_2(\mathbf{r}, \theta, t) + \mathcal{O}\left(\alpha^3\right).$$

From now on, we adapt the computations led in section (6.4), with an extra stochastic term. Integrating (6.30) over the orientation variable yield at leading order in α

$$\partial_t \rho_\epsilon + \int \mathrm{d}\theta\, \mathbf{e}_\theta \cdot \nabla(g_1) = \mathcal{O}(\alpha)\,, \tag{6.31}$$

but this time the leading order term of (6.30) contains a stochastic part

$$\frac{1}{2\pi}\mathbf{e}_\theta \cdot \nabla \rho_\epsilon = L[g_1] + \sqrt{\alpha^2 \epsilon}\eta\left[\frac{\rho_\epsilon}{2\pi}\right].$$

We know define g_d and g_s where

$$L[g_d] = \frac{\mathbf{e}_\theta \cdot \nabla \rho_\epsilon}{2\pi},$$

accounts for the deterministic part of g_1 and

$$L[g_s] = -\sqrt{\alpha^2 \epsilon}\eta\left[\frac{\rho_\epsilon}{2\pi}\right],$$

accounts for the stochastic part of g_1, such that

$$g_d + g_s = g_1. \tag{6.32}$$

In the deterministic case of section 6.4, we had $g_1 = g_d$, and we already computed its expression, hence

$$g_d = \frac{1}{2\pi}\frac{\mathbf{e}_\theta \cdot \nabla \rho_\epsilon}{\hat{P}_1 - 1}. \tag{6.33}$$

To compute g_s, we also need to invert L. This is possibly if and only if $\int \mathrm{d}\theta\, \eta = 0$, i.e. if $\eta \in (\ker L)^\perp$. This the case as a consequence of the conservation of the total mass at the level of the kinetic LDP, i.e. any realization of the kinetic noise η that violates mass conservation has zero probability. Hence, we obtain

$$g_s = -\sqrt{\alpha^2 \epsilon} L^{-1}\left[\eta\left[\frac{\rho_\epsilon}{2\pi}\right]\right]. \tag{6.34}$$

Combining (6.32-6.34) and (6.31) yield the SPDE for ρ_N

$$\partial_t \rho_\epsilon = D\Delta\rho_\epsilon + \sqrt{\alpha^2\epsilon}\nabla\cdot\boldsymbol{\xi}\left[\rho_\epsilon\right](\mathbf{r},t) + \mathcal{O}(\alpha), \tag{6.35}$$

with

$$\boldsymbol{\xi}\left[\rho_\epsilon\right](\mathbf{r},t) = -\int \mathrm{d}\theta\, \mathbf{e}_\theta L^{-1}\left[\eta\left[\frac{\rho_\epsilon}{2\pi}\right]\right].$$

In order to compare our result (6.35) with the Dean-Kawasaki equation, we need to characterize the correlation structure of the Gaussian noise term ξ.

6.5.3. Correlation function of the noise

Since L^{-1} is self-adjoint with respect to the scalar product (6.13), and using $L^{-1}\left[\mathbf{e}_\theta\right] = \left(\hat{P}_1 - 1\right)\mathbf{e}_\theta$ we can rewrite the noise term

$$\boldsymbol{\xi}\left[\rho_\epsilon\right](\mathbf{r},t) = \frac{-1}{\hat{P}_1 - 1}\int \mathrm{d}\theta\, \mathbf{e}_\theta \eta\left[\frac{\rho_\epsilon}{2\pi}\right], \tag{6.36}$$

where we used $L^{-1}\left[\mathbf{e}_\theta\right] = \mathbf{e}_\theta / \left(\hat{P}_1 - 1\right)$. We can then use the formula (6.29) to compute the autocorrelation function of ξ. We first notice that

$$Q_{\rho_\epsilon/(2\pi)}\left[\varphi\right] = \frac{1}{2\pi}\frac{\delta H^{(2)}}{\delta p}\left[\rho_\epsilon, \varphi\right] = -\frac{2}{\pi}\rho_\epsilon L\left[\varphi\right].$$

As a consequence introducing (6.36) into (6.29) yields,

$$\mathbb{E}\left(\boldsymbol{\xi}\left[\rho_\epsilon\right](\mathbf{r},t)\otimes\boldsymbol{\xi}\left[\rho_\epsilon\right](\mathbf{r}',t')\right) = \frac{-2}{\pi\left(\hat{P}_1 - 1\right)^2}\delta(\mathbf{r}-\mathbf{r}')\int \mathrm{d}\theta\, \rho_\epsilon \mathbf{e}_\theta \otimes L\left[\mathbf{e}_\theta\right]\delta(t-t')$$

Now we use $L\left[\mathbf{e}_\theta\right] = \left(\hat{P}_1 - 1\right)\mathbf{e}_\theta$ to obtain

$$\mathbb{E}\left(\boldsymbol{\xi}\left[\rho_\epsilon\right](\mathbf{r},t)\otimes\boldsymbol{\xi}\left[\rho_\epsilon\right](\mathbf{r}',t')\right) = 2D\rho_\epsilon \mathrm{Id}\delta(\mathbf{r}-\mathbf{r}')\delta(t-t').$$

Introducing the delta-correlated tridimensional Gaussian field $\boldsymbol{\zeta}$ such that

$$\mathbb{E}\left(\boldsymbol{\zeta}(\mathbf{r},t)\otimes\boldsymbol{\zeta}(\mathbf{r}',t')\right) = \mathrm{Id}\delta(\mathbf{r}-\mathbf{r}')\delta(t-t'),$$

we can recast the fluctuating hydrodynamics (6.35) into

$$\partial_t \rho_\epsilon = D\Delta\rho_\epsilon + \nabla\cdot\left(\sqrt{2\alpha^2\epsilon D\rho_\epsilon}\boldsymbol{\zeta}\right) + \mathcal{O}(\alpha), \tag{6.37}$$

which is the expected equation from the Dean-Kawasaki theory[6], with the precision that $\gamma = \alpha^2$. The value of this coefficient γ is important to assess the asymptotic regime where the fluctuating hydrodynamics gives a relevant description of the particle system. Here, the interpretation of (6.37) is delicate because it does not grant that the next deterministic terms in the Chapman-Enskog expansion of higher order in α are negligible compared to the noise term. This SPDE is useful to assess rare trajectories of the empirical density, driven by large realization of the noise term. A regularized version of the Dean-Kawasaki equation may also be able to describe small fluctuations around the hydrodynamic evolution, as it is widely used to do so by physicists and justified in [76, 77]. However, from our computations there is no indication that this is the case. We only consider it a rephrasing of the underlying quadratic hydrodynamic LDP for the empirical density. We derive this hydrodynamic LDP directly from the kinetic LDP in the next section.

6.6. Convergence of the large deviation functionals and contraction principle

In this section, we obtain fluctuating hydrodynamics as a LDP for the evolution paths of the empirical density, as in (6.7-6.9). This is done by studying the small α asymptotics of the kinetic LDP.

We know that the hydrodynamic evolution of the density field is obtained after a double limit

$$\rho\left(\mathbf{r},t\right) = \lim_{\alpha\to 0}\lim_{\epsilon\to 0}\int \mathrm{d}\theta\, f_\epsilon^\alpha\left(\mathbf{r},\theta,t\right).$$

Now, we are not only interested in the most probable evolution path for the the empirical density

$$\rho_\epsilon^\alpha\left(\mathbf{r},t\right) = \int \mathrm{d}\theta\, f_\epsilon^\alpha\left(\mathbf{r},\theta,t\right), \tag{6.38}$$

which is given by the hydrodynamic equation for the density (6.25), but we want to quantify the large deviations of such a field in the small α limit. In other words, we want to estimate the asymptotics of

$$\lim_{\epsilon\to 0}\left(-\epsilon\log\mathbb{P}\left(\{\rho_\epsilon^\alpha(t)\}_{0\le t<T} = \{\rho(t)\}_{0\le t<T}\right)\right),$$

[6] This is actually a dimensionless version of the Dean-Kawasaki equation. Inverting the change of variable we made to obtain the kinetic and the hydrodynamic equations and dropping higher order terms in α, (6.37) would yield in physical units

$$\partial_t\rho_N = \tilde{D}\Delta\rho_N + \nabla\cdot\left(\sqrt{2\tilde{D}\rho_N}\boldsymbol{\zeta}\right),$$

where the empirical density is normalized such that $\int \mathrm{d}\mathbf{r}\,\rho_N = N$, and where $\tilde{D} = v_0^2 D/\lambda$ with v_0 being the velocity of the particles, and λ their tumbling rate.

as α goes to zero.

Under the parabolic rescaling (6.10), the kinetic rate function (6.4) that we rename I_T^α to emphasize its dependence on α reads

$$I_T^\alpha[f] = \frac{1}{\alpha^4}\int_0^T \mathrm{d}t \sup_p \left(\int \mathbf{r}\mathrm{d}\theta\, p\left(\alpha^2\partial_t f - \alpha \mathbf{e}_\theta\cdot\nabla f\right) - H_{\text{tumb}}[f,p]\right). \tag{6.39}$$

The time T in the time integral is also rescaled by α^2, but we abusively redefine it to keep the same notations, since it does not play any role in the following. Our goal is to derive a LDP for the empirical density $\rho_\epsilon = \int \mathrm{d}\theta\, f_\epsilon$ in the small α limit, to describe dynamical fluctuations of the density field. Using a contraction principle (see section 3.2.3), we expect such a LDP to read

$$\mathbb{P}\left(\{\rho_\epsilon^\alpha(\mathbf{r},t)\}_{0\leq t<T} = \{\rho(t)\}_{0\leq t<T}\right) \underset{\epsilon\to 0}{\asymp} \mathrm{e}^{-\frac{1}{\epsilon}\inf\limits_{\int \mathrm{d}\theta\, f=\rho} I_T^\alpha[f]}. \tag{6.40}$$

However, in general there is no simple way to compute $\inf\limits_{\int \mathrm{d}\theta\, f=\rho} I_T^\alpha[f]$. The key point here, is that in the hydrodynamical limit as α goes to zero, the dynamics of the empirical measure concentrates close to local equilibria of the kinetic equation. In this case, as α goes to zero we expect the minimizers of $I_T^\alpha[f]$ to be distributions that are uniform in angle. Then, the constraint $\int \mathrm{d}\theta\, f = \rho$ in the infimum amounts to specifying the density profile associated with a uniform in angle distribution that minimizes $I_T^\alpha[f]$. The object of this section is then to study the small α asymptotics of (6.40), by solving the following variational problem in the small α limit:

$$\inf_{\int \mathrm{d}\theta\, f=\rho} I_T^\alpha[f]. \tag{6.41}$$

For convenience, we introduce

$$I_{\text{hydro}}[\rho] = \lim_{\alpha\downarrow 0} \alpha^\nu \inf_{\int \mathrm{d}\theta\, f=\rho} I_T^\alpha[f] \tag{6.42}$$

the leading order term of (6.41) as α goes to zero, where ν has to be determined so the limit is finite.

In this section, we do not assume any hypothesis about the Gaussianity of the large deviation functional and we explain how it arises from the computations. Our goal is to compute $I_{\text{hydro}}[\rho]$ the leading order term in α of (6.41).

6.6.1. Optimization on p

Let us start by computing the supremum on p in (6.39), i.e. by rephrasing the Hamiltonian formulation of the rate function into a Lagrangian formulation. To do so, we use a Taylor series representation of the tumbling Hamiltonian with respect to the conjugate momentum p:

$$H_{\text{tumb}}[f,p] = \int \mathbf{r}\mathrm{d}\theta\, pL[f] + H^{(2)}[f,p] + H^{(3)}[f,p] + H^{(h.o.)}[f,p],$$

where $L[f]$ is the collision operator and is defined in (6.2), $H^{(2)}$ gathers the terms that are quadratic in p; $H^{(3)}$, the cubic terms in p,and $H^{(h.o.)}$ the terms that are at least quartic. For instance,

$$H^{(2)}[f,p] = \frac{1}{2}\int \mathrm{d}\mathbf{r}\mathrm{d}\theta\mathrm{d}\theta' \, f(\mathbf{r},\theta,t)P_t(\theta-\theta')\left(-p(\mathbf{r},\theta,t)+p(\mathbf{r},\theta',t)\right)^2 .$$

We then have to compute

$$\sup_p \left(\int \mathrm{d}\mathbf{r}\mathrm{d}\theta \, p\left(\alpha^2\partial_t f + \alpha \mathbf{e}_\theta\cdot\nabla f - L[f]\right) - H^{(2)}[f,p] - H^{(3)}[f,p] - H^{(h.o.)}[f,p]\right). \tag{6.43}$$

A differentiation with respect to p in (6.43) yields an equation on the optimal p

$$\alpha^2\partial_t f + \alpha\mathbf{e}_\theta\cdot\nabla f - L[f] = \frac{\delta H^{(2)}}{\delta p}[f,p] + \frac{\delta H^{(3)}}{\delta p}[f,p] + \frac{\delta H^{(h.o.)}}{\delta p}[f,p]. \tag{6.44}$$

If $L[f]$ is of order one ($\mathcal{O}(1)$ as α goes to zero), the optimal p solving (6.44) is of order one too ($\mathcal{O}(1)$ as α goes to zero), since $\frac{\delta H^{(2)}}{\delta p}[f,p]$ is linear in p. This would make the rate functional $I_T^\alpha[f]$ (6.39) of order one as well. However, in order to minimize $I_T^\alpha[f]$, a better choice would be to have the optimal p solving (6.43) of order α, thus making $I_T^\alpha[f]$ of order α^2. This can be done by imposing $L[f]$ to be of order α, i.e. by having f to be close to a local equilibrium of the kinetic equation. Note that we cannot have the optimal p to be smaller than α because of the presence of terms of order α on the r.h.s. of (6.44). Hence, the optimal f minimizing (6.41) can be written $f = f^0 + \mathcal{O}(\alpha)$, where $f^0 \in \ker L$.

Using the constraint on the infimum: $\int \mathrm{d}\theta\, f = \rho$, the local equilibrium f^0 has to be $\rho/(2\pi)$. We then expand f up to order 2 in α

$$f = \frac{1}{2\pi}\rho + \alpha g_1 + \alpha^2 g_2 + o\left(\alpha^2\right), \tag{6.45}$$

with the constraint that $\int \mathrm{d}\theta\, g_1 = 0$ and $\int \mathrm{d}\theta\, g_2 = 0$ to ensure $\int \mathrm{d}\theta\, f = \rho$. Thanks to this remark, the computation of the supremum on p (6.43) becomes easier and we show in the following that it only involves the quadratic part of the large deviation Hamiltonian.

The optimal p (6.44) then solves

$$\alpha^2\frac{\partial_t\rho}{2\pi} + \frac{\alpha}{2\pi}\mathbf{e}_\theta\cdot\nabla\rho + \alpha^2\mathbf{e}_\theta\cdot\nabla g_1 - \alpha L[g_1] - \alpha^2 L[g_2] = \frac{\delta H^{(2)}}{\delta p}[f,p] + \frac{\delta H^{(3)}}{\delta p}[f,p] + \frac{\delta H^{(h.o.)}}{\delta p}[f,p] + o\left(\alpha^2\right). \tag{6.46}$$

Since $\frac{\delta H^{(2)}}{\delta p}[f,p]$ is linear in p, p has to be of order α for the l.h.s. and the r.h.s. to be equated, as wished for[7]. We then look for p order by order in α:

$$p = \alpha p_1 + \alpha^2 p_2 + o\left(\alpha^2\right).$$

[7] It is crucial to remark that this reasoning collapses when the gradients are not of order one in (6.46). For instance, the transport term $\mathbf{e}_\theta\cdot\nabla\rho$ can be of order $1/\alpha$, if the hydrodynamic description allows shock solutions over such scales.

A posteriori, we realize that we do not p_2 as a consequence of the mass conservation property of the collision operator L, however at this stage there is no reason to omit it. All in all, at order α^2 the optimal (p_1, p_2) solves

$$\alpha^2 \frac{\partial_t \rho}{2\pi} + \frac{\alpha}{2\pi} \mathbf{e}_\theta \cdot \nabla \rho + \alpha^2 \mathbf{e}_\theta \cdot \nabla g_1 - \alpha L[g_1] - \alpha^2 L[g_2] = \\ \frac{\alpha}{2\pi} \frac{\delta H^{(2)}}{\delta p}[\rho, p_1] + \alpha^2 \frac{\delta H^{(2)}}{\delta p}[g_1, p_1] + \frac{\alpha^2}{2\pi} \frac{\delta H^{(2)}}{\delta p}[\rho, p_2] + \frac{\alpha^2}{2\pi} \frac{\delta H^{(3)}}{\delta p}[\rho, p_1] + o\left(\alpha^2\right).$$

Noticing that the term involving the cubic part of the Hamiltonian vanishes[8]

$$\frac{\delta H^{(3)}}{\delta p}[\rho, p_1] = 0$$

and

$$\frac{\delta H^{(2)}}{\delta p}[\rho, p_1] = -2\rho L[p_1],$$

the optimal (p_1, p_2) has to solve

$$\alpha \frac{\partial_t \rho}{2\pi} + \frac{1}{2\pi} \mathbf{e}_\theta \cdot \nabla \rho + \alpha \mathbf{e}_\theta \cdot \nabla g_1 - L[g_1] - \alpha L[g_2] = \\ -\frac{1}{\pi} \rho L[p_1] + \alpha \frac{\delta H^{(2)}}{\delta p}[g_1, p_1] + \frac{\alpha}{2\pi} \frac{\delta H^{(2)}}{\delta p}[\rho, p_2] + o(\alpha).$$

This is actually a crucial part of the computation, as it makes valid the a priori quadratization of the kinetic large deviation Hamiltonian. In order to compute p_1 in the expression above, we have to invert L. This is possible only if

$$\alpha \frac{\partial_t \rho}{2\pi} + \frac{1}{2\pi} \mathbf{e}_\theta \cdot \nabla \rho + \alpha \mathbf{e}_\theta \cdot \nabla g_1 - L[g_1] - \alpha L[g_2] - \alpha \frac{\delta H^{(2)}}{\delta p}[g_1, p_1] - \frac{\alpha}{2\pi} \frac{\delta H^{(2)}}{\delta p}[\rho, p_2] \quad (6.47)$$

is in $(\ker L)^\top$, which is satisfied if $\int \mathrm{d}\theta$ (6.47) $= 0$, i.e. if

$$\partial_t \rho + \int \mathrm{d}\theta \, \mathbf{e}_\theta \cdot \nabla g_1 = 0.$$

We note than p_2 does not play a role here and we can adjust only p_1 in order to optimize (6.43). Then, the optimal p_1 satisfies at leading order

$$-\frac{1}{\pi} \rho L[p_1] = \frac{1}{2\pi} \mathbf{e}_\theta \cdot \nabla \rho - L[g_1],$$

[8] In all the cases studied in his manuscript, $H^{(3)}$ does not play a role in the hydrodynamical limit, for various reasons: the hydrodynamic variable is not a conserved quantity, or a supplementary symmetry cancels $H^{(3)}$. Here, $H^{(3)}[\rho, p_1] = 0$ as a consequence of the symmetry of the tumbling distribution: $P(\theta) = P(-\theta)$, which among other grants the time-reversibility of the microscopic dynamics.

i.e.

$$p_1 = \frac{\pi}{\rho} g_1 - \frac{1}{2\rho} L^{-1} \left[\mathbf{e}_\theta \cdot \nabla \rho \right]$$

with the constraint that

$$\partial_t \rho = \int \mathrm{d}\theta \, \mathbf{e}_\theta \cdot \nabla g_1. \tag{6.48}$$

Introducing the optimal p_1 in (6.39), we can compute the infimum of the large deviation functional $I_T^\alpha [f]$ at leading order in α, we obtain

$$I_{\text{hydro}} [\rho] = \lim_{\alpha \downarrow 0} \alpha^2 \inf_{\int \mathrm{d}\theta \, f = \rho} I_T^\alpha [f] = \inf_{g_1} \left\{ \frac{-1}{2\pi} \int_0^T \mathrm{d}t \int \mathbf{d}\mathbf{r}\mathrm{d}\theta \left(\rho p_1 L \left[p_1 \right] \right), \quad \partial_t \rho = \int \mathrm{d}\theta \, \mathbf{e}_\theta \cdot \nabla g_1 \right\}, \tag{6.49}$$

with

$$p_1 = \frac{\pi}{\rho} g_1 - \frac{1}{2\rho} L^{-1} \left[\mathbf{e}_\theta \cdot \nabla \rho \right].$$

We remark that the correct scaling in (6.42) is $\nu = 2$. At this point, the problem of finding the optimal f minimizing (6.41) can be seen as an optimization on g_1 and g_2 given the Chapman-Enskog like expansion of f (6.45).

6.6.2. Minimization of the Lagrangian and negative Sobolev norm H_{-1}

Now, we want to connect the hydrodynamic rate function (6.49) with the Dean-Kawasaki LDP (6.7-6.9). We introduce g_d and g_s such that

$$g_d = \frac{1}{2\pi} L^{-1} \left[\mathbf{e}_\theta \cdot \nabla \rho \right],$$

$$g_s = \frac{\rho}{\pi} p_1$$

and $g_d + g_s = g_1$[9]. Doing so, the rate function for ρ reads

$$I_{\text{hydro}} [\rho] = \inf_{g_s} \left\{ \frac{-\pi}{2} \int_0^T \mathrm{d}t \int \mathbf{d}\mathbf{r}\mathrm{d}\theta \frac{g_s L \left[g_s \right]}{\rho}, \quad \partial_t \rho - \frac{1}{2\pi} \int \mathrm{d}\theta \, \mathbf{e}_\theta \cdot \nabla L^{-1} \left[\mathbf{e}_\theta \cdot \nabla \rho \right] = \int \mathrm{d}\theta \, \mathbf{e}_\theta \cdot \nabla g_s \right\},$$

However, recalling the computation (6.33) of section 6.5, we know that the constraint can be rewritten:

$$\partial_t \rho - D \Delta \rho = \int \mathrm{d}\theta \, \mathbf{e}_\theta \cdot \nabla g_s.$$

[9] We use a decomposition of g_1 similar to the one we made during the noisy Chapman-Enskog expansion in section 6.5.

All in all, we have the hydrodynamic LDP for the evolution paths of the empirical density

$$\mathbb{P}\left(\{\rho_\epsilon^\alpha(\mathbf{r},t)\}_{0\le t<T}=\{\rho(t)\}_{0\le t<T}\right)\underset{\epsilon\to 0}{\asymp}\mathrm{e}^{-\frac{1}{\epsilon\alpha^2}I_{\text{hydro}}[\rho]}, \tag{6.50}$$

with

$$I_{\text{hydro}}[\rho]=\inf_{g_s}\left\{\frac{-\pi}{2}\int_0^T\mathrm{d}t\int\mathbf{dr}\mathrm{d}\theta\frac{g_sL[g_s]}{\rho},\ \ \partial_t\rho-D\Delta\rho=\int\mathrm{d}\theta\,\mathbf{e}_\theta\cdot\nabla g_s\right\}. \tag{6.51}$$

To compute this infimum, we use that L is diagonal on the Fourier basis, as seen in (6.20). On one hand, we have

$$\frac{-\pi}{2}\int\mathrm{d}\theta\,\frac{g_sL[g_s]}{\rho}=\frac{1}{4\rho}\sum_k\hat{g}_s^{-k}\hat{g}_s^k\left(1-\hat{P}_k\right). \tag{6.52}$$

On the other hand, the constraint can be rewritten using the Fourier modes of g_s as following

$$\partial_t\rho-D\Delta\rho=\nabla\cdot\begin{pmatrix}\Re\hat{g}_s^{-1}\\ \Im\hat{g}_s^{-1}\end{pmatrix}, \tag{6.53}$$

where $\Re,\Im$ denote the real and imaginary parts. From (6.53), it is clear that the constraint on g_s only apply to its Fourier modes $k=-1,1$. A first step in order to minimize (6.52) is to take $\hat{g}_s^k=0$ for all $k\notin\{-1,1\}$. Then, the minimization of (6.52) amounts to minimizing

$$\frac{-\pi}{2}\int\mathrm{d}\theta\,\frac{g_sL[g_s]}{\rho}=\frac{|\hat{g}_s^{-1}|^2}{4D\rho},$$

with the constraint on $\hat{g}_s^{-1}$ given by (6.53). This optimization problem is nothing else than the definition of the H_{-1} Sobolev norm of $\partial_t\rho-D\Delta\rho$. We can then write (6.51),

$$I_{\text{hydro}}[\rho]=\frac{1}{2}\int_0^T\mathrm{d}t\int\mathbf{dr}\ \|\partial_t\rho-D\Delta\rho\|^2_{-1,2D\rho}, \tag{6.54}$$

where the norm is defined by

$$\|a\|^2_{-1,h}=\inf_\varphi\left\{\int\mathbf{dr}\,\frac{|\varphi|^2}{h},\ \ \nabla\cdot\varphi=a\right\}. \tag{6.55}$$

This norm also has a dual formulation

$$\|a\|^2_{-1,h}=2\sup_\psi\left\{\int\mathbf{dr}\,a\psi-\frac{1}{2}\int\mathbf{dr}\,h\,|\nabla\psi|^2\right\},$$

allowing to bridge from (6.54) to the Hamiltonian formulation predicted in (6.8). We find that our result (6.54) is consistent with the Dean-Kawasaki theory, with $\gamma=\alpha^2$, as also

predicted by the SPDE approach of the previous section. This is not surprising, given that the Sobolev norm (6.55) is deeply related to the Wasserstein distance [179], which is known to be the right tool to describe distances in the space of empirical density of N Brownian diffusions[10] [110]. The approach we took here was based on the contraction principle, but it could be rephrased in terms of Γ-convergence of the kinetic large deviation functionals in the small α limit. We refer to [27, 155, 16, 1] that discuss the relevance of Γ-convergence approaches to compute large deviation functionals.

6.7. Outline of the part

In this second part of the manuscript, we apply the framework we presented here to obtain fluctuating hydrodynamics for various systems, with sometimes additional challenges. In chapter 7, starting from the LDP associated with the Boltzmann equation, we derive the fluctuating compressible and incompressible Navier-Stokes equations. In chapter 8, we derive the kinetic LDP, and the associated fluctuating hydrodynamics for a system of active particles with alignment interaction. For such a system, there exists a hydrodynamic field (the orientation field), that is not associated with a conservation law. In chapter 9, we focus on the large deviation theory of scalar conservation laws. Such PDEs are known to exhibit shock solutions and the application of the approach detailed in the present chapter fails to describe the probability of those.

[10] It is well-known than a Run-and-Tumbling particle and a Brownian diffusing particle are described by the same diffusion equation for the density at the level of deterministic hydrodynamics [180, 195]. This computation also indicates that their description in terms of large deviations for the empirical density is similar.

7. Microscopical derivation of the fluctuating (in)compressible Navier-Stokes equations

In this chapter, we derive the fluctuating compressible and incompressible Navier-Stokes equations, starting from the large deviation principle associated with the Boltzmann, describing the probability of evolution paths of the empirical measure of N particles of a dilute gas. The results are the following set of SPDEs for the density ρ, velocity $\mathbf{u}$ and temperature θ fields[1]. Within the hyperbolic scaling, we obtain the fluctuating compressible Navier-Stokes system

$$\begin{cases} \partial_t \rho + \nabla \cdot (\rho \mathbf{u}) = 0, \\ \rho \partial_t \mathbf{u} + \rho \left(\mathbf{u} \cdot \nabla\right) \mathbf{u} + \frac{k_B}{m} \nabla(\rho\theta) = \frac{1}{2} \nabla \cdot \left(\nu \boldsymbol{\sigma}\left(\mathbf{u}\right)\right) + \nabla \cdot \mathbf{J}, \\ \frac{3}{2} k_B \left(\rho \partial_t \theta + \rho\theta \nabla \cdot \mathbf{u} + \frac{3}{2} \rho \left(\mathbf{u} \cdot \nabla\right) \theta\right) = \nabla \cdot (\kappa \nabla \theta) + \frac{1}{2} m \nu \boldsymbol{\sigma}\left(\mathbf{u}\right) : \boldsymbol{\sigma}\left(\mathbf{u}\right) + \nabla \cdot \left(m \mathbf{u} \cdot \mathbf{J} + \mathbf{q}\right), \end{cases}$$

where $\mathbf{J}$ and $\mathbf{q}$ are Gaussian random fluxes characterized by their correlation functions

$$\mathbb{E}(J_{ij}\left(\mathbf{r}, t\right) J_{kl}\left(\mathbf{r}', t'\right)) = \frac{2\nu k_B \theta}{m} \left[\delta_{ik}\delta_{jl} + \delta_{il}\delta_{jk} - \frac{2}{3}\delta_{ij}\delta_{kl}\right] \delta(t - t')\delta(\mathbf{r} - \mathbf{r}'),$$

$$\mathbb{E}(q_i\left(\mathbf{r}, t\right) q_j\left(\mathbf{r}', t'\right)) = 2\kappa k_B^2 \theta^2 \delta_{ij} \delta(t - t')\delta(\mathbf{r} - \mathbf{r}'),$$

and

$$\mathbb{E}(q_i\left(\mathbf{r}, t\right) J_{kl}\left(\mathbf{r}', t'\right)) = 0,$$

where k_B is the Boltzmann constant, m the mass of a particle, κ and ν are diffusive coefficients that can be related to the microscopic dynamics, and $\boldsymbol{\sigma}$ is the stress tensor that will be defined later. Within the parabolic scaling, we obtain the fluctuating incompressible Navier-Stokes system

$$\begin{cases} \nabla\left(\rho + \theta\right) = 0, \\ \partial_t \mathbf{u} + \mathbf{u} \cdot \nabla \mathbf{u} + \nabla\left(\frac{P}{\rho_0}\right) = \nu \Delta \mathbf{u} + \nabla \cdot \mathbf{J}, \\ \nabla \cdot \mathbf{u} = 0, \\ \partial_t \theta + \mathbf{u} \cdot \nabla \theta = \kappa \Delta \theta + \nabla \cdot \mathbf{q}, \end{cases}$$

[1] More precisely, the unknowns of these SPDEs are the empirical hydrodynamical fields and they still depend on the number of particles. For the sake of clarity, and in agreement with commonly used notations, in this chapter and the next one, we omit the $_N$ subscript to denote them.

with

$$\mathbb{E}(J_{ij}(\mathbf{r},t)\,J_{kl}(\mathbf{r}',t')) = \frac{2\nu k_B T_0}{\rho_0}\left[\delta_{ik}\delta_{jl}+\delta_{il}\delta_{jk}-\frac{2}{3}\delta_{ij}\delta_{kl}\right]\delta(t-t')\delta(\mathbf{r}-\mathbf{r}'),$$

$$\mathbb{E}(q_i(\mathbf{r},t)\,q_j(\mathbf{r}',t')) = \frac{2\kappa T_0^2}{\rho_0}\delta_{ij}\delta(t-t')\delta(\mathbf{r}-\mathbf{r}'),$$

where ρ_0 is the average density and T_0 the average temperature.

In section 7.1, we recall the large deviation principle associated with the Boltzmann equation and the different scalings leading to the compressible and incompressible Navier-Stokes equations. We also justify the quadratization of the kinetic large deviation Hamiltonian in the hydrodynamical limit. This allows to translate the LDP for the Boltzmann equation into a fluctuating Boltzmann equation, that will be the starting point of the Chapman-Enskog expansion. In section 7.2, we show that using a hyperbolic rescaling, the hydrodynamical limit of the fluctuating Boltzmann equation is the fluctuating compressible Navier-Stokes equations. In section 7.3, within the parabolic rescaling we obtain the fluctuating incompressible Navier-Stokes equations as a hydrodynamical limit. In section 7.4, we connect our results to the ones of the literature by introducing back the physical dimensions of the different fields. In section 7.5, we discuss the gradient-flow structures associated with the compressible and incompressible fluctuating Navier-Stokes equations. This microscopical derivation of the fluctuating Navier-Stokes equations is one of the first that actually starts from the particle dynamics without assuming the noise terms from fluctuation-dissipation theorems. A more detailed bibliographical account about the derivations of the fluctuating Navier–Stokes equations and its applications is given in the introductive chapter.

In this chapter, all the derivations are carried out at the level of the SPDEs, using a noisy Chapman-Enskog expansion of the fluctuating Boltzmann equation. However, they are essentially a large deviation result, and they could also be led at the level of the large deviation functionals, in the spirit of the derivation of section 6.6.

7.1. Path large deviations for the empirical measure and the Boltzmann equation

In this section, we summarize the result of [50] on the dynamical large deviations from the Boltzmann equation. In section 7.1.1, we present the large deviation Hamiltonian that characterizes the probabilities of evolution paths for the empirical measure on the μ-space for a dilute gas of N particles. This Hamiltonian is non quadratic in the conjugate momentum variable, thus it characterizes non Gaussian fluctuations of the μ-space empirical measure. However, in sections 7.1.2 and 7.1.3, we show that formally, when looking at the hydrodynamical limit, i.e. for small Knudsen number, only the quadratic part of this Hamiltonian plays a role. As a consequence, in section 7.1.4 we rephrase the dynamical large deviation principle for the Boltzmann equation as a fluctuating Boltzmann equation with Gaussian noise.

7.1.1. Hamiltonian for the Boltzmann fluctuations

Our starting point is the large deviation principle for the empirical measure of particles derived in [50], already introduced in section 5.3.1 (with slightly different notations). We call N the total number of particles, V the total volume, ℓ the mean free path. $\epsilon = (N\ell^3/V)^{-1}$ is the inverse of the typical number of particles inside a volume of linear size the mean free path. We consider a Boltzmann-Grad limit, that is $\epsilon \to 0$, $N \to \infty$, with $\epsilon N \geq 1$ (ϵN can be much larger than 1).

We denote $(\mathbf{r}_i(t), \mathbf{v}_i(t))_{1\leq i\leq N}$ the positions and velocities of the particles We use the thermal velocity $v_T = \sqrt{k_B T_0/m}$ as the velocity unit, ℓ as the space unit, and the typical time between collisions ℓv_T as the time unit. In this context, it is shown in [50] that the rescaled empirical measure

$$f_\epsilon(\mathbf{r}, \mathbf{v}, t) = \epsilon \sum_{i=1}^{N} \delta(\mathbf{r} - \mathbf{r}_i(t))\delta(\mathbf{v} - \mathbf{v}_i(t))$$

satisfies a large deviation principle

$$\mathbb{P}\left(\{f_\epsilon(\mathbf{r}, \mathbf{v}, t)\}_{0\leq t\leq T} = \{f(\mathbf{r}, \mathbf{v}, t)\}_{0\leq t\leq T}\right) \underset{\epsilon\downarrow 0}{\asymp} e^{-\frac{1}{\epsilon}\left\{\int_0^T \mathrm{d}t \sup_{\mathrm{p}}\left[\int \mathbf{drdv}\, p\partial_t f - H[f,p]\right]\right\}},$$

with rate ϵ and Hamiltonian

$$H[f, p] = H_T[f, p] + H_C[f, p],$$

where $p(\mathbf{r}, \mathbf{v})$ is the conjugate momentum field, ans H_T and H_C are the Hamiltonians associated with free transport and collisions respectively:

$$H_T[f, p] = -\int \mathbf{drdv}\, p(\mathbf{r}, \mathbf{v})\mathbf{v} \cdot \nabla f \tag{7.1}$$

and

$$H_C[f, p] = \frac{1}{2}\int \mathbf{drdv}_1\mathbf{dv}_2\mathbf{dv}_1'\mathbf{dv}_2'\, w(\mathbf{v}_1', \mathbf{v}_2'; \mathbf{v}_1, \mathbf{v}_2)\, f(\mathbf{r}, \mathbf{v}_1)f(\mathbf{r}, \mathbf{v}_2) \times \left[e^{p(\mathbf{r},\mathbf{v}_1')+p(\mathbf{r},\mathbf{v}_2')-p(\mathbf{r},\mathbf{v}_1)-p(\mathbf{r},\mathbf{v}_2)} - 1\right], \tag{7.2}$$

where w is the collision rate. The large deviation functional is then

$$I_T[f] = \int_0^T \mathrm{d}t \left\{\sup_p \int \mathbf{drdv}\, p(\mathbf{r}, \mathbf{v})\partial_t f - H_T[f, p] - H_C[f, p]\right\}.$$

The deterministic evolution is given by $\partial_t f = \left(\delta\left(H_T + H_C\right)/\delta p\right)[f, p = 0]$, and is, as it should, Boltzmann equation:

$$\partial_t f + \mathbf{v} \cdot \nabla f = Q(f, f), \tag{7.3}$$

with the collision operator

$$Q(f,f)(\mathbf{r},\mathbf{v}) = \int \mathrm{d}\mathbf{v}_2 \mathrm{d}\mathbf{v}_1' \mathrm{d}\mathbf{v}_2' \, w(\mathbf{v}_1', \mathbf{v}_2'; \mathbf{v}, \mathbf{v}_2) \, \left[f(\mathbf{r},\mathbf{v}_1') f(\mathbf{r},\mathbf{v}_2') - f(\mathbf{r},\mathbf{v}) f(\mathbf{r},\mathbf{v}_2) \right].$$

This collision operator vanishes on the Maxwellian functions $M_{\rho,\mathbf{u},\theta}$, parameterized by a local density, velocity and temperature fields $\rho(\mathbf{r},t), \mathbf{u}(\mathbf{r},t), \theta(\mathbf{r},t)$:

$$M_{\rho,\mathbf{u},\theta}(\mathbf{v}) = \frac{\rho}{(2\pi\theta)^{\frac{3}{2}}} e^{-\frac{1}{2}\frac{(\mathbf{v}-\mathbf{u})^2}{\theta}}. \tag{7.4}$$

Those Maxwellian functions are the local equilibria of the Boltzmann equation, and the hydrodynamical fields indexing the local equilibria are related to mass, momentum, and energy conservation at the level of the microscopic dynamics.

We are interested in the large time and large scale dynamics: we shall then use appropriate time and space scales, rescaled with the Knudsen number $\alpha = \ell/L$, where L is a typical macroscopic length scale. Our goal in the following two subsections is to argue that under the appropriate scaling for the compressible and incompressible Navier-Stokes equation respectively, it is legitimate to truncate this Hamiltonian at quadratic order. This argument is similar to the one used in section 6.6 to justify the quadratization of the Hamiltonian in the hydrodynamical limit.

7.1.2. Quadratic approximation for the Hamiltonian: compressible Navier-Stokes equations

We first use the appropriate hyperbolic scaling discussed in section 6.2 to derive the compressible Euler and Navier-Stokes equations. We introduce the macroscopic space and time variables $\tilde{\mathbf{r}}, \tilde{t}$

$$\tilde{\mathbf{r}} = \alpha \mathbf{r} \ , \ \tilde{t} = \alpha t \ .$$

To avoid cumbersome notations, we remove the tildes in the following. The effect of the new variables is to introduce α factors in the large deviation rate function, which becomes

$$I_T^\alpha[f] = \frac{1}{\alpha^4} \int_0^T \mathrm{d}t \left\{ \sup_p \iint \mathbf{drdv} \, \alpha p(\mathbf{r},\mathbf{v}) \partial_t f - \alpha H_T[f,p] - H_C[f,p] \right\}. \tag{7.5}$$

H_C can be written as a sum of three terms

$$H_C[f,p] = H_C^{(1)}[f,p] + H_C^{(2)}[f,p] + H_C^{(\mathrm{h.o.})}[f,p] \tag{7.6}$$

where $H_C^{(1)}, H_C^{(2)}, H_C^{(\mathrm{h.o.})}$ are respectively linear in p, quadratic in p and higher order in p. In particular

$$H_C^{(1)}[f,p] = \iint \mathbf{drdv} \, p Q(f,f), \tag{7.7}$$

where $Q(f,f)$ is the deterministic collision term. In the following we compute the supremum in p in (7.5) perturbatively in the small α limit.

The supremum in p in (7.5) requires to solve in p the equation:

$$\frac{\delta H_C^{(2)}}{\delta p} + \frac{\delta H_C^{(\mathrm{h.o.})}}{\delta p} = \alpha \partial_t f + \alpha \mathbf{v}\cdot\nabla f - Q(f,f). \tag{7.8}$$

We are interested in computing the large deviation rate for functions f close to be hydrodynamical solutions, that is

$$f(\mathbf{r},\mathbf{v},t) = M_{\rho,\mathbf{u},\theta}(\mathbf{r},\mathbf{v},t) + \mathcal{O}(\alpha), \tag{7.9}$$

where $M_{\rho,\mathbf{u},\theta}$ is the Maxwellian (7.4). Since $Q(M_{\rho,\mathbf{u},\theta}, M_{\rho,\mathbf{u},\theta}) = 0$, we have $Q(f,f) = \mathcal{O}(\alpha)$. The right hand side in (7.8) is then of order α. The first term in the left hand side is linear in p; we conclude that the optimal p is of order α:

$$p^{\mathrm{opt}} = \alpha p^{(1)} + \mathcal{O}(\alpha^2),$$

and furthermore the leading order $p^{(1)}$ is entirely determined by $H_C^{(2)}$, the quadratic term of the collision Hamiltonian. From (7.5), we conclude that the leading order (in α) of the large deviation function is $\mathcal{O}(1)$, and does not involve $H_C^{(\mathrm{h.o.})}$. However, this leading order corresponds to compressible Euler equations, the leading order of the hydrodynamical equations in the scaling we have used; compressible Navier-Stokes equations require to go one step further in the expansion in α, which corresponds to order α in the large deviation function. A priori, this order includes a term $H_C^{(3)}[f,p^{(1)}]$, where $H_C^{(3)}[f,p]$ is the cubic in p term of H_C. Using (7.9), this term is at leading order

$$\int \mathbf{dr}\mathbf{dv}_1\mathbf{dv}_2\mathbf{dv}_1'\mathbf{dv}_2'\, w(\mathbf{v}_1', d\mathbf{v}_2'; \mathbf{v}_1, \mathbf{v}_2) M_{\rho,\mathbf{u},\theta}(\mathbf{r},\mathbf{v}_1) M_{\rho,\mathbf{u},\theta}(\mathbf{r},\mathbf{v}_2) \\ \times \left[p(\mathbf{r},\mathbf{v}_1') + p(\mathbf{r},\mathbf{v}_2') - p(\mathbf{r},\mathbf{v}_1) - p(\mathbf{r},\mathbf{v}_2)\right]^3,$$

where $M_{\rho,\mathbf{u},\theta}$ is the appropriate Maxwellian, and it should be eventually evaluated at $p = p^{(1)}$. We use now symmetry properties of w and energy conservation:

$$M_{\rho,\mathbf{u},\theta}(\mathbf{r},\mathbf{v}_1) M_{\rho,\mathbf{u},\theta}(\mathbf{r},\mathbf{v}_2) w(\mathbf{v}_1',\mathbf{v}_2';\mathbf{v}_1,\mathbf{v}_2) = M_{\rho,\mathbf{u},\theta}(\mathbf{r},\mathbf{v}_1') M_{\rho,\mathbf{u},\theta}(\mathbf{r},\mathbf{v}_2') w(\mathbf{v}_1',\mathbf{v}_2';\mathbf{v}_1,\mathbf{v}_2),$$

to conclude that this term vanishes[2]. Hence, up to order α in the large deviation function, which is the relevant order for compressible Navier-Stokes equations, the terms of order more than quadratic in p play no role in the hydrodynamical limit. We shall then neglect them, and consider the noise is Gaussian already at kinetic level.

An important remark is in order: throughout the above discussion, we have tacitly assumed that f does not change on temporal or spatial scales of order α, so that $\partial_t f$, $\mathbf{v}\cdot\nabla f$ are of order 1. This rules out the possibility of hydrodynamical shocks. Hence the statistical weight of such shock profiles may not be correctly described by this quadratic Hamiltonian. We shall detail this observation in chapter 9.

[2]Similarly to the case of independent Run-and-Tumbling particles, the symmetry of w canceling the cubic term of the Hamiltonian is linked to the microscopic time-reversibility of the particle dynamics.

7.1.3. Quadratic approximation for the Hamiltonian: incompressible Navier-Stokes equations

The appropriate macroscopic space and time variables $(\tilde{\mathbf{r}}, \tilde{t})$ to derive the incompressible Navier-Stokes equations is parabolic

$$\tilde{\mathbf{r}} = \alpha \mathbf{r} \ , \ \tilde{t} = \alpha^2 t \ .$$

The effect of these new variables is to introduce α factors in the large deviation rate function, which becomes (again removing the tildes for convenience):

$$I_T^\alpha[f] = \frac{1}{\alpha^5} \int_0^T \mathrm{d}t \left\{ \sup_p \iint \mathbf{dr dv}\, \alpha^2 p(\mathbf{r}, \mathbf{v}) \partial_t f - \alpha H_T[f, p] - H_C[f, p] \right\} . \quad (7.10)$$

We introduce some definitions. $M(\mathbf{v})$ is the reference Maxwellian:

$$M(\mathbf{v}) = \frac{1}{(2\pi)^{\frac{3}{2}}} e^{-\frac{1}{2}\mathbf{v}^2}. \quad (7.11)$$

We are interested in computing the large deviation rate for distributions f close to the reference Maxwellian, that is

$$f(\mathbf{r}, \mathbf{v}, t) = M(\mathbf{v})\big(1 + \alpha g + O(\alpha^2)\big), \quad (7.12)$$

where g is

$$g = \rho(\mathbf{r}, t) + \mathbf{u}(\mathbf{r}, t) \cdot \mathbf{v} + \theta(\mathbf{r}, t) \frac{\mathbf{v}^2 - 3}{2} + O(\alpha) \quad (7.13)$$

We define the operators $\mathcal{Q}$ (quadratic) and $\mathcal{L}$ (linear):

$$\mathcal{Q}(g, g) = \frac{1}{M} Q(Mg, Mg) \ , \ \mathcal{L}[g] = -\frac{2}{M} Q(M, Mg); \quad (7.14)$$

we shall use in the velocity space the scalar product weighted with M:

$$\langle f, g \rangle_M = \int \mathbf{dv}\, f g M$$

With this scalar product, $\mathcal{L}$ is self-adjoint. Furthermore,

$$\mathrm{Ker}\mathcal{L} = \mathrm{Span}(1, \mathbf{v}, \mathbf{v}^2).$$

Then the function g (7.13) is in $\mathrm{Ker}\mathcal{L}$, and for f as in (7.12):

$$Q(f, f) = \alpha^2 M \mathcal{Q}(g, g) + O(\alpha^3), \quad (7.15)$$

Equation (7.8) becomes

$$\frac{\delta H_C^{(2)}}{\delta p} + \frac{\delta H_C^{(\mathrm{h.o.})}}{\delta p} = \alpha^3 \partial_t g + \alpha^2 \mathbf{v} \cdot \nabla g - Q(f, f). \quad (7.16)$$

with $Q(f,f) = O(\alpha^2)$ because of (7.15). Hence the optimal p is now a priori of order α^2:

$$p^{\mathrm{opt}} = \alpha^2 p^{(2)} + O(\alpha^3).$$

Incompressible Navier-Stokes equation (and its fluctuations) appear at order α^3, when the $\partial_t g$ term comes into play. We see on (7.10) that this corresponds to an order α^2 for I_T^α. But $H^{(\mathrm{h.o})}[f, p^{\mathrm{opt}}]$ is of order at least α^3, hence it does not contribute to the hydrodynamical large deviation function. We conclude again that all non Gaussian terms in the noise formally disappear in the hydrodynamical limit. We will then assume that the noise is Gaussian at the kinetic level, i.e. keep only the quadratic approximation for the collision Hamiltonian.

As already noted at the end of paragraph 7.1.2, this quadratic approximation assumes that the profile f of which we want to estimate the probability does not have too steep gradients.

7.1.4. A SPDE formulation

Large deviation principles associated with quadratic in p Hamiltonians can be rewritten as Ito stochastic PDEs with small Gaussian noise. Let us proceed first formally. Consider the large deviation principle for the spatio-temporal stochastic process $f_\lambda(\mathbf{r}, t)$ with speed λ and quadratic Hamiltonian $H[f,p]$, with a deterministic dynamics $\partial_t f + K(f) = 0$:

$$\mathbb{P}\left(\{f_\lambda(t)\}_{0\le t\le T} = \{f(t)\}_{0\le t\le T}\right) \underset{\lambda\downarrow 0}{\asymp} e^{-\frac{1}{\lambda}\left\{\int_0^T \mathrm{d}t \sup_{\mathrm{p}}\left[\int \mathrm{d}\mathbf{r}\, p(\partial_t f + K(f)) - H[f,p]\right]\right\}}.$$

Performing the optimization over p, one gets

$$\mathbb{P}\left(\{f_\lambda(t)\}_{0\le t\le T} = \{f(t)\}_{0\le t\le T}\right) \underset{\lambda\downarrow 0}{\asymp} e^{-\frac{1}{4\lambda}\int_0^T \mathrm{d}t \int \mathrm{d}\mathbf{r}\left(\partial_t f + K(f)\right) L_f^{-1}\left(\partial_t f + K(f)\right)},$$

where L_f is the linear operator such that $\frac{\delta H}{\delta p}[f,p] = 2L_f(p)$. The following stochastic PDE formally recovers the same large deviation principle:

$$\partial_t f + K(f) = \sqrt{\lambda}\eta(\mathbf{r}, t),$$

where η is a Gaussian noise with correlations

$$\mathbb{E}\left(\eta(\mathbf{r},t)\eta(\mathbf{r}',t')\right) = 2\delta(t-t')\delta(\mathbf{r}-\mathbf{r}')L_f.$$

The expression above for the correlations has to be understood with respect to test functions ψ and φ of the space variable as following

$$\int \mathrm{d}\mathbf{r}\mathrm{d}\mathbf{r}'\, \psi(\mathbf{r})\,\varphi(\mathbf{r}')\,\mathbb{E}\left(\eta(\mathbf{r},t)\eta(\mathbf{r}',t')\right) = \delta(t-t')\int \mathrm{d}\mathbf{r}\,\psi(\mathbf{r})\,L_f(\varphi)(\mathbf{r}).$$

In the following, we apply this formalism to express the Boltzmann large deviation principle for the empirical measure as a stochastic PDE. Although it may be difficult to give a

precise mathematical meaning to the obtained nonlinear stochastic PDE, it will be easier to manipulate at the formal level than the Large Deviation Principle. In both scalings leading to the compressible and incompressible Navier-Stokes equations, we showed in section 7.1.3 that at leading order in the Knudsen number α, we can assume the large deviation Hamiltonian is quadratic in p and only retain its quadratic part:

$$H_Q[f,p] = H_T[f,p] + H_C^{(1)}[f,p] + H_C^{(2)}[f,p],$$

where H_T and $H_C^{(1)}$ are linear in p and are defined in equations (7.1-7.7) and

$$H_C^{(2)}[f,p] = \int \mathbf{dr}\mathbf{dv}_1\mathbf{dv}_2\mathbf{dv}_1'\mathbf{dv}_2'\, w(\mathbf{v}_1',\mathbf{v}_2';\mathbf{v}_1,\mathbf{v}_2)\, f(\mathbf{r},\mathbf{v}_1) f(\mathbf{r},\mathbf{v}_2) \times \left(p(\mathbf{r},\mathbf{v}_1') + p(\mathbf{r},\mathbf{v}_2') - p(\mathbf{r},\mathbf{v}_1) - p(\mathbf{r},\mathbf{v}_2)\right)^2.$$

Stochastic PDE for compressible Navier-Stokes equations. With the hyperbolic scaling that leads to the compressible Navier–Stokes equations, the kinetic deterministic equation is

$$\alpha(\partial_t f + \mathbf{v}\cdot\nabla f) - Q(f) = 0, \tag{7.17}$$

which contains a small parameter α. The large deviation rate is $\lambda = \epsilon\alpha^4$. The associated stochastic PDE is

$$\alpha(\partial_t f + \mathbf{v}\cdot\nabla f) - Q(f) = \lambda^{\frac{1}{2}}\eta[f] \tag{7.18}$$

which can be rewritten

$$\partial_t f + \mathbf{v}\cdot\nabla f - \frac{1}{\alpha}Q(f) = \left(\epsilon\alpha^2\right)^{\frac{1}{2}}\eta[f], \tag{7.19}$$

where

$$\mathbb{E}\left(\eta[f](\mathbf{r},\mathbf{v},t)\,\eta[f](\mathbf{r}',\mathbf{v}',t')\right) = 2\delta(t-t')\delta(\mathbf{r}-\mathbf{r}')\,L_f \tag{7.20}$$

with

$$\begin{aligned} L_f(p)(\mathbf{r},\mathbf{v},t) &= \frac{\delta H_C^{(2)}}{\delta p(\mathbf{r},\mathbf{v},t)}[f,p], \\ &= -f(\mathbf{v})\int \mathbf{dr}\mathbf{dv}_2\mathbf{dv}_1'\mathbf{dv}_2'\, w(\mathbf{v}_1',\mathbf{v}_2';\mathbf{v},\mathbf{v}_2) f(\mathbf{v}_2)\left[p(\mathbf{v}_1') + p(\mathbf{v}_2') - p(\mathbf{v}) - p(\mathbf{v}_2)\right]. \end{aligned}$$

When the distribution function f is a Maxwellian $M_h = M_{\rho,\mathbf{u},\theta}$ (with $h = (\rho,\mathbf{u},\theta)$); we have $L_{M_h}\cdot g = M_h\mathcal{L}_{M_h}$ where $\mathcal{L}_{M_h} = -\frac{2}{M_h}Q(M_h, M_h g)$. This will be useful later as $\mathcal{L}_{M_h}$ appears naturally when linearizing the collision operator close to a Maxwellian.

Stochastic PDE for incompressible Navier-Stokes equations. With the parabolic scaling that leads to the incompressible Navier–Stokes equations, the kinetic deterministic equation is

$$\alpha^3 \partial_t g + \alpha^2 \mathbf{v} \cdot \nabla g + \alpha \mathcal{L}(g) - \alpha^2 \mathcal{Q}(g,g) = 0, \tag{7.21}$$

and the large deviation rate is $\epsilon\alpha^5$. The associated SPDE is

$$\alpha^3 \partial_t g + \alpha^2 \mathbf{v} \cdot \nabla g + \alpha \mathcal{L}(g) - \alpha^2 \mathcal{Q}(g,g) = (\epsilon\alpha^5)^{\frac{1}{2}} \frac{\eta[M]}{M},$$

or

$$\alpha \partial_t g + \mathbf{v} \cdot \nabla g + \alpha^{-1} \mathcal{L}(g) - \mathcal{Q}(g,g) = (\epsilon\alpha)^{\frac{1}{2}} \frac{\eta[M]}{M}, \tag{7.22}$$

where the correlations for η are given by

$$\mathbb{E}\left(\eta[M](\mathbf{r},\mathbf{v},t)\,\eta[M](\mathbf{r}',\mathbf{v}',t')\right) = 2M\delta(t-t')\delta(\mathbf{r}-\mathbf{r}')\,\mathcal{L}. \tag{7.23}$$

In the above equations, operators $\mathcal{Q}, \mathcal{L}$ are defined in (7.14). To express (7.23), we have used that when the distribution function f is the absolute Maxwellian M defined in (7.11) we have $L_M = M\mathcal{L}$. When dropping the non-linear term, equation (7.22) is the fluctuating Boltzmann equation derived in [191] from a central limit theorem approach.

7.2. Derivation of the fluctuating compressible Navier–Stokes and Euler equations

In this section, we derive the fluctuating compressible Navier–Stokes system using the SPDE formalism introduced in section 6.5; the starting point is the fluctuating Boltzmann equation (7.19) with Gaussian noise in the hyperbolic scaling with respect to the Knudsen number

$$\partial_t f + \mathbf{v} \cdot \nabla f = \frac{1}{\alpha} Q(f,f) + \sqrt{\epsilon\alpha^2}\eta[f]\,. \tag{7.24}$$

The strategy is to follow the standard deterministic computations, as in [14], adding the noise term in the expansion.

7.2.1. Chapman–Enskog expansion

At leading order for small α, we obtain $Q(f^0, f^0) = 0$, which ensures that f^0 has the following Maxwellian form:

$$f^0(\mathbf{r},\mathbf{v},t) = M_h(\mathbf{r},\mathbf{v},t) = \frac{\rho}{(2\pi\theta)^{3/2}} e^{-\frac{1}{2}\frac{(\mathbf{v}-\mathbf{u})^2}{\theta}}, \tag{7.25}$$

where $h(\mathbf{r},t) = (\rho(\mathbf{r},t), \mathbf{u}(\mathbf{r},t), \theta(\mathbf{r},t))$ are the hydrodynamical fields, respectively the density, velocity and temperature fields.

The goal of the Chapman–Enskog expansion is to reduce the evolution of the distribution function f to the evolution of its hydrodynamical fields $(\rho(\mathbf{r},t), \mathbf{u}(\mathbf{r},t), \theta(\mathbf{r},t))$ as the Knudsen number tends to 0. We shall look for an expansion in α: $f = f^0 + O(\alpha)$. We recall the definition of the linearized kinetic operator

$$\mathcal{L}_{M_h} : g \mapsto -\frac{2}{M_h} Q(M_h, M_h g), \tag{7.26}$$

which is self adjoint with respect to the L^2 weighted scalar product

$$\langle a, b \rangle_{M_h} = \int \mathrm{d}\mathbf{v}\, a(\mathbf{v})\, b(\mathbf{v})\, M_h,$$

its kernel is $\mathrm{span}(1, \mathbf{v}, v^2)$[3] as explained in appendix B.1. It satisfies a Fredholm alternative, i.e. the equation

$$\mathcal{L}_{M_h}[g] = a$$

has a solution only if $a \in \ker(\mathcal{L}_{M_h})^\perp$ and in this case this solution is unique if ones adds the condition $g \in \ker(\mathcal{L}_{M_h})^\perp$. We will write this solution as $g = \mathcal{L}_{M_h}^{-1}[a]$. We denote Π the projection operator on hydrodynamical modes

$$\Pi[f] = \begin{pmatrix} \int f d\mathbf{v} \\ \int \mathbf{v} f d\mathbf{v} \\ \frac{1}{2}\int v^2 f d\mathbf{v} \end{pmatrix}. \tag{7.27}$$

Note that $g \in \ker(\mathcal{L}_{M_h})^\perp$ is equivalent to $\Pi[M_h g] = 0$. We now build a Chapman-Enskog expansion to solve the fluctuating Boltzmann equation (7.24):

$$f = M_h(1 + \alpha g_\alpha^1 + \alpha^2 g_\alpha^2 + \mathcal{O}(\alpha^3)). \tag{7.28}$$

We require that $\Pi[M_h g^k] = 0$ for any $k \geq 1$: this means that all the "hydrodynamical content of f is captured by M_h; this condition requires that the g^k (and also M_h) keep a dependence in α, emphasized as an index in (7.28).

Inserting (7.28) into the fluctuating Boltzmann equation (7.24) yields

$$(\partial_t + \mathbf{v}\cdot\nabla)[M_h] = -M_h \mathcal{L}_{M_h}[g_\alpha^1] + \sqrt{\epsilon\alpha^2}\eta\,[M_h] + \mathcal{O}(\alpha). \tag{7.29}$$

We note that at leading order in α, the noise term only depends on M_h and not on the full distribution function. Now, applying Π to (7.29), using the conservation laws of the kinetic equation (i.e. $\ker(\mathcal{L}_{M_h}^\dagger) = \ker(\mathcal{L}_{M_h}) = \mathrm{span}(1, \mathbf{v}, v^2)$) and the conservation properties obeyed by the noise (B.2) (see appendix B.1) , we are left with

$$\Pi[(\partial_t + \mathbf{v}\cdot\nabla)[M_h]] = \mathcal{O}(\alpha). \tag{7.30}$$

[3] $\mathrm{span}(1, \mathbf{v}, \mathbf{v}^2)$ denotes the span of the functions of the velocity variable $\mathbf{v} \mapsto 1$, $\mathbf{v} \mapsto \mathbf{v}$, and $\mathbf{v} \mapsto v^2$.

If we drop the $\mathcal{O}(\alpha)$ terms, (7.30) is the compressible Euler system for the hydrodynamical fields[4]:

$$\partial_t \rho + \nabla \cdot (\rho \mathbf{u}) = 0, \tag{7.31}$$

$$\partial_t (\rho \mathbf{u}) + \nabla \cdot (\rho \mathbf{u} \otimes \mathbf{u}) + \nabla(\rho\theta) = 0, \tag{7.32}$$

$$\frac{3}{2}\rho\partial_t\theta + \rho\theta\nabla\cdot\mathbf{u} + \frac{3}{2}\rho\left(\mathbf{u}\cdot\nabla\right)\theta = 0. \tag{7.33}$$

It is worth noticing the equation on the temperature θ (7.33) can be rephrased as the conservation of energy equation:

$$\partial_t\left(\frac{3}{2}\rho\theta + \frac{1}{2}u^2\right) + \nabla\cdot\left(\left(\frac{5}{2}\rho\theta + \frac{1}{2}u^2\right)\mathbf{u}\right) = 0,$$

where the first term is the time-derivative of the total energy, and the second term is the divergence of the enthalpy flux. We note that at this order in the Knudsen number α, there is no noise term. To obtain dissipative and noise terms, we have to push the expansion further in α. To do so, we need to solve for g^1_α in (7.29):

$$\mathcal{L}_{M_h}[g^1_\alpha] = -\frac{(\partial_t + \mathbf{v}\cdot\nabla)[M_h]}{M_h} + \sqrt{\epsilon\alpha^2}\frac{\eta}{M_h} + O(\alpha).$$

We expand $g^1_\alpha = g^1 + O(\alpha)$, where g^1 is the unique solution of

$$\mathcal{L}_{M_h}[g^1] = -\frac{(\partial_t + \mathbf{v}\cdot\nabla)[M_h]}{M_h} + \sqrt{\epsilon\alpha^2}\frac{\eta}{M_h},\ \Pi[M_h g^1] = 0.$$

Decomposing g^1 into a deterministic and a stochastic part, we write

$$g = g^{1,d} + g^{1,s}$$

where

$$\mathcal{L}_{M_h}[g^{1,d}] = -\frac{(\partial_t + \mathbf{v}\cdot\nabla)[M_h]}{M_h}, \tag{7.34}$$

and

$$\mathcal{L}_{M_h}[g^{1,s}] = \sqrt{\epsilon\alpha^2}\frac{\eta}{M_h}. \tag{7.35}$$

We first focus on the deterministic term. The explicit form of M_h (7.25) and the compressible Euler equations (7.31-7.32) yield

$$\frac{(\partial_t + \mathbf{v}\cdot\nabla)[M_h]}{M_h} = \mathbf{A}(\mathbf{V})\cdot\frac{\nabla\theta}{\sqrt{\theta}} + \frac{1}{2}\mathbf{B}(\mathbf{V}) : \boldsymbol{\sigma}(\mathbf{u}),.$$

[4]It is interesting to note that the derivation of the compressible Euler system only requires the knowledge of: the local equilibria that cancel the collision operator, and the content of the kernel of the adjoint of its linearization close to a local equilibrium. In other words, a different collision operator, sharing the same local equilibria and conserved quantities would yield the exact same hydrodynamical limit, at order 1 in the Knudsen number. The BGK collision operator $Q(f) = -f + f_0$ where $f_0 = M_h$ with $h = \Pi[f]$, satisfies these requirements [38].

where we introduced the reduced velocity $\mathbf{V} = (\mathbf{v} - \mathbf{u})/\sqrt{\theta}$, the vector

$$\mathbf{A}(\mathbf{V}) = \frac{1}{2}\left(V^2 - 5\right)\mathbf{V}, \tag{7.36}$$

the tensor

$$\mathbf{B}(\mathbf{V}) = \mathbf{V} \otimes \mathbf{V} - \frac{1}{3}V^2 \mathrm{Id}, \tag{7.37}$$

and the stress tensor $\boldsymbol{\sigma}$ whose components are given by

$$\sigma_{ij}(\mathbf{u}) = \partial_j u_i + \partial_i u_j - \frac{2}{3}\delta_{ij}\partial_k u_k \tag{7.38}$$

Since $\mathbf{A}$ and $\mathbf{B}$ are in $(\ker \mathcal{L}_{M_h})^\perp$, we can compute $\mathcal{L}_{M_h}^{-1}[\mathbf{A}]$ and $\mathcal{L}_{M_h}^{-1}[\mathbf{B}]$. According to [14], and using similar notations, we have

$$\mathcal{L}^{-1}[\mathbf{A}](\mathbf{V}) = -a(V)\mathbf{A}(\mathbf{V})\ ,\ \mathcal{L}^{-1}[\mathbf{B}](\mathbf{V}) = -b(V)\mathbf{B}(\mathbf{V})\ .$$

With these new definitions, we can rephrase (7.34)

$$g^{1,d} = a(V)\,\mathbf{A}(\mathbf{V}) \cdot \frac{\nabla\theta}{\sqrt{\theta}} + \frac{1}{2}b(V)\mathbf{B}(\mathbf{V})) : \boldsymbol{\sigma}(\mathbf{u})\,. \tag{7.39}$$

The stochastic term can also be explicitly obtained by inverting $\mathcal{L}_{M_h}$

$$g^{1,s} = \sqrt{\epsilon\alpha^2}\mathcal{L}_{M_h}^{-1}\left[\frac{\eta}{M_h}\right]. \tag{7.40}$$

The inversion is possible because of the conservation properties of the noise (B.2)[5]. From there, we can compute g^1 at leading order in α in (7.29) and push the expansion (7.28) to the Navier-Stokes (dissipative) order. In order to do so, we once again look for a solution of the fluctuating Boltzmann equation as a Chapman-Enskog expansion close to a local equilibrium M_h. In other words, we insert (7.28) into (7.24), but this time, we also gather terms of order α, yielding

$$(\partial_t + \mathbf{v}\cdot\nabla)[M_h] + \alpha(\partial_t + \mathbf{v}\cdot\nabla)[g^1] = -M_h\mathcal{L}_{M_h}\left[g_\alpha^1\right] - M_h\mathcal{L}_{M_h}\left[g_\alpha^2\right] + \alpha M_h\mathcal{Q}(g_\alpha^1, g_\alpha^1) + \sqrt{\epsilon\alpha^2}\eta + \mathcal{O}(\alpha^2).$$

Applying Π, the r.h.s. furnishes only a $O(\alpha^2)$ term. Hence

$$\Pi[(\partial_t + \mathbf{v}\cdot\nabla)[M_h]] + \alpha\Pi[\mathbf{v}\cdot\nabla g^1] = O(\alpha^2). \tag{7.41}$$

We have also used that Π and ∂_t commute, and that $\Pi[g^1] = 0$. Dropping the $O(\alpha^2)$ remainder, (7.41) is the fluctuating compressible Navier-Stokes system, where $g^1 = g^{1,d} + g^{1,s}$ is given by (7.39-7.40). It can be rewritten more explicitly

$$\partial_t\rho + \nabla\cdot(\rho\mathbf{u}) + \alpha\nabla\cdot\left(\int \mathrm{d}\mathbf{v}\,\mathbf{v}g^1 M_h\right) = 0, \tag{7.42}$$

$$\rho\partial_t\mathbf{u} + \rho(\mathbf{u}\cdot\nabla)\mathbf{u} + \nabla(\rho\theta) + \alpha\nabla\cdot\left(\int \mathrm{d}\mathbf{v}\,\mathbf{v}\otimes\mathbf{v}g^1 M_h\right) = 0, \tag{7.43}$$

$$\frac{3}{2}\rho\partial_t\theta + \rho\theta\nabla\cdot\mathbf{u} + \frac{3}{2}\rho(\mathbf{u}\cdot\nabla)\theta + \frac{1}{2}\alpha\nabla\cdot\left(\int \mathrm{d}\mathbf{v}\,v^2\mathbf{v}g^1 M_h\right) = 0. \tag{7.44}$$

[5] More precisely, a noise realization for the fluctuating kinetic equation that violates mass, momentum or energy conservation would be associated with a zero probability.

Recalling that $\Pi[g^1 M_h] = 0$, we see that the terms of order α vanish in the equations for ρ. Hence there is no dissipation nor noise in the first equation. The explicit computations of the terms involving g^1 is given in appendix B.2. The final result reads

$$\partial_t \rho + \nabla \cdot (\rho \mathbf{u}) = 0 \tag{7.45}$$

$$\rho \partial_t \mathbf{u} + \rho \left(\mathbf{u} \cdot \nabla\right) \mathbf{u} + \nabla(\rho\theta) = \alpha \nabla \cdot (\nu \boldsymbol{\sigma}) + \sqrt{\epsilon \alpha^4} \nabla \cdot \mathbf{J}, \tag{7.46}$$

$$\frac{3}{2}\rho \partial_t \theta + \rho\theta \nabla \cdot \mathbf{u} + \frac{3}{2}\rho \left(\mathbf{u} \cdot \nabla\right) \theta = \alpha \left(\nabla \cdot (\kappa \nabla \theta) + \frac{\nu}{2} \boldsymbol{\sigma} : \boldsymbol{\sigma}\right) + \sqrt{\epsilon \alpha^4} \nabla \cdot \mathbf{J}^\theta, \tag{7.47}$$

where

$$\sigma_{ij}\left(\mathbf{u}\right) = \partial_j u_i + \partial_i u_j - \frac{2}{3}\delta_{ij} \partial_k u_k,$$

$$J_{ij} = \theta^{5/2} \int \mathrm{d}\mathbf{V}\, b\left(V\right) B_{ij}\left(\mathbf{V}\right) \eta\left(\sqrt{\theta}\mathbf{V} + \mathbf{u}\right),$$

and

$$J_j^\theta = \theta^{5/2} \int \mathrm{d}\mathbf{V}\, \left(\theta^{1/2} a\left(V\right) A_j\left(\mathbf{V}\right) + u_i b\left(V\right) B_{ij}(\mathbf{V})\right) \eta\left(\sqrt{\theta}\mathbf{V} + \mathbf{u}\right).$$

The expressions for ν (7.48) and κ (7.49) are given in the next paragraph and derived in Appendix B.2.

7.2.2. Noise correlations

The noise terms in (7.46-7.47) are Gaussian and delta-correlated in space and time. To obtain explicit form of the fluctuating compressible Navier-Stokes system, we now only have to compute their correlations. We have to compute $\mathbb{E}\left[J_{ij} J_{kl}\right]$ and $\mathbb{E}\left[J_i^\theta J_j^\theta\right]$. We forget now the dependency on space and time, since it is trivial.We will need to compute quantities such as

$$\int \varphi(\mathbf{v}) \psi(\mathbf{v}') \mathbb{E}[\eta(\mathbf{v}) \eta(\mathbf{v}')] \mathrm{d}\mathbf{v} \mathrm{d}\mathbf{v}'.$$

Going back to the correlations of η (7.23), we have that

$$\int \varphi(\mathbf{v}) \psi(\mathbf{v}') \mathbb{E}[\eta(\mathbf{v}) \eta(\mathbf{v}')] \mathrm{d}\mathbf{v} \mathrm{d}\mathbf{v}' = 2 \int M_h \varphi \mathcal{L}_{M_h}[\psi] \mathrm{d}\mathbf{v}.$$

The correlation functions of the noise terms are computed in section B.2.4. The result reads

$$\mathbb{E}\left(J_{ij}\left(\mathbf{r}, t\right) J_{kl}\left(\mathbf{r}', t'\right)\right) = 2\theta\nu \left(\delta_{ik}\delta_{jl} + \delta_{il}\delta_{jk} - \frac{2}{3}\delta_{ij}\delta_{kl}\right) \delta\left(\mathbf{r} - \mathbf{r}'\right) \delta\left(t - t'\right)$$

and

$$\mathbb{E}\left(J_i^\theta\left(\mathbf{r}, t\right) J_j^\theta\left(\mathbf{r}', t'\right)\right) = 2\left(\theta^2 \kappa \delta_{ij} + \theta\nu B_{ij}\left(\mathbf{u}\right)\right) \delta\left(\mathbf{r} - \mathbf{r}'\right) \delta\left(t - t'\right),$$

where

$$\nu = -\frac{2}{15}\frac{\rho\theta}{\sqrt{2\pi}}\int_0^\infty dV\, V^6 b\left(V\right)\mathrm{e}^{-V^2/2}, \tag{7.48}$$

and

$$\kappa = -\frac{1}{6}\frac{\rho\theta}{\sqrt{2\pi}}\int_0^\infty dV\, V^4\left(V^2-5\right)^2 a\left(V\right)\mathrm{e}^{-V^2/2}. \tag{7.49}$$

a and b are negative functions of the norm of the reduced velocity V [14]. As a consequence the viscosity ν and the thermal diffusivity κ are positive. Because the collision operator $Q(f)$ is quadratic in the distribution function, we can show that a and b are proportional to the inverse of the density ρ. An alternate way to rewrite the fluctuating compressible Navier–Stokes equations is to introduce the stochastic flux $\mathbf{q}$ that is Gaussian and satisfies

$$\mathbb{E}\left(q_i\left(\mathbf{r},t\right)q_j\left(\mathbf{r}',t'\right)\right) = 2\theta^2\kappa\delta_{ij}\delta\left(\mathbf{r}-\mathbf{r}'\right)\delta\left(t-t'\right).$$

Doing so, the compressible Navier–Stokes system reads

$$\begin{aligned}
\partial_t\rho + \nabla\cdot\left(\rho\mathbf{u}\right) &= 0 && (7.50)\\
\rho\partial_t\mathbf{u} + \rho\left(\mathbf{u}\cdot\nabla\right)\mathbf{u} + \nabla(\rho\theta) &= \alpha\nabla\cdot\left(\nu\boldsymbol{\sigma}\right) + \sqrt{\epsilon\alpha^4}\nabla\cdot\mathbf{J}, && (7.51)\\
\frac{3}{2}\rho\partial_t\theta + \rho\theta\nabla\cdot\mathbf{u} + \frac{3}{2}\rho\left(\mathbf{u}\cdot\nabla\right)\theta &= \alpha\nabla\cdot\left(\kappa\nabla\theta\right) + \alpha\frac{\nu}{2}\boldsymbol{\sigma}:\boldsymbol{\sigma} + \sqrt{\epsilon\alpha^4}\nabla\cdot\left(\mathbf{u}\cdot\mathbf{J}+\mathbf{q}\right) && (7.52)
\end{aligned}$$

In the following, we call $\mathbf{J}$ the fluctuating stress and $\mathbf{q}$ the fluctuating heat density flux. It is straightforward to check that the stochastic fluxes $\mathbf{u}\cdot\mathbf{J}+\mathbf{q}$ and $\mathbf{J}^\theta$ have the same correlation structure. In addition to this, the cross-correlation between $\mathbf{J}$ and $\mathbf{q}$ vanishes: $\mathbb{E}\left(\mathbf{J}\otimes\mathbf{q}\right) = 0$.

These equations are expressed in a set of physical units in section 7.4. To our knowledge, this is the first derivation of the fluctuating compressible Navier-Stokes equations starting from the microscopic dynamics (in the sense that the noise in the fluctuating Boltzmann equation stems from the underlying kinetic large deviation principle rather than thermodynamic considerations).

7.3. Derivation of the fluctuating incompressible Navier–Stokes equations

In this section, we derive the fluctuating incompressible Navier–Stokes system starting from (7.22), the Chapman-Enskog expansion of the fluctuating Boltzmann equation within the parabolic rescaling.

7.3.1. Chapman–Enskog expansion

Let us recall first that when investigating the incompressible limit, we look for a solution of the Boltzmann equation as a Chapman-Enskog expansion close to an absolute Maxwellian:

$$f(\mathbf{r},\mathbf{v},t) = M(\mathbf{v})\big(1+\alpha g + O(\alpha^2)\big), \quad \text{with} \quad M(\mathbf{v}) = \frac{1}{(2\pi)^{\frac{3}{2}}} e^{-\frac{1}{2}\mathbf{v}^2}.$$

Making $\alpha \to 0$ in (7.22) imposes that $g \in \mathrm{Ker}\mathcal{L}$ at leading order, that is at leading order

$$g = \rho + \mathbf{u}\cdot\mathbf{v} + \theta\frac{\mathbf{v}^2-3}{2}, \tag{7.53}$$

as was already anticipated in the section (7.1).

As shown in appendix (B.1), $\mathcal{Q}(g,g)$ and $\frac{1}{M}\eta$ are in $(\ker\mathcal{L})^\perp$ with respect to the L^2 scalar product weighted by the absolute Maxwellian

$$\langle a,b\rangle_M = \int \mathrm{d}\mathbf{v}\, a(\mathbf{v})\, b(\mathbf{v})\, M(\mathbf{v}).$$

Hence, taking the scalar product of (7.22) against the elements of $\ker\mathcal{L}$ and making $\alpha \to 0$, we obtain the incompressibility and Boussinesq equations (we obtain only 4 equations, since the elements of $\ker\mathcal{L}$ $\mathbf{v}\mapsto 1$ and $\mathbf{v}\mapsto v^2$ both yield the incompressibility equation):

$$\nabla\cdot\mathbf{u} = 0, \tag{7.54}$$

$$\nabla(\rho+\theta) = 0. \tag{7.55}$$

These equations do not contain any noise term.

Now let us look at the order 1 term in α in (7.22). Taking the scalar product of (7.22) with $\mathbf{v}$, and dividing by α, we have

$$\partial_t\langle\mathbf{v},g\rangle_M + \frac{1}{\alpha}\langle\mathbf{v}\otimes\mathbf{v},g\rangle_M = 0,$$

which we rewrite

$$\partial_t\langle\mathbf{v},g\rangle_M + \nabla P + \frac{1}{\alpha}\nabla\langle\mathbf{B}(\mathbf{v}),g\rangle_M = 0,$$

where $P = (1/\alpha)\,\langle v^2 g/3\rangle_M$ is the pressure and $\mathbf{B}$ is the tensor defined in (7.37). Using the expression for g (7.53), we obtain that the first term above tends to $\partial_t\mathbf{u}$ when $\alpha\to 0$. To compute the third one, we use that $\mathcal{L}$ is self adjoint, and that $\mathbf{B}(\mathbf{v})$ is in $(\ker\mathcal{L})^\perp$

$$\langle\mathbf{B}(\mathbf{v}),g\rangle_M = \langle\mathcal{L}^{-1}[\mathbf{B}](\mathbf{v}),\mathcal{L}[g]\rangle_M.$$

Going back to (7.22), we use

$$\frac{1}{\alpha}\mathcal{L}[g] = -\mathbf{v}\cdot\nabla g + \mathcal{Q}(g,g) + \frac{\sqrt{\epsilon\alpha}}{M}\eta + O(\alpha). \tag{7.56}$$

Thus

$$\frac{1}{\alpha}\langle \mathbf{B}, g\rangle_M = -\nabla\langle \mathcal{L}^{-1}[\mathbf{B}]\otimes\mathbf{v}, g\rangle_M + \langle \mathcal{L}^{-1}[\mathbf{B}], \mathcal{Q}(g,g)\rangle_M + \sqrt{\epsilon\alpha}\langle \mathcal{L}^{-1}[\mathbf{B}], \frac{1}{M}\eta\rangle_M + O(\alpha). \tag{7.57}$$

To compute these scalar products, we need to invert $\mathcal{L}^{-1}$ on $(\ker\mathcal{L})^\perp$. This was already done in the last section, and we recall the notations

$$\mathcal{L}^{-1}[\mathbf{A}](\mathbf{v}) = -a(v)\mathbf{A}(\mathbf{v})\ ,\ \mathcal{L}^{-1}[\mathbf{B}](\mathbf{v}) = -b(v)\mathbf{B}(\mathbf{v})\ .$$

Then, the first (resp. second) term on the r.h.s. of (7.57) yields the viscosity (resp. inertial) term in the momentum equation of the Navier-Stokes system. The third term provides the noise. The final equation is

$$\partial_t\mathbf{u} + \mathbf{u}\cdot\nabla\mathbf{u} + \nabla P = \nu\Delta\mathbf{u} + \sqrt{\epsilon\alpha}\nabla\cdot\mathbf{J} \tag{7.58}$$

where

$$\nu = -\frac{2}{15}\frac{1}{\sqrt{2\pi}}\int_0^\infty \mathrm{d}v\, b\,(v)\, v^6 \mathrm{e}^{-v^2/2}. \tag{7.59}$$

and the fluctuating stress tensor reads

$$J_{ij} = \langle \left(\mathcal{L}^{-1}[\mathbf{B}]\right)_{ij}, \frac{1}{M}\eta(\mathbf{r},\mathbf{v},t)\rangle_M.$$

We follow the same route to obtain the equation for θ: taking the scalar product of (7.22) with $(v^2-5)/2$, and dividing by α:

$$\partial_t\langle\frac{(v^2-5)}{2}, g\rangle_M + \frac{1}{\alpha}\nabla\cdot\langle\mathbf{A}(\mathbf{v}), g\rangle_M = 0,$$

where $\mathbf{A}$ is defined in (7.36). Now, again using that $\mathcal{L}$ is self adjoint, and that $\mathbf{A}(\mathbf{v})$ is in $(\ker\mathcal{L})^\perp$, we have

$$\langle\mathbf{A}(\mathbf{v}), g\rangle_M = \langle\mathcal{L}^{-1}[\mathbf{A}](\mathbf{v}), \mathcal{L}[g]\rangle_M.$$

With (7.56), we obtain, since $\langle\frac{(v^2-5)}{2}, g\rangle_M$ tends to $3\theta/2-\rho$:

$$\partial_t\left(\frac{3\theta}{2}-\rho\right) = \partial_i\partial_j\langle\mathcal{L}^{-1}[\mathbf{A}]_i v_j, g\rangle_M - \partial_i\langle\mathcal{L}^{-1}[\mathbf{A}]_i, \mathcal{Q}(g,g)\rangle_M - \sqrt{\epsilon\alpha}\partial_i\langle\mathcal{L}^{-1}[\mathbf{A}]_i, \frac{1}{M}\eta\rangle_M.$$

The first term in the r.h.s. above yields the temperature diffusion, together with an explicit expression for the thermal diffusivity; the second term yields the temperature advection. The third term is the fluctuating heat density flux. With $\partial_t\rho = 0$, the final equation is

$$\partial_t\theta + \mathbf{u}\cdot\nabla\theta = \kappa\Delta\theta + \sqrt{\epsilon\alpha}\nabla\cdot\mathbf{q}, \tag{7.60}$$

where

$$\kappa = -\frac{1}{6}\frac{1}{\sqrt{2\pi}}\int_0^\infty \mathrm{d}v\, a\,(v)\, v^4\left(v^2-5\right)^2\mathrm{e}^{-v^2/2}, \tag{7.61}$$

and

$$\mathbf{q}_i = -\frac{2}{3}\langle\left(\mathcal{L}^{-1}[\mathbf{A}]\right)_i, \frac{1}{M}\eta(\mathbf{r},\mathbf{v},t)\rangle_M.$$

7.3.2. Noise correlations

Computations very similar to the one done in section B.2.4 give the correlation of the stochastic fluxes:

$$\mathbb{E}(J_{ij}(\mathbf{r},t)\,J_{kl}(\mathbf{r}',t')) = 2\nu\left[\delta_{ik}\delta_{jl}+\delta_{il}\delta_{jk}-\frac{2}{3}\delta_{ij}\delta_{kl}\right]\delta(t-t')\delta(\mathbf{r}-\mathbf{r}'), \tag{7.62}$$

and

$$\mathbb{E}\left(q_i(\mathbf{r},t)\,q_j(\mathbf{r}',t')\right) = 2\kappa\delta_{ij}\delta(t-t')\,\delta(\mathbf{r}-\mathbf{r}'), \tag{7.63}$$

where ν and κ are the diffusive coefficients defined in (7.59-7.61). We note that the cross-correlations vanish: $\mathbb{E}(\mathbf{J}(\mathbf{r},t)\otimes\mathbf{q}(\mathbf{r}',t')) = 0$. We connect the result (7.58-7.62) with the literature in section 7.4 by expressing it in a set of physical units rather than the dimensionless ones we have used so far.

7.4. Connection between the microscopic non-dimensional and the macroscopic set of units

In the following, we denote by a subscript φ the variables $(\mathbf{r}_\varphi, \mathbf{v}_\varphi, t_\varphi)$ expressed in physical units. To obtain the Boltzmann equation (7.3), we used the following set of variable suited to the kinetic description, subscripted by a k

$$\mathbf{r}_k = \mathbf{r}_\varphi/\ell,\;\; \mathbf{v}_k = \mathbf{v}_\varphi/v_T,\;\; t_k = v_T t_\varphi/\ell,$$

where ℓ is the mean free path of particle, and $v_T = \sqrt{k_B T_0/m}$ is the thermal velocity, where k_B is the Boltzmann constant, T_0 the average temperature, and m the mass of particle.

7.4.1. Compressible Navier–Stokes equations in physical units

To obtain the compressible Navier–Stokes equations, we rescaled the kinetic time and space units by the Knudsen number $\alpha = \ell/L$ as following

$$\tilde{\mathbf{r}} = \alpha\mathbf{r}_k,\;\; \tilde{t} = \alpha t_k.$$

Thus the dictionary between physical units and the set of dimensionless units used in section 7.2 is:

$$\tilde{\mathbf{r}} = \mathbf{r}_\varphi/L,\;\; \tilde{t} = v_T t_\varphi/L,$$

$$\rho = \rho_\varphi/\rho_0,\;\; \mathbf{u} = \mathbf{u}_\varphi/v_T,\;\; \nu = \nu_\varphi/\left(\rho_0\ell v_T\right),\;\; \theta = k_B\theta_\varphi/(mv_T^2),\;\; \kappa = \kappa_\varphi/\left(\rho_0\ell v_T\right)$$

where $\rho_0 = N/L^3$ is the average density. Expressing equations (7.50-7.52) with the set of physical units introduced above, and dropping the $_\varphi$ subscripts yield

$$\begin{cases} \partial_t \rho + \nabla \cdot (\rho \mathbf{u}) = 0, \\ \rho \partial_t \mathbf{u} + \rho \left(\mathbf{u} \cdot \nabla\right) \mathbf{u} + \frac{k_B}{m} \nabla(\rho\theta) = \frac{1}{2} \nabla \cdot \left(\nu \boldsymbol{\sigma}\left(\mathbf{u}\right)\right) + \nabla \cdot \left(\sqrt{\frac{\nu k_B \theta}{m}} \mathbf{J}\right), \\ \frac{3}{2} k_B \left(\rho \partial_t \theta + \rho\theta \nabla \cdot \mathbf{u} + \frac{3}{2} \rho \left(\mathbf{u} \cdot \nabla\right) \theta\right) = \nabla \cdot \left(\kappa \nabla \theta\right) + \frac{1}{2} m \nu \boldsymbol{\sigma}\left(\mathbf{u}\right) : \boldsymbol{\sigma}\left(\mathbf{u}\right) + \nabla \cdot \left(\sqrt{m \nu k_B \theta} \mathbf{u} \cdot \mathbf{J} + \sqrt{\kappa k} \right. \end{cases}$$

with

$$\mathbb{E}(J_{ij}\left(\mathbf{r}, t\right) J_{kl}\left(\mathbf{r}', t'\right)) = 2 \left[\delta_{ik}\delta_{jl} + \delta_{il}\delta_{jk} - \frac{2}{3}\delta_{ij}\delta_{kl}\right] \delta(t - t')\delta(\mathbf{r} - \mathbf{r}'),$$

$$\mathbb{E}(q_i\left(\mathbf{r}, t\right) q_j\left(\mathbf{r}', t'\right)) = 2\delta_{ij}\delta(t - t')\delta(\mathbf{r} - \mathbf{r}'),$$

and

$$\mathbb{E}(q_i\left(\mathbf{r}, t\right) J_{kl}\left(\mathbf{r}', t'\right)) = 0.$$

This is exactly the fluctuating compressible Navier-Stokes system employed in the computational fluid dynamics literature [96, 95, 9].

7.4.2. Incompressible Navier–Stokes equations in physical units

To obtain the incompressible Navier–Stokes equations, we rescaled kinetic time and space units by the Knudsen number $\alpha = \ell/L$ as following

$$\tilde{\mathbf{r}} = \alpha \mathbf{r}_k, \quad \tilde{t} = \alpha^2 t_k.$$

Thus the dictionary between physical units and our set of units is:

$$\mathbf{r} = \mathbf{r}_\varphi / L, \quad t = \ell v_T t_\varphi / L^2, \quad \mathbf{u} = \mathbf{u}_\varphi / (\alpha v_T),$$

$$\theta = k_B \theta_\varphi / (\alpha m v_T^2), \quad \kappa = \kappa_\varphi / (\ell v_T), \quad \nu = \nu_\varphi / (\ell v_T).$$

Using that $v_T^2 = k_B T_0 / m$, where T_0 is the average temperature of the system, we can rephrase the fluctuating incompressible Navier–Stokes equation for the velocity (7.58) in physical units dropping the $_\varphi$ as following

$$\partial_t \mathbf{u} + \mathbf{u} \cdot \nabla \mathbf{u} + \nabla \left(\frac{P}{\rho_0}\right) = \nu \Delta \mathbf{u} + \nabla \cdot \mathbf{J}, \tag{7.64}$$

where

$$\mathbb{E}(J_{ij}\left(\mathbf{r}, t\right) J_{kl}\left(\mathbf{r}', t'\right)) = \frac{2\nu k_B T_0}{\rho_0} \left[\delta_{ik}\delta_{jl} + \delta_{il}\delta_{jk} - \frac{2}{3}\delta_{ij}\delta_{kl}\right] \delta(t - t')\delta(\mathbf{r} - \mathbf{r}'),$$

and $\rho_0 = N/L^3$. The temperature equation (7.60) in physical units reads

$$\partial_t \theta + \mathbf{u} \cdot \nabla \theta = \kappa \Delta \theta + \sqrt{\epsilon \alpha} \nabla \cdot \mathbf{q},$$

with

$$\mathbb{E}(q_i(\mathbf{r}, t)\, q_j(\mathbf{r}', t')) = \frac{2\kappa T_0^2}{\rho_0} \delta_{ij} \delta(t - t') \delta(\mathbf{r} - \mathbf{r}').$$

Linearizing those equations close to a uniform temperature and velocity profile yields the linearized Landau-Lifshitz-Navier-Stokes system, historically reported in [147].

7.5. Gradient-flow structure for the Navier–Stokes equation

From the fluctuating hydrodynamics equations derived in the previous sections, one obtains a transverse-gradient-flow structure both for the incompressible and compressible Navier-Stokes equations. These gradient flow structures are natural in the sense that they emerge from the underlying microscopic dynamics [160].

We expect that we can write the incompressible Navier-Stokes equation as following

$$\partial_t \mathbf{u} = -\mathbb{P}(\mathbf{u} \cdot \nabla \mathbf{u}) - \mathrm{Grad}_{\mathbf{u}} K[\mathbf{u}], \tag{7.65}$$

where

$$K[\mathbf{u}] = \frac{1}{2} \int \mathrm{d}\mathbf{r}\, \mathbf{u}^2$$

is the total kinetic energy, $\mathbb{P}$ is the Leray projector on the space of divergence-free vector fields, and $\mathrm{Grad}_{\mathbf{u}}$ is the gradient with respect to a $\mathbf{u}$-dependent norm that has to be determined and that will be linked to the correlation structure of the noise term in the fluctuating incompressible Navier-Stokes equation.

For the compressible Navier-Stokes system, we expect the energy functional for the gradient-flow to be the negative of the total entropy $S[\rho, \mathbf{u}, \theta]$, so that the compressible Navier-Stokes equations can be rewritten as

$$\partial_t \begin{pmatrix} \rho \\ \mathbf{u} \\ \theta \end{pmatrix} = -\mathcal{T} \cdot \begin{pmatrix} \rho \\ \mathbf{u} \\ \theta \end{pmatrix} - \mathrm{Grad}_{\rho, \mathbf{u}, \theta} (-S[\rho, \mathbf{u}, \theta]), \tag{7.66}$$

where $\mathcal{T}$ is a transport operator (or equivalently the compressible Euler operator). The transport terms in both the compressible and incompressible Navier-Stokes equations also satisfy a transversality (orthogonality) condition with the dissipative terms with respect to the L^2 scalar product, granting that the transport terms do not increase nor decrease the quasipotential. The gradient-flow energy functional can be obtained either

from equilibrium thermodynamics, from the quasipotential for the Boltzmann large deviation principle, or from the large deviation structure underlying the fluctuating Navier-Stokes equations. In this section, we use the latter option to obtain (7.65-7.66).

In section 7.5.1, we explain how starting from a small noise SPDE describing the evolution of a macroscopic field, whose underlying microscopic dynamics is time-reversible one can uncover the gradient-flow structure for the noiseless deterministic PDE. In section 7.5.2, we derive the gradient-flow structure for the incompressible Navier-Stokes equations. In section 7.5.3, we obtain the gradient-flow structure for the compressible Navier-Stokes equations.

7.5.1. Generic transverse gradient-flow structure of a SPDE whose large deviations are Gaussian

This section is a reminder of the results of [160] on the relationship between the LDP and gradient-flow structures. Consider a macroscopic field[6] $\phi_\lambda(\mathbf{r},t)$ that takes values in a vector space E, and whose evolution is ruled by a small-noise SPDE:

$$\partial_t \phi_\lambda = -\mathcal{T}[\phi_\lambda] + \mathcal{D}[\phi_\lambda] + \sqrt{2\lambda}\Sigma \cdot \eta[\phi_\lambda], \tag{7.67}$$

such that

$$\mathbb{E}\left(\eta[\phi_\lambda](\mathbf{r},t) \otimes \eta[\phi_\lambda](\mathbf{r}',t')\right) = \mathcal{C}[\phi_\lambda](\mathbf{r},\mathbf{r}')\,\delta(t-t'),$$

where $\eta[\phi_\lambda]$ takes values in another vector field F, Σ is a linear operator from F to E, $\mathcal{C}[\phi_\lambda](\mathbf{r},\mathbf{r}')$ is a linear operator on F. When the SPDE is conservative, Σ would typically be a divergence operator. $\mathcal{T}$ is a linear operator on E that represents a transport term. $\mathcal{D}$ is an operator on E (that is not necessarily linear), it could be a diffusion term. From the Freidlin-Wentzell theory result [115] introduced in section 3.2.2, that we here apply to an infinite-dimensional setting, we know that the probability of the evolution paths of the field ϕ_λ follows a large deviation principle in the small noise regime

$$\mathbb{P}\left(\{\phi_\lambda(t)\}_{0\le t\le T} = \{\phi(t)\}_{0\le t\le T}\right) \underset{\lambda\downarrow 0}{\asymp} e^{-\frac{1}{\lambda}\left\{\int_0^T \mathrm{d}t \sup_{\mathrm{p}}\left[\int \mathrm{d}\mathbf{r}\, p\partial_t\phi - H[\phi,p]\right]\right\}}, \tag{7.68}$$

with a quadratic large deviation Hamiltonian

$$H[\phi,p] = H^{(1)}[\phi,p] + H^{(2)}[\phi,p],$$

$$H^{(1)}[\phi,p] = \int \mathrm{d}\mathbf{r}\, p\left(-\mathcal{T}[\phi] + \mathcal{D}[\phi]\right),$$

and

$$H^{(2)}[\phi,p] = \int \mathrm{d}\mathbf{r}\mathrm{d}\mathbf{r}'\, p(\mathbf{r},t)\,\mathcal{A}[\phi_\lambda](\mathbf{r},\mathbf{r}')\,p(\mathbf{r}',t),$$

[6] A field whose evolution equation has been obtained by the coarse-graining of a certain microscopic dynamics.

where

$$\mathcal{A}\left[\phi_\lambda\right](\mathbf{r},\mathbf{r}') = \Sigma^\top \mathcal{C}\left[\phi_\lambda\right](\mathbf{r},\mathbf{r}')\,\Sigma.$$

This discussion is a reformulation of the one of section 7.1.4, where we adapted the notation for the noise term in order to take into account that the noise coming into play in the fluctuating Navier-Stokes equations can be written as the divergence of a random tensor or vector.

We assume that we know the quasipotential U associated with the LDP (7.68). We also assume that the LDP satisfies a detailed balance condition, such that the relation (3.20) holds with respect to the quasipotential U. As explained in section 3.4, U solves the stationary Hamilton-Jacobi equation

$$H\left[\phi, \frac{\delta U}{\delta \phi}\right] = 0.$$

Under these assumptions, we can then write the relaxation path (the noiseless PDE) associated with (7.67) as a transverse gradient-flow decomposition. Introducing the ϕ-dependent scalar product,

$$\left\langle \varphi, \psi \right\rangle_\phi = \int \mathbf{dr}\mathbf{dr}'\, \varphi(\mathbf{r},t)\, \mathcal{A}\left[\phi\right](\mathbf{r},\mathbf{r}')\, \psi(\mathbf{r}',t)\,, \tag{7.69}$$

the relaxation path associated with (7.67) (the noiseless PDE) can be rewritten

$$\partial_t \phi = -\mathcal{T}\left[\phi\right] + \mathcal{D}\left[\phi\right], \tag{7.70}$$

with

$$\mathcal{D}\left[\phi\right] = -\mathrm{Grad}_\phi U = -\int \mathbf{dr}'\, \mathcal{A}\left[\phi\right](\mathbf{r},\mathbf{r}')\, \frac{\delta U}{\delta \phi(\mathbf{r}',t)},$$

and the transversality condition with respect to the L^2 scalar product

$$\int \mathbf{dr}\, \mathcal{T}\left[\phi\right] \frac{\delta U}{\delta \phi} = 0, \tag{7.71}$$

where U is the quasipotential associated with (7.68). This is the transverse gradient-flow decomposition for the PDE (7.70). More precisely, it decomposes the r.h.s. of the PDE (7.70) as the sum of a transport term, that does not modify the quasipotential U, and a dissipative term, that is the negative of the gradient of the quasipotential with respect to the ϕ-dependent scalar product (7.69). With respect to the L^2 scalar product (7.71), the transport term and the dissipative terms are orthogonal, as a consequence of the Hamilton-Jacobi equation. Such a structure highlights the geometry of the dissipation of the quasipotential U along the trajectories of (7.70)[7]. In particular, if ϕ is a solution of

[7] The trajectories of the noiseless PDE (7.70) are the relaxation paths associated with the dynamics (7.67). The decrease of the quasipotential along those trajectories was then already expected from the property 4. of section 3.4.

the PDE (7.70), we can obtain an estimate for the decrease of the quasipotential involving the ϕ-dependent scalar product (7.69). Indeed, the chain's rule yields

$$\frac{\mathrm{d}}{\mathrm{d}t}U\left[\phi\right] = \int \mathrm{d}\mathbf{r}\, \partial_t \phi \frac{\delta U}{\delta \phi}.$$

Then using that ϕ is a solution of (7.70) and the transversality condition (7.71), we are left with

$$\frac{\mathrm{d}}{\mathrm{d}t}U\left[\phi\right] = \int \mathrm{d}\mathbf{r}\, \mathcal{D}\left[\phi\right] \frac{\delta U}{\delta \phi} = -\int \mathrm{d}\mathbf{r}\mathrm{d}\mathbf{r}'\, \frac{\delta U}{\delta \phi\left(\mathbf{r},t\right)} \mathcal{A}\left[\phi\right]\left(\mathbf{r},\mathbf{r}'\right) \frac{\delta U}{\delta \phi\left(\mathbf{r}',t\right)}.$$

We conclude by noticing the r.h.s. can be expressed with the ϕ-dependent scalar product (7.69) :

$$\frac{\mathrm{d}}{\mathrm{d}t}U\left[\phi\right] = \left\langle \frac{\delta U}{\delta \phi}, \frac{\delta U}{\delta \phi} \right\rangle_{\phi} \leq 0. \tag{7.72}$$

We expect in the compressible case the quasipotential to be the negative of the entropy, and in the incompressible case, the quasipotential should be the kinetic energy. In both cases, ϕ will be the hydrodynamic fields, $\mathcal{T}\left[\phi\right]$ the transport terms in the fluid equations, and $\mathcal{D}\left[\phi\right]$ the diffusive terms. The two next sections are dedicated to bridge from the fluctuating (in)compressible Navier-Stokes equations that are SPDEs with small noises to large deviation principles with quadratic Hamiltonian, from which we can directly deduce a transverse-gradient-flow structure. We will check that the conjectured quasipotentials are the good ones in each case, by verifying that they satisfy the required Hamilton-Jacobi equation (see the discussion of equation (3.14)).

7.5.2. Gradient structure for the incompressible Navier–Stokes equations

We first consider the incompressible Navier–Stokes equation without the temperature equation. This is legitimate, as the velocity equation is not coupled to the temperature equation, neither for the deterministic terms, nor for the noise terms. In this section, we use the set of non-dimensional units adapted to the derivation of the hydrodynamics equation. We start from the equations

$$\partial_t \mathbf{u} + \left(\mathbf{u}\cdot\nabla\right)\mathbf{u} + \nabla P = \nu\Delta\mathbf{u} + \sqrt{\epsilon\alpha}\nabla\cdot\mathbf{J} \text{ and } \nabla\cdot\mathbf{u} = 0,$$

where ν is the kinematic viscosity, and ϵ is the small kinetic parameter, α the Knudsen number, so that $\epsilon\alpha$ is also a small parameter. $\mathbf{J}$ is the fluctuating stress tensor, with Gaussian statistics, and correlation function given in (7.62).

Following the reasoning of section 7.5.1, it is possible to write the quadratic large deviation Hamiltonian associated with a SPDE with Gaussian noise. We apply this general result to the stochastic incompressible Navier-Stokes equation. In order to properly take into account the incompressibility condition, we consider the Leray projector onto

the space of divergence free vector fields, denoted $\mathbb{P}$. We then write the incompressible stochastic Navier–Stokes equations as

$$\partial_t \mathbf{u} + \mathbb{P}\left(\mathbf{u}\cdot\nabla\mathbf{u}\right) = \nu\Delta\mathbf{u} + \sqrt{\epsilon\alpha}\mathbb{P}\nabla\cdot\mathbf{J}. \tag{7.73}$$

The remaining of the implementation of the program of section 7.5.1 is detailed in appendix B.3.1. Briefly, we start by bridging from the small noise SPDE (7.73), to the corresponding Gaussian LDP. Then, we check that the kinetic energy is indeed the quasipotential for this LDP. Finally, we identify the quadratic part of the large deviation Hamiltonian, defining the geometry of the dissipation of the kinetic energy as generically explained in the previous section.

The result of this program is the following transverse gradient-flow decomposition of the incompressible Navier-Stokes equation

$$\partial_t \mathbf{u} = \underbrace{-\mathbb{P}\left(\left(\mathbf{u}\cdot\nabla\right)\mathbf{u}\right)}_{\text{transport}} - \underbrace{\int \mathrm{d}\mathbf{r}'\,\mathcal{A}\left(\mathbf{r},\mathbf{r}'\right)\frac{\delta K}{\delta\mathbf{u}\left(\mathbf{r}',t\right)}}_{\text{gradient of the kinetic energy}}, \tag{7.74}$$

where the quasipotential K is the total kinetic energy

$$K\left[\mathbf{u}\right] = \frac{1}{2}\int \mathrm{d}\mathbf{r}\,\mathbf{u}^2,$$

and the operator $\mathcal{A}$ is

$$\mathcal{A}\left(\mathbf{r},\mathbf{r}'\right) = -\nu\Delta\delta\left(\mathbf{r}-\mathbf{r}'\right).$$

The transversality condition for the transport part of (7.74) reads

$$\int \mathrm{d}\mathbf{r}\left(\frac{\delta K}{\delta\mathbf{u}}\right)\cdot\left(\left(\mathbf{u}\cdot\nabla\right)\mathbf{u}\right) = 0, \tag{7.75}$$

where the dot is the $\mathbb{R}^3$ Euclidean scalar product, which is nothing else than the conservation energy relation for the incompressible Euler (inviscid) equation. The dissipation of the kinetic energy is then best described within the geometry induced by the following scalar product related to the quadratic part of the large deviation Hamiltonian:

$$\left(\mathbf{a},\mathbf{b}\right)_i = \nu\int \mathrm{d}\mathbf{r}\,\left\langle\nabla\mathbb{P}\mathbf{a},\nabla\mathbb{P}\mathbf{b}\right\rangle_i \quad\text{with}\quad \left\langle\mathbf{T},\mathbf{R}\right\rangle_i = \frac{1}{2}\mathrm{Tr}\left(\left(\mathbf{T}+\mathbf{T}^\top\right)\left(\mathbf{R}+\mathbf{R}^\top\right)\right).$$

This scalar product is positive definite on the space of vectors that have non-zero Leray projection. If we note T_{kl} the components of a tensor $\mathbf{T}$, we have

$$\left\langle\mathbf{T},\mathbf{T}\right\rangle_i = 2\sum_{k,l} T_{kl}^2 > 0,$$

unless $\mathbf{T}=0$. As a consequence of the transverse-gradient flow decomposition (7.74-7.75), we obtain the following kinetic energy dissipation inequality

$$\frac{\mathrm{d}}{\mathrm{d}t}K\left[\mathbf{u}\right] = -\left(\mathbf{u},\mathbf{u}\right)_i \leq 0, \tag{7.76}$$

when the velocity field solves (7.74). We note than the scalar product in (7.76) does not depend on the field $\mathbf{u}$ itself, as a consequence of the additive nature of the noise in the fluctuating incompressible Navier-Stokes equation.

7.5.3. Gradient structure for the compressible Navier–Stokes equations

We now check that the entropy is the negative of the quasipotential for the fluctuating compressible Navier–Stokes equations and we look for the associated gradient-flow structure. For the sake of generality, in this section we do not assume the fluid is an ideal nor a monoatomic gas. We still assume that the fluctuating compressible Navier–Stokes equations we derived in section 7.2 hold in this context.

Density, velocity, entropy formulation of the compressible Navier-Stokes equations. To work in this more general context, we consider as independent variables the density, velocity and entropy, and we work in the same set of non-dimensional units as in section 7.2. We start from the equations

$$\partial_t \rho + \nabla \cdot (\rho \mathbf{u}) = 0, \tag{7.77}$$

$$\partial_t \mathbf{u} + \mathbf{u} \cdot \nabla \mathbf{u} = -\frac{\nabla P}{\rho} + \alpha \frac{\nabla \cdot \mathbf{\Pi}}{\rho}, \tag{7.78}$$

$$\rho\theta \left(\partial_t s + \mathbf{u} \cdot \nabla s\right) = \nabla \cdot (\mathbf{u} \cdot \mathbf{\Pi}) - \alpha \nabla \cdot \mathbf{\Xi}, \tag{7.79}$$

where $\mathbf{\Pi}$ is the rank 2 tensor

$$\mathbf{\Pi} = \nu \boldsymbol{\sigma}\left(\mathbf{u}\right) + \zeta \left(\nabla \cdot \mathbf{u}\right) \mathrm{Id} + \sqrt{\epsilon \alpha^2}\mathbf{J},$$

where ν is the shear viscosity, ζ the bulk viscosity[8], and $\mathbf{\Xi}$ the vector

$$\mathbf{\Xi} = -\kappa \nabla \theta + \sqrt{\epsilon \alpha^2}\mathbf{q},$$

and where the fluctuating stress tensor $\mathbf{J}$ and fluctuating heat density flux $\mathbf{q}$ are respectively a Gaussian random rank 2 tensor and a Gaussian random vector with correlations functions

$$\mathbb{E}\left(J_{ij}\left(\mathbf{r}, t\right) J_{kl}\left(\mathbf{r}', t'\right)\right) = 2\nu\theta \left(\delta_{ik}\delta_{jl} + \delta_{il}\delta_{jk} + \left(\gamma - \frac{2}{3}\right)\delta_{ij}\delta_{kl}\right) \delta\left(\mathbf{r} - \mathbf{r}'\right) \delta\left(t - t'\right), \tag{7.80}$$

$$\mathbb{E}\left(q_i\left(\mathbf{r}, t\right) q_j\left(\mathbf{r}', t'\right)\right) = 2\kappa\theta^2 \delta_{ij} \delta(t - t') \delta(\mathbf{r} - \mathbf{r}'), \tag{7.81}$$

[8] For a monoatomic gas, the bulk viscosity is zero $\zeta = 0$. However, the gradient-flow structure of the compressible Navier-Stokes system applies in a more general framework than the one we used to derive it from the Boltzmann equation. For the sake of generality, we keep the contribution of ζ in the stress tensor.

with $\gamma = \zeta/\nu$ and $\mathbb{E}\left(\mathbf{J} \otimes \mathbf{q}\right) = 0$. We also note that the entropy s per unit mass, energy ϵ per unit mass, enthalpy w per unit mass, pressure P and density ρ are related through the thermodynamic relations $\mathrm{d}\epsilon = \theta \mathrm{d}s + P\mathrm{d}\rho/\rho^2$, $\omega = \epsilon + P/\rho$ and $\mathrm{d}\omega = \mathrm{d}P/\rho$. As an example, for a perfect gas, we have $s = -\log\left(P/\theta^{3/2}\right) + \mathrm{Cst}$, $\epsilon = 3\theta/2$, $w = 5\theta/2$, and $P = \rho\theta$. With the perfect gas assumption and a vanishing bulk viscosity $\zeta = 0$, the equations (7.77-7.79) can be recast into (7.45-7.47). We now discuss the physical insights gained from this formulation of the fluctuating compressible Navier-Stokes system.

In order to first discuss the conservation laws, we write the hydrodynamic equations (7.78-7.79) in their conservative form. We have

$$\partial_t \left(\rho \mathbf{u}\right) + \nabla \cdot \left(\rho \mathbf{u} \otimes \mathbf{u}\right) = \nabla \cdot \left(-P + \alpha \mathbf{\Pi}\right),$$

and

$$\partial_t \left(\frac{1}{2}\rho u^2 + \rho\epsilon\right) + \nabla . \left[\rho \mathbf{u} \left(\frac{1}{2}\rho u^2 + \rho w\right)\right] = \alpha \nabla \cdot \left(\mathbf{u} \cdot \mathbf{\Pi} - \mathbf{\Xi}\right).$$

These equations show that the fluctuating stress $\mathbf{J}$ and heat density flux $\mathbf{q}$ act on the fluxes but do not break the structure of the local conservation laws. As a consequence, mass, momentum and energy are local and global conservation laws, as should be expected.

We now apply the result of the discussion of section 7.5.1 to the fluctuating compressible Navier–Stokes equations (7.77-7.79). The momenta conjugated to the fields ρ, $\mathbf{u}$ and s are denoted p_ρ, $\mathbf{p_u}$, and p_s respectively. The detailed computations can be found in appendix B.3.2.

The result reads

$$\partial_t \begin{pmatrix} \rho \\ \mathbf{u} \\ s \end{pmatrix} = \underbrace{\begin{pmatrix} -\nabla \cdot (\rho \mathbf{u}) \\ -\mathbf{u} \cdot \nabla \mathbf{u} - \frac{\nabla P}{\rho} \\ \mathbf{u} \cdot \nabla s \end{pmatrix}}_{\text{transport terms}} - \underbrace{B_{(\rho,\mathbf{u},s)} \left[-\frac{\delta S}{\delta \rho}, -\frac{\delta S}{\delta \mathbf{u}}, -\frac{\delta S}{\delta s}\right]}_{\text{gradient of the negentropy}},$$

where

$$B_{(\rho,\mathbf{u},s)}\left[p_\rho, \mathbf{p_u}, p_s\right] = \alpha \left(0, B^{p_\mathbf{u}}_{(\rho,\mathbf{u},s)}\left[p_\rho, \mathbf{p_u}, p_s\right], B^{p_s}_{(\rho,\mathbf{u},s)}\left[p_\rho, \mathbf{p_u}, p_s\right]\right),$$

with

$$B^{p_\mathbf{u}}_{(\rho,\mathbf{u},s)}\left[p_\rho, \mathbf{p_u}, p_s\right] = -\frac{1}{\rho}\nabla . \left\{\nu\theta\left[\nabla\left(\frac{\mathbf{p_u}}{\rho}\right) + \left(\nabla\left(\frac{\mathbf{p_u}}{\rho}\right)\right)^\top\right] + \frac{\eta\nu p}{\rho}\left[\nabla\mathbf{u} + (\nabla\mathbf{u})^\top\right]\right\} + \frac{1}{\rho}\nabla\left\{\left(\zeta - \frac{2}{3}\nu\right)\left[-\theta\nabla . \left(\frac{\mathbf{p_u}}{\rho}\right) + \frac{p_s}{\rho}\nabla.\mathbf{u}\right]\right\},$$

and

$$B^{p_s}_{(\rho,\mathbf{u},s)}\left[p_\rho, \mathbf{p_u}, p_s\right] = -\frac{\nu}{\rho}. \left\{\nabla\mathbf{u}. \left[\nabla\left(\frac{\mathbf{p_u}}{\rho}\right) + \left(\nabla\left(\frac{\mathbf{p_u}}{\rho}\right)\right)^\top\right]\right\} + \frac{\nu p_s}{\rho^2\theta}\nabla\mathbf{u}. \left[\nabla\mathbf{u} + (\nabla\mathbf{u})^\top\right] - \frac{1}{\rho}\left(\zeta - \frac{2}{3}\nu\right)\nabla . \left(\frac{\mathbf{p_u}}{\rho}\right)\nabla.\mathbf{u} + \frac{p_s}{\rho^2\theta}\left(\zeta - \frac{2}{3}\nu\right)(\nabla.\mathbf{u})^2 - \nabla . \left[\kappa\theta^2\nabla\left(\frac{p_s}{\rho\theta}\right)\right],$$

and where the quasipotential is the negative of the total entropy up to conservation laws[9]

$$-U = \begin{cases} S = \int \mathrm{d}\mathbf{r}\, \rho s \ \text{ if } \ \int \mathrm{d}\mathbf{r}\, \rho = M \ \text{ and } \ \int \mathrm{d}\mathbf{r}\, \left(\frac{1}{2}\mathbf{u}^2 + \frac{3}{2}\theta\right) = E, \\ -\infty \ \text{ otherwise.} \end{cases}.$$

The transversality condition reads

$$\int \mathrm{d}\mathbf{r} \begin{pmatrix} -\nabla\cdot(\rho\mathbf{u}) \\ -\mathbf{u}\cdot\nabla\mathbf{u} - \frac{\nabla P}{\rho} \\ \mathbf{u}\cdot\nabla s \end{pmatrix} \cdot \begin{pmatrix} -\frac{\delta S}{\delta \rho} \\ -\frac{\delta S}{\delta \mathbf{u}} \\ -\frac{\delta S}{\delta s} \end{pmatrix} = 0.$$

This time, the norm defined by the dissipative operator $B_{(\rho,\mathbf{u},s)}$ depends on the hydrodynamical fields, as a consequence of the multiplicativity of the noise term in the fluctuating compressible Navier-Stokes equations.

7.6. Conclusion

In this chapter, we derived the fluctuating incompressible and compressible Navier-Stokes equations starting from the large deviation principle associated with the Boltzmann equation. Within the incompressible scaling, we retrieve the fluctuating incompressible Navier-Stokes equations with additive noise that is usually found in the literature. Within the compressible scaling, we derive the fluctuating compressible Navier-Stokes equations with a multiplicative noise that acts on the equations for the velocity and the temperature. In both cases, it is to our knowledge the first derivation of noise terms from the microscopic dynamics for the fluctuating Navier-Stokes equations that does not rely on linearization of the equations nor fluctuation-dissipation relations. The computation is done at the level of the SPDEs using a noisy Chapman-Enskog expansion but the result should be interpreted as the underlying quadratic (Gaussian) large deviation principle for the empirical hydrodynamical fields. In particular, when looking at typical realization of the noise in the fluctuating hydrodynamics, it might be negligible compared to the terms of higher order in α that could enter the Chapman-Enskog expansion (the so-called Burnett terms [61]). This structure allows to obtain a tranverse gradient-flow decomposition for the Navier-Stokes equations. This structure naturally illustrates the geometry of the kinetic energy dissipation in the incompressible case, and of the entropy creation in the compressible case. It should be noted that all these derivations were made using small α (Knudsen number) expansions. Some of the arguments may break down in the presence of shocks (gradient of the hydrodynamic fields may become of order $1/\alpha$). Such singularities are ubiquitous for hyperbolic conservation laws PDEs. In chapter 9, studying a simpler particle system whose hydrodynamic limit is a 1D conservation law, we explain that the fluctuating hydrodynamics we obtain using the techniques presented in this manuscript may not be adequate to compute the probability of non-entropic shocks.

[9] One should also account for momentum conservation, depending on the boundary conditions.

8. Fluctuating hydrodynamics for dilute active gases

This chapter is adapted from [105]. It deals with the derivation of a kinetic large deviation principle and the corresponding fluctuating hydrodynamics for a system of active particles where particles interact through binary collisions. The result is a set of SPDEs (8.25, 8.27, 8.28), that describe the evolution of the density and orientation fields of the particles, with a noise term in the orientation equation accounting for finite N fluctuations, that is derived from the microscopic dynamics. The novelty of this chapter, compared to the derivation of fluctuating hydrodynamics led in chapter 6 and 7, is that the microscopic dynamics only conserves the total number of particles. To obtain an equation for the orientation field despite the lack of conservation laws, we use the notion of Generalized Collision Invariant (GCI), first introduced in [87].

8.1. Introduction: hydrodynamical theories for active matter

Active systems are composed of units able to extract non-thermal energy from the environment and dissipate it to self-propel [152]. Examples span a broad range of scales, from bacteria to animals in the biological world, and significant effort has been devoted recently to build synthetic active systems in the laboratory using self-propelled granular particles [90], Janus particles [173] or Quincke rollers [60] to name just a few examples. Active systems break detailed balance microscopically, as opposed to more classical non-equilibrium systems where detailed balance is broken by boundary driving. As such, they are capable of novel collective behaviours that are impossible in equilibrium systems, whose characterization and control attracted a significant attention recently [152]. When the dominant interaction among particles is to align their direction of motion, which can be caused by collision when particles have anisotropic shape, or by reaction to sensing, a well-known collective behavior of active systems emerges: flocking. This is a ferromagnetic-like state where all particles move in average along a given direction; broken detailed balance allows for long range order even in two-dimensions and a scale-free structure giving rise to long-range correlations without the need of fine-tuning to criticality [209, 198].

One of the main tools used to investigate the collective behavior of active systems are fluctuating hydrodynamic theories. These theories can be derived via two complementary paths. On one hand, they can be written on the basis of symmetry arguments [152, 200, 67]; this approach is particularly useful for studying active systems,

given that their complexity often does not allow to build first-principle models even at the microscopic level; it had great success to unveil new generic and universal (i.e. qualitative and quantitative properties independent of system details) physics induced by activity. It has two shortcomings though: first, symmetries do not allow to relate microscopic parameters to those entering in the fluctuating hydrodynamics. Second, in active systems the noise term is not constrained by the fluctuation-dissipation theorem, and it is unclear how to specify it a-priori, except when dealing with critical systems (cases in which Renormalization Group arguments allow to discard irrelevant nonlinearities). It should be noted that this feature is at variance not only with equilibrium systems, but also with non-equilibrium ones weakly driven by the boundaries; in these, at least for weak coupling, the noise term is constrained by linear response theory [32]. Hence, this makes the approach to fluctuating hydrodynamics we adopt in this dissertation extremely relevant to active systems. There is something to learn from linking the microscopic and macroscopic descriptions of active systems even if the starting point are phenomenological particle models often chosen only on the basis of simplicity. Several works in the literature have been indeed focused on this program [31, 30, 87, 71].

Kinetic and hydrodynamic theories have been widely employed for describing systems of self-propelled particles interacting via alignment. This route has indeed been followed both within the weak-interactions limit [87] and within the Boltzmann-like framework of dilute systems [31, 30, 71]. The Dean-Kawasaki approach has been widely employed to derive the fluctuating kinetic theory and fluctuating hydrodynamics of microscopic active matter models. This is justified when interactions are long-ranged, as it happens for dilute microswimmer suspensions in which the primary source of interactions are low-Reynolds fluid flows created by the motion of the swimmers [181, 194, 190]. Yet, the fact that hydrodynamics noise is independent of interactions within the Dean approach motivated some authors to use it even for short-ranged aligning particles [29], even if these systems are clearly out of the regime of applicability of the method. For dilute systems, indeed, although particle diffusion will give rise to a Dean-like noise, one can expect another contribution from particle-particle collisions.

In this chapter, we describe how to derive the fluctuating kinetic theory and the corresponding fluctuating hydrodynamics of active particles that interact by aligning after undergoing binary collisions. The fluctuating kinetic theory is obtained in the dilute limit, analogous to the Boltzmann-Grad limit of perfect gases. This leads to a noise term at kinetic level that is not Gaussian. We then derive the corresponding fluctuating hydrodynamics. This result extends to the dilute limit, both at the deterministic and fluctuating levels, previous results that have been obtained in the weak-interactions limit [87], and it is valid when the Knudsen number is small. We also quickly explain how to extend to the fluctuating level the hydrodynamical limit obtained in [31, 30] in the limit as the distance to the order-disorder phase transition goes to zero. Interestingly, the noise entering at the fluctuating level is Gaussian, and we explicitly compute its variance. The latter turns out to be proportional to the square of the density field and to depend explicitly on the interactions among particles; both these facts differentiate our conclusion from the results obtained in the Dean-Kawasaki approach, where the noise variance is linear in the density and independent from particle-particle interactions [29].

The chapter is organized as follows. In section 8.2 we specify the particle-based model we consider and, under an extended molecular chaos type hypothesis, derive its kinetic theory and the associated fluctuating kinetic theory, described as a kinetic LDP. The large deviation Hamiltonian we obtain is not quadratic, which corresponds to a fluctuating kinetic theory with a non Gaussian noise. In section 8.3, we start from the fluctuating kinetic theory to derive fluctuating hydrodynamic equations at leading order in the Knudsen number α. In particular, we show that in this limit $\alpha \to 0$, the noise becomes Gaussian.

8.2. Definition of the particle-based model, kinetic theory and dynamical large deviations

We start by introducing the particle-based model we consider, that we term the Boltzmann–Vicsek particle model, in section 8.2.1; in section 8.2.2 we describe its well-known kinetic description at the deterministic level (known as Boltzmann–Vicsek equation). We then introduce a suited non-dimensional system of units that allows to investigate fluctuations at the kinetic level in section 8.2.3. Adapting the arguments of [50], we derive in section 8.2.4 the fluctuating kinetic theory associated with the particle-based model as a large deviation principle.

8.2.1. Boltzmann-Vicsek particle model

We consider N particles evolving in a periodic two-dimensional box of size $L \times L$. We denote $(\mathbf{r}_i, \theta_i)_{1\leq i\leq N}$ their positions and orientations according to some arbitrary axis. The dynamics is the one first introduced in [31]. Particles move ballistically with constant speed v_0: $\mathrm{d}\mathbf{r}_i/\mathrm{d}t = v_0(\cos\theta_i, \sin\theta_i)$, until they collide. When two particles i and j are close enough (i.e. $|\mathbf{r}_i - \mathbf{r}_j| \leq 2R$, R being the interaction radius) a collision occurs with a rate $(v_0/R)K(\theta_i - \theta_j)$ where K is a cross-section chosen to mimic hard-sphere collisions. This rate is furthermore chosen so that when two particles meet, they have a probability to interact of order 1. When a collision occurs, particles update their orientation according to the following rule

$$\theta_i^{\text{out}} = \bar{\theta} + \zeta_i, \quad \theta_j^{\text{out}} = \bar{\theta} + \zeta_j,$$

where $\bar{\theta} = \arg\left(\mathrm{e}^{i\theta_i^{\text{in}}} + \mathrm{e}^{i\theta_j^{\text{in}}}\right)$ and the superscript "in" (resp. "out") denotes incoming (resp. outcoming) orientations. ζ_i and ζ_j are independent random variables distributed according to $P_\sigma(\theta)$ over $[-\pi, \pi)$ with variance σ^2. At low variance of the noise, this interaction favors the polar alignment of particles.

It should be observed that in the model, at variance with the standard Vicsek model that is often considered in computational works [209, 70], only binary collisions are considered. The collision process is schematically presented in figure 8.1. In the following, this model is called the Boltzmann-Vicsek particle model.

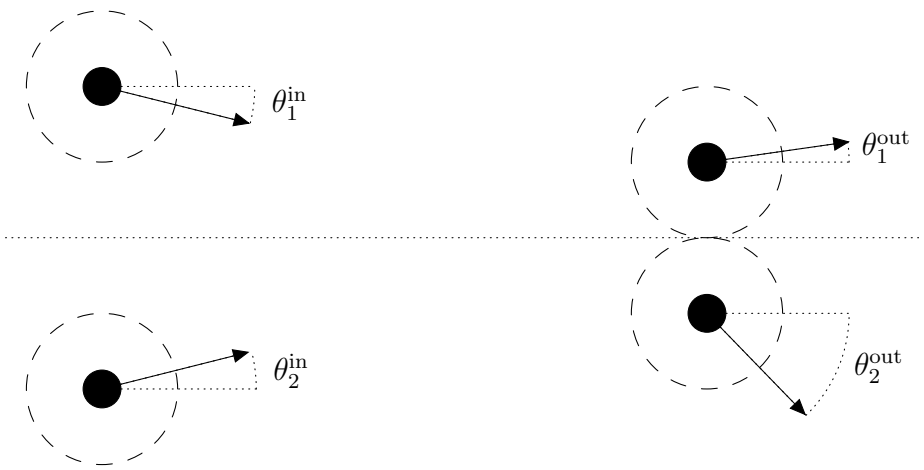


Figure 8.1.: Schematic representation of a collision event. In this specific case, $\bar{\theta} = \arg\left(\mathrm{e}^{i\theta_1^{\text{in}}} + \mathrm{e}^{i\theta_2^{\text{in}}}\right) = 0$ with respect to the dotted axis, $\zeta_1 = \theta_1^{\text{out}}$, and $\zeta_2 = \theta_2^{\text{out}}$.

8.2.2. Boltzmann-Vicsek equation

The deterministic kinetic description associated with the Boltzmann–Vicsek particle model was derived in [31] and reads

$$\partial_t f_e(\mathbf{r},\theta,t) + v_0 \mathbf{e}_\theta \cdot \nabla f_e(\mathbf{r},\theta,t) = v_0 R \mathcal{I}_{\text{col}}[f_e](\mathbf{r},\theta,t) \tag{8.1}$$

where $f_e(\mathbf{r},\theta,t)$ is the one-particle distribution function in the phase-space (representing the number of particles at a position $\mathbf{r}$, with orientation θ at a certain time t) normalized such that $\int \mathrm{d}\mathbf{r}\mathrm{d}\theta\, f_e = N$. In (8.1) the collision term is given by

$$\mathcal{I}_{\text{col}}[f_e](\mathbf{r},\theta,t) = \iint \mathrm{d}\theta_1 \mathrm{d}\theta_2\, f_e(\mathbf{r},\theta_1,t) f_e(\mathbf{r},\theta_2,t) K(\theta_2 - \theta_1) \left\{ P_\sigma(\theta - \Psi(\theta_1,\theta_2)) - \delta(\theta - \theta_1) \right\}, \tag{8.2}$$

where $K(\theta_2 - \theta_1) = 2\left|\sin\left(\frac{\theta_2-\theta_1}{2}\right)\right|$ is the scattering cross-section, and $\Psi(\theta_1,\theta_2) = \arg\left(e^{i\theta_1} + e^{i\theta_2}\right)$ is the average of the orientations (θ_1,θ_2).

The Boltzmann–Vicsek equation (8.1) relies on the molecular chaos hypothesis and it is expected to be a valid description of the particle system in the limit of a large number of particles in the Boltzmann-Grad limit, as is made explicit in the next section. Quantitative arguments in favor of the validity of the molecular chaos hypothesis for a locally mean-field Vicsek-like particle model can be found in [75, 132], when the mean free path is much larger than the interaction radius.

8.2.3. The rescaled Boltzmann–Vicsek equation

We introduce a set of units that are suited to investigate the kinetic limit: space is measured in units of the mean free path $\ell = 1/(R\rho_0)$, where $\rho_0 = N/L^2$ is the mean

density, and time in units of ℓ/v_0, which is the average time between two collisions. We also define $\epsilon = (\rho_0 \ell^2)^{-1}$, the inverse of the number of particles in a region of surface ℓ^2. By performing a space-time rescaling $\mathbf{r}' = \mathbf{r}/\ell$, $t' = tv_0/\ell$ and by rescaling the distribution function $f(\mathbf{r}', \theta, t') = \epsilon f_e(\mathbf{r}', \theta, t')$ (primes are dropped afterwards), the Boltzmann–Vicsek equation reads

$$\partial_t f + \mathbf{e}_\theta \cdot \nabla f = \mathcal{I}_{\text{col}}[f]. \tag{8.3}$$

As we shall see below, the Boltzmann–Vicsek equation is a valid description of the microscopic model in the limit $N \to +\infty$, $\epsilon \to 0$ (and under the molecular chaos hypothesis). It should be noticed that $\epsilon = R/\ell = NR^2/L^2$, meaning that the limit yielding a Boltzmann-type kinetic description is opposite to a weak-interaction limit for which the number of particles in an interaction radius goes to infinity.

In the next section, we go beyond this law of large numbers, taking into account fluctuations by determining the LDP for the empirical measure.

8.2.4. Large deviations from the Boltzmann–Vicsek equation

We now aim at deriving the fluctuating kinetic theory associated with the microscopic model introduced in section 8.2.1, along the same lines as in 3.7.2 where we derived the LDP for N independent Run-and-Tumbling particles. We expect a LDP for the rescaled empirical measure

$$f_\epsilon(\mathbf{r}, \theta, t) = \epsilon \sum_{n=1}^{N} \delta(\mathbf{r}_n(t) - \mathbf{r}) \, \delta(\theta_n(t) - \theta), \tag{8.4}$$

in the form

$$\mathbb{P}\left[\{f_\epsilon(t)\}_{0 \le t < T} = \{f(t)\}_{0 \le t < T}\right] \underset{\epsilon \downarrow 0}{\asymp} \exp\left(-\frac{1}{\epsilon} J_T[f]\right), \tag{8.5}$$

where

$$J_T[f] = \int_0^T \mathrm{d}t \sup_p \left(\int \mathbf{r}\mathrm{d}\theta \, \partial_t f p - H_{BV}[f, p] \right), \tag{8.6}$$

$$H_{BV}[f, p] = \lim_{\epsilon \downarrow 0} \epsilon G_f \left[\mathrm{e}^{\frac{1}{\epsilon} \int \mathbf{r}\mathrm{d}\theta \, p f_\epsilon} \right] \mathrm{e}^{-\frac{1}{\epsilon} \int \mathbf{r}\mathrm{d}\theta \, p f}, \tag{8.7}$$

and where G_f the infinitesimal generator of the stochastic process for the empirical measure of N particles whose dynamics is the one described in section 8.2.1. In (8.5) and in every other equivalences that involve $\epsilon \to 0$, we also implicitly take the $N \to +\infty$ limit.

We start from the definition of the infinitesimal generator (3.24) and apply it to compute the infinitesimal generator of the stochastic process for the empirical measure. This time, the expectation $\mathbb{E}_f$ denotes an expectation over the stochastic process of the

rescaled empirical measure f_ϵ of N particles submitted to the Boltzmann–Vicsek dynamics conditioned by $f_\epsilon(t=0)=f$. We can decompose the infinitesimal generator in two terms

$$G_f = G_{f,\mathcal{T}} + G_{f,\mathrm{col}},$$

where $G_{f,\mathcal{T}}$ is the infinitesimal generator accounting for free transport, already computed in (3.54), and $G_{f,\mathrm{col}}$ accounts for two-body collisions. To evaluate $G_{f,\mathrm{col}}$, we need the rate of two-body collisions, which change the orientation of two particles from (θ_1,θ_2) to (θ_1',θ_2') in the volume element $\mathrm{d}\mathbf{r}$ centered at point $\mathbf{r}$. If f is the rescaled empirical measure, this rate reads

$$\frac{1}{2\epsilon}K(\theta_2-\theta_1)f(\mathbf{r},\theta_1,t)f(\mathbf{r},\theta_2,t)P_\sigma\left(\theta_1'-\Psi(\theta_1,\theta_2)\right)P_\sigma\left(\theta_2'-\Psi(\theta_1,\theta_2)\right)\mathrm{d}\theta_1\mathrm{d}\theta_2\mathrm{d}\theta_1'\mathrm{d}\theta_2'\mathrm{d}\mathbf{r}. \tag{8.8}$$

As we did to justify the Boltzmann–Vicsek equation (8.1), we assumed the molecular chaos hypothesis to express the rate (8.8) as a function of the one-particle distribution function only. As for tumbling events, collisions change the empirical measure; $f(\mathbf{r},\theta)$ is changed into

$$\begin{aligned} f(\mathbf{r},\theta) - \epsilon\delta(\mathbf{r}-\mathbf{r}_1)\delta(\theta-\theta_1) - \epsilon\delta(\mathbf{r}-\mathbf{r}_1)\delta(\theta-\theta_2) \\ + \epsilon\delta(\mathbf{r}-\mathbf{r}_1)\delta(\theta-\theta_1') + \epsilon\delta(\mathbf{r}-\mathbf{r}_1)\delta(\theta-\theta_2'). \end{aligned} \tag{8.9}$$

The infinitesimal generator term accounting for collisions thus reads

$$\begin{aligned} G_{f,\mathrm{col}}[\phi] = \frac{1}{2\epsilon}\int \mathrm{d}\theta_1\mathrm{d}\theta_2\mathrm{d}\theta_1'\mathrm{d}\theta_2'\mathrm{d}\mathbf{r}\; K(\theta_2-\theta_1) \\ \times f(\mathbf{r},\theta_1,t)f(\mathbf{r},\theta_2,t)P_\sigma\left(\theta_1'-\Psi(\theta_1,\theta_2)\right)P_\sigma\left(\theta_2'-\Psi(\theta_1,\theta_2)\right)\left(\phi[\tilde{f}]-\phi[f]\right). \end{aligned} \tag{8.10}$$

where $\tilde{f}(\mathbf{r}_0,\theta,t) = f(\mathbf{r}_0,\theta,t)+\epsilon\delta(\mathbf{r}_0-\mathbf{r})\left(-\delta(\theta-\theta_1)-\delta(\theta-\theta_2)+\delta(\theta-\theta_1')+\delta(\theta-\theta_2')\right)$. The large deviation Hamiltonian is deduced using (8.7)

$$H_{BV}[f,p] = H_{\mathcal{T}}[f,p] + H_{\mathrm{col}}[f,p], \tag{8.11}$$

where $H_{\mathcal{T}}$ is given by

$$H_{\mathcal{T}}[f,p] = -\int \mathrm{d}\mathbf{r}\mathrm{d}\theta\, p(\mathbf{r},\theta,t)\mathbf{e}_\theta\cdot\nabla f(\mathbf{r},\theta,t), \tag{8.12}$$

and the collision term of the Hamiltonian reads

$$\begin{aligned} H_{\mathrm{col}}[f,p] = \frac{1}{2}\int \mathrm{d}\theta_1\mathrm{d}\theta_2\mathrm{d}\theta_1'\mathrm{d}\theta_2'\mathrm{d}\mathbf{r}\; K(\theta_2-\theta_1)f(\mathbf{r},\theta_1,t)f(\mathbf{r},\theta_2,t)\times \\ P_\sigma\left(\theta_1'-\Psi(\theta_1,\theta_2)\right)P_\sigma\left(\theta_2'-\Psi(\theta_1,\theta_2)\right)\left\{e^{-p(\mathbf{r},\theta_1,t)-p(\mathbf{r},\theta_2,t)+p(\mathbf{r},\theta_1',t)+p(\mathbf{r},\theta_2',t)}-1\right\}. \end{aligned} \tag{8.13}$$

Equation (8.11) along with (8.12,8.13) is the fluctuating kinetic theory for the Boltzmann-Vicsek model. The most probable evolution path satisfies the deterministic evolution equation given by the Hamilton equation associated with H_{BV}

$$\partial_t f(\mathbf{r},\theta,t) = \frac{\delta H_{BV}}{\delta p(\mathbf{r},\theta,t)}[f,0] \; = -\mathbf{e}_\theta \cdot \nabla f(\mathbf{r},\theta,t) + \mathcal{I}_{\text{col}}[f](\mathbf{r},\theta,t) \tag{8.14}$$

which is the *deterministic* Boltzmann–Vicsek equation (8.3).

Just as in the Run-and-Tumble case, collisions conserve locally the number of particles, and this is reflected in the fact that $\int \mathbf{r}\mathrm{d}\theta\, \delta H_{\text{col}}/\delta p(\mathbf{r},\theta) = 0$. Furthermore, H_{BV} is again non-quadratic in the conjugated momentum p. This means that dynamical large deviations of the empirical measure are non-Gaussian. Contrary to the tumbling Hamiltonian (3.57), the Hamiltonian for collisions is quadratic in f, because collisions considered in the Boltzmann–Vicsek dynamics are binary. The Hamiltonian H_{BV} share some similarities with the one derived in [50] for the Boltzmann equation describing the dynamics of a passive dilute gas: quadraticity in the distribution function f and exponential dependence on the conjugated momentum. At variance with that case, however, the collision rules of the Vicsek-Boltzmann model break time-reversal symmetry, and does not conserve momentum nor kinetic energy.

8.3. Fluctuating hydrodynamics in the ordered phase

In this section, we derive the fluctuating hydrodynamics from the Boltzmann–Vicsek LDP given by (8.5) and (8.11). This is done as a Chapman-Enskog expansion of the fluctuating kinetic equation, i.e. a perturbative expansion in a small parameter, the Knudsen number $\alpha = \ell/L$, where ℓ is the mean free path and L is the system size. α is also the time scale to reach a local equilibrium[1]. As a first step, we introduce in section 8.3.1 the macroscopic scaling with the Knudsen number, and associate a fluctuating Boltzmann–Vicsek equation with the Boltzmann–Vicsek LDP. From there we adapt to the fluctuating case the framework developed in a deterministic setting in [87]. In section 8.3.2 we discuss the local equilibria of the Boltzmann–Vicsek equation. These local equilibria are characterized by two slow modes: the density field, and the orientational order field. Then, in section 8.3.3 we obtain fluctuating hydrodynamic equations for these two slow modes. Further, we show that at leading order in the Knudsen number α, the noise appearing in these hydrodynamic equations is Gaussian. In section 8.3.4, we connect our result with the Toner-Tu equations, widely used in the active matter community to describe large scale behavior of aligning active systems.

[1] This derivation can also without any supplementary efforts lead at the level of the large deviation functional.

8.3.1. Macroscopic scaling and rephrasing of the Large Deviation Principle as a Stochastic PDE

Since we are interested in large scales and long times, we introduce the macroscopic variables $\tilde{t} = \alpha t, \tilde{\mathbf{r}} = \alpha \mathbf{r}$, and define $\tilde{f}(\tilde{\mathbf{r}}, \theta, \tilde{t}) = f(\alpha^{-1}\tilde{\mathbf{r}}, \theta, \alpha^{-1}\tilde{t})$, $\tilde{p}(\tilde{\mathbf{r}}, \theta) = p(\alpha^{-1}\tilde{\mathbf{r}}, \theta)$. Then

$$H_{\mathcal{T}}[f,p] = \frac{1}{\alpha}\tilde{H}_{\mathcal{T}}[\tilde{f},\tilde{p}] \tag{8.15}$$

$$H_{\mathrm{col}}[f,p] = \alpha^{-2}\tilde{H}_{\mathrm{col}}[\tilde{f},\tilde{p}], \int \mathbf{dr}\mathrm{d}\theta\, p\partial_t f = \frac{1}{\alpha}\int \mathrm{d}\tilde{\mathbf{r}}\mathrm{d}\theta\, \tilde{p}\partial_{\tilde{t}}\tilde{f}; \tag{8.16}$$

we remove the tildes in the following. Isolating the linear part in p (which contributes to the deterministic evolution), the collision Hamiltonian can be written

$$H_{\mathrm{col}}[f,p] = \int \mathbf{dr}\mathrm{d}\theta\, p(\mathbf{r},\theta)\mathcal{I}_{\mathrm{col}}[f](\mathbf{r},\theta) + H_{\mathrm{col,stoch}},$$

where $H_{\mathrm{col,stoch}}$ gathers all terms of order at least 2 in p. The empirical measure then satisfies a large deviation principle with speed ϵ^{-1} and rate function

$$J_T[f] = \frac{1}{\alpha^3}\int_0^T \mathrm{d}t \sup_p \left\{ \int \mathbf{dr}\mathrm{d}\theta\, p(\mathbf{r},\theta)\big(\alpha\partial_t f + \alpha e_\theta\cdot\nabla f - \mathcal{I}_{\mathrm{col}}[f]\big) - H_{\mathrm{col,stoch}}[f,p]\right\}. \tag{8.17}$$

Notice the overall factor α^{-3} coming from the change of time and space variables; the final time T and the system size have also been rescaled. Formally, this LDP can be recast as a stochastic PDE:

$$\alpha\big(\partial_t f + e_\theta\cdot\nabla f\big) - \mathcal{I}_{\mathrm{col}}[f] = \xi(\mathbf{r},\theta,t), \tag{8.18}$$

where the left hand side is the deterministic Boltzmann-Vicsek equation, and the right hand side is a noise whose distribution satisfies the LDP

$$\mathbb{P}\left[\{\xi(t)\}_{0\le t<T} = \{u(t)\}_{0\le t<T}\right] \underset{\epsilon\downarrow 0}{\asymp} \exp\left(-\frac{1}{\epsilon\alpha^3}J_f[u]\right), \tag{8.19}$$

with

$$J_f[u] = \int_0^T \mathrm{d}t \sup_p \left(\int \mathbf{dr}\mathrm{d}\theta\, pu - H_{\mathrm{col,stoch}}[f,p]\right). \tag{8.20}$$

A consequence of (8.19) is that we can express the variance of ξ through the large deviation Hamiltonian

$$\mathbb{E}\left[\xi\left[f\right](\mathbf{r},\theta,t)\,\xi\left[f\right](\mathbf{r}',\theta',t')\right] = \epsilon\alpha^3\frac{\delta^2 H_{BV}}{\delta p(\mathbf{r},\theta,t)\delta p(\mathbf{r}',\theta',t')}\left[f,p=0\right]. \tag{8.21}$$

Note that only $H_{\mathrm{col,stoch}}$ contributes to the second functional derivative of H_{BV} with respect to p. From the original LDP, which is a statement on the probability distribution

of f, to the above statement about the probability distribution of ξ, there is a change of variable, which should introduce a Jacobian factor. At the large deviations level however, this factor is negligible. We stress that the noise ξ bears several features that are in stark contrast with the fluctuating kinetic theories derived in the weak-interaction limit [86, 32]: it is multiplicative at the kinetic level (since its distribution depends on f), it is non-Gaussian (this is encoded in the fact that H_{BV} is not quadratic in p), and it depends explicitly on the particle-particle interactions.

Finally, the local conservation of the number of particles implies that whenever $\int \mathrm{d}\theta\, u\left(\mathbf{r},\theta\right) \neq 0$, $J_f[u] = +\infty$. Indeed, take any momentum field $p(\mathbf{r})$ independent of θ; then $H_{\mathrm{col,stoch}}[f,p] = 0$ and $\int \mathrm{d}\theta\, u(\mathbf{r},\theta)p(\mathbf{r}) = p(\mathbf{r}) \int \mathrm{d}\theta\, u \neq 0$. A good choice of $p(\mathbf{r})$ then makes the supremum in (8.20) as large as we wish. In the stochastic PDE (8.18), this translates in the fact that the noise conserves the number of particles:

$$\int \mathrm{d}\theta\, \xi(\mathbf{r},\theta,t) = 0. \tag{8.22}$$

Contrary to the case of passive dilute gases (where also momentum and energy are conserved), there is no other conservation law, reflecting the absence of these conservation laws at the level of the microscopic collisions.

8.3.2. Local equilibria

We now discuss the local equilibria of the Boltzmann-Vicsek equation, i.e. distributions f that make the collision kernel vanish $\mathcal{I}_{\mathrm{col}}[f] = 0$. This is the crucial ingredient to derive the fluctuating hydrodynamics deeply in the ordered state because any initial condition should relax fastly (over time scales of order α^{-1}) towards these local equilibria.

For clarity, we choose the noise distribution P_σ in the collision kernel (8.2) to be a Von Mises distribution $P_\sigma\left(\theta\right) = V_s(\theta) = \left(2\pi I_0\left(s\right)\right)^{-1} \exp\left(s\cos\theta\right)$, but any other choice for P_σ with similar qualitative characteristics would be admissible. This distribution has a circular variance $\sigma^2\left(s\right) = 1 - I_1(s)/I_0(s)$, where I_j is the modified Bessel function of order j. The variance σ^2 is a decreasing function of s.

The local equilibria are the solutions of the integral equation

$$\mathcal{I}_{\mathrm{col}}[f]\left(\theta\right) = 0 \iff f\left(\theta\right) = \frac{\iint \mathrm{d}\theta_1 \mathrm{d}\theta_2\, f\left(\theta_1\right) f\left(\theta_2\right) K\left(\theta_2-\theta_1\right) V_s\left(\theta - \Psi\left(\theta_1,\theta_2\right)\right)}{\int \mathrm{d}\theta_1\, f\left(\theta_1\right) K\left(\theta_1-\theta\right)}. \tag{8.23}$$

The homogeneous isotropic state (f independent of the angle) is always a solution. This is the unique one when $\sigma > \sigma_c$: here the system is described by a single hydrodynamic variable, the density $\rho(\mathbf{r},t)$. We are interested in the regime $\sigma < \sigma_c$, when non isotropic local equilibria emerge. By rotation invariance, they are indexed by a local angle $\varphi(\mathbf{r},t)$; the local equilibria are then of the form $\rho(\mathbf{r},t)M_{\varphi(\mathbf{r},t)}$ and there are two hydrodynamic fields: ρ and φ. By rotational symmetry, the dependence on φ is simple: there exists a function m such that $M_\varphi(\theta) = m(\theta-\varphi)$.

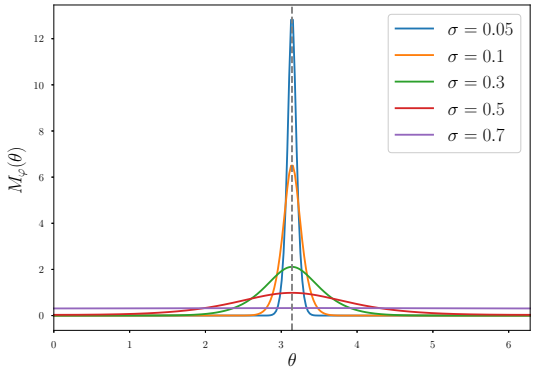


Figure 8.2.: Profile of the local equilibria $M_\varphi(\theta)$ for different values of σ and $\varphi = \pi$.

Although $M_{\varphi(\mathbf{r},t)}$ cannot be found analytically when $\sigma < \sigma_c$, finding it numerically is straightforward using the fixed-point formulation (8.23). We did this by implementing a fixed-point iteration method. For $\sigma > \sigma_c$, our algorithm correctly converges towards a constant solution, while for $\sigma < \sigma_c$, we obtain a solution for (8.23) which carries a preferential orientation. Our numerical solutions for $M_{\varphi(\mathbf{r},t)}$ as a function of σ is provided in Fig. 8.2. As it should be, the weaker this noise is, the narrower the local equilibrium M_φ is around the local orientation φ. Obtaining $M_{\varphi(\mathbf{r},t)}$ with this method is very fast computationally, requiring only a few iterations unless σ is set very close to σ_c. The value of σ_c can be computed analytically [30]. To do so, one has to assess the linear stability of the collision operator $\mathcal{I}_{\text{col}}$ linearized close to a uniform in angle distribution $f(\mathbf{r},\theta,t) = \rho(\mathbf{r},t)$. With the specific choice of a Von Mises distribution for the microscopical noise distribution P_σ, we have $\sigma_c = \sqrt{3}/3 \approx 0.58$.

8.3.3. Chapman–Enskog expansion close to a local equilibrium

In order to get the fluctuating hydrodynamics, we now want to compute evolution equations for the density ρ and the orientation field φ that specify the local equilibria. To do so, we look for solutions to the kinetic equation (8.18) as a Chapman–Enskog expansion close to a local equilibrium. This amounts to expand f for small α as

$$f(\mathbf{r},\theta,t) = \rho(\mathbf{r},t)\, M_{\varphi(\mathbf{r},t)}(\theta) + \alpha g(\mathbf{r},\theta,t) + \mathcal{O}\left(\alpha^2\right).$$

At leading order in α, we obtain from (8.18) that

$$\left(\partial_t + \mathbf{e}_\theta \cdot \nabla\right)(\rho M_\varphi) - \rho L_\varphi[g] = \frac{1}{\alpha}\xi\left[\rho M_\varphi\right], \tag{8.24}$$

where L_φ is the linearization of $\mathcal{I}_{\text{col}}$ close to ρM_φ:

$$L_\varphi[g](\theta) = \iint \mathrm{d}\theta_1 \mathrm{d}\theta_2\, M_\varphi(\theta_1)\, g(\theta_2)\, K(\theta_2 - \theta_1)\left\{2V_s\left(\theta - \Psi(\theta_1,\theta_2)\right) - \delta(\theta - \theta_1) - \delta(\theta - \theta_2)\right\}.$$

Classically, the Chapman–Enskog expansion then proceeds integrating (8.24) against conserved quantities, over the velocity variables (here the angle θ). Each conserved quantity then yields an evolution equation for a hydrodynamic mode.

A difference with respect to the classical case arises here: we only have a single conserved quantity (density) and want to obtain evolution equations for both the density ρ and the orientation field φ. Such problem was already discussed and solved in [87] noting that, to obtain the evolution equation for the slow modes, we only need to integrate against quantities χ that are in the kernel of $L_\varphi^\dagger$, the adjoint operator of L_φ. The elements of the kernel of $L_\varphi^\dagger$ which do not correspond to conservation laws are known as Generalized Collisional Invariant (GCI).

8.3.3.1. Equation for the density field.

We observe that constants are in the kernel of $L_\varphi^\dagger$. Hence, integrating the fluctuating kinetic equation (8.24) over θ yields the hydrodynamic equation for the density field

$$\partial_t \rho + c_1 \nabla \cdot (\rho \mathbf{e}_\varphi) = 0, \tag{8.25}$$

where $c_1 = \int \mathrm{d}\theta \, \cos(\theta - \varphi)\, m(\theta - \varphi)$, and $\mathbf{e}_\varphi = (\cos\varphi, \sin\varphi)$ is the orientational order field. We have used the density preserving property of the noise (8.22).

8.3.3.2. Equation for the orientational order field.

In order to obtain a second hydrodynamic equation for the orientation field, we need to find another element of $\ker L_\varphi^\dagger$ to integrate (8.24) against. In the classical kinetic theory of passive gases, this second element is usually the velocity variable [14], which is a manifestation of momentum conservation at the level of the kinetic equation. For active particles, momentum conservation is broken and a GCI is needed.

Since $\mathcal{I}_{\mathrm{col}}[M_\varphi] = 0$ for all φ, $\mathcal{I}_{\mathrm{col}}[M_{\varphi+\delta\varphi}] = 0$ for any perturbation $\delta\varphi$. This implies that not only $M_\varphi \in \ker L_\varphi$ but also $\frac{\partial M_\varphi}{\partial \varphi} = -m'(\theta - \varphi) \in \ker L_\varphi$, which provides two elements in $\ker L_\varphi$ as soon as the system is locally ordered. Hence $\ker L_\varphi^\dagger$ is also two-dimensional, spanned by the constants and another element which we call ψ_φ: this is the GCI.

As it was the case for M_φ, ψ_φ cannot be found analytically, but it can be determined numerically. In order to compute ψ_φ, we numerically solve the equation $L_\varphi^\dagger[\psi_\varphi] = 0$ by discretizing $[0, 2\pi)$. Then, $L_\varphi^\dagger[\psi_\varphi] = 0$ is a simple matrix equation that one can solve for ψ_φ. Observe that by rotational symmetry, the generalized collision invariant satisfies $\psi_\varphi(\theta) = -\psi_{-\varphi}(-\theta)$. In figure 8.3, we plot ψ_φ for $\varphi = \pi$ and for several values of σ.

Integrating (8.24) over θ and against ψ_φ and using that $L_\varphi^\dagger[\psi_\varphi] = 0$ yields the hydrodynamic equation for the orientation field

$$\alpha \int \mathrm{d}\theta \, \psi_\varphi \left(\partial_t + e_\theta \cdot \nabla_{\mathbf{r}} \cdot \rho M_\varphi\right) = \int \mathrm{d}\theta \, \psi_\varphi \xi \left[\rho M_\varphi\right], \tag{8.26}$$

We see that for a smooth evolution of the orientation field $\varphi(\mathbf{r}, t)$, the left hand side is of order α, which corresponds to the noise $\alpha\eta = \int \mathrm{d}\theta \, \psi_\varphi \xi \left[\rho M_\varphi\right]$ to be of order α as

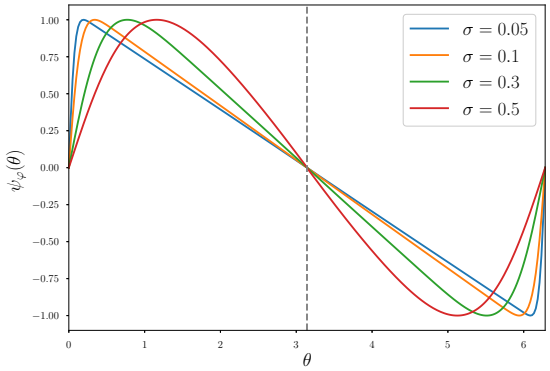


Figure 8.3.: Profile of the GCI $\psi_\varphi(\theta)$ for different values of σ and $\varphi = \pi$. This quantity is defined whenever $\sigma < \sigma_c$.

well. Contracting the probability distribution of ξ given in (8.18) and (8.19) to obtain the distribution of $\alpha\eta$, and expanding for small α, it is easy to see that only the quadratic part of the distribution of $\alpha\eta$ contributes to leading order in α. This is equivalent to saying that the noise becomes Gaussian in the hydrodynamic limit at leading order in α.

The explicit computation of the different terms in (8.26) yields the fluctuating hydrodynamic equation for the orientational order:

$$\rho\left(\partial_t \mathbf{e}_\varphi + c_2 \mathbf{e}_\varphi \cdot \nabla \mathbf{e}_\varphi\right) + c_3 \nabla_\perp \rho = \eta \mathbf{e}_\perp + \mathcal{O}(\alpha), \tag{8.27}$$

where the $\mathcal{O}(\alpha)$ term represents the error committed in neglecting the higher order terms in the Chapman-Enskog expansion. In (8.27), $\mathbf{e}_\perp = \mathbf{e}_{\varphi+\pi/2}$, $\nabla_\perp \rho = (\mathbf{e}_\perp \cdot \nabla\rho)\mathbf{e}_\perp$ is the gradient of ρ along the direction which is orthogonal to $\mathbf{e}_\varphi$ and

$$c_4 = \frac{-1}{\int \mathrm{d}\theta\, \psi_\varphi(\theta)\, m'(\theta - \varphi)},$$

$$c_2 = -c_4 \int \mathrm{d}\theta\, \psi_\varphi(\theta) \cos(\theta - \varphi)\, m'(\theta - \varphi),$$

and

$$c_3 = c_4 \int \mathrm{d}\theta\, \psi_\varphi(\theta) \sin(\theta - \varphi)\, m(\theta - \varphi).$$

Using the two-point correlations for ξ (8.21), we can characterize the Gaussian noise η

$$\mathbb{E}\left[\eta(\mathbf{r}, t)\, \eta(\mathbf{r}', t')\right] = \alpha\epsilon C \rho^2(\mathbf{r}, t)\, \delta(\mathbf{r} - \mathbf{r}')\, \delta(t - t') + \mathcal{O}(\alpha^2), \tag{8.28}$$

and

$$C = c_4^2 \left(C_1 + C_2 + C_3 + C_4 + C_5\right),$$

with

$$C_1 = \int \mathrm{d}\theta \mathrm{d}\theta' \, \psi_\varphi(\theta)^2 \, M_\varphi(\theta) \, M_\varphi(\theta') \, K(\theta - \theta') \,,$$

$$C_2 = \int \mathrm{d}\theta \mathrm{d}\theta' \, \psi_\varphi(\theta) \, \psi_\varphi(\theta') \, M_\varphi(\theta) \, M_\varphi(\theta') \, K(\theta - \theta') \,,$$

$$C_3 = \int \mathrm{d}\theta \mathrm{d}\theta_1' d\theta_2' \, \psi_\varphi(\theta)^2 \, M_\varphi(\theta_1') \, M_\varphi(\theta_2') \, K(\theta_1' - \theta_2') \, V_s(\theta - \Psi(\theta_1', \theta_2')) \,,$$

$$C_4 = \int \mathrm{d}\theta \mathrm{d}\theta' \mathrm{d}\theta_1' \mathrm{d}\theta_2' \, \psi_\varphi(\theta) \, \psi_\varphi(\theta') \, M_\varphi(\theta_1') \, M_\varphi(\theta_2') \, K(\theta_1' - \theta_2') \, V_s(\theta - \Psi(\theta_1', \theta_2')) \, V_s(\theta' - \Psi(\theta_1', \theta_2')) \,,$$

$$C_5 = -4 \int \mathrm{d}\theta \mathrm{d}\theta' \mathrm{d}\theta_1 \, \psi_\varphi(\theta) \, \psi_\varphi(\theta') \, M_\varphi(\theta) \, M_\varphi(\theta_1) \, K(\theta_1 - \theta) \, V_s(\theta' - \Psi(\theta, \theta_1)) \,.$$

Although it is not apparent from the above expressions, we have checked numerically that C is positive and an increasing function of σ, as expected.

The structure of the fluctuating equation for the local orientation field (8.27) is not usual. In relation with the lack of momentum conservation, (8.27) contains a noise term but no diffusive terms. These would give corrections at $\mathcal{O}(\alpha)$ in (8.27) and we expect that they can be obtained by similar lines as in [88] where they were derived for the Vicsek model within the weak-interaction limit; we leave this for future investigations. We should however observe that (8.27) allows already to obtain the path probability for $\mathbf{e}_\varphi$ to first order in α, which is the central result of this Section.

The two main novelties of our results are the following. First, we obtain the hydrodynamics of self-propelled aligning particles for dilute systems, deeply in the ordered phase, which was not even known at the deterministic level, since the results of [87] were derived in the weak-interaction limit. Second, we obtained also the hydrodynamics at the fluctuating level. The fact that we work in the dilute regime implies that the hydrodynamic noise variance is proportional to ρ^2, and that the noise depends explicitly on the collision rules (interactions) among particles. Both of these facts are at variance with the fluctuating hydrodynamics obtained in the weak-interaction regime – the regime where one particle interacts with many others and noise comes from angular diffusion rather than collisions [29]. For the sake of clarity, we only consider noise that stems from collisions. Adding angular diffusion to the model would slightly modify the kinetic equation by adding a diffusion term as well as a Dean-like noise. At the deterministic hydrodynamics level, this would result in a modification of the linearized collision kernel L_φ, the shape of the local equilibrium M_φ, and thus of the hydrodynamic coefficients. At the fluctuating level, there would be a new noise term whose variance is proportional to ρ instead of ρ^2. We expect this noise to be the dominant one at low densities.

8.3.4. Connection with the Toner-Tu equations

In [31, 30, 29, 177], the authors derive Toner-Tu like fluid equations starting from the Boltzmann-Vicsek kinetic equation. They derive the fluid equations by using that when

approaching the phase transition exhibited by the Boltzmann-Vicsek equation, the polar order parameter

$$\mathbf{p} = (p_x, p_y) = \left(\int \mathrm{d}\theta \, f \cos\theta, \int \mathrm{d}\theta \, f \sin\theta \right),$$

associated with the distribution function f, becomes a hydrodynamic mode. However, this derivation do not include the noise term. We define the distance to the phase transition $\mu\left(\sigma\right) = \sigma_c - \sigma$. In our paper [105], we derive in the small but positive μ limit, the fluctuating Toner-Tu equations from the Boltzmann-Vicsek equation. Our result is the following set of SPDEs for the polar order parameter and and the density fluctuation $\delta\rho$ around a stationary and uniform profile ρ_0

$$\partial_t \delta\rho + \nabla \cdot \mathbf{p} = 0, \tag{8.29}$$

$$\partial_t \mathbf{p} + \lambda_1 \left(\mathbf{p} \cdot \nabla\right) \mathbf{p} + \lambda_2 \left(\nabla \cdot \mathbf{p}\right) \mathbf{p} - \frac{\lambda_2}{2} \nabla \left(\mathbf{p}^2\right) = \left(a - b\mathbf{p}^2\right) \mathbf{p} - c_3 \nabla \delta\rho + D_T \Delta \mathbf{p} + \eta, \tag{8.30}$$

and $\eta = \left(\eta_i\right)_{i=1,2}$ is an isotropic Gaussian white noise whose correlations read

$$\mathbb{E}[\eta_i(\mathbf{r}, t)\eta_j(\mathbf{r}', t')] = \frac{1}{2}\zeta\left(\epsilon, \alpha, \mu\right) \rho_0^2 \delta(t - t')\delta(\mathbf{r} - \mathbf{r}'), \tag{8.31}$$

where $\zeta\left(\epsilon, \alpha, \mu\right)$ is a small parameter whose size depends on the smallness of ϵ the kinetic parameter, α the Knudsen number, and μ the distance to the transition. The exact value of ζ is derived from the microscopic dynamics for the first time in the section 4 of [105], where we also recall the main steps to derive the Toner-Tu system.

Although the Toner-Tu equations are derived in the limit where the system is close to the phase transition, they are widely used deeply in the ordered phase [200]. We now examine the connection between the Toner-Tu system and the equation we derive for the orientation field in the previous section (8.27). Assuming the norm of the polarity field to be fixed to $p_0 = \sqrt{a/b}$, which is reasonable deep in the ordered phase, we look for solutions with uniform magnitude of the local polar order $\mathbf{p} = p_0 \mathbf{e}_\varphi$, where $\mathbf{e}_\varphi$ is a unit 2d-vector parametrized by the angle φ. Projecting (8.30) onto $\mathbf{e}_\perp = \mathbf{e}_{\varphi+\pi/2}$ yields

$$p_0 \partial_t \mathbf{e}_\varphi + \lambda_1 p_0^2 \Big[(\mathbf{e}_\varphi \cdot \nabla)\mathbf{e}_\varphi \Big] = -c_3 \nabla_\perp \delta\rho + D_T p_0 (\mathbf{e}_\perp \cdot \Delta \mathbf{e}_\varphi)\mathbf{e}_\perp + (\mathbf{e}_\perp \cdot \eta)\mathbf{e}_\perp \tag{8.32}$$

We recognize in (8.32) all the terms present in (8.27). However these two equations differ for two reasons. First, the dependence of the parameters entering the hydrodynamic description on the microscopic ones differs in the two cases, both at deterministic and fluctuating level. Second, the Laplacian term in (8.32) is of the same order as transport terms, while these Laplacian terms were subdominant (and hence neglected) in (8.27).

8.4. Conclusions

We focused on active matter systems where polar alignment is the dominant interaction in the dilute regime. Within this framework, we have extended the Boltzmann-Vicsek deterministic kinetic theory to its fluctuating counterpart. This is best described through a large deviation theory formalism, given that fluctuations in the kinetic theory are not Gaussian. The large deviation Hamiltonian associated with it is given in (8.11), (8.13). Our fluctuating Boltzmann-Vicsek equation has the same regime of validity as the original Boltzmann-Vicsek equation: $\epsilon \ll 1$, where $\epsilon^{-1} = \rho_0 \ell^2$ is the number of particles in an area equal to the square of the mean free path ℓ.

We have then derived the associated fluctuating hydrodynamics. Our final result is (8.25), (8.27), (8.28), which allows to obtain the path probability of the density and the orientational field to leading order in the Knudsen number $\alpha = \ell/L$, where L is a macroscopic length-scale (e.g. the size of the system). In this regime and for dilute systems, even the derivation of the deterministic hydrodynamics was not known. We stopped the perturbative expansion at leading order in α, which corresponds to neglecting diffusive terms, but the same technique could be employed to obtained them, along the lines of the computations previously done in the weak-interactions regime [87]. These diffusive terms might be important to help better define the solutions of the deterministic and fluctuating hydrodynamic equations we derived.

The derivation of the hydrodynamic noise in the dilute regime differs in two important aspects from the one obtained in the weak-interactions regime [86, 29]. First, it depends explicitly on the particle interactions and, reflecting the binary nature of the collisions, its variance is quadratic in the density.

We conclude with three remarks. First, we have presented results on polar particles with polar aligning interactions, but we expect that these can be generalized to polar particles with nematic interactions or to fully active nematic systems. Second, in most real systems stochasticity at hydrodynamic level can originate both from interactions and from single-particle diffusion; independent spatial diffusion of every particles would just add a "Dean-Kawasaki like" noise term to the hydrodynamic equations, whose variance is proportional to ρ rather than ρ^2. Lastly, while our derivation of the hydrodynamic theory deeply in the ordered state can be considered controlled from a mathematical viewpoint, it should be noted that our results assume a small noise on top of a smooth evolution at the hydrodynamic level: our scaling hypothesis might break down in the presence of shocks. The analysis of large deviations in their presence is a much harder problem that is addressed in the next chapter.

9. Large deviations for scalar conservation laws

In this chapter, we assess the ability of a fluctuating hydrodynamics approach to estimate the probability of density profiles that are (non-entropic) weak solutions of the fluid equations for a particle system whose hydrodynamical limit is a scalar conservation law. This is motivated by the questions raised in the derivation of the fluctuating hydrodynamics in the previous two chapters. More precisely, in chapter 7, we derive the fluctuating compressible Navier-Stokes equations, starting from the Large Deviation Principle (LDP) associated with the Boltzmann equation. We did so by using a Gaussian approximation of the kinetic LDP, allowing to rephrase the LDP in terms of a fluctuating Boltzmann equation with Gaussian noise. We then used a Chapman-Enskog expansion of the fluctuating Boltzmann equation to obtain the fluctuating compressible Navier-Stokes equations in the small Knudsen number (α) limit, in agreement with the literature. However, this expansion as well as the Gaussianity assumption on the LDP does not seem to hold when the distribution function changes on length and time scales of order α, yielding gradient of order $1/\alpha$, seemingly ruling out the possibility of hydrodynamic shocks. We can also rephrase the fluctuating compressible Navier-Stokes equation into a large deviation principle for the empirical hydrodynamic fields. Another question is whether we can study the vanishing diffusion and noise limit $\alpha \to 0$ in this large deviation principle to characterize the probability of weak solutions to the compressible Euler (inviscid) system.

To explore these questions, in this chapter we turn to the study of a simpler particle system in one dimension, that is described at the hydrodynamic level by a scalar conservation law. To do so, we study a system of N particles undergoing a Run-and-Tumble dynamics on the real line, with a tumbling rate that depends on the local density. We derive the fluctuating hydrodynamics for this system as a large deviation principle for the empirical density, using a small Knudsen number expansion. From there, we compute the probability of observing a certain non-entropic shock density profile and we retrieve the classical Jensen-Varadhan result characterizing the probability of non-entropic shock density profiles in the limit of vanishing noise and diffusion. However, in the presence of a shock, it is not obvious that the small Knudsen number expansion still makes sense. We find that there is no reason for the Jensen-Varadhan result to hold in general. We show that it can be retrieved in a "quasi-incompressible" regime.

9.1. Introduction: scalar conservation laws

We consider a scalar conservation law

$$\partial_t \rho + \partial_x \left(a \left(\rho \right) \right) = 0, \tag{9.1}$$

where $\rho = \rho \left(x, t \right)$ with $x \in \mathbb{R}$, and we assume $a : \rho \mapsto a(\rho)$ to be convex. It is known that the Cauchy problem for (9.1) in general does not have globally defined smooth solutions [93]. We call $\rho(x,t)$ a weak solution of (9.1) if for all regular enough functions $\varphi(x,t)$ with compact support in $\mathbb{R} \times \mathbb{R}^+$, the following identity holds

$$\int_{\mathbb{R}} \mathrm{d}x \int_0^\infty \mathrm{d}t \ \left(\partial_t \rho + \partial_x \left(a \left(\rho \right) \right) \right) \varphi = 0.$$

Note that if ρ is not regular enough, we make sense of this previous identity with partial integration:

$$- \int_{\mathbb{R}} \mathrm{d}x \int_0^\infty \mathrm{d}t \ \left(\rho \partial_t \varphi + a \left(\rho \right) \partial_x \varphi \right) - \int_{\mathbb{R}} \mathrm{d}x \, \rho \left(x, 0 \right) \varphi \left(x, 0 \right) = 0. \tag{9.2}$$

When all weak solutions to (9.2) are considered, uniqueness fails for the initial value problem, which indicates that (9.1) misses some relevant physics. Among those weak solutions, (9.1) is known to exhibit weak shock solutions of the form:

$$\rho(x,t) = \begin{cases} \rho_L & \text{if } x \leq v_s t, \\ \rho_R & \text{if } x > v_s t, \end{cases}$$

where v_s is the speed of the shock, given by the Rankine-Hugoniot relation: $v_s = \left(a \left(\rho_L \right) - a \left(\rho_R \right) \right) / \left(\rho_L - \rho_R \right)$. In the following, we assume ρ_L and ρ_R to be positive.

In this chapter, we understand (9.1) as the hydrodynamic limit of a certain particle system. More precisely, we consider ρ as a density and $a(\rho)$ as a particle flux. $a'(\rho)$ is the velocity at density ρ. The convexity of a implies that $a'(\rho_L) > a'(\rho_R)$ iff $\rho_L > \rho_R$. Then, this shock solution is a physical solution iff $\rho_L > \rho_R$: the particles on the left "catch up" on the particles on the right. This is why we designate such solutions as *shocks*, whereas shock solution with $\rho_L < \rho_R$ are called *antishocks* [1]. Both situations are qualitatevely depicted in figure 9.1. We explain how a shock solution can emerge in the specific case of the Burgers' equation (i.e. (9.1) with $a \left(\rho \right) = \rho^2 / 2$) with a Gaussian initial condition in figure 9.2.

[1] The situation is more complicated when a is neither convex nor concave.

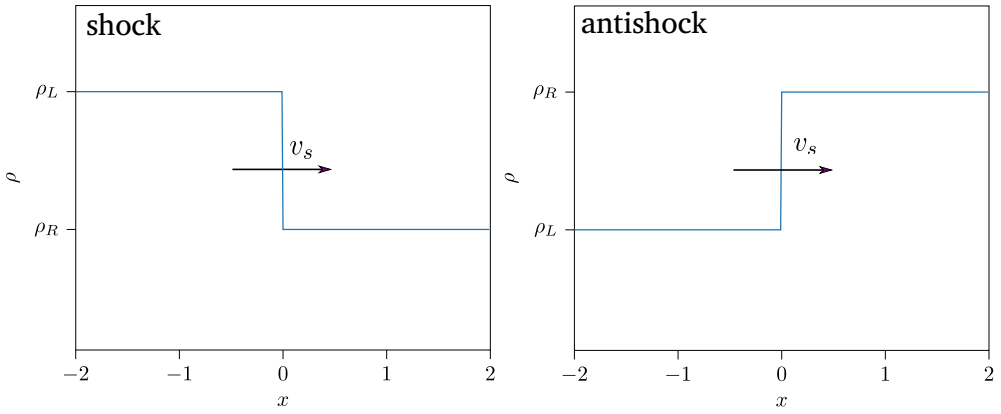
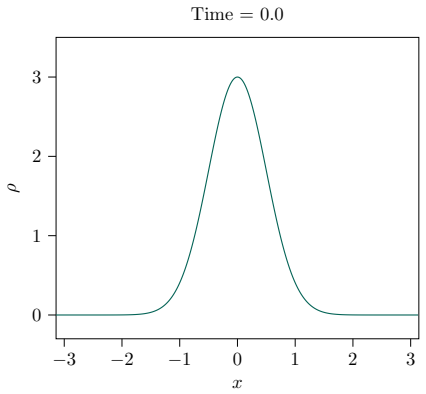
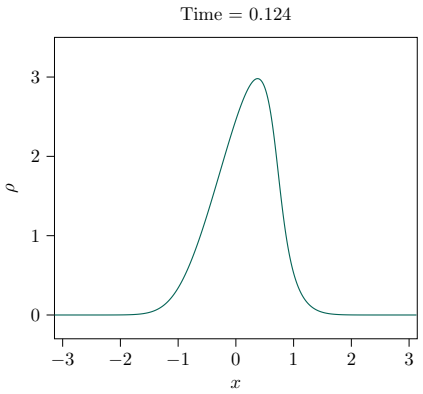


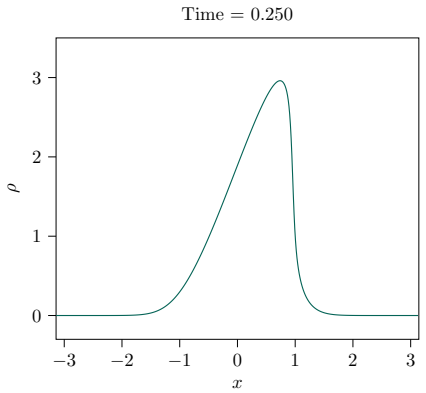
Figure 9.1.: A shock and an antishock weak solutions to the scalar conservation law.



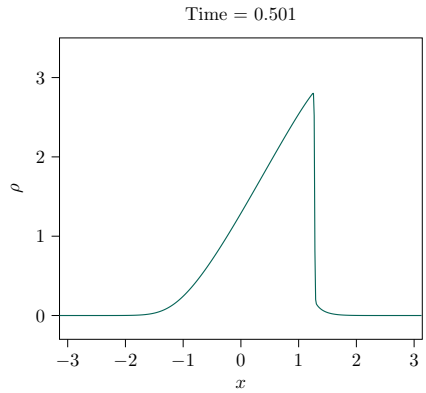
(a) The density is initially normally distributed.



(b) Since the flux function $\rho \mapsto a(\rho)$ is convex, the local velocity $\rho \mapsto a'(\rho)$ is an increasing function of the density.



(c) The mass initially located around $x = 0$ travels faster toward the positive x than the rest of the mass.



(d) Ultimately, the mass acumulates behind a frontline separating a high and a low density zone and leads to the formation of a shock.

Figure 9.2.: Shock formation in the Burgers equation ($\partial_t \rho + \partial_x (a(\rho)) = 0$ with $a(\rho) = \rho^2/2$) with a Gaussian initial density profile $\rho(x, 0) = 3e^{-2x^2}$. The plots are snapshots of a simulation using a first-order upwind scheme [78].

A way to discriminate shocks from antishocks, is to introduce a small viscosity term:

$$\partial_t \rho + \partial_x \left(a \left(\rho \right) \right) = \alpha \partial_x \left(D \left(\rho \right) \partial_x \rho \right) . \tag{9.3}$$

This is natural when thinking about (9.1) as the leading order term in a small α (Knudsen number) Chapman-Enskog expansion. In the small α limit, we retrieve the conservation law. When α is non zero, regularized shocks are still solutions to (9.3) but regularized antishocks are not anymore [116]. Now, when thinking about the conservation laws as the hydrodynamic limit of a particle system, it makes sense to take into account finite size effects by adding a small conservative noise to (9.3):

$$\partial_t \rho_N + \partial_x \left(a \left(\rho_N \right) \right) = \alpha \partial_x \left(D \left(\rho_N \right) \partial_x \rho_N \right) + \sqrt{\alpha^\nu / N} \partial_x \left(\sigma \left(\rho_\epsilon \right) \eta \right) , \tag{9.4}$$

where η is Gaussian and fully characterized by

$$\mathbb{E} \left(\eta \left(x, t \right) \eta \left(x', t' \right) \right) = \delta \left(x - x' \right) \delta \left(t - t' \right) ,$$

and ν is an exponent to be determined. This setting raises another question: what is the probability to observe a given spatio-temporal profile $\rho_N(x,t)$, which is not necessarily a solution of (9.3)? In the small noise and viscosity limit $(\alpha \to 0, N \to +\infty)$, it turns out that weak solutions, shocks and antishocks, are overwhelmingly more probable than other profiles, and that shocks are overwhelmingly more probable than antishocks. How to derive a large deviation principle characterizing this fact is the topic of this chapter.

Once we established that shocks and solutions of (9.4) are overwhelming more probable than antishocks, to compute the probability of a certain spatio-temporal density profile that is a weak solution to the conservation law (9.1), we only have to compute the weight of an antishock. We then retrieve the weight of a generic weak solution by additivity. Such a work has been first led by Jensen and Varadhan [133, 205] that obtained a large deviation principle for the probability to observe an antishock for the density profile whose underlying particle dynamics is the TASEP, a lattice exclusion model that is a continuous-time Markov process on $\{0,1\}^{\mathbb{Z}}$. Their result is the derivation of the rate function encoding the probability of an antishock defined by a couple of densities (ρ_L, ρ_R) , the so-called Jensen-Varadhan functional and it reads

$$I_{JV} \left[\rho^A \right] = \frac{1}{4} \int_{\mathbb{R}} \mathrm{d}x \int_{\rho_L}^{\rho_R} \mathrm{d}u \, \frac{D(u)}{\sigma^2 \left(u \right)} \left(v_s \rho_L - a \left(\rho_L \right) - v_s u + a(u) \right) , \tag{9.5}$$

where D and σ are the diffusive coefficients of the conservation law with a small noise and diffusion (9.4). It is important to note that the TASEP does not admit a kinetic description and the tools to analyze its hydrodynamical limit are different that the one presented in this manuscript. As we explain in this chapter, starting from a particle dynamics, that admits several velocities and evolves on a continuum space is a very different problem. The derivation of the Jensen-Varadhan functional (9.5) encoding the probability of antishocks starting from (9.4) is the question addressed in [154, 20], and then [15, 21] in more than one dimension. In this manuscript, we are interested in the derivation of the Jensen-Varadhan functional (9.5) starting from a certain particle

dynamics, that can be described non-trivially at the kinetic level (at variance with the TASEP). We explain in this chapter than even if the derivation of the Jensen-Varadhan from the fluctuating hydrodynamics description (9.4) is well-understood, it seems that the assumptions one has to use to derive the fluctuating hydrodynamics (9.4) from certain particle dynamics break down in the presence of steep gradients for the density profile.

More generally, the study of fluctuations within the hydrodynamical limit for systems whose macroscopic description is hyperbolic or ballistic (rather than diffusive) has been a very active topic, motivated by the study of conservation laws and transport phenomena. Notable results include the fluctuating hydrodynamics description of the Weakly Asymmetric Exclusion principle [34, 33], and the study of its associated shock solutions [44, 99]. As discussed in chapter 8, such systems are also of interest in active matter. In [2, 3], the authors study fluctuations in the hydrodynamic limit for an active lattice particle system whose fluid limit is a transport equation. From the point of view of integrable systems, progress has also recently been made toward a Ballistic Macroscopic Fluctuation Theory (in reference to the MFT for diffusive systems described in [32]) based on fluctuation-dissipation theorems.

In this chapter, we explain that the assumptions typically made to obtain the fluctuating conservation law with small diffusion (9.4) and used throughout the manuscript to obtain fluctuating hydrodynamics collapse in the presence of shocks. As a consequence, the Jensen-Varadhan description of antishocks does not hold for the particle model we consider. The outline of the chapter is summarized in figure 9.3. In section 9.2, we introduce the particle model as well as its kinetic description (via a LDP for the empirical measure). Ignoring the possible presence of shocks, we show in section 9.3 that we can derive the fluctuating hydrodynamics description from the particle dynamics, as a LDP for the empirical density that is equivalent to (9.4). Ignoring the effect of steep gradients in the small Knudsen number expansions, we then explain in section 9.4 how to obtain the Jensen-Varadhan LDP quantifying the probability of antishocks as a small Knudsen number convergence of the hydrodynamical large deviation functional, reproducing the computations from [154, 20]. In section 9.5, considering the effects of shocks in the asymptotic expansions that led to obtaining fluctuating hydrodynamics, we explain that this derivation is no longer possible. We present the steps to obtain a large deviation result characterizing antishocks directly from the particle dynamics, and show that in general we do not obtain the Jensen-Varadhan functional. Remarkably, we find that within a quasi-incompressible regime (where the shocks are regularized on length scales much larger than the microscopic scales), we recover the Jensen-Varadhan result.

9.2. Microscopic and kinetic model

In this section, we introduce a simple particle toy-model admitting the conservation law (9.1) as a hydrodynamical limit, and which large deviation structure is well-known. It can be seen as a one-dimensional version of the Run-and-Tumble model introduced in chapter 3, with density dependent tumbling rates. Run-and-Tumble dynamics are widely

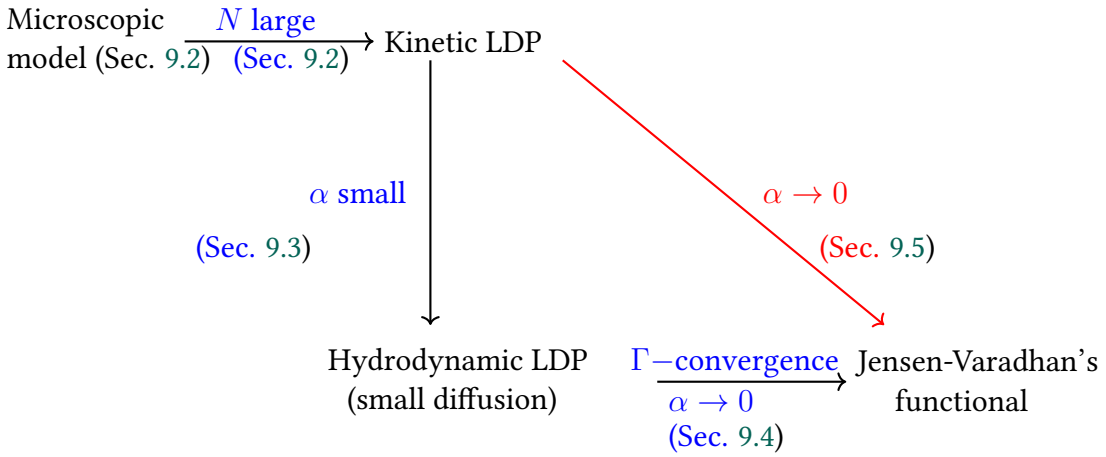


Figure 9.3.: Synoptic scheme of the chapter. In section 9.2, we introduce the microscopic model and the associated kinetic description. In section 9.3 we derive from the kinetic large deviation principle the fluctuating hydrodynamics description in the form of a LDP for the empirical density. In section 9.4, we derive the Jensen-Varadhan functional giving the probability to observe an antishock profile for the density as a $\Gamma-$convergence of the LDP for the empirical density. In section 9.5, we compute the probability of an antishock starting directly from the kinetic LDP. However, the Jensen-Varadhan's functional is only retrieved with the supplementary assumption of "quasi-incompressibility".

used in biology and biophysics to describe the behavior of bacteria (see for instance [24, 23, 180]); we only use it here as a simple tractable model. The results of this section are the derivation of the kinetic equation describing the distribution of position and velocity of the particles, and of a large deviation principle quantifying the probability of evolution paths of the $\mu-$space empirical measure. Because it stems from a jump process, the associated large deviation Hamiltonian is non quadratic with respect to the conjugated momentum, making the large deviations non Gaussian. We discuss the appropriate macroscopic scaling to obtain the hydrodynamical limit and the validity of the truncation of the Hamiltonian to its quadratic part within this limit.

Microscopic model. We consider a model of N particles in a domain of size L with positions $(x_n)_{1\leq n\leq N} \in \mathbb{R}^N$. There are two kinds of particles: particles with velocity u and particles with velocity $-u$. Particles switch velocity at a rate depending on the local density $\bar{\rho}_{N,R}(x,t)$:

$$\bar{\rho}_{N,R}(x,t) = \frac{L}{NR}\sum_{n=1}^{N} \mathbf{1}_{B(x,R)}\left(x_n\left(t\right)\right),$$

where $\mathbf{1}_{B(x,R)}$ is the indicator function of $\{y \in \mathbb{R} \mid |y-x| \leq R\}$. The particles velocities evolve according to the Markov jump process:

$$\begin{array}{lll} +u & \overset{\lambda g_-\left(\bar{\rho}_{N,R}\right)}{\longrightarrow} & -u, \\ -u & \overset{\lambda g_+\left(\bar{\rho}_{N,R}\right)}{\longrightarrow} & +u, \end{array} \tag{9.6}$$

where the subtext on the arrows indicates the transition rates. $g_\pm$ are dimensionless functions, chosen so that for any y: $g_+(y) + g_-(y) = 1$; λ is a rate. Writing $x_n(t), v_n(t)$ for the position and velocity of particle n ($v_n = \pm u$), the positions dynamics is simply $\dot{x}_n = v_n$. To be complete, we should define the boundary conditions; we take for instance periodic boundary conditions: $(x_n)_{1\leq n\leq N} \in (\mathbb{R}/L\mathbb{Z})^N$, but they do not play an important role in the following.

This model has three length scales: the interaction range R, the size of the system L and the mean free path

$$\ell = \frac{u}{\lambda}.$$

We assume in the following $R \ll \ell \ll L$.

Kinetic equation. In an appropriate large N limit, this microscopic model can be described by a kinetic equation.

We use in this paragraph the typical time between velocity switches λ^{-1} as time unit and the mean free path ℓ as space unit, so that the particles' velocities are ± 1. We define the empirical measures on the μ-space, i.e. the one particle phase-space which is $\{-1,1\} \times \mathbb{R}/L\mathbb{Z}$,

$$f_{N,\pm}(x,t) = \frac{L}{N\ell} \sum_{i=1}^{N} \delta\big(x - x_i(t)\big)\, \delta\left(v_i(t), \pm 1\right) \tag{9.7}$$

where L is the size of the system. $\varepsilon^{-1} = N\ell/L$ is the typical number of particles in an interval of size the mean free path; we assume this number to be large. With this normalization, the phase space densities $f_{N,\pm}$ typically take values of order 1.

In the limit $\varepsilon \to 0$, the empirical measures $f_{N,\pm}$ approach the limiting functions $f_\pm$, which satisfy the kinetic equation:

$$\begin{cases} \partial_t f_+ + \partial_x f_+ &= -g_- f_+ + g_+ \left(\mathbf{1}_R * \rho\right) f_- \\ \partial_t f_- - \partial_x f_- &= -g_+ f_- + g_- \left(\mathbf{1}_R * \rho\right) f_+ \end{cases},$$

where $\rho(x,t) = f_+(x,t) + f_-(x,t)$, and $\mathbf{1}_R(x) = \frac{L}{R}\mathbf{1}_{B(0,1)}\left(\frac{x}{R}\right)$ is the rescaled indicator function of $[-R,R]$.

Then, in the limit of vanishing interaction radius $R \to 0$ (which corresponds in physical units to the limit $R \ll \ell$), $\mathbf{1}_R * \rho$ tends to ρ, and the kinetic equation becomes

$$\begin{cases} \partial_t f_+ + \partial_x f_+ &= -f_+ + M_+(\rho) \\ \partial_t f_- - \partial_x f_- &= -f_- + M_-(\rho) \end{cases}, \tag{9.8}$$

where $M_\pm(\rho) = \rho g_\pm(\rho)$ (we have used here $g_+(\rho) + g_-(\rho) - = 1$). This last kinetic equation is the starting point for many mathematical works (see for instance [59, 7]), which are often interested in proving the hydrodynamical limit in an appropriate scaling, and sometimes look for efficient numerical methods to simulate conservation laws. The kinetic equation (9.8) can also be interepreted as a BGK-like kinetic equation, for a system with two velocities and $M_\pm$ playing the role of the Maxwellian distribution.

Large deviations. Since the microscopic dynamics is a jump process, we can also characterize dynamical fluctuations of the empirical measure with the following large deviation principle, as done for instance in chapter 3 for the 2D Run-and-Tumble model or in chapter 8 for the Boltzmann-Vicsek model. The result is the following LDP for the empirical measures

$$\mathbb{P}\left(\{f_{N,+}(t), f_{N,-}(t)\}_{0\le t\le T} = \{f_+(t), f_-(t)\}_{0\le t\le T}\right) \underset{N\to+\infty}{\asymp} \mathrm{e}^{-NI_T[f]}, \tag{9.9}$$

with $f = (f_+, f_-)$. The large deviation functional reads

$$I_T[f] = \int_0^T \mathrm{d}t \int_{\mathbb{R}} \mathrm{d}x \sup_p \{p_+\partial_t f_+ + p_-\partial_t f_- - H[f,p]\} \tag{9.10}$$

where $p = (p_+, p_-)$ and

$$H[f,p] = H_T[f,p] + H_Q[f,p].$$

H_T is the transport Hamiltonian

$$H_T[f,p] = -p_+\partial_x f_+ + p_-\partial_x f_-, \tag{9.11}$$

and H_Q is the jump Hamiltonian

$$H_Q[f,p] = \frac{f_+ M_-(\mathbf{1}_R * \rho)}{\mathbf{1}_R * \rho}\left(\mathrm{e}^{-p_+ + p_-} - 1\right) + \frac{f_- M_+(\mathbf{1}_R * \rho)}{\mathbf{1}_R * \rho}\left(\mathrm{e}^{-p_- + p_+} - 1\right). \tag{9.12}$$

According to the hypothesis $R \ll 1$ (i.e. the interaction radius is much smaller than the mean free path $R \ll \ell$ in physical units), we may take the small R limit in (9.12): the convolution $\mathbf{1}_R * \rho$ is replaced by ρ and the Hamiltonian becomes purely local.

Macroscopic scaling. To study the hydrodynamical limit, we focus in situations where the size of the system L is much larger than the mean free path ℓ. Hence it makes sense to consider profiles $f_\pm$ which vary over length and time scales much larger than ℓ and λ^{-1}. We then introduce the Knudsen number $\alpha = \ell/L$, where L is a macroscopic length, and rescale space and time as $\tilde{t} = \alpha t$, $\tilde{x} = \alpha x$: this is a hyperbolic rescaling. The kinetic equation becomes:

$$\alpha\left(\partial_t f_\pm \pm \partial_x f_\pm\right) = -f_\pm + M_\pm(\rho). \tag{9.13}$$

In the small α limit, one then expects the phase space distributions $f_\pm$ to be close to the functions $M_\pm(\rho)$. At leading order in α, one then obtains the equation for $\rho = f_+ + f_-$:

$$\partial_t \rho + \partial_x\big(a(\rho)\big) = 0, \text{ with } a(\rho) = M_+(\rho) - M_-(\rho). \tag{9.14}$$

This is a nonlinear conservation law, and plays the role of Euler equation in standard hydrodynamics. An expansion in the parameter α would add a diffusive term of order α to (9.14), and turn it to a one-dimensional analogue of compressible Navier-Stokes equations.

Under this hyperbolic rescaling, the rate function (9.10) reads

$$I_T^\alpha[f] = \alpha^{-2} \int_0^T \mathrm{d}t \int_{\mathbb{R}} \mathrm{d}x \sup_p \left\{\alpha\left(\partial_t f_+ p_+ + \partial_t f_- p_- + p_+ \partial_x f_+ - p_- \partial_x f_-\right) - H_Q[f,p]\right\}. \tag{9.15}$$

The Hamiltonian H_Q contains a linear in p part which contributes to the deterministic kinetic equation (9.13), and a part of order quadratic in p or higher which describes the stochastic fluctuations around (9.13). It is convenient to separate both terms, so we rewrite the rate function:

$$\begin{aligned} I_T^\alpha[f] = \alpha^{-2} \int_0^T \mathrm{d}t \int_{\mathbb{R}} \mathrm{d}x \sup_p \Big\{&\alpha\left(\partial_t f_+ p_+ + \partial_t f_- p_- + p_+ \partial_x f_+ - p_- \partial_x f_-\right) \\ &+ (f_+ - M_+)p_+ + (f_- - M_-)p_- - \tilde{H}_Q[f,p]\Big\}, \end{aligned} \tag{9.16}$$

where we have and defined $\tilde{H}_Q$ by removing the linear in p part of H_Q:

$$\tilde{H}_Q[f,p] = H_Q[f,p] - (f_+ - M_+)p_+ - (f_- - M_-)p_-.$$

Quadratic approximation. The microscopic jump process naturally creates a Poissonian noise, expressed by the Hamiltonian (9.12). In the macroscopic scaling however, this Poissonian noise is often replaced by a Gaussian approximation, which amounts to use a quadratic approximation to the Hamiltonian. For instance, we showed in chapter 6 that this approximation was valid when investigating the diffusive dynamics of N independent Run-and-Tumbling particles.

This quadratic approximation for the Hamiltonian is valid as long as the conjugated momentum p remains small. For a given profile $f = (f_+, f_-)$, the corresponding momenta p_+, p_- maximizing the supremum in (9.16) solve the equation

$$\alpha\left(\partial_t f_\pm \pm \partial_x f_\pm\right) + f_+ - M_\pm = \frac{\delta \tilde{H}_Q}{\delta p_\pm},$$

where the leading order at small p on the right hand side is linear. From this equation we see that in the small α regime, p remains small under the two following hypotheses:

1. $f_\pm$ is close to $M_\pm$: this amounts to consider profiles which are close to local equilibrium;
2. $\alpha(\partial_t f_\pm \pm \partial_x f_\pm)$ is small: this amounts to consider profiles which do not vary too steeply in space and time.

In the following, we shall use that quadratic approximation for the Hamiltonian and discuss its validity; in particular, we can check with the above criterion that our computations are consistent. The jump Hamiltonian truncated at quadratic order reads:

$$H_Q[f,p] = -p_+(f_+ - M_+) - p_-(f_- - M_-) + \frac{1}{2\rho}(f_+M_- + f_-M_+)(p_+ - p_-)^2 . \quad (9.17)$$

Lagrangian formulation of the large deviation functional. Under the quadratic approximation for the Hamiltonian (9.17), it is easy to solve the optimization on p in (9.10), and to obtain a Lagrangian expression for the kinetic rate function. The optimization in p is

$$\sup_p \Big\{ \alpha(\partial_t f_+ p_+ + \partial_t f_- p_- + p_+ \partial_x f_+ - p_- \partial_x f_-) + (f_+ - M_+)p_+ + (f_- - M_-)p_- - \frac{1}{2\rho}(f_+M_- + f_-M_+)(p_+ - p_-)^2 \Big\} .$$

By differentiation with respect to p_+ and p_-, we have that the optimal $p = (p_+, p_-)$ satisfies

$$\alpha(\partial_t f_+ + \partial_x f_+) + f_+ - M_- = \frac{1}{\rho}(f_+M_- + f_-M_+)(p_+ - p_-),$$
$$\alpha(\partial_t f_- - \partial_x f_-) + f_- - M_- = -\frac{1}{\rho}(f_+M_- + f_-M_+)(p_+ - p_-).$$

Summing these two equalities, we obtain a constraint that has to be satisfied in order for the supremum to exist

$$\partial_t \rho + \partial_x (f_+ - f_-) = 0. \quad (9.18)$$

Using the constraint (9.18), we notice that the quantity to maximize can be rewritten as following

$$\alpha(\partial_t f_+ p_+ + \partial_t f_- p_- + p_+ \partial_x f_+ - p_- \partial_x f_-) + (f_+ - M_+)p_+ + (f_- - M_-)p_- = (\alpha(\partial_t f_+ + \partial_x f_+) + f_+ - M_+)(p_+ - p_-).$$

As a consequence, we can express the supremum over p only as a function of the optimal

$$p_+ - p_- = \frac{\rho}{f_+M_- + f_-M_+}\{\alpha(\partial_t f_+ + \partial_x f_+) + f_+ - M_+\}. \quad (9.19)$$

From there, the kinetic rate function can be expressed as follows:

$$I_T^\alpha[f] = \alpha^{-2}\int_0^T \mathrm{d}t \int_{\mathbb{R}} \mathrm{d}x \, \frac{\rho}{4(f_+M_- + f_-M_+)}\{\alpha(\partial_t f_+ + \partial_x f_+) + f_+ - M_+\}^2 , \quad (9.20)$$

if $\partial_t \rho + \partial_x(f_+ - f_-) = 0$ and $I_T[f] = +\infty$ otherwise.

9.3. Fluctuating hydrodynamics from the kinetic LDP (without shocks)

In this section, we start from the rate function (9.20) of the kinetic LDP, obtained in the hyperbolic scaling and in the quadratic approximation. Our goal is to derive a fluctuating hydrodynamics description in terms of a large deviation principle for the empirical density field $\rho_N = f_{N,+} + f_{N,-}$ in the small α limit. At the deterministic level, we have seen that one obtains in the small α limit a Euler-like equation at leading order (9.14). The next to leading order in α is a Navier-Stokes-like equation, which includes a diffusion term of order $O(\alpha)$. From (9.20), we want to compute both this diffusion term and the stochastic fluctuations around this Navier-Stokes-like equation. To be more precise, we fix a density profile $\rho(x,t)$, which we assume to be regular. Our goal is to compute at the large deviation level and in the small α limit the probability to observe ρ. As discussed in section 6.6 of chapter 6, the hydrodynamic LDP that allows to quantify the probability to observe a given density profile ρ stems from the contraction principle in the small α limit:

$$\mathbb{P}\left(\{f_{N,+}(t), f_{N,-}(t)\}_{0\leq t\leq T} = \{f_+(t), f_-(t)\}_{0\leq t\leq T} \text{ s.t.} f_+ + f_- = \rho\right) \underset{\epsilon\to 0}{\asymp} \mathrm{e}^{-\frac{1}{\epsilon}\inf_{f_++f_-=\rho} I_T^\alpha[f]}. \tag{9.21}$$

In other words the probability of a certain density profile ρ is given by the probability of the most probable couple of distribution functions (f_+, f_-) according to the kinetic LDP 9.9, that satisfies $f_+ + f_- = \rho$. The goal of this section is then to estimate the small α asymptotics of $\inf_{f_++f_-=\rho} I_T^\alpha[f]$.

Let us first assume that

$$\partial_t\rho + \partial_x\big(a(\rho)\big) = \mathcal{O}(1). \tag{9.22}$$

In other words, ρ is far from being an approximate solution of Euler equation (9.14). Then it is not possible to choose (f_+, f_-) to be close to the local equilibrium $(M_+(\rho), M_-(\rho))$: indeed the constraint $\partial_t\rho + \partial_x\left(f_+ - f_-\right) = 0$ would impose $\partial_t\rho + \partial_x\big(a(\rho)\big)$ to be small. We conclude that the minimal $I_T^\alpha[f]$ (9.20) is of order α^{-2}, which eventually becomes infinite in the small α limit.

We now assume that

$$\partial_t\rho + \partial_x\big(a(\rho)\big) = \mathcal{O}(\alpha). \tag{9.23}$$

It is then possible to choose (f_+, f_-) to be close to the local equilibrium $(M_+(\rho), M_-(\rho))$, and we can anticipate that the minimal $I_T^\alpha[f]$ (9.20) is of order 1 in α (the integrand is of order α^2 and compensates the α^{-2} prefactor). We conclude that density profiles ρ that are approximate solutions of the Euler equation (9.14) are in the small α limit overwhelmingly more probable than density profiles which are not. We now compute the leading order of $I_T^\alpha[f]$.

Define $g = (g_+, g_-)$ such that

$$f_\pm = M_\pm(\rho) + \alpha g_\pm + \mathcal{O}\left(\alpha^2\right), \tag{9.24}$$

where $g_+ + g_- = 0$ (so that $M_\pm$ captures all the hydrodynamical content of $f_\pm$: $\rho = f_+ + f_- = M_+(\rho) + M_-(\rho)$). At leading order in α, we can rewrite the rate function (9.20) as following

$$I_T^\alpha[f] = \int_0^T \mathrm{d}t \int_{\mathbb{R}} \mathrm{d}x \, \frac{\rho}{8M_+M_-} \left\{\partial_t M_+ + \partial_x M_+ + g_+ + \mathcal{O}(\alpha)\right\}^2,$$

with the constraint

$$\partial_t \rho + \partial_x \left(a(\rho)\right) + \alpha \partial_x \left(g_+ - g_-\right) = 0,$$

where we recall $a(\rho) = M_+(\rho) - M_-(\rho)$. Now, instead of minimizing over $f = (f_+, f_-)$ such that $f_+ + f_- = \rho$, we optimize on $g = (g_+, g_-)$ such that $g_+ + g_- = 0$. We further split $g_\pm$ in a deterministic and a stochastic part: $g_\pm = g_\pm^d + g_\pm^s$, where the deterministic parts are fixed

$$g_\pm^d = -\left(\partial_t M_\pm \pm \partial_x M_\pm\right),$$

and we still have to optimize over the stochastic parts $g_\pm^s$. A quick computation gives

$$g_+^d - g_-^d = -D(\rho)\, \partial_x \rho$$

where

$$D(\rho) = 1 - a'(\rho)^2.$$

With these new notations, the optimization of (9.20) on $f_\pm$ becomes an optimization on g_+^s

$$\inf_{f_+ + f_- = \rho} I_T^\alpha[f] = \inf_{g_+^s} \int_0^T \mathrm{d}t \int_{\mathbb{R}} \mathrm{d}x \, \frac{\rho}{8M_+M_-} \left\{g_+^s + \mathcal{O}(\alpha)\right\}^2,$$

with the constraint

$$\partial_t \rho + \partial_x \left(a(\rho)\right) - \alpha \partial_x \left(D(\rho)\, \partial_x \rho\right) + \alpha \partial_x \left(g_+^s - g_-^s\right) = 0.$$

Noticing that $g_+^s + g_-^s = \mathcal{O}(\alpha)$, we finally get that the constraint reads

$$\alpha g_+^s = \frac{1}{2} \int_x \left(\partial_t \rho + \partial_x \left(a(\rho)\right) - \alpha \partial_x \left(D(\rho)\, \partial_x \rho\right)\right) + \text{cte}.$$

All in all, we can compute the leading order of the rate function as α goes to zero and the final result reads

$$\inf_{f_+ + f_- = \rho} I_T^\alpha[f] = \frac{1}{\alpha^2} I_{\text{hydro}}^\alpha[\rho], \tag{9.25}$$

where we introduce the hydrodynamical large deviation functional

$$I^{\alpha}_{\text{hydro}}[\rho] = \int_0^T \mathrm{d}t \int_{\mathbb{R}} \mathrm{d}x \, \frac{\rho}{8M_+M_- (u_2-u_1)^2} \left\{ \int_x \left(\partial_t \rho + \partial_x (a(\rho)) - \alpha \partial_x (D(\rho) \partial_x \rho) \right) \right\}^2 . \tag{9.26}$$

where the constant in the primitive is chosen so as to minimize $I^{\alpha}_{\text{hydro}}$. In other words, $I^{\alpha}_{\text{hydro}}$ describes the large deviation of the rescaled empirical density $\rho_\epsilon(x,t) = \epsilon \sum \delta(x - x_n(t))$, through the following LDP in the small α limit

$$\mathbb{P}\left(\{\rho_\epsilon(x,t)\}_{0\le t\le T} = \{\rho(x,t)\}_{0\le t\le T} \right) \underset{\epsilon\to 0}{\asymp} \mathrm{e}^{-\frac{1}{\alpha^2\epsilon} I^{\alpha}_{\text{hydro}}[\rho]}. \tag{9.27}$$

We see from (9.26) that if ρ satisfies (9.23) (i.e. ρ is an approximate solution of the Euler equation), $I^{\alpha}_{\text{hydro}}$ is of order α^2, meaning that the associated probability in the LDP (9.27) is of order 1. We also recover from (9.26-9.27) that if ρ satisfies (9.22), i.e. if ρ is not an approximate solution of the Euler equation, then $I^{\alpha}_{\text{hydro}}$ is of order 1, and the associated probability in (9.27) is exponentially small. However, we must keep in mind that although this order of magnitude is correct, the expression of (9.26) is not if $\partial_t\rho + \partial_x(a(\rho))$ is of order one.

A SPDE for the empirical density with the large deviation behavior required by (9.26) would read

$$\partial_t \rho_\epsilon + \partial_x (a(\rho_\epsilon)) = \alpha \partial_x (D(\rho) \partial_x \rho_\epsilon) + \partial_x \left(\sqrt{\frac{2\alpha^2 \epsilon M_+ M_-}{\rho_\epsilon}} \eta \right) = 0, \tag{9.28}$$

where

$$\mathbb{E}(\eta(x,t)\eta(x',t')) = \delta(x-x')\delta(t-t').$$

The SPDE (9.28) is the equivalent of the fluctuating compressible Navier-Stokes equation when the particle dynamics is the one of a dilute gas. Equation (9.28) is also the starting point of [154, 20] to derive the Jensen-Varadhan functional.

We have used in this computation the quadratic approximation to the Hamiltonian. We may question whether the conditions listed in 9.2 to use this approximation are fulfilled. Clearly, they are not when ρ satisfies (9.22). However, when ρ satisfies (9.23), we have seen that the optimal kinetic function $f = (f_+, f_-)$ that minimizes $I_T[f]$ with $f_+ + f_- = \rho$ is close to a local equilibrium, so the first condition is met. The second condition requires that the space and time derivatives of ρ remain of order 1, or at least smaller than α^{-1}. This is actually a very stringent condition put on the profiles ρ, because solutions of conservation laws (9.14) typically develop shocks.

9.4. Jensen-Varadhan large deviation functional

Section 9.3 provides the large deviation speed and rate function for density profiles which are approximate solutions of the scalar conservation law (9.1) and are regular

enough. We start from the hydrodynamic LDP (9.26) assuming it is also valid for steep density profiles, and use it to compute the weight of antishocks when $\alpha \to 0$. In this context, we recover the Jensen-Varadhan functional that quantifies the probability of antishocks. We know it may not be correct, but it will provide a comparison with the direct computations which follow.

First, we fix an antishock ρ^A, and we compute $\liminf_{\rho^\alpha \to \rho^A} I^\alpha_{\text{hydro}}[\rho^\alpha]$, i.e. we look for a sequence of regularized profiles ρ^α approaching the steep antishock profile ρ^A while maximizing their probability according to the hydrodynamic LDP (9.26). Technically, this is a $\Gamma-$ convergence result for the rate function (9.25). This is essentially a "physicist's view" of the results of Mariani et al [154, 20], which provide an almost complete proof of the $\Gamma-$ convergence. We shall obtain in the end the same Jensen-Varadhan's functional as in [154, 20].

Let ρ^A be an antishock between ρ_L and ρ_R, with speed $v_s = (a(\rho_R) - a(\rho_L))/(\rho_R - \rho_L)$. We have to find a family (ρ^α) of regularized profiles approximating ρ^A in the $\alpha \to 0$ limit in an optimal way (in the sense that they minimize $I^\alpha_{\text{hydro}}[\rho^\alpha]$).

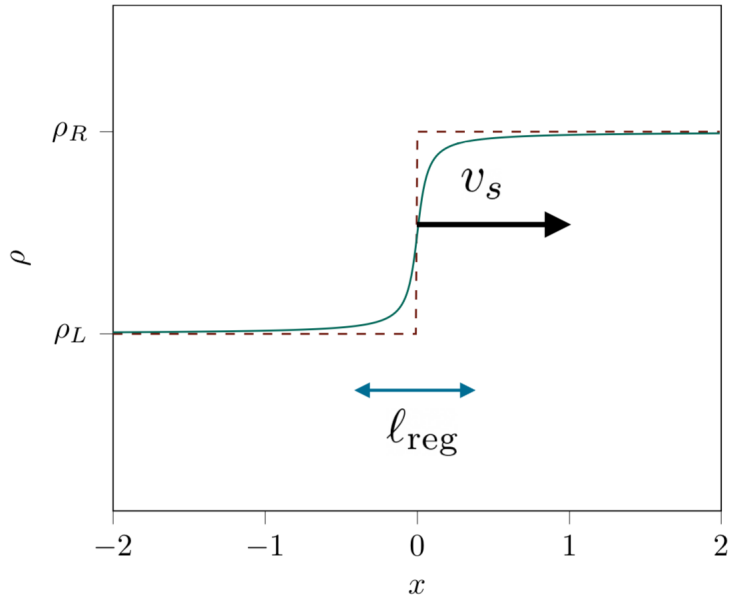


Figure 9.4.: An antishock profile ρ^A (dashed line) between ρ_L and ρ_R and a density profile ρ^α approximating the antishock with a regularization length ℓ_{reg} (solid line).

First assume that (ρ^α) regularizes ρ^A over a spatial scale ℓ_{reg}. The regularization length of a regularized profile ρ^α is the length needed for ρ^α to vary smoothly from ρ_L to ρ_R (see figure 9.4). Then far from the discontinuity, ρ^α is uniform and does not contribute to the rate function (9.26). In a window of width ℓ_{reg} around the discontinuity, $\partial_t \rho^\alpha + \partial_x a(\rho^\alpha)$ and $\partial_x \left(D(\rho^\alpha)\partial_x \rho^\alpha\right)$ are of order ℓ_{reg}^{-1} and ℓ_{reg}^{-2} respectively. After taking the primitive, the square and integrating over space we see that the hydrodynamic rate function (9.26) is of order $\ell_{\text{reg}} + \alpha^2 \ell_{\text{reg}}^{-1}$: this order of magnitude is clearly smallest for $\ell_{\text{reg}} \propto \alpha$. We have proved that the optimal spatial scale over which ρ^α regularizes the antishock ρ^A is α, in the sense that any smoother or steeper regularization corresponds to a much larger

value of the rate function.

Hence we may then parameterize ρ^α by (the opposite of) its associated diffusion coefficient $\tilde{D}$, where $\tilde{D}$ is defined by the equation:

$$\partial_t \rho^\alpha + \partial_x \left(a\left(\rho^\alpha\right)\right) = -\alpha \partial_x \left(\tilde{D}\left(\rho^\alpha\right) \partial_x \rho^\alpha \right). \tag{9.29}$$

We also define $\sigma(\rho) = \sqrt{\frac{4M_+M_-}{\rho}}$. The goal is now to find the best possible sequence ρ^α, or equivalently the best possible $\tilde{D}$, and compute the limit when $\alpha \to 0$ of $I^\alpha_{\text{hydro}}[\rho]$. In other words, we want to compute the leading order in α of

$$\inf_{\tilde{D}|\rho^\alpha \to \rho^A} I^\alpha_{\text{hydro}}\left[\rho^\alpha\right], \tag{9.30}$$

i.e. infimum of the hydrodynamic rate function $I^\alpha_{\text{hydro}}[\rho^\alpha]$ over the regularized density profiles ρ^α (parametrized by $\tilde{D}$) approaching the antishock ρ^A in the small α limit. This rate function will ultimately give the probability to observe a certain antishock profile ρ^A.

With these new notations, the rate function reads

$$\inf_{\tilde{D}|\rho^\alpha \to \rho^A} I^\alpha_{\text{hydro}}\left[\rho^\alpha\right] = \inf_{\tilde{D}} \frac{\alpha^2}{4} \int_0^T \mathrm{d}t \int_{\mathbb{R}} \mathrm{d}x \, \frac{1}{\sigma^2\left(\rho^\alpha\right)} \left(\left(\tilde{D}\left(\rho^\alpha\right) + D\left(\rho^\alpha\right) \right) \partial_x \rho^\alpha \right)^2. \tag{9.31}$$

We introduce the new variables: $z = x - v_s t$, $\rho_\alpha(x,t) = U(z/\alpha)$. z is a position variable that follows the antishock, and U parametrizes the profile of the antishock. Then, we can recast the definition (9.29) of $\tilde{D}$ as follows:

$$-v_s U' + a'(U)U' = -\left(\tilde{D}(U) U' \right)',$$

where the primes denote derivatives. Integrating the previous identity gives

$$\tilde{D}(U) U' - v_S U + a(U) = C, \tag{9.32}$$

where C is a constant. We can compute this constant C for instance by looking at $z \to -\infty$, we obtain: $C = -v_s \rho_L + a(\rho_L)$. With the change of variables $t \to z = x - v_s t$ and using (9.32) we have the following identity

$$\left(\partial_x \rho^\alpha\right)^2 = U'^2 = U' \left(-v_s \rho_L + a(\rho_L) - a(U) + v_s U \right) / \tilde{D}(U).$$

Introducing this identity in the rate function (9.31) yields

$$\inf_{\tilde{D}|\rho^\alpha \to \rho^A} I^\alpha_{\text{hydro}}\left[\rho^\alpha\right] = \inf_{\tilde{D}} \frac{\alpha^2}{4} \int_{\mathbb{R}} \mathrm{d}x \int_{\alpha^{-1}x}^{\alpha^{-1}(x - v_s T)} \mathrm{d}z \, \frac{1}{\sigma^2(U)} \frac{\left(D + \tilde{D}\right)^2}{\tilde{D}} U' \left(-v_s \rho_L + a(\rho_L) + v_s U - a(U) \right).$$

Finally, we introduce the following change of variable: $u = U(z)$, and we have

$$\inf_{\tilde{D}|\rho^\alpha \to \rho^A} I^\alpha_{\text{hydro}}\left[\rho^\alpha\right] = \inf_{\tilde{D}} \frac{\alpha^2}{4} \int_{\mathbb{R}} \mathrm{d}x \int_{\rho_L}^{\rho_R} \mathrm{d}u \, \frac{1}{\sigma^2(u)} \frac{\left(D(u) + \tilde{D}(u)\right)^2}{\tilde{D}(u)} \left(-v_s \rho_L + a(\rho_L) + v_s u - a(u) \right).$$

(9.33)

We see that for the infimum to be non-trivial in (9.33) we need to introduce the rescaled rate functional:

$$I_{JV}\left[\rho^A\right] = \inf_{\tilde{D}|\rho^\alpha \to \rho^A} \frac{1}{\alpha^2} I^\alpha_{\text{hydro}}\left[\rho^\alpha\right]. \tag{9.34}$$

Now, we want to compute (9.34), i.e. to perform the minimization on $\tilde{D}$. Then the optimal $\tilde{D}$ that minimizes (9.33) is obtained by derivation with respect to $\tilde{D}(u)$ and has to satisfy $\tilde{D}(u) = D(u)$. This extremum is indeed a minimum, because $\frac{1}{\sigma^2(u)} > 0$ and by convexity of $a : \rho \mapsto a(\rho)$, $-v_s\rho_L + a\left(\rho_L\right) + v_s u - a(u) \geq 0$.

The final result is the Jensen-Varadhan large deviation functional

$$I_{JV}\left[\rho^A\right] = \frac{1}{4}\int_{\mathbb{R}} \mathrm{d}x \int_{\rho_L}^{\rho_R} \mathrm{d}u \, \frac{D(u)}{\sigma^2\left(u\right)} \left(v_s\rho_L - a\left(\rho_L\right) - v_s u + a(u)\right), \tag{9.35}$$

that quantifies the probability of a certain antishock, defined by its densities (ρ_L, ρ_R) to be observed through the following LDP in the small α limit

$$\mathbb{P}\left(\rho^A = (\rho_L, \rho_R)\right) \underset{\epsilon \to 0}{\asymp} \mathrm{e}^{-\frac{1}{\epsilon} I_{JV}\left[\rho^A\right]}.$$

This rate function measures the "entropy production", with the entropy function s, such that $s''(u) = D(u)/\sigma^2(u)$. This is the Jensen-Varadhan functional found in [154] starting from the hydrodynamic LDP (9.26).

9.5. Weight of an antishock directly from the kinetic LDP

In section 9.3 we have obtained, under appropriate hypotheses, the rate function for the density at the diffusive (Navier-Stokes) level, for small but finite Knudsen number α; then in section 9.4 we have taken the limit $\alpha \to 0$ to obtain the Jensen-Varadhan functional. This requires in particular that the optimal kinetic function f remains close to a local equilibrium of the kinetic equation, which is a priori not guaranteed for an antishock. In order to shed light on the validity of the rate function (9.35), in this section we start directly from the kinetic rate function (9.20), and we compute the probability of an antishock. Technically, we need to perform a contraction from the kinetic functions "$f-$space" to the density functions "$\rho-$space, with the extra difficulty that the target density ρ is not regular. We show that there is no reason that the optimal kinetic function f corresponding to the antishock remains close to a local equilibrium, and no reason that the Jensen-Varadhan's functional (9.35) remains valid.

In general, the large deviation rate function replacing (9.35) that we obtain is not very explicit. However, we also identify the regime where (9.35) is valid: it corresponds to the cases where the length over which shocks and antishocks are regularized is large with respect to the mean free path; it also corresponds to a quasi incompressible regime.

The starting point is the kinetic rate function

$$I_T^\alpha[f] = \int_0^T \mathrm{d}t \int_{\mathbb{R}} \mathrm{d}x \, \frac{\rho^\alpha}{4\left(f_- M_+ + f_+ M_-\right)} \left\{\alpha\left(\partial_t f_+ + \partial_x f_+\right) + f_+ - M_+\right\}^2, \quad (9.36)$$

if $\partial_t(f_+ + f_-) + \partial_x\left(f_+ - f_-\right) = 0$ and $I_T[f] = +\infty$ otherwise.

Let ρ^A be an antishock between ρ_L and ρ_R, with speed $v_s = \left(a\left(\rho_R\right) - a\left(\rho_L\right)\right) / \left(\rho_R - \rho_L\right)$. In principle, our goal is to perform a contraction from the kinetic LDP, ie to compute

$$\inf_{f_+ + f_- = \rho} \left(I_T[f],\ f_+ + f_- = \rho^A\right).$$

However, ρ^A is singular; thus the possible f_+, f_- would be singular too, and would correspond to an infinite value for the rate function. We then introduce (ρ^α) a family of regularized profiles approximating ρ^A in the $\alpha \to 0$ limit, to be determined. We parameterize the family (ρ^α) by the diffusion coefficient $\tilde{D}(\rho)$, through the equation

$$\partial_t \rho^\alpha + \partial_x(a(\rho^\alpha)) = -\alpha \partial_x \left(\tilde{D}(\rho^\alpha)\partial_x \rho^\alpha\right).$$

Note that since ρ^α regularizes an antishock, the diffusion is negative. Furthermore, ρ^α regularizes the antishock ρ^A over a lengthscale

$$\ell_{\mathrm{reg}} \sim \alpha \frac{D}{a'}. \quad (9.37)$$

Our goal is to compute

$$I_h\left[\rho^\alpha\right] = \lim_{\alpha \to 0} \inf_{f_+ + f_- = \rho^\alpha} \left(I_T[f],\ f_+ + f_- = \rho^\alpha\right), \quad (9.38)$$

and to minimize it over the approximating profile ρ^α, that is minimizing it over $\tilde{D}(\rho)$ which characterizes ρ^α.

Let $f_\pm = M_\pm(\rho^\alpha) + g_\pm$, without assuming a priori that $g_\pm$ is of order α. $g_\pm$ are the deviations with respect to the local equilibrium. Since $f_+ + f_- = M_+(\rho^\alpha) + M_-(\rho^\alpha) = \rho^\alpha$, we have $g_+ + g_- = 0$.

We now split $g_\pm$ between a deterministic and a stochastic part $g_\pm = g_\pm^d + g_\pm^s$, with

$$g_+^d + \alpha(\partial_t + \partial_x) g_+^d = -\alpha(\partial_t + \partial_x) M_+ \quad (9.39)$$
$$g_-^d + \alpha(\partial_t - \partial_x) g_-^d = -\alpha(\partial_t - \partial_x) M_- \quad (9.40)$$

Introducing the notations $\mathcal{T}_\pm h = (\partial_t \pm \partial_x) h$, this is solved as

$$g_\pm^d = -\alpha\left(\mathrm{Id} + \mathcal{T}_\pm^{-1}\right) \cdot \mathcal{T}_\pm M_\pm.$$

Furthermore, the constraint for the kinetic large deviation functional to be finite reads

$$\partial_t \rho^\alpha + \partial_x\left(a(\rho^\alpha)\right) + \partial_x(g_+^d - g_-^d) = -\partial_x(g_+^s - g_-^s)$$

i.e.

$$g_+^s - g_-^s = \tilde{D}\partial_x \rho^\alpha - (g_+^d - g_-^d);$$

the constant which appears in the integration over x is seen to vanish by considering the behavior far from the antishock: there $g_\pm = 0$. Using $g_+^s + g_-^s = -(g_+^d + g_-^d)$, we conclude

$$g_+^s = -g_+^d + \frac{1}{2}\tilde{D}\partial_x\rho^\alpha \tag{9.41}$$

$$g_-^s = -g_-^d - \frac{1}{2}\tilde{D}\partial_x\rho^\alpha \tag{9.42}$$

We can now compute the integrand of the rate function (9.38). First

$$\begin{aligned}\alpha\left(\partial_t f_+ + \partial_x f_+\right) + f_+ - M_+ &= (\mathrm{Id} + \mathcal{T}_+)g_+^s \\ &= \mathcal{T}_+ M_+ + \frac{1}{2}(\mathrm{Id} + \alpha\mathcal{T}_+)\tilde{D}\partial_x\rho^\alpha \\ &= \frac{1}{2}(D(\rho^\alpha) + \tilde{D}(\rho^\alpha))\partial_x\rho^\alpha \\ &\quad + \frac{1}{2}\alpha\left[\mathcal{T}_+\tilde{D}\partial_x\rho^\alpha - (1+a')\partial_x(\tilde{D}\partial_x\rho^\alpha)\right].\end{aligned} \tag{9.43}$$

In the above computation, we have used the definition of D: $D(\rho) = 1 - a'(\rho)^2$.

The final step is to rewrite (9.36) using (9.43) and minimize it with respect to the diffusion coefficient $\tilde{D}$. This is in general a difficult task. One thing is clear however: the result is *not* the Jensen-Varadhan functional as found in 9.4. We also remark that if, for the optimal $\tilde{D}$, the regularization length (9.37) is much larger than α, then the second term on the right hand side in (9.43) is much smaller than the first one: indeed, $\alpha\partial_x\rho^\alpha \sim \alpha/\ell_{\mathrm{reg}} \ll 1$. By the same reasoning, in this case $g_\pm^d$ and $g_\pm^s$ are small, so that local equilibrium holds. We have seen in 9.4 that in such a situation the optimal $\tilde{D}$ is $\tilde{D} = D$, and that the limit rate function becomes at leading order Jensen-Varadhan functional. If $\tilde{D} = D$, the $\ell_{\mathrm{reg}} \gg \alpha$ hypothesis rewrites:

$$\frac{1 - a'^2}{|a'|} \gg 1 \Leftrightarrow |a'| \ll 1.$$

This condition should be satisfied for all densities spanned by the antishock, ie $[\rho_R, \rho_L]$. $a'(\rho)$ is of the same order of magnitude as the antishock velocity; it can be interpreted as a typical "macroscopic velocity". Hence the above condition amounts to a *small Mach number*. We have shown here that this small Mach number condition, which is not surprising if one wants to ensure local equilibrium for typical density profiles, is actually also sufficient for local equilibrium to hold for non typical density profiles, at large deviation level. Finally, from (9.36) and (9.43), it is not difficult to compute the first correction to the Jensen-Varadhan functional, of order $\alpha/\ell_{\mathrm{reg}}$. It is not however particularly illuminating.

To summarize, we have shown:

1. In general, the Jensen-Varadhan functional (9.35) does not describe the large deviation of the density.

2. However, in the regime where shocks are regularized over length scales much larger than the mean free path, which corresponds to small Mach numbers, the Jensen-Varadhan functional for the large deviation of the density is recovered.

9.6. Conclusions

In the context of a toy-model whose hydrodynamical limit is a conservation law, we have shown that in general the fluctuating hydrodynamics approach fails to describe the probability of the density to be an antishock weak solution of the conservation law. This is because, when gradients become steep in the Chapman-Enskog expansion (or generally in the hydrodynamical limit computations), several assumptions collapse: at the deterministic level, the distribution function does not have to remain close to a local equilibrium, at the fluctuating level, the noise term has no reason to become Gaussian. However, in a quasi-incompressible regime where the shocks are regularized at scales much larger than the microscopic scale, implying that their velocity is small compared to the microscopical one (i.e. the Mach number is small), we showed that the the previously mentioned assumptions still hold. In the context of our $1D$ toy-model, we recover the Jensen-Varadhan large deviation functional quantifying the probability of an antishock.

Even if we are far from understanding the possible shocks of the Navier-Stokes equations, these results seem to indicate that the fluctuating hydrodynamics we derived in chapter (7) should not be able to describe the probability of hydrodynamical profiles in the presence of shock, at least in the compressible case. Besides the questions related to the shocks for the Navier-Stokes equations, the understanding of hydrodynamic fluctuations around non-regular hydrodynamic profiles can be of importance for the study of transport phenomena exhibiting dynamical phase transitions. In [22] the authors study a 1D system similar to the one discussed in this chapter, except the particles evolve on a lattice and change velocities according to a local Ising rule. Such a system exhibits a flocking state (all the particles locally have the same velocity) that can rarely reverse its direction, driven by finite N fluctuations that propagate through the flock with a non-regular front.

10. Conclusions

In this final chapter, we summarize the content of the thesis manuscript and discuss the perspectives emanating from this work.

10.1. Summary

This thesis discusses the derivation of fluctuating hydrodynamics starting from the microscopic description of the particle dynamics. Fluctuating hydrodynamics can describe the evolution of macroscopic, coarse-grained fields while still taking into account fluctuations induced by finite particle number effects. Such a result can either be expressed as a stochastic PDE for the (empirical) hydrodynamic fields, or as a large deviation principle for the same fields. The derivation of fluctuating hydrodynamics is two-fold, as reflected by the structure of this dissertation. First, one needs to bridge from the particle description to a kinetic large deviation principle, that describes dynamical fluctuations of the empirical measure, whose most probable path (law of large numbers) is predicted by the kinetic equation. Then, we obtain a fluctuating hydrodynamics description by studying either the asymptotics of the kinetic large deviation principle within the hydrodynamic limit, or the asymptotics of the associated fluctuating kinetic equation.

More precisely, in the first part of the manuscript, we introduced the general framework of the large deviation approach to kinetic theory. We also derived two original results that are large deviation principles that estimate the probability of any evolution path for the empirical measure of a Hamiltonian systems of N particles coupled by a long-range pair potential, in the large N limit, in the general case, and within the Landau approximation for plasmas. These two results extend the classical Balescu-Guernsey-Lenard and Landau kinetic theories. Alongside other works on the large deviations associated with the Boltzmann kinetic theory [184, 50, 45, 46], these results complete the picture of kinetic large deviation principles for Hamiltonian systems whose kinetic theory is well-known.

In the second part of the manuscript, we explained how to derive fluctuating hydrodynamics starting from kinetic large deviation principles. We review two methods: one based on the generalization of the Chapman-Enskog expansion to fluctuating kinetic equations, that allows to compute fluctuating hydrodynamics as SPDEs for the hydrodynamic fields. The other method consists in studying the asymptotics of the kinetic large deviation functional in the hydrodynamical limit, through the lens of the contraction principle, to obtain a large deviation principle for the evolution paths of the empirical hydrodynamical fields. In both cases, we argue that in some of the examples studied in this manuscript, the resulting hydrodynamical large deviation principle is Gaussian, regard-

less of the Gaussianity of the underlying kinetic large deviation principle. This allowed us to derive the compressible and incompressible fluctuating Navier-Stokes equations, SPDEs describing thermal fluctuations for fluids, starting from the large deviation principle for the Boltzmann equation. This is to our knowledge one of the first microscopic derivation of the stochastic fluxes in these equations. We also derived the fluctuating hydrodynamics for a dilute gas of active particles aligning through binary collisions. In this case, the microscopic derivation allowed to obtain the correlation structure of the noise, which appeared to be quadratic in the density. This highlights the relevance of the microscopic derivation of fluctuating hydrodynamics when the shape of the noise terms cannot be obtained by equilibrium thermodynamics considerations. In the last chapter of this manuscript, we bring a nuance to our approach when the hydrodynamic limit is a conservation law, in the case of a one-dimensional toy model. In this context, it is known that the fluid equation admits shock solutions as weak solutions. We show that in this case, the asymptotic developments carried out to obtain the fluctuating hydrodynamics have no more reason to be valid. However, in a quasi-incompressible limit, it becomes possible to quantify the probability of hydrodynamic profiles including non-entropic shocks.

10.2. Prospects

We discuss here the perspectives opened by the work presented in the first part of the manuscript. It is surprising that the derivation of the large deviation principle associated with the Balescu-Guernsey-Lenard equation lead to explicit expressions for the large deviation Hamiltonian, through the use of the Szegö-Widom theorem. It is then interesting to wonder if such approaches can be applied to other systems. There is a wide variety of systems whose kinetic description is based on a similar slow-fast averaging, for which the understanding of large deviations is crucial and could be achieved through the techniques presented in this manuscript. Here, we focus on systems related to long-range interacting particle systems. We obtained conclusive results not listed in this document for the extension to inhomogeneous systems with long-range interactions, and to long-rang interacting particles forced out-of-equilibrium by a stochastic external field. This last system offers a wide non-equilibrium phenomenology (bistability, phase transitions) [166, 167] and a large deviation approach could give concrete insights to characterize those dynamical phase transitions through the estimations of transition time, or the computations of typical transition paths. Ultimately, the system discussed in [166, 167] is partially motivated by its deep connection with the kinetic reduction used to study the mid-latitude atmospheric fluid dynamics in geophysics [53]. It is then a natural perspective to obtain dynamical large deviation principles for such a system, that also exhibits dynamical phase transitions of importance for the study of the climate.

Then, the large deviation approach to the derivation of fluctuating hydrodynamics opens both theoretical and physical questions. The theoretical aspects are largely discussed in this dissertation and the formalization of the notion of convergence of the

kinetic large deviation principle to a hydrodynamic large deviation principle plays a central role in it. We used the contraction principle to obtain such results, but the $\Gamma-$convergence approach seems to yield similar result, as well as a starting point to rigorous approaches [47, 83, 16, 155] and more systematic studies of fluctuating hydrodynamics. Another point raised in this manuscript is that all the stochastic PDEs derived are rephrasings of underlying large deviation principles. As a consequence, they are appropriate do describe rare trajectories of the hydrodynamical evolution driven by extreme realization of the noise term, but they might not accurately describe small fluctuations. However, it has been observed that the fluctuating Navier-Stokes equations accurately describe small thermal fluctuations close to the deterministic evolution. This implies that there might be an argument that makes our large deviation approach relevant to describe small fluctuations close to the hydrodynamic evolution.

From a more physical perspective, the most exciting perspectives for the derivations of fluctuating hydrodynamics concern non equilibrium systems. Typically, in active matter, the role of fluctuations is prominent due to the relatively small size of the systems, and the different fluctuation induced phase transitions that have been observed [156, 92]. Large deviations approaches are natural to study such phenomena, providing tools to compute transition paths and frequency.

Active matter systems being deeply out-of-equilibrium, there is no way to infer the expression of the noise term in fluctuating hydrodynamics description with respect to microscopic parameters on the basis of thermodynamics. Our first-principle approach is then relevant for them, and the derivation of fluctuating hydrodynamics for other classes of active systems, that either display an interesting phenomenology, or offer useful applications; such as active nematics [29], or active particles in a quenched disorder [176] is a natural follow-up to our work.

In conclusion, it should be noted that this work is based on the kinetic and hydrodynamic scaling limits approach to statistical mechanics. The deterministic macroscopic equations are obtained as a law of large numbers from particle dynamics. From there, it is possible to study fluctuations around the deterministic limit thanks to the usual tools of probability theory: the central limit theorem and the large deviation principle. However, it is not obvious that this paradigm holds for some physical systems because of the strong assumptions needed to derive the kinetic equations. Typically, the kinetic approach is mathematically rigorous when the particle system is in the dilute limit, or in the opposite mean-field interacting limit. This is far from being true for most physical fluids, such as liquid water, and remains a physically unattainable limit in general. Using asymptotic descriptions to describe physical systems that do not quite approach them is of course common in physics, and often yields useful results. However, in [13] the authors suggest that fluctuating hydrodynamics may be relevant on scales as small as a fraction of the Kolmogorov length, which is much larger than the molecular scale (the mean free path). This does not disqualify the derivation of hydrodynamic LDPs presented in this thesis. On the contrary, it raises interesting questions about how to interpret them. Even if the formal mapping from SPDE to LDP seems easy to grasp, one of the key points is how to interpret the noise term, e.g. how to set a relevant cut-off for a numerical implementation. Answering this question would allow to clarify the

range of validity of the scaling limit approach to fluctuating hydrodynamics undertaken in this thesis, i.e. at which scales it is possible to consider fluctuating hydrodynamics as a small correction to deterministic hydrodynamics. So far, these remarks are not supported by any experimental observations and an attempt to address these problems from an experimental point of view would be an interesting continuation of this work.

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A. Appendices relative to the first part

We report here the appendices relative to the first part of the dissertation.

A.1. The relative entropy for N independent diffusions solves the stationary Hamilton–Jacobi equation

We consider the relative entropy

$$\mathcal{S}_{\text{rel}}[f] = -\int \mathbf{drdv}\, f \log\left(f/f_{\text{eq}}\right),$$

where f_{eq} is the equilibrium distribution. In this appendix, we shows that $-\mathcal{S}_{\text{rel}}$ solves the stationary Hamilton-Jacobi equation ($H_{MF}[f, -\delta\mathcal{S}_{\text{rel}}/\delta f] = 0$), for the case of N independent diffusions (3.37). We recall that $H_{MF}[f, -\delta\mathcal{S}_{\text{rel}}/\delta f] = 0$ is a necessary condition for $-\mathcal{S}_{\text{rel}}$ to be the quasipotential. By contrast, when those N diffusions are coupled in a mean field way (in 3.43) and the drift and diffusion coefficients depend actually on f, we are no more able to conclude that $H_{MF}[f, -\delta\mathcal{S}_{\text{rel}}/\delta f] = 0$ and we believe this is actually wrong in general.

In both cases, the large deviation Hamiltonian for the empirical density f_N reads

$$H_{MF}[f,p] = H_T[f,p] + H_{MF,h}[f,p],$$

where

$$H_T[f,p] = \int \mathbf{drdv}\, f\mathbf{v}\cdot\frac{\partial p}{\partial \mathbf{r}},$$

and

$$H_{MF,h}[f,p] = \int \mathbf{drdv}\, f\left\{\mathbf{b}[f].\frac{\partial p}{\partial \mathbf{v}} + \frac{\partial}{\partial \mathbf{v}}\left(\mathbf{D}[f]\frac{\partial p}{\partial \mathbf{v}}\right) + \mathbf{D}[f] : \frac{\partial p}{\partial \mathbf{v}}\frac{\partial p}{\partial \mathbf{v}}\right\}.$$

In the simple case where the N diffusions are independent, the drift and the diffusion coefficients do not depend on the actual distribution f: $\mathbf{b}[f] = \mathbf{b}$ and $\mathbf{D}[f] = \mathbf{D}$. In order to check that the relative entropy $\mathcal{S}_{\text{rel}}$ is the opposite of the quasipotential,

according to property 11 from section 3.4, we shall check that it solves the stationary Hamilton–Jacobi equation

$$H_{MF}\left[f, -\delta\mathcal{S}_{\text{rel}}/\delta f\right] = 0 \tag{A.1}$$

We have

$$\begin{aligned} -\frac{\partial}{\partial \mathbf{r}}\left(\frac{\delta\mathcal{S}_{\text{rel}}}{\delta f}\right) &= \frac{1}{f}\frac{\partial f}{\partial \mathbf{r}} - \frac{1}{f_{\text{eq}}}\frac{\partial f_{\text{eq}}}{\partial \mathbf{r}}, \\ -\frac{\partial}{\partial \mathbf{v}}\left(\frac{\delta\mathcal{S}_{\text{rel}}}{\delta f}\right) &= \frac{1}{f}\frac{\partial f}{\partial \mathbf{v}} - \frac{1}{f_{\text{eq}}}\frac{\partial f_{\text{eq}}}{\partial \mathbf{v}}, \end{aligned} \tag{A.2}$$

and f_{eq} solves the stationary Fokker–Planck equation

$$-\mathbf{v}\cdot\frac{\partial f_{\text{eq}}}{\partial \mathbf{r}} + \frac{\partial}{\partial \mathbf{v}}\cdot\left(\mathbf{D}\left[f_{\text{eq}}\right]\cdot\frac{\partial f_{\text{eq}}}{\partial \mathbf{v}} - \mathbf{b}\left[f_{\text{eq}}\right] f_{\text{eq}}\right) = 0. \tag{A.3}$$

Using (A.2) we have

$$\begin{aligned} H_{MF}\left[f, -\frac{\delta\mathcal{S}_{\text{rel}}}{\delta f}\right] = \int \mathrm{d}\mathbf{r}\mathrm{d}\mathbf{v}\, \Bigg\{ &-\frac{f}{f_{\text{eq}}}\mathbf{v}\cdot\frac{\partial f_{\text{eq}}}{\partial \mathbf{r}} + \mathbf{b}\left[f\right]\cdot\frac{\partial f}{\partial \mathbf{v}} - \frac{f}{f_{\text{eq}}}\frac{\partial f_{\text{eq}}}{\partial \mathbf{v}}\cdot\mathbf{b}\left[f\right] \\ &+\mathbf{D}\left[f\right]\cdot\frac{\partial f_{\text{eq}}}{\partial \mathbf{v}}\frac{1}{f_{\text{eq}^2}}\cdot\left(\frac{\partial f}{\partial \mathbf{v}} f_{\text{eq}} - \frac{\partial f_{\text{eq}}}{\partial \mathbf{v}} f\right)\Bigg\}. \end{aligned}$$

Now, we integrate by parts the first and the last term of the expression above, noting that

$$\frac{1}{f_{\text{eq}^2}}\left(\frac{\partial f}{\partial \mathbf{v}} f_{\text{eq}} - \frac{\partial f_{\text{eq}}}{\partial \mathbf{v}} f\right) = \frac{\partial}{\partial \mathbf{v}}\left(\frac{f}{f_{\text{eq}}}\right),$$

and

$$-f\frac{\partial \mathbf{b}\left[f\right]}{\partial \mathbf{v}} - \frac{f}{f_{\text{eq}}}\frac{\partial f_{\text{eq}}}{\partial \mathbf{v}}\mathbf{b}\left[f\right] = -\frac{f}{f_{\text{eq}}}\frac{\partial}{\partial \mathbf{v}}\left(\mathbf{b}\left[f\right] f_{\text{eq}}\right).$$

We obtain

$$H_{MF}\left[f, -\frac{\delta\mathcal{S}_{\text{rel}}}{\delta f}\right] = \int \mathrm{d}\mathbf{v}\, \frac{f}{f_{\text{eq}}}\left\{-\mathbf{v}\cdot\frac{\partial f_{\text{eq}}}{\partial \mathbf{r}} + \frac{\partial}{\partial \mathbf{v}}\cdot\left(\mathbf{D}\left[f\right]\frac{\partial f_{\text{eq}}}{\partial \mathbf{v}} - \mathbf{b}\left[f\right] f_{\text{eq}}\right)\right\}.$$

We see that if for any f

$$-\mathbf{v}\cdot\frac{\partial f_{\text{eq}}}{\partial \mathbf{r}} + \frac{\partial}{\partial \mathbf{v}}\cdot\left(\mathbf{D}\left[f\right]\frac{\partial f_{\text{eq}}}{\partial \mathbf{v}} - \mathbf{b}\left[f\right] f_{\text{eq}}\right) = 0, \tag{A.4}$$

then $H_{MF}\left[f, -\frac{\delta\mathcal{S}_{\text{rel}}}{\delta f}\right] = 0$ for any f. When $\mathbf{b}\left[f\right] = \mathbf{b}$ and $\mathbf{D}\left[f\right] = \mathbf{D}$ do not depend of f, i.e. when the N diffusions are independent, this identity is equivalent to the stationary

Fokker–Planck equation (A.3). It thus holds. It follows that the Hamilton–Jacobi equation (A.1) is verified and that the negative of the relative entropy solves the stationary Hamilton–Jacobi equation, for the case of N independent diffusions.

However, when the drift and the diffusion coefficient do depend on the distribution, (A.4) is no more true for any f. Then, we cannot conclude anymore that the relative entropy solves the stationary Hamilton–Jacobi equation.

An interesting remark is that in the specific case where $\mathbf{b}[f]$ and $\mathbf{D}[f]$ are chosen to mimic a Balescu-Guernsey-Lenard dynamics as in (4.15), with the precision that

$$\mathbf{B}(\mathbf{v},\mathbf{v}')\cdot(\mathbf{v}-\mathbf{v}')=0$$

to ensure momentum conservation, then the identity (A.4) holds for all f with

$$f_{\mathrm{eq}}(\mathbf{v})=\frac{\beta^{3/2}}{(2\pi)^{3/2}}\exp\left(-\beta\frac{\mathbf{v}^2}{2}\right).$$

A.2. Long time large deviations for quadratic observables of Gaussian processes, functional determinants and the Szegö–Widom theorem for Fredholm determinants

In this appendix, we explain how we can use the Szegö–Widom theorem in order to evaluate the large time asymptotics of Fredholm determinants that appears when computing the cumulant generating function of a quadratic observable of a Gaussian process. We follow the ideas in [57], adapting the discussion for the case of Gaussian processes with complex variables.

Let Y_t be a stationary $\mathbb{C}^n$-valued Gaussian process with correlation matrix $C(t)=\mathbb{E}(Y_t\otimes Y_0^*)$ and with a zero relation matrix $R(t)=\mathbb{E}(Y_t\otimes Y_0)=0$, let $M\in\mathcal{M}_n(\mathbb{C})$ be a $n\times n$ Hermitian matrix. The aim of this appendix is to prove that

$$\log\mathbb{E}\exp\left(\int_0^T \mathrm{d}t\, Y_t^{*\intercal}MY_t\right)\underset{T\to\infty}{\sim}-\frac{T}{2\pi}\int \mathrm{d}\omega\,\log\det\left(I_n-M\tilde{C}(\omega)\right), \tag{A.5}$$

where $\tilde{C}(\omega)=\int_{\mathbb{R}}\mathrm{e}^{i\omega t}C(t)\,\mathrm{d}t$ is the Fourier transform of the correlation matrix $C(t)$ and I_n is the $n\times n$ identity matrix. We note that the determinant of the r.h.s. of (A.5) is a real number. Indeed, as Y_t is a stationary process, $\tilde{C}(\omega)$ and M are Hermitian matrices, then the determinant is the determinant of a Hermitian operator and is a real number.

For pedagogical reasons, in this appendix the result (A.5) is stated for a process Y_t that takes values in a finite-dimensional space. However with adapted hypotheses, this result can be generalized when Y_t is a stationary $\mathcal{H}$-valued Gaussian process, where $\mathcal{H}$ is a Hilbert space, and where M is a Hermitian operator on $\mathcal{H}$.

In section A.2.1, we state the Szegö–Widom theorem. In section A.2.2, we explain that the left hand side of (A.5) is the log of the determinant of a Gaussian integral,

that this quantity can be expressed as a functional determinant for linear operators on $L^2([0,T],\mathbb{C}^n)$, and that Szegö–Widom theorem reduces it to the computation of frequency integrals of determinants of operators on the space $\mathbb{C}^n$, as expressed by (A.5).

A.2.1. The Szegö–Widom theorem

We first define integral operators on $L^2([0,T],\mathbb{C}^n)$. We considers maps $\varphi : [0,T] \to \mathbb{C}^n$ and $K : \mathbb{R} \to \mathcal{M}_n(\mathbb{C})$, where $\mathcal{M}_n(\mathbb{C})$ is the set of $n \times n$ complex matrices. We define the integral operator $\mathbf{K}_T$ by

$$\mathbf{K}_T\varphi(t) = \int_0^T K(t-s)\,\varphi(s)\,\mathrm{d}s, \tag{A.6}$$

$\mathbf{K}_T$ is a linear operator of $L^2([0,T],\mathbb{C}^n)$. K is called the kernel of the operator $\mathbf{K}_T$.

The Szegö–Widom theorem allows to compute large T asymptotics of the logarithm of the Fredholm determinant of the integral operator $\mathrm{Id} + \mathbf{K}_T$. The result is

$$\log \det_{[0,T]} (\mathrm{Id} + \mathbf{K}_T) \underset{T\to\infty}{\sim} \frac{T}{2\pi} \int \mathrm{d}\omega\, \log\det \left(I_n + \int_{\mathbb{R}} \mathrm{e}^{i\omega t} K(t)\,\mathrm{d}t \right), \tag{A.7}$$

where I_n is the $n \times n$ identity matrix. Whereas the determinant on the l.h.s. of this expression, denoted by the subscript $[0,T]$ is a Fredholm determinant, the determinant on the r.h.s. is a matrix determinant which can be more easily computed. Further details about this theorem and its possible applications can be found in [57].

A.2.2. Expectation of functionals of Gaussian processes

Let Y_t be a $\mathbb{C}^n$-valued stationary Gaussian process with correlation matrix

$$C(t) = \mathbb{E}(Y_t \otimes Y_0^*),$$

and with zero relation matrix

$$R(t) = \mathbb{E}(Y_t \otimes Y_0) = 0.$$

We will compute the large time asymptotics of

$$\mathcal{U}(T) = \log \mathbb{E} \exp \left(\int_0^T \mathrm{d}t\, Y_t^{*\intercal} \mathbf{M}_T Y_t \right),$$

where $\mathbf{M}_T$ is an integral operator on $L^2([0,T],\mathbb{C}^n)$ whose integral kernel is given by $M(t)$ (see the definition (A.6)). We assume that for all times t, $M(t)$ is a $n \times n$ Hermitian matrix. As Y_t is a Gaussian process we can compute the expectation as a Gaussian integral. It is straightforward to check that

$$\mathbb{E} \exp \left(\int_0^T \mathrm{d}t\, Y_t^{*\intercal} \mathbf{M}_T Y_t \right) = \det_{[0,T]} (\mathrm{Id} - (\mathbf{MC})_T)^{-1},$$

where $(\mathbf{MC})_T$ is the integral operator whose kernel is $(M \star C)(t)$ the convolution product on $[0,T]$ of the kernels $M(t)$ and $C(t)$.

Then, we can deduce the following expression for u

$$\mathcal{U}(T) = -\log \det_{[0,T]} (\mathrm{Id} - (\mathbf{MC})_T),$$

where the determinant is the Fredholm determinant of the integral operator $\mathrm{Id} - (\mathbf{MC})_T$. Generally, it is not obvious how to compute this kind of Fredholm determinant. Fortunately, we can use the Szegö–Widom theorem to obtain an expression for large T asymptotics as a finite-dimensional determinant. Using the result (A.7) from section A.2.1, we get

$$\mathcal{U}(T) \underset{T\to\infty}{\sim} -\frac{T}{2\pi} \int \mathrm{d}\omega \, \log\det \left(I_n - \int_{\mathbb{R}} \mathrm{e}^{-i\omega t} (M \star C)(t) \, \mathrm{d}t \right).$$

In the special case when $\mathbf{M}_T$ is a diagonal integral operator, i.e. when its kernel is $M(t) = M\delta(t)$, we can write

$$\mathcal{U}(T) \underset{T\to\infty}{\sim} -\frac{T}{2\pi} \int \mathrm{d}\omega \, \log\det \left(I_n - M \int_{\mathbb{R}} \mathrm{e}^{-i\omega t} C(t) \, \mathrm{d}t \right),$$

which is the result (A.5). In these expressions, the determinant to be computed on the r.h.s. is the determinant of a $n \times n$ matrix.

A.3. Computation of the determinant of the operator $u_{\mathbf{k},\omega}$

In this appendix, we compute the determinant of the operator $u_{\mathbf{k},\omega}$, encountered in section 4.5.3, and defined by

$$u_{\mathbf{k},\omega}[\varphi](\mathbf{v}_1) = \varphi(\mathbf{v}_1) - \int \mathrm{d}\mathbf{v}_2 \mathrm{d}\mathbf{v}_3 \, M(\mathbf{k}, \mathbf{v}_1, \mathbf{v}_2) \, \widetilde{\mathcal{C}_{GG}}(\mathbf{k}, \omega, \mathbf{v}_2, \mathbf{v}_3) \, \varphi(\mathbf{v}_3),$$

for any $\varphi \in \mathcal{H}_{\mathbf{v}}$, $\mathcal{H}_{\mathbf{v}}$ being the Hilbert space of complex functions over the velocity space. Using equation (4.40), we can simplify this expression

$$u_{\mathbf{k},\omega}[\varphi](\mathbf{v}_1) = \varphi(\mathbf{v}_1) - i\hat{W}(\mathbf{k})\,\mathbf{k} \cdot \int \mathrm{d}\mathbf{v}_2 \mathrm{d}\mathbf{v}_3 \, \widetilde{\mathcal{C}_{GG}}(\mathbf{k}, \omega, \mathbf{v}_2, \mathbf{v}_3) \left\{ \frac{\partial p}{\partial \mathbf{v}}(\mathbf{v}_2) - \frac{\partial p}{\partial \mathbf{v}}(\mathbf{v}_1) \right\} \varphi(\mathbf{v}_3). \tag{A.8}$$

We note that the operator $u_{\mathbf{k},\omega}$ has the form

$$u_{\mathbf{k},\omega} : \varphi \longmapsto \varphi - \langle w, \mathbf{Q}\varphi \rangle \, v - \langle v, \mathbf{Q}\varphi \rangle \, w, \tag{A.9}$$

where $\mathbf{Q}$ is a Hermitian operator over $\mathcal{H}_{\mathbf{v}}$, w and v are complex functions over the velocity space, and $\langle ., . \rangle$ denotes the Hermitian product: $\langle a, b \rangle = \int \mathrm{d}\mathbf{v} \, a^*(\mathbf{v}) \, b(\mathbf{v})$.

The connection is made between formulas (A.8) and (A.9) by setting $v(\mathbf{v}) = -i\mathbf{k}.\frac{\partial p}{\partial \mathbf{v}}$, $w(\mathbf{v}) = \hat{W}(\mathbf{k})$ and $\mathbf{Q}[\phi](\mathbf{v}_1) = \int d\mathbf{v}_2 \widetilde{\mathcal{C}_{GG}}(\mathbf{k}, \omega, \mathbf{v}_1, \mathbf{v}_2)\phi(\mathbf{v}_2)$. Using (4.35), we see that Q is a Hermitian operator. We note that, whenever $\frac{\partial p}{\partial \mathbf{v}}$ is not a constant in the velocity space, v and w are linearly independent.

Formula (A.9) shows that $u_{\mathbf{k},\omega} - \mathrm{Id}$ is a rank two linear operator. Then $\det_{\mathcal{H}_\mathbf{v}} u_{\mathbf{k},\omega}$ is the determinant of the operator $u_{\mathbf{k},\omega}$ restricted to $\mathrm{span}(v, w)$:

$$\det_{\mathcal{H}_\mathbf{v}} u_{\mathbf{k},\omega} = \begin{vmatrix} 1 - \langle w, \mathbf{Q}v\rangle & -\langle w, \mathbf{Q}w\rangle \\ -\langle v, \mathbf{Q}v\rangle & 1 - \langle v, \mathbf{Q}w\rangle \end{vmatrix}.$$

Then

$$\det_{\mathcal{H}_\mathbf{v}} u_{\mathbf{k},\omega} = 1 - 2\Re\left[\langle v, \mathbf{Q}w\rangle\right] + \langle v, \mathbf{Q}w\rangle \langle v, \mathbf{Q}w\rangle^* - \langle w, \mathbf{Q}w\rangle \langle v, \mathbf{Q}v\rangle.$$

where we have used $\langle w, \mathbf{Q}v\rangle = \langle \mathbf{Q}w, v\rangle = \langle v, \mathbf{Q}w\rangle^*$, as $\mathbf{Q}$ is an Hermitian operator.

We can explicitly compute the determinant of (A.8). We have

$$\langle v, \mathbf{Q}v\rangle = \int d\mathbf{v}_1 d\mathbf{v}_2\, \mathbf{k}.\frac{\partial p}{\partial \mathbf{v}_1}\mathbf{k}.\frac{\partial p}{\partial \mathbf{v}_2}\widetilde{\mathcal{C}_{GG}}(\mathbf{k}, \omega, \mathbf{v}_1, \mathbf{v}_2),$$

$$\langle v, \mathbf{Q}w\rangle = i\int d\mathbf{v}_1\, \mathbf{k}.\frac{\partial p}{\partial \mathbf{v}_1}\widetilde{\mathcal{C}_{VG}}(\mathbf{k}, \omega, \mathbf{v}_1)^*,$$

and

$$\langle w, \mathbf{Q}w\rangle = \widetilde{\mathcal{C}_{VV}}(\mathbf{k}, \omega),$$

where $\widetilde{\mathcal{C}_{VG}}$, $\widetilde{\mathcal{C}_{VV}}$ and $\widetilde{\mathcal{C}_{GG}}$ are the two-point correlations functions of the quasi-linear problem computed in section 4.4.2, and we have used (4.36-4.37).

We conclude that

$$\det_{\mathcal{H}_\mathbf{v}}(u_{\mathbf{k},\omega}) = 1 + 2\int d\mathbf{v}_1\, \mathbf{k}.\frac{\partial p}{\partial \mathbf{v}_1}\Im\left(\widetilde{\mathcal{C}_{VG}}(\mathbf{k}, \omega, \mathbf{v}_1)\right)$$
$$+ \int d\mathbf{v}_1 d\mathbf{v}_2\, \mathbf{k}.\frac{\partial p}{\partial \mathbf{v}_1}\mathbf{k}.\frac{\partial p}{\partial \mathbf{v}_2}\left\{\widetilde{\mathcal{C}_{VG}}(\mathbf{k}, \omega, \mathbf{v}_1)\widetilde{\mathcal{C}_{VG}}(\mathbf{k}, \omega, \mathbf{v}_2)^* - \widetilde{\mathcal{C}_{VV}}(\mathbf{k}, \omega)\widetilde{\mathcal{C}_{GG}}(\mathbf{k}, \omega, \mathbf{v}_1, \mathbf{v}_2)\right\}.$$

A.4. Current formulation of the large deviation principle

Because the particle number is conserved, it is clear that the dynamics of the empirical density has a conservative form $\frac{\partial f_N}{\partial t} + \frac{\partial}{\partial \mathbf{v}} \cdot \mathbf{j}_N = 0$. For the microscopic dynamics (before time averaging), this is a consequence of equations (4.22) or (4.26) with

$$\mathbf{j}_N(\mathbf{v}, t) = -\frac{1}{NL^3}\int \mathbf{dr}\left(\frac{\partial V[\delta g_N]}{\partial \mathbf{r}}\delta g_N\right).$$

After time averaging, we could have obtained the path large deviations by studying the large deviations of the time averaged current. Alternatively, we can rephrase our large deviation principle as a large deviation principle for the current, through a change of variable. This is the subject of this appendix.

The conservative nature of the dynamics is visible because the large deviation Hamiltonian H (4.56) does depend on the conjugate momentum p only through its gradient $\partial p/\partial \mathbf{v}$. We define $\tilde{H}$ as $\tilde{H}\left[f, \partial p/\partial \mathbf{v}\right] = H\left[f, p\right]$. We start from the definition of the large deviation Lagrangian

$$L\left[f, \dot{f}\right] = \mathrm{Sup}_p \left\{ \int \mathrm{d}\mathbf{v}\, \dot{f} p - H[f,p] \right\}.$$

Writing $\dot{f}$ as the divergence of a current $\dot{f} + \partial/\partial \mathbf{v} \cdot \mathbf{j} = 0$, we have

$$L\left[f, \dot{f}\right] = \sup_{\left\{\mathbf{j} | \dot{f} + \frac{\partial}{\partial \mathbf{v}} \cdot \mathbf{j} = 0\right\}} \mathrm{Sup}_p \left\{ - \int \mathrm{d}\mathbf{v}\, p \frac{\partial}{\partial \mathbf{v}} \cdot \mathbf{j} - H[f,p] \right\}.$$

Using $H\left[f,p\right] = \tilde{H}\left[f, \partial p/\partial \mathbf{v}\right]$, and integrating by part, we have

$$L\left[f, \dot{f}\right] = \sup_{\left\{\mathbf{j} | \dot{f} + \frac{\partial}{\partial \mathbf{v}} \cdot \mathbf{j} = 0\right\}} \tilde{L}\left[f, \mathbf{j}\right]$$

with

$$\tilde{L}\left[f, \mathbf{j}\right] = \sup_{\mathbf{E}} \left\{ \int \mathrm{d}\mathbf{v}\, \mathbf{j} \cdot \mathbf{E} - \tilde{H}[f, \mathbf{E}] \right\}.$$

where $\mathbf{E}$ designates the conjugate quantity of the current $\mathbf{j}$.

We thus have the large deviation principle

$$\mathbf{P}\left(\{f_N(\tau)\}_{0\leq\tau\leq T} = \{f(\tau)\}_{0\leq\tau\leq T}\right) \underset{N\to\infty}{\asymp} \mathbf{e}^{-NL^3 \sup\limits_{\left\{\mathbf{j} | \dot{f} + \frac{\partial}{\partial \mathbf{v}} \cdot \mathbf{j} = 0\right\}} \int_0^T \mathrm{d}\tau\, \tilde{L}[f, \mathbf{j}]} \mathbf{e}^{-NI_0[f(\tau=0)]}. \tag{A.10}$$

We note that we can also write a large deviation principle for the joint probability of the empirical density and the time averaged current $\mathbf{j}_N\left(\tau\right)$

$$\mathbf{P}\left(\{f_N(\tau), \mathbf{j}_N\left(\tau\right)\}_{0\leq t\leq T} = \{f(\tau), \mathbf{j}\left(\tau\right)\}_{0\leq t\leq T}\right) \underset{N\to\infty}{\asymp} \mathbf{e}^{-N\mathcal{A}[f,\mathbf{j}]} \mathbf{e}^{-NI_0[f(\tau=0)]},$$

with

$$\mathcal{A}\left[f, \mathbf{j}\right] = \begin{cases} L^3 \int_0^T \mathrm{d}\tau\, \tilde{L}\left[f, \mathbf{j}\right] & \text{if } \dot{f} + \frac{\partial}{\partial \mathbf{v}} \cdot \mathbf{j} = 0, \\ +\infty & \text{otherwise.} \end{cases}$$

A.5. Consistence of the two definitions of the tensor $\mathbf{B}$

We prove that for Coulomb interaction the two expressions for $\mathbf{B}$, (5.17) and (??) are equal.

The first expression for $\mathbf{B}$, (5.17), is

$$\mathbf{B}(\mathbf{v}_1, \mathbf{v}_2) = \frac{1}{2}\Lambda \int \mathrm{d}\mathbf{q}\, w(\mathbf{v}_1, \mathbf{v}_2; \mathbf{q}) \mathbf{q} \otimes \mathbf{q},$$

Expressing w in terms of the cross-section σ_0 through (5.8) with $\gamma = (\lambda_D/L)^3$, using (5.7), and choosing for σ_0 the Rutherford diffusion cross-section

$$\sigma_0(\mathbf{v}_1 + \mathbf{q}, \mathbf{v}_2 - \mathbf{q}; \mathbf{v}_1, \mathbf{v}_2) = \frac{1}{4\pi^2 \Lambda^2 q^4},$$

for two-body collisions of particles with electrostatic interactions [189], we obtain

$$\mathbf{B}(\mathbf{v}_1, \mathbf{v}_2) = \int \mathrm{d}\mathbf{q}\, \frac{\mathbf{q} \otimes \mathbf{q}}{8\pi^2 q^4} \delta\left(2\mathbf{q}.\left(\mathbf{v}_2 - \mathbf{v}_1\right)\right). \tag{A.11}$$

We perform the integration over $\mathbf{q}$ angle in (A.11) to get

$$\mathbf{B}(\mathbf{v}_1, \mathbf{v}_2) = C \frac{g^2 \mathrm{Id} - \mathbf{g}\mathbf{g}}{g^3},$$

with $C = (8\pi)^{-1} \int_0^\infty q^{-1} \mathrm{d}q$, $\mathbf{g} = \mathbf{v}_2 - \mathbf{v}_1$, and where Id is the identity matrix in three-dimension. We note that $\mathbf{B}(\mathbf{v}_1, \mathbf{v}_2)$ is proportional to $g^2\mathrm{Id} - \mathbf{g} \otimes \mathbf{g}$, which is the projector on the plane orthogonal to $\mathbf{v}_2 - \mathbf{v}_1$. This should have been expected as a consequence of symmetries.

In order to obtain the proportionality coefficient C we follow equations (6.3.15-6.3.21) in chapter 6.3 of Schram's textbook [189]. This chapter explains how one can deal with the logarithmic divergence arising in the computation of C. Briefly, one has to regularize the Coulomb interaction at large and small scales by introducing cut-offs, justified by the geometry of grazing collision at small scales, and by the Debye shielding at large scales. The final result reads

$$\mathbf{B}(\mathbf{v}_1, \mathbf{v}_2) = \frac{1}{8\pi} \ln \Lambda \frac{g^2 \mathrm{Id} - \mathbf{g}\mathbf{g}}{g^3}. \tag{A.12}$$

Following the computations in chapter 8.4 of Schram's textbook [189], we can show in a similar way that the definition of $\mathbf{B}$ given by (5.5) is also equal to (A.12). We have thus conclude that the two expression for $\mathbf{B}$, (5.17) and 5.5 are equal.

A.6. Symmetries and conservation laws associated with the collision kernels

A.6.1. The Boltzmann collision kernel

The time reversal symmetry of the microscopic Hamiltonian dynamics imposes that

$$w_0(\mathbf{v}_1', \mathbf{v}_2'; \mathbf{v}_1, \mathbf{v}_2) = w_0(-\mathbf{v}_1, -\mathbf{v}_2; -\mathbf{v}_1', -\mathbf{v}_2'). \tag{A.13}$$

The space rotation symmetry imposes that for any rotation $\mathbf{R}$ that belongs to the orthogonal group $SO(3)$

$$w_0(\mathbf{v}_1', \mathbf{v}_2'; \mathbf{v}_1, \mathbf{v}_2) = w_0(\mathbf{R}\mathbf{v}_1, \mathbf{R}\mathbf{v}_2; \mathbf{R}\mathbf{v}_1', \mathbf{R}\mathbf{v}_2').$$

The combination of the time reversal symmetry and of the space rotation symmetry for $\mathbf{R} = -\mathbf{I}$, where $\mathbf{I}$ is the identity operator, implies the inversion symmetry

$$w_0(\mathbf{v}_1', \mathbf{v}_2'; \mathbf{v}_1, \mathbf{v}_2) = w_0(\mathbf{v}_1, \mathbf{v}_2; \mathbf{v}_1', \mathbf{v}_2'). \tag{A.14}$$

The local conservation of momentum and energy implies that

$$w_0(\mathbf{v}_1', \mathbf{v}_2'; \mathbf{v}_1, \mathbf{v}_2) = \sigma(\mathbf{v}_1', \mathbf{v}_2'; \mathbf{v}_1, \mathbf{v}_2)\delta\left(\mathbf{v}_1 + \mathbf{v}_2 - \mathbf{v}_1' - \mathbf{v}_2'\right)\delta\left(\mathbf{v}_1^2 + \mathbf{v}_2^2 - \mathbf{v}'^2_1 - \mathbf{v}'^2_2\right), \tag{A.15}$$

where σ is the diffusion cross-section. σ is of the order of a^2 where a is a typical atom size.

A.6.2. The Landau collision kernel

The tensor $\mathbf{B}$ defined by

$$\mathbf{B}(\mathbf{v}_1, \mathbf{v}_2) = \frac{\Lambda}{2}\int \mathrm{d}\mathbf{q}\, w(\mathbf{v}_1, \mathbf{v}_2; \mathbf{q})\mathbf{q}\otimes\mathbf{q}, \tag{A.16}$$

involved in the Landau equation (5.15) has properties related to the symmetry and conservation properties of the collision process. In equation (A.16), $w(\mathbf{v}_1, \mathbf{v}_2; \mathbf{q})$ is an approximation at order zero of the collision kernel $w(\mathbf{v}_1 + \mathbf{q}/2, \mathbf{v}_2 - \mathbf{q}/2; \mathbf{q})$ associated with the collision of two particles with momenta $(\mathbf{v}_1, \mathbf{v}_2)$ that exchange a momentum $\mathbf{q}$. We have:

1. $w(\mathbf{v}_1, \mathbf{v}_2; \mathbf{q}) = w(\mathbf{v}_2, \mathbf{v}_1; \mathbf{q})$ because the incident particles are indiscernible,
2. $\mathbf{q}.(\mathbf{v}_1 - \mathbf{v}_2) = 0$ at leading order in $\mathbf{q}$ because of the energy conservation condition $\mathbf{v}_1^2 + \mathbf{v}_2^2 = (\mathbf{v}_1 + \mathbf{q})^2 + (\mathbf{v}_2 - \mathbf{q})^2$,
3. $w(\mathbf{v}_1, \mathbf{v}_2; \mathbf{q}) = w(\mathbf{v}_1, \mathbf{v}_2; -\mathbf{q})$, which is a direct consequence of (A.14) and the definition of w (5.8).

We notice that the momentum conservation is already built-in in the definition of w. The first property implies $\mathbf{B}(\mathbf{v}_1, \mathbf{v}_2) = \mathbf{B}(\mathbf{v}_2, \mathbf{v}_1)$. The second property implies $\mathbf{B}(\mathbf{v}_1, \mathbf{v}_2).(\mathbf{v}_1 - \mathbf{v}_2) = 0$. In addition to that, $\mathbf{B}(\mathbf{v}_1, \mathbf{v}_2)$ is by construction a symmetric tensor for every pair $(\mathbf{v}_1, \mathbf{v}_2)$.

A.7. Asymptotic expansions leading to the Landau equation and its large deviation Hamiltonian

A.7.1. Asymptotic expansions leading to the Landau equation

In this appendix, we start from the collision operator of the Boltzmann equation (the right hand side of equation (5.16)), we develop it at order 2 in $\mathbf{q}$, and we prove that we recover the collision term of the Landau equation (5.15).

We start from the expression of I in equation (5.16). Noting that $[f(\mathbf{v}+\mathbf{q})f(\mathbf{v}_2-\mathbf{q})-f(\mathbf{v})f(\mathbf{v}_2)]$ has no term of order zero, in order to compute an expansion at order 2 in $q=|\mathbf{q}|$, it will be sufficient to work with the expansions:

$$\begin{cases} w(\mathbf{v}+\frac{1}{2}\mathbf{q},\mathbf{v}_2-\frac{1}{2}\mathbf{q};\mathbf{q}) & = w(\mathbf{v},\mathbf{v}_2;\mathbf{q})+\frac{1}{2}\left(\frac{\partial w}{\partial \mathbf{v}}-\frac{\partial w}{\partial \mathbf{v}_2}\right).\mathbf{q}+\mathcal{O}(q^2), \text{ and} \\ f(\mathbf{v}+\mathbf{q})f(\mathbf{v}_2-\mathbf{q})-f(\mathbf{v})f(\mathbf{v}_2) & = \left(\frac{\partial f}{\partial \mathbf{v}}f(\mathbf{v}_2)-\frac{\partial f}{\partial \mathbf{v}_2}f(\mathbf{v})\right).\mathbf{q}+ \\ & \quad +\left(\frac{\partial^2 f}{\partial \mathbf{v}\partial \mathbf{v}}f(\mathbf{v}_2)+\frac{\partial^2 f}{\partial \mathbf{v}_2\partial \mathbf{v}_2}f(\mathbf{v})-2\frac{\partial f}{\partial \mathbf{v}}\frac{\partial f}{\partial \mathbf{v}_2}\right):\mathbf{q}\mathbf{q}+\mathcal{O}(q^3). \end{cases}$$

Let us now compute the collision integral $I(\mathbf{v})$ order by order. We directly notice that there is no term of order zero in $\mathbf{q}$. Let us compute $I^{(1)}(\mathbf{v})$ the term of order 1 of the collision integral

$$I^{(1)}(\mathbf{v})=\Lambda\int \mathrm{d}\mathbf{v}_2\mathrm{d}\mathbf{q}\, w(\mathbf{v},\mathbf{v}_2;\mathbf{q})\left(\frac{\partial f}{\partial \mathbf{v}}f(\mathbf{v}_2)-\frac{\partial f}{\partial \mathbf{v}_2}f(\mathbf{v})\right).\mathbf{q}.$$

We use that $w(\mathbf{v},\mathbf{v}_2;\mathbf{q})$ is an even function of $\mathbf{q}$ (point 3 of appendix (A.6.2)). This makes the integrand an odd function of $\mathbf{q}$, and implies that $I^{(1)}(\mathbf{v})=0$.

At order 2 in $\mathbf{q}$ we have

$$I(\mathbf{v})=\frac{\Lambda}{2}\int \mathrm{d}\mathbf{v}_2\mathrm{d}\mathbf{q}\left\{\left(\frac{\partial w}{\partial \mathbf{v}}-\frac{\partial w}{\partial \mathbf{v}_2}\right)\left(\frac{\partial f}{\partial \mathbf{v}}f(\mathbf{v}_2)-\frac{\partial f}{\partial \mathbf{v}_2}f(\mathbf{v})\right)\right.$$
$$\left.+w\left(\frac{\partial^2 f}{\partial \mathbf{v}\partial \mathbf{v}}f(\mathbf{v}_2)+\frac{\partial^2 f}{\partial \mathbf{v}_2\partial \mathbf{v}_2}f(\mathbf{v})-2\frac{\partial f}{\partial \mathbf{v}}\frac{\partial f}{\partial \mathbf{v}_2}\right)\right\}:\mathbf{q}\mathbf{q}.$$

To obtain the Landau equation, we have to write $I(\mathbf{v})$ as a divergence involving the tensor $\mathbf{B}$. In order to do so, we integrate by parts the term involving $\frac{\partial w}{\partial \mathbf{v}_2}$ while keeping the terms involving $\frac{\partial w}{\partial \mathbf{v}}$. This gives

$$I(\mathbf{v})=\frac{\Lambda}{2}\int \mathrm{d}\mathbf{v}_2\mathrm{d}\mathbf{q}\left\{\frac{\partial w}{\partial \mathbf{v}}\left(\frac{\partial f}{\partial \mathbf{v}}f(\mathbf{v}_2)-\frac{\partial f}{\partial \mathbf{v}_2}f(\mathbf{v})\right)+w\frac{\partial}{\partial \mathbf{v}}\left(\frac{\partial f}{\partial \mathbf{v}}f(\mathbf{v}_2)-\frac{\partial f}{\partial \mathbf{v}_2}f(\mathbf{v})\right)\right\}:\mathbf{q}\mathbf{q}.$$

Now, by noting that $I(\mathbf{v})$ can be written as a total divergence with respect to $\mathbf{v}$ and using equation 5.17 we obtain

$$I(\mathbf{v})=\frac{\partial}{\partial \mathbf{v}}\int \mathrm{d}\mathbf{v}_2\mathbf{B}(\mathbf{v},\mathbf{v}_2)\left(-\frac{\partial f}{\partial \mathbf{v}_2}f(\mathbf{v})+\frac{\partial f}{\partial \mathbf{v}}f(\mathbf{v}_2)\right)+o\left(q^2\right), \tag{A.17}$$

with $\mathbf{B}(\mathbf{v},\mathbf{v}_2)=\Lambda\int \mathrm{d}\mathbf{q}\, w(\mathbf{v},\mathbf{v}_2;\mathbf{q})\mathbf{q}\otimes\mathbf{q}/2$ (see equation (5.17)), and $o\left(q^2\right)$ means that we omitted terms of order larger than 2. The term of order 2 is the collision operator of the Landau equation (5.15).

A.7.2. Asymptotic expansions leading to the large deviation Hamiltonian associated to the Landau equation

In this section, we detail the computation of the large deviation Hamiltonian for the Landau equation starting from the Hamiltonian (5.19) for the Boltzmann equation and using the grazing collision limit.

First, let us rewrite this Hamiltonian

$$H[f,p] = \frac{\Lambda}{2}\int \mathbf{dr}\mathbf{dv_1}\mathbf{dv}_2\mathbf{dq}\, w\left(\mathbf{v}_1+\frac{1}{2}\mathbf{q},\mathbf{v}_2-\mathbf{q};\mathbf{q}\right) f(\mathbf{v}_1)f(\mathbf{v}_2)\left\{\mathrm{e}^{[-p(\mathbf{v}_1)-p(\mathbf{v}_2)+p(\mathbf{v}_1+\mathbf{q})+p(\mathbf{v}_2-\mathbf{q})]}-1\right\}.$$

In order to obtain a Hamiltonian associated with the Landau equation, we will use the same hypothesis of grazing collisions and a Taylor expansion in $\mathbf{q}$ to the same order

$$\begin{cases} w(\mathbf{v}_1+\frac{1}{2}\mathbf{q},\mathbf{v}_2-\frac{1}{2}\mathbf{q};\mathbf{q}) & = w(\mathbf{v}_1,\mathbf{v}_2;\mathbf{q})+\frac{1}{2}\left(\frac{\partial w}{\partial \mathbf{v}_1}-\frac{\partial w}{\partial \mathbf{v}_2}\right).\mathbf{q}+\mathcal{O}(q^2) \\ \mathrm{e}^{[-p(\mathbf{v}_1)-p(\mathbf{v}_2)+p(\mathbf{v}_1+\mathbf{q})+p(\mathbf{v}_2-\mathbf{q})]}-1 & = \left(\frac{\partial p}{\partial \mathbf{v}_1}-\frac{\partial p}{\partial \mathbf{v}_2}\right).\mathbf{q}+ \\ & \quad +\frac{1}{2}\left\{\frac{\partial^2 p}{\partial \mathbf{v}_1\partial \mathbf{v}_1}+\frac{\partial^2 p}{\partial \mathbf{v}_2\partial \mathbf{v}_2}+\left(\frac{\partial p}{\partial \mathbf{v}_1}-\frac{\partial p}{\partial \mathbf{v}_2}\right)\left(\frac{\partial p}{\partial \mathbf{v}_1}-\frac{\partial p}{\partial \mathbf{v}_2}\right)\right\}:\mathbf{qq}+\mathcal{O}(q^3). \end{cases}$$

We evaluate the terms of H order by order. There is no term of order zero. The term of order one in $\mathbf{q}$ is

$$\frac{\Lambda}{2}\int \mathbf{dr}\mathbf{dv_1}\mathbf{dv}_2\mathbf{dq}\, w(\mathbf{v}_1,\mathbf{v}_2;\mathbf{q})f(\mathbf{v}_1)f(\mathbf{v}_2)\left(\frac{\partial p}{\partial \mathbf{v}_1}-\frac{\partial p}{\partial \mathbf{v}_2}\right).\mathbf{q},$$

which is zero because $w(\mathbf{v}_1,\mathbf{v}_2;\mathbf{q})$ is an even function of $\mathbf{q}$ (see point 3 of appendix (A.6.2)). At second order in $\mathbf{q}$ the Hamiltonian reads

$$\begin{aligned} H_{\text{Landau}}[f,p] &= \frac{\Lambda}{4}\int \mathbf{dr}\mathbf{dv}_1\mathbf{dv}_2\mathbf{dq}\, f(\mathbf{v}_1)f(\mathbf{v}_2)\left\{w\left[\frac{\partial^2 p}{\partial \mathbf{v}_1\partial \mathbf{v}_1}+\frac{\partial^2 p}{\partial \mathbf{v}_2\partial \mathbf{v}_2}+\left(\frac{\partial p}{\partial \mathbf{v}_1}-\frac{\partial p}{\partial \mathbf{v}_2}\right)\left(\frac{\partial p}{\partial \mathbf{v}_1}-\frac{\partial p}{\partial \mathbf{v}_2}\right)\right]\right. \\ &+ \left.\left(\frac{\partial p}{\partial \mathbf{v}_1}-\frac{\partial p}{\partial \mathbf{v}_2}\right)\left(\frac{\partial w}{\partial \mathbf{v}_1}-\frac{\partial w}{\partial \mathbf{v}_2}\right)\right\}:\mathbf{qq}. \end{aligned}$$

In this expression, in order to make appear the tensor $\mathbf{B}(\mathbf{v},\mathbf{v}_2)=\Lambda\int \mathbf{dq}\, w(\mathbf{v},\mathbf{v}_2;\mathbf{q})\mathbf{qq}/2$ (see equation (5.17)), we integrate by parts the terms involving $\frac{\partial w}{\partial \mathbf{v}_1}$ and $\frac{\partial w}{\partial \mathbf{v}_2}$, we develop the derivatives of products generated by partial integration, we use equation (5.17) and we obtain

$$\begin{aligned} H_{\text{Landau}}[f,p] &= \frac{1}{2}\int \mathbf{dr}\mathbf{dv}_1\mathbf{dv}_2\,\mathbf{B}(\mathbf{v}_1,\mathbf{v}_2)\left\{f(\mathbf{v}_1)f(\mathbf{v}_2)\left(\frac{\partial p}{\partial \mathbf{v}_1}-\frac{\partial p}{\partial \mathbf{v}_2}\right)\left(\frac{\partial p}{\partial \mathbf{v}_1}-\frac{\partial p}{\partial \mathbf{v}_2}\right)+\right. \\ &+ \left.\left(\frac{\partial p}{\partial \mathbf{v}_1}-\frac{\partial p}{\partial \mathbf{v}_2}\right)\left(\frac{\partial f}{\partial \mathbf{v}_2}f(\mathbf{v}_1)-\frac{\partial f}{\partial \mathbf{v}_1}f(\mathbf{v}_2)\right)\right\}. \end{aligned}$$

Using the property that $\mathbf{B}(\mathbf{v}_1,\mathbf{v}_2)=\mathbf{B}(\mathbf{v}_2,\mathbf{v}_1)$ (see appendix A.6.2), we have for every function g of $(\mathbf{v}_1,\mathbf{v}_2)$: $\int \mathbf{dv_1}\mathbf{dv}_2\mathbf{B}(\mathbf{v}_1,\mathbf{v}_2)g(\mathbf{v}_1,\mathbf{v}_2)=\int \mathbf{dv_1}\mathbf{dv}_2\mathbf{B}(\mathbf{v}_1,\mathbf{v}_2)g(\mathbf{v}_2,\mathbf{v}_1)$. Using this property we have

$$H_{\text{Landau}}[f,p] = \int \mathbf{dr}\mathbf{dv}_1\mathbf{dv}_2\, \mathbf{B}(\mathbf{v}_1,\mathbf{v}_2) \left\{ f(\mathbf{v}_1)f(\mathbf{v}_2) \left(\frac{\partial p}{\partial \mathbf{v}_1}\frac{\partial p}{\partial \mathbf{v}_1} - \frac{\partial p}{\partial \mathbf{v}_1}\frac{\partial p}{\partial \mathbf{v}_2} \right) + \frac{\partial p}{\partial \mathbf{v}_1}\frac{\partial f}{\partial \mathbf{v}_2} f(\mathbf{v}_1) - \frac{\partial p}{\partial \mathbf{v}_1}\frac{\partial f}{\partial \mathbf{v}_1} f(\mathbf{v}_2) \right\}.$$

We integrate by parts the last term with respect to $\mathbf{v}_1$ to obtain

$$\begin{aligned} H_{\text{Landau}}[f,p] \;=\; & \int \mathbf{dr}\mathbf{dv}_1\mathbf{dv}_2\, f(\mathbf{v}_1) \left\{ \frac{\partial p}{\partial \mathbf{v}_1}\mathbf{B}(\mathbf{v}_1,\mathbf{v}_2)\frac{\partial f}{\partial \mathbf{v}_2} \right. \\ & \left. + \frac{\partial p}{\partial \mathbf{v}_1}\frac{\partial p}{\partial \mathbf{v}_1}\mathbf{B}(\mathbf{v}_1,\mathbf{v}_2) f(\mathbf{v}_2) + \frac{\partial}{\partial \mathbf{v}_1}\left(\mathbf{B}(\mathbf{v}_1,\mathbf{v}_2) f(\mathbf{v}_2) \frac{\partial p}{\partial \mathbf{v}_1} \right) \right\} \\ & - \int \mathbf{dr}\mathbf{dv}_1\mathbf{dv}_2\, f(\mathbf{v}_1)f(\mathbf{v}_2) \frac{\partial p}{\partial \mathbf{v}_1}\frac{\partial p}{\partial \mathbf{v}_2}\mathbf{B}(\mathbf{v}_1,\mathbf{v}_2). \end{aligned}$$

From here, using equation (4.15) we obtain

$$H_{\text{Landau}}[f,p] = H_{MF}[f,p] + H_I[f,p], \tag{A.18}$$

with

$$H_{MF}[f,p] = \int \mathbf{dr}\mathbf{dv}_1 f \left\{ \mathbf{b}[f] . \frac{\partial p}{\partial \mathbf{v}_1} + \frac{\partial}{\partial \mathbf{v}_1}\left(\mathbf{D}[f] \frac{\partial p}{\partial \mathbf{v}_1} \right) + \mathbf{D}[f] : \frac{\partial p}{\partial \mathbf{v}_1}\frac{\partial p}{\partial \mathbf{v}_1} \right\},$$

and

$$H_I[f,p] = -\int \mathbf{dr}\mathbf{dv}_1\mathbf{dv}_2 f(\mathbf{v}_1)f(\mathbf{v}_2) \frac{\partial p}{\partial \mathbf{v}_1}\frac{\partial p}{\partial \mathbf{v}_2} : \mathbf{B}(\mathbf{v}_1,\mathbf{v}_2).$$

A.8. From the Balescu–Guernsey–Lenard Hamiltonian to the Landau Hamiltonian

In this appendix, we show that the Hamiltonian describing the large deviations associated with the Landau equation can be recovered from the one describing the large deviations associated with the Balescu–Guernsey–Lenard equation, within the Landau approximation. In section A.8.1, we perform a series expansion of the logarithm in the large deviation Hamiltonian for the Balescu–Guernsey–Lenard equation. In section A.8.2, we show that within the Landau approximation, only the first two terms of the series expansion are relevant, and we recover the quadratic large deviation Hamiltonian associated with the Landau equation.

A.8.1. Series expansion of the logarithm

In this appendix, we expand H from the formula (5.28) in powers of p. This amounts at a cumulant expansion for the statistics of the fluctuations. We expand the logarithm in formula (5.28) to obtain

$$H[f,p] = \frac{1}{4\pi L^3} \sum_{\mathbf{k}} \int \mathrm{d}\omega \sum_{n=1}^{+\infty} \frac{1}{n} \left(\mathcal{J}[f,p](\mathbf{k},\omega)\right)^n = \sum_{n=1}^{+\infty} H^{(n)}[f,p]. \tag{A.19}$$

The second equality defines $H^{(n)}$ as being the terms homogeneous of order n in p in this expansion. It is the n-th cumulant.

We also define $\mathbf{B}^{(m)}$ as

$$\mathbf{B}^{(m)}(\mathbf{v}_1,\dots,\mathbf{v}_{2m}) = \frac{(2\pi)^{2m}}{4\pi m L^3} \sum_{\mathbf{k}} \int_{\Gamma} \mathrm{d}\omega \, \frac{W(\mathbf{k})^{2m}}{|\varepsilon(\mathbf{k},\omega)|^{2m}} \mathbf{k}^{\otimes 2m} \prod_{i=1}^{2m} \delta(\omega - \mathbf{k}.\mathbf{v}_i).$$

$\mathbf{B}^{(m)}$ is a rank $2m$ tensor. $l^{(k)}$ and $q^{(k)}$ are defined by the relations. We have $\mathcal{J}[f,p] = \mathcal{L}[f,p] + Q[f,p,p]$, where $\mathcal{L}$ and Q are defined in equations (4.53) and (4.54). We will need to compute $(\mathcal{L}[f,p])^k$, which is $\mathcal{L}[f,p]$ to the power k. We define $l^{(k)}$ and $q^{(k)}$ by

$$(\mathcal{L}[f,p])^k = \int \mathrm{d}\mathbf{v}_1 \cdots \mathrm{d}\mathbf{v}_{2k} \, l^{(k)}[f,p] \prod_{j=1}^{k} \mathbf{A}(\mathbf{k},\omega,\mathbf{v}_{2j-1},\mathbf{v}_{2j}),$$

and

$$(Q[f,p,p])^k = \int \mathrm{d}\mathbf{v}_1 \cdots \mathrm{d}\mathbf{v}_{2k} \, q^{(k)}[f,p,p] \prod_{j=1}^{k} \mathbf{A}(\mathbf{k},\omega,\mathbf{v}_{2j-1},\mathbf{v}_{2j}).$$

$l^{(k)}$ and $q^{(k)}$ are both tensors of order $2k$. $l^{(k)}$ depends on p as a homogeneous function of order k. $q^{(k)}$ depends on p as a homogeneous function of order $2k$.

In the expansion of $(\mathcal{J}[f,p])^n$ using $\mathcal{J}[f,p] = \mathcal{L}[f,p] + Q[f,p,p]$, we see that for all $m \in [n/2,n] \cap \mathbb{N}$, $\mathcal{L}^{2m-n}[f,p]\, Q^{n-m}[f,p,p]$ is homogeneous of order n in p. Using this remark, from equation (A.19) we obtain

$$H^{(n)}[f,p] = \sum_{m \in [n/2,n] \cap \mathbb{N}} \int \mathrm{d}\mathbf{v}_1 \cdots \mathrm{d}\mathbf{v}_{2m} \begin{pmatrix} m \\ 2m-n \end{pmatrix} \frac{1}{(2\pi)^{2m}} \times \mathbf{B}^{(m)}(\mathbf{v}_1,\dots,\mathbf{v}_{2m}) : l^{(2m-n)}[f,p]\, q^{(n-m)}[f,p,p], \tag{A.20}$$

where the symbol " : " means a contraction of a tensor of order $2m$ with another tensor of order $2m$.

A.8.2. Hierarchy of the series expansion within the Landau approximation

Let us first recall that we can obtain the Landau equation from the Balescu–Guernsey–Lenard equation. The collision kernel for the Balescu–Guernsey–Lenard equation converges to the Landau collision kernel in the limit where all the wavevectors in (**??**) satisfy $k\lambda_D \gg 1$. In our system of plasma unit, where the length unit is renormalized by the Debye length, this means that the Balescu–Guernsey–Lenard collision kernel converges toward the Landau collision kernel in the limit of infinitely large wavevectors. In a similar way, we obtain the large deviation Hamiltonian for the Landau equation H_{Landau} from the large deviation Hamiltonian H (A.19) of the empirical measure of N Coulomb interacting particles using the same limit. In the expression of the tensor $\mathbf{B}^{(1)} = \mathbf{B}$

$$\mathbf{B}^{(1)} = \mathbf{B}(\mathbf{v}_1, \mathbf{v}_2) = \pi \left(\frac{\lambda_D}{L}\right)^3 \int_{-\infty}^{+\infty} \mathrm{d}\omega \sum_{\mathbf{k}} \frac{\mathbf{k}\mathbf{k}}{k^{4n} \left|\varepsilon[f](\omega, \mathbf{k})\right|^2} \delta(\omega - \mathbf{k}.\mathbf{v}_1)\, \delta(\omega - \mathbf{k}.\mathbf{v}_2)\,,$$

the Landau approximation implies that $k \gg 1$. In this context, we can consider that the dielectric function ε is equal to one. From there, a clear hierarchy appears in the cumulant series expansion (A.19) . For $n \geq 2$, the terms involving

$$\mathbf{B}^{(n)}(\mathbf{v}_1, \ldots, \mathbf{v}_{2n}) = \frac{(2\pi)^{2n}}{4\pi n} \left(\frac{\lambda_D}{L}\right)^3 \sum_{\mathbf{k}} \int_\Gamma \mathrm{d}\omega \, \frac{\mathbf{k}^{\otimes 2n}}{k^{4n} \left|\varepsilon(\mathbf{k}, \omega)\right|^{2n}} \prod_{i=1}^{2n} \delta(\omega - \mathbf{k}.\mathbf{v}_i)$$

will be negligible with respect to the terms involving $\mathbf{B}^{(1)} = \mathbf{B}$.

Let us define

$$\mathbf{B}_{\mathbf{k}}^{(n)}(\mathbf{v}_1, \ldots, \mathbf{v}_{2n}) = \int_\Gamma \mathrm{d}\omega \, \frac{\mathbf{k}^{\otimes 2n}}{k^{4n} \left|\varepsilon(\mathbf{k}, \omega)\right|^{2n}} \prod_{i=1}^{2n} \delta(\omega - \mathbf{k}.\mathbf{v}_i)\,,$$

such that

$$\mathbf{B}^{(n)}(\mathbf{v}_1, \ldots, \mathbf{v}_{2n}) = \frac{(2\pi)^{2n}}{4\pi n} \sum_{\mathbf{k}} \left(\frac{\lambda_D}{L}\right)^3 \mathbf{B}_{\mathbf{k}}^{(n)}(\mathbf{v}_1, \ldots, \mathbf{v}_{2n})\,.$$

Let us evaluate the size of $\mathbf{B}_{\mathbf{k}}^{(n)}$ in terms of the wavevectors $\mathbf{k}$. We have,

$$\mathbf{B}_{\mathbf{k}}^{(n)}(\mathbf{v}_1, \ldots, \mathbf{v}_{2n}) = k^{1-4n} \frac{\mathbf{m}^{\otimes 2n}}{\left|\varepsilon(\mathbf{k}, \omega)\right|^{2n}} \prod_{i=2}^{2n} \delta(\mathbf{m}.(\mathbf{v}_1 - \mathbf{v}_i))\,,$$

where $\mathbf{m} = \mathbf{k}/k$. Then,

$$\left(\frac{\lambda_D}{L}\right)^3 \mathbf{B}_{\mathbf{k}}^{(n)} \underset{k \gg 1}{=} \mathcal{O}\left(\left(\frac{\lambda_D}{Lk}\right)^3 \left(\frac{1}{k}\right)^{4n-4}\right), \tag{A.21}$$

where $\mathcal{O}(k^m)$ means that the term is of order k^m.

Furthermore, we note the wavevectors $\mathbf{k}$ are of the form $2\pi\left(\lambda_D/L\right)\mathbf{l}$ with $\mathbf{l} \in \mathbb{Z}^3$. Then $\left(\frac{\lambda_D}{Lk}\right)^3$ is of order one at most. Thus, we can conclude that within the Landau approximation ($k \gg 1$ within the set of non-dimensional plasma units) all the tensors $\mathbf{B}^{(n)}$ are negligible except for $\mathbf{B}^{(1)} = \mathbf{B}$. We have presented all the computation and this estimation in a finite box of length L. However similar reasoning generalize easily to an infinite box.

As a conclusion, at leading order, we can just keep the terms involving $\mathbf{B}^{(1)}$ in the cumulant series expansion, and the large deviations Hamiltonian for the Landau equation reads

$$\begin{aligned} H_{\text{Landau}}\left[f,p\right] &= \int \mathbf{dr}\mathbf{dv}_1 f \left\{ \mathbf{b}\left[f\right].\frac{\partial p}{\partial \mathbf{v}_1} + \frac{\partial}{\partial \mathbf{v}_1}\left(\mathbf{D}\left[f\right]\frac{\partial p}{\partial \mathbf{v}_1}\right) + \mathbf{D}\left[f\right] : \frac{\partial p}{\partial \mathbf{v}_1}\frac{\partial p}{\partial \mathbf{v}_1} \right\} \\ &- \int \mathbf{dr}\mathbf{dv}_1\mathbf{dv}_2 f(\mathbf{v}_1) f(\mathbf{v}_2) \frac{\partial p}{\partial \mathbf{v}_1}\frac{\partial p}{\partial \mathbf{v}_2} : \mathbf{B}\left(\mathbf{v}_1,\mathbf{v}_2\right). \end{aligned} \tag{A.22}$$

This is exactly the Hamiltonian we derived from the Boltzmann equation large deviation Hamiltonian in section 5.3.3.

B. Appendices relative to the second part

In these appendices, we detail the computations relative to the microscopic derivation of the fluctuating Navier-Stokes equations and the ensuing gradient-flow structure.

B.1. Properties of the kinetic noise and the linearized kinetic operator

We first discuss conservation properties of the fluctuating Boltzmann equation.

B.1.1. Conservation laws for the kinetic equation

The Boltzmann equation (7.3) preserves total mass, momentum and energy

$$M[f] = \int \mathrm{d}\mathbf{v}\, f, \quad \mathbf{P}[f] = \int \mathrm{d}\mathbf{v}\, \mathbf{v} f, \quad E[f] = \int \mathrm{d}\mathbf{v}\, \frac{v^2}{2} f,$$

as a consequence of the symmetries of its collision kernel, explained in appendix A.6.1. These conservation properties can been seen at the level of the collision operator

$$\Pi[Q(f,f)]] = \begin{pmatrix} \int \mathrm{d}\mathbf{v}\, Q(f,f) \\ \int \mathrm{d}\mathbf{v}\, \mathbf{v} Q(f,f) \\ \int \mathrm{d}\mathbf{v}\, \frac{\mathbf{v}^2}{2} Q(f,f) \end{pmatrix} = 0. \tag{B.1}$$

As a consequence of (B.1) and the definition (7.26) of $\mathcal{L}_{M_h}$, we have that $\{1, \mathbf{v}, \mathbf{v^2}/2\} \subset \ker\left(\mathcal{L}^\dagger_{M_h}\right) = \ker\left(\mathcal{L}^\dagger_{M_h}\right)$ for the scalar product weighted by the Maxwellian M_h.

B.1.2. Conservation laws for the kinetic noise

As a consequence of the microscopical conservation laws of the system (mass, momentum, energy), the kinetic noise η satisfies the following conservation properties:

$$\Pi[\eta] = 0. \tag{B.2}$$

This is a consequence of the symmetry at the level of the large deviation Hamiltonian, explained in 9. of section 3.7.2.3. Then, realizations of η violating mass, momentum, or energy conservation is then associated with a zero probability.

B.2. Computation of the viscous and noise terms for the compressible Navier–Stokes equations

In this section, we present the explicit computation that allows to bridge from equations (7.31-7.33) to the compressible fluctuation Navier–Stokes system. The computation of the deterministic term is essentially the one presented in [14]. The novelty here is the computation of the stochastic term coming from the noise term in the fluctuating Boltzmann equation. The starting point of this appendix is

$$\partial_t \rho + \nabla \cdot (\rho \mathbf{u}) + \alpha \nabla \cdot \left(\int \mathrm{d}\mathbf{v}\, \mathbf{v} g^1 M_h \right) = 0, \tag{B.3}$$

$$\rho \partial_t \mathbf{u} + \rho \left(\mathbf{u} \cdot \nabla \right) \mathbf{u} + \nabla(\rho\theta) + \alpha \nabla \cdot \left(\int \mathrm{d}\mathbf{v}\, \mathbf{v} \otimes \mathbf{v} g^1 M_h \right) = 0, \tag{B.4}$$

$$\frac{3}{2}\rho \partial_t \theta + \rho\theta \nabla \cdot \mathbf{u} + \frac{3}{2}\rho \left(\mathbf{u} \cdot \nabla \right) \theta + \frac{\alpha}{2} \nabla \cdot \left(\int \mathrm{d}\mathbf{v}\, v^2 \mathbf{v} g^1 M_h \right) = 0, \tag{B.5}$$

where the order α terms can be computed through

$$g^1 = g^{1,d} + g^{1,s},$$

where

$$\mathcal{L}_{M_h}[g^{1,d}] = -\frac{(\partial_t + \mathbf{v} \cdot \nabla)[M_h]}{M_h}, \tag{B.6}$$

$$\mathcal{L}_{M_h}[g^{1,s}] = \sqrt{\epsilon\alpha^2}\frac{\eta}{M_h}. \tag{B.7}$$

B.2.1. Equation for the density

We start by computing the order one in α terms of the density equation (B.3). We define

$$C_{\rho,d} = \nabla \cdot \left(\int \mathrm{d}\mathbf{v}\, \mathbf{v} g^{1,d} M_h \right), \text{ and } C_{\rho,s} = \nabla \cdot \left(\int \mathrm{d}\mathbf{v}\, \mathbf{v} g^{1,s} M_h \right)$$

which account respectively for the deterministic and the stochastic order α correction in the density equation (B.3), such as

$$\nabla \cdot \left(\int \mathrm{d}\mathbf{v}\, \mathbf{v} g^1 M_h \right) = C_{\rho,d} + C_{\rho,s}.$$

It is straightforward to show that $C_{\rho,s}$ vanishes because $g^{1,s} = \sqrt{\epsilon\alpha^2}\mathcal{L}_{M_h}^{-1}\left[\frac{\eta}{M_h}\right] \in \ker\left(\mathcal{L}_{M_h}\right)^\top$. To compute $C_{\rho,d}$ we use

$$\mathbf{A}' = \mathcal{L}_{M_h}^{-1}[\mathbf{A}] = -a\mathbf{A}\ ,\ \mathbf{B}' = \mathcal{L}_{M_h}^{-1}[\mathbf{B}] = -b\mathbf{B},$$

where a and b are negative functions depending on ρ, θ and V the norm of the reduced velocity $\mathbf{V} = \theta^{-1/2}(\mathbf{v} - \mathbf{u})$. In the following, we omit the dependence in ρ and θ when writing $a(V)$ and $b(V)$. To compute $C_{\rho,d}$, the first step is to use the change of variable $\mathbf{V} = \theta^{-1/2}(\mathbf{v} - \mathbf{u})$ in the integral over $\mathbf{v}$. Then, using parity and symmetry arguments such as

$$\int \mathrm{d}\mathbf{V} V_i V_j b(V) \mathrm{e}^{-V^2/2} = \frac{1}{3}\delta_{ij} \int \mathrm{d}\mathbf{V} V^2 b(V) \mathrm{e}^{-V^2/2}, \tag{B.8}$$

and

$$\int \mathrm{d}\mathbf{V} V^4 a(V) \mathrm{e}^{-V^2/2} = 5 \int \mathrm{d}\mathbf{V} V^2 a(V) \mathrm{e}^{-V^2/2}, \tag{B.9}$$

one can show that $C_{\rho,d}$ also vanishes. In conclusion, the density equation has no correction term of order α and it still reads

$$\partial_t \rho + \nabla \cdot (\rho \mathbf{u}) = 0$$

in the compressible Navier–Stokes system.

B.2.2. Equation for the velocity

To compute the order α correction in the velocity equation (B.4), we define

$$\mathbf{C}_{\mathbf{u},d} = \nabla \cdot \left(\int \mathrm{d}\mathbf{v}\, \mathbf{v} \otimes \mathbf{v} g^{1,d} M_h \right), \quad \text{and} \quad \mathbf{C}_{\mathbf{u},s} = \nabla \cdot \left(\int \mathrm{d}\mathbf{v}\, \mathbf{v} \otimes \mathbf{v} g^{1,s} M_h \right).$$

Computation of the viscous (deterministic) term. We start by computing the deterministic contribution $\mathbf{C}_{\mathbf{u},d}$. Once again, we start by change of variable $\mathbf{V} = \theta^{-1/2}(\mathbf{v} - \mathbf{u})$ in the integral over $\mathbf{v}$ and we use

$$g^{1,d} = a(V) \frac{\nabla\theta}{\sqrt{\theta}} \cdot \mathbf{A}(\mathbf{V}) + \frac{1}{2} b(V) \mathbf{B}(\mathbf{V}) : \boldsymbol{\sigma}(\mathbf{u}). \tag{B.10}$$

Using parity arguments and the symmetry relation (B.8), we obtain

$$(\mathbf{C}_{\mathbf{u},d})_i = \partial_j \left\{ \frac{\theta}{2(2\pi)^{3/2}} \rho \sigma_{kl} \int \mathrm{d}\mathbf{V}\, V_i V_j \left(V_k V_l - \frac{1}{3} V^2 \delta_{kl} \right) b(V) \mathrm{e}^{-V^2/2} \right\}, \tag{B.11}$$

where Einstein summation is implied and $(\mathbf{C}_{\mathbf{u},d})_i$ denotes the i-th component of $\mathbf{C}_{\mathbf{u},d}$. Because b only depends on the norm of the reduced velocity $\mathbf{V}$, it is possible to show

$$\int \mathrm{d}\mathbf{V}\, V_i V_j V_k V_l b(V) \mathrm{e}^{-V^2/2} = \frac{1}{15} \int \mathrm{d}\mathbf{V}\, V^4 b(V) \mathrm{e}^{-V^2/2} \left\{ \delta_{ij}\delta_{kl} + \delta_{ik}\delta_{jl} + \delta_{il}\delta_{jk} \right\}.$$

Inserting this symmetry relation in (B.11) leads to the viscous term

$$(\mathbf{C}_{\mathbf{u},d})_i = -\partial_j \left\{ \frac{1}{2} \nu \sigma_{kl}(\mathbf{u}) \left(\delta_{ik}\delta_{jl} + \delta_{il}\delta_{jk} - \frac{2}{3}\delta_{ij}\delta_{kl} \right) \right\}, \tag{B.12}$$

where we introduced the viscosity

$$\nu = \frac{-2}{15}\frac{\rho\theta}{\sqrt{2\pi}}\int_0^\infty \mathrm{d}V\, V^6 b\left(V\right)\mathrm{e}^{-V^2/2}. \tag{B.13}$$

(in agreement with Bardos-Golse-Levermore). Note that the integral in (B.13) is performed over the norm of the velocity, rather than the 3d velocity vector itself. Recalling the definition of the stress tensor

$$\sigma_{ij}\left(\mathbf{u}\right) = \partial_j u_i + \partial_i u_j - \frac{2}{3}\delta_{ij}\partial_k u_k, \tag{B.14}$$

we have

$$\sigma_{kl}\left(\mathbf{u}\right)\left(\delta_{ik}\delta_{jl} + \delta_{il}\delta_{jk} - \frac{2}{3}\delta_{ij}\delta_{kl}\right) = 2\sigma_{ij}\left(\mathbf{u}\right).$$

We conclude that the viscous term (B.12) reads

$$\mathbf{C}_{\mathbf{u},d} = -\nabla\cdot\left\{\nu\boldsymbol{\sigma}\left(\mathbf{u}\right)\right\}.$$

Computation of the stochastic term. Using

$$g^{1,s} = \sqrt{\epsilon\alpha^2}\mathcal{L}_{M_h}^{-1}\left[\frac{\eta}{M_h}\right],$$

the stochastic term in the velocity equation (B.4) reads

$$\mathbf{C}_{\mathbf{u},s} = \sqrt{\epsilon\alpha^2}\nabla\cdot\left(\int \mathrm{d}\mathbf{v}\,\mathbf{v}\otimes\mathbf{v}\mathcal{L}_{M_h}^{-1}\left[\frac{\eta}{M_h}\right]M_h\right).$$

Performing the change of variable $\mathbf{V} = \theta^{-1/2}\left(\mathbf{v}-\mathbf{u}\right)$ yields

$$\mathbf{C}_{\mathbf{u},s} = \sqrt{\epsilon\alpha^2}\nabla\cdot\left\{\frac{\rho}{\left(2\pi\right)^{3/2}}\int \mathrm{d}\mathbf{V}\,\left(\theta\left(\mathbf{B}\left(\mathbf{V}\right)+\frac{1}{3}V^2\mathrm{Id}\right)+\mathbf{u}\otimes\mathbf{u}\right.\right.$$
$$\left.\left.+\sqrt{\theta}\left(\mathbf{u}\otimes\mathbf{V}+\mathbf{V}\otimes\mathbf{u}\right)\right)\mathcal{L}_M^{-1}\left[\frac{\eta}{M}\right]\mathrm{e}^{-V^2/2}\right\},$$

where $\mathcal{L}_M^{-1}\left[\frac{\eta}{M}\right]$ is evaluated in the velocity $\sqrt{\theta}\mathbf{V}+\mathbf{u}$ and where we used $M_h\left(\sqrt{\theta}\mathbf{V}+\mathbf{u}\right) = \rho\theta^{-3/2}M\left(\mathbf{V}\right)$ where M is the absolute Maxwellian (7.11). Now, we recall that $\mathcal{L}_M^{-1}\left[\frac{\eta}{M}\right]\in\ker\mathcal{L}^\top$ for the scalar product weighted by the absolute Maxwellian distribution and that $\mathcal{L}_M^{-1}$ is self-adjoint with respect to this same scalar product. Hence,

$$\mathbf{C}_{\mathbf{u},s} = -\sqrt{\epsilon\alpha^2}\nabla\cdot\left\{\theta^{5/2}\int \mathrm{d}\mathbf{V}\, b\left(V\right)\mathbf{B}\left(\mathbf{V}\right)\eta\left(\sqrt{\theta}\mathbf{V}+\mathbf{u}\right)\right\}.$$

Thus, the velocity equation in the compressible Navier–Stokes system reads

$$\rho\partial_t\mathbf{u} + \rho\left(\mathbf{u}\cdot\nabla\right)\mathbf{u} + \nabla(\rho\theta) = \frac{\alpha}{2}\nabla\cdot\left(\nu\boldsymbol{\sigma}\left(\mathbf{u}\right)\right) + \sqrt{\epsilon\alpha^4}\nabla\cdot\left(\sqrt{\theta}\mathbf{J}\right), \tag{B.15}$$

with

$$J_{ij} = \theta^2\int \mathrm{d}\mathbf{V}\, b\left(V\right)B_{ij}\left(\mathbf{V}\right)\eta\left(\sqrt{\theta}\mathbf{V}+\mathbf{u}\right).$$

B.2.3. Equation for the temperature

To compute the order α correction in the temperature equation (B.5), we define

$$C_{\theta,d} = \frac{1}{2}\nabla\cdot\left(\int \mathrm{d}\mathbf{v}\, v^2\mathbf{v} g^{1,d} M_h\right), \quad \text{and} \quad C_{\theta,s} = \frac{1}{2}\nabla\cdot\left(\int \mathrm{d}\mathbf{v}\, v^2\mathbf{v} g^{1,s} M_h\right).$$

Computation of the deterministic term. The first step is to write $C_{\theta,d}$ in reduced velocity variable and to use the formula (B.10) for $g^{1,d}$

$$C_{\theta,d} = -\frac{1}{2}\nabla\cdot\left\{\frac{\rho}{(2\pi)^{3/2}}\int \mathrm{d}\mathbf{V}\,\left(\theta V^2 + u^2 + 2\sqrt{\theta}\mathbf{u}\cdot\mathbf{V}\right)\left(\sqrt{\theta}\mathbf{V}+\mathbf{u}\right)\right.$$
$$\left.\times\left(a\left(V\right)\frac{\nabla\theta}{\sqrt{\theta}}\cdot\mathbf{A}(\mathbf{V}) + \frac{1}{2}b\left(V\right)\mathbf{B}(\mathbf{V}):\boldsymbol{\sigma}(\mathbf{u})\right)\mathrm{e}^{-V^2/2}\right\}.$$

Then, using parity and symmetry arguments, we can decompose $C_{\theta,d}$ such as

$$C_{\theta,d} = C_\theta^A + C_\theta^B,$$

where C_θ^A is the part yielding the thermal diffusion term

$$C_\theta^A = -\frac{1}{2}\nabla\cdot\left\{\nabla\theta\frac{\rho\theta}{6\left(2\pi\right)^{3/2}}\int \mathrm{d}\mathbf{V}\, a\left(V\right)V^4\left(V^2-5\right)\mathrm{e}^{-V^2/2}\right\},$$

and C_θ^B is the term yielding the viscous term

$$C_\theta^B = -\frac{1}{2}\partial_j\left\{\frac{\rho\theta u_i\sigma_{kl}(\mathbf{u})}{2\left(2\pi\right)^{3/2}}\int \mathrm{d}\mathbf{V}\, b\left(V\right)V_iV_jB_{kl}\left(\mathbf{V}\right)\mathrm{e}^{-V^2/2}\right\}.$$

We define the thermal diffusivity in agreement with [14]

$$\kappa = -\frac{1}{6}\frac{\rho\theta}{\left(2\pi\right)^{1/2}}\int_0^\infty \mathrm{d}V\, a\left(V\right)V^4\left(V^2-5\right)^2\mathrm{e}^{-V^2/2}. \tag{B.16}$$

Using the symmetry relation (B.9), we establish

$$C_\theta^A = -\nabla\cdot\left(\kappa\nabla\theta\right).$$

The computation of the viscous term is very close to the one of the velocity equation and the result is

$$C_\theta^B = -\nabla\cdot\left(\nu\mathbf{u}\cdot\boldsymbol{\sigma}\left(\mathbf{u}\right)\right).$$

Recalling that $\boldsymbol{\sigma}$ is a traceless symmetric tensor and using its definition (B.14), we note $2\nabla\cdot\left(\nu\mathbf{u}\cdot\boldsymbol{\sigma}\left(\mathbf{u}\right)\right) = \nu\boldsymbol{\sigma}\left(\mathbf{u}\right):\boldsymbol{\sigma}\left(\mathbf{u}\right)$. Finally the order α deterministic correction to the temperature equation reads

$$C_{\theta,d} = -\nabla\cdot\left(\kappa\nabla\theta\right) - \frac{1}{2}\nu\boldsymbol{\sigma}\left(\mathbf{u}\right):\boldsymbol{\sigma}\left(\mathbf{u}\right).$$

Computation of the stochastic term. Using

$$g^{1,s} = \sqrt{\epsilon\alpha^2}\mathcal{L}_{M_h}^{-1}\left[\frac{\eta}{M_h}\right],$$

the stochastic term in the energy equation (B.5) reads

$$C_{\theta,s} = \frac{1}{2}\sqrt{\epsilon\alpha^2}\nabla\cdot\left(\int \mathrm{d}\mathbf{v}\, v^2\mathbf{v}\mathcal{L}_{M_h}^{-1}\left[\frac{\eta}{M_h}\right]M_h\right).$$

Performing the change of variable $\mathbf{V} = \theta^{-1/2}(\mathbf{v}-\mathbf{u})$ yields

$$C_{\theta,s} = \frac{1}{2}\sqrt{\epsilon\alpha^2}\nabla\cdot\left\{\frac{\rho}{(2\pi)^{3/2}}\int \mathrm{d}\mathbf{V}\,\left(\theta V^2+u^2+2\sqrt{\theta}\mathbf{u}\cdot\mathbf{V}\right)\left(\sqrt{\theta}\mathbf{V}+\mathbf{u}\right)\mathcal{L}_{M_h}^{-1}\left[\frac{\eta}{M_h}\right]\mathrm{e}^{-V^2/2}\right\},$$

where M_h and η are evaluated in the velocity $\sqrt{\theta}\mathbf{V}+\mathbf{u}$. Now, we recall that $\mathcal{L}_{M_h}^{-1}\left[\frac{\eta}{M_h}\right] \in \ker\mathcal{L}^\top$ for the scalar product weighted by the absolute Maxwellian distribution and that $\mathcal{L}_{M_h}^{-1}$ is self adjoint with respect to this same scalar product. Hence,

$$C_{\theta,s} = \frac{1}{2}\sqrt{\epsilon\alpha^2}\nabla\cdot\left\{\frac{\rho}{(2\pi)^{3/2}}\int \mathrm{d}\mathbf{V}\,\left(\theta^{3/2}V^2\mathbf{V}+2\theta\left(\mathbf{u}\cdot\mathbf{V}\right)\mathbf{V}\right)\mathcal{L}_{M_h}^{-1}\left[\frac{\eta}{M_h}\right]\mathrm{e}^{-V^2/2}\right\}.$$

Let us recall that $V^2\mathbf{V} = 2\mathbf{A}(\mathbf{V})+5\mathbf{V}$ and $\mathbf{V}\otimes\mathbf{V} = \mathbf{B}(\mathbf{V})+\frac{1}{3}V^2\mathrm{Id}$ to express the stochastic term $C_{\theta,s}$ in terms of the vector $\mathbf{A}$ and the tensor $\mathbf{B}$

$$C_{\theta,s} = \frac{1}{2}\sqrt{\epsilon\alpha^2}\nabla\cdot\left\{\frac{\rho}{(2\pi)^{3/2}}\int \mathrm{d}\mathbf{V}\,\left(2\theta^{3/2}A(\mathbf{V})+2\theta\mathbf{u}\cdot\mathbf{B}(\mathbf{V})\right)\mathcal{L}_{M_h}^{-1}\left[\frac{\eta}{M_h}\right]\mathrm{e}^{-V^2/2}\right\}.$$

Using the fact that $\mathcal{L}_{M_h}^{-1}$ is self-adjoint, we obtain

$$C_{\theta,s} = -\sqrt{\epsilon\alpha^2}\nabla\cdot\left\{\theta^{3/2}\int \mathrm{d}\mathbf{V}\,\left(\theta^{3/2}a(V)\mathbf{A}(\mathbf{V})+\theta b(V)\mathbf{u}\cdot\mathbf{B}(\mathbf{V})\right)\eta\left(\sqrt{\theta}\mathbf{V}+\mathbf{u}\right)\right\}.$$

In conclusion, the energy equation of the compressible Navier–Stokes system reads

$$\frac{3}{2}\rho\partial_t\theta+\rho\theta\nabla\cdot\mathbf{u}+\frac{3}{2}\rho\left(\mathbf{u}\cdot\nabla\right)\theta = \alpha\nabla\cdot(\kappa\nabla\theta)+\alpha\frac{\nu}{2}\boldsymbol{\sigma}(\mathbf{u}):\boldsymbol{\sigma}(\mathbf{u})+\sqrt{\epsilon\alpha^4}\nabla\cdot\left(\mathbf{J}^\theta\right), \quad \text{(B.17)}$$

with

$$\mathbf{J}^\theta = \theta^{3/2}\int \mathrm{d}\mathbf{V}\,\left(\theta^{3/2}a(V)\mathbf{A}(\mathbf{V})+\theta b(V)\mathbf{u}\cdot\mathbf{B}(\mathbf{V})\right)\eta\left(\sqrt{\theta}\mathbf{V}+\mathbf{u}\right). \quad \text{(B.18)}$$

B.2.4. Computation of the correlation functions

In this section, we show how to compute the correlation functions of the stochastic fluxes $\mathbf{J}$ and $\mathbf{J}^\theta$.

B.2.4.1. Correlation function for the velocity.

In this paragraph, we compute the correlation function $\mathbb{E}\left(J_{ij}\left(\mathbf{r},t\right)J_{kl}\left(\mathbf{r}',t'\right)\right)$ of the velocity noise flux of the fluctuating compressible Navier-Stokes equation (B.15). We recall the expression for the components of the tensor $\mathbf{J}$

$$J_{ij}\left(\mathbf{r},t\right)=\theta^{2}\int\mathrm{d}\mathbf{V}\,b\left(V\right)B_{ij}\left(\mathbf{V}\right)\eta\left(\sqrt{\theta}\mathbf{V}+\mathbf{u}\left(\mathbf{r},t\right),\mathbf{r},t\right).$$

The correlation structure of the noise η is given by the operator $\mathcal{L}_{M_h}$ according to (7.20). More precisely, we can compute correlations between functions φ and ψ of the reduced velocity $\mathbf{V}$ as following

$$\begin{aligned}&\int\mathrm{d}\mathbf{V}\mathrm{d}\mathbf{V}'\,\varphi\left(\mathbf{V}\right)\psi\left(\mathbf{V}'\right)\mathbb{E}\left(\theta^{2}\eta\left(\sqrt{\theta}\mathbf{V}+\mathbf{u}\left(\mathbf{r},t\right),\mathbf{r},t\right)\eta\left(\sqrt{\theta}\mathbf{V}'+\mathbf{u}\left(\mathbf{r}',t'\right),\mathbf{r}',t'\right)\right)\\&=2\delta\left(\mathbf{r}-\mathbf{r}'\right)\delta\left(t-t'\right)\int\mathrm{d}\mathbf{V}\,\varphi\left(\mathbf{V}\right)\mathcal{L}_{M_h}\left(\psi\right)\left(\mathbf{V}\right)M_h\left(\sqrt{\theta}\mathbf{V}+\mathbf{u}\left(\mathbf{r},t\right)\right).\end{aligned}\tag{B.19}$$

Then,

$$\mathbb{E}\left(J_{ij}\left(\mathbf{r},t\right)J_{kl}\left(\mathbf{r}',t'\right)\right)=-2\delta\left(\mathbf{r}-\mathbf{r}'\right)\delta\left(t-t'\right)\frac{\rho\theta^{2}}{\left(2\pi\right)^{3/2}}\int\mathrm{d}\mathbf{V}\,b\left(V\right)B_{ij}\left(\mathbf{V}\right)B_{kl}\left(\mathbf{V}\right)\mathrm{e}^{-V^{2}/2}.$$

We already computed this integral to find the viscous terms of the Navier–Stokes equation, the result reads

$$\frac{-\rho\theta}{\left(2\pi\right)^{3/2}}\int\mathrm{d}\mathbf{V}\,b\left(V\right)B_{ij}\left(\mathbf{V}\right)B_{kl}\left(\mathbf{V}\right)\mathrm{e}^{-V^{2}/2}=\nu\left(\delta_{ik}\delta_{jl}+\delta_{il}\delta_{jk}-\frac{2}{3}\delta_{ij}\delta_{kl}\right).$$

We conclude

$$\mathbb{E}\left(J_{ij}\left(\mathbf{r},t\right)J_{kl}\left(\mathbf{r}',t'\right)\right)=2\theta\nu\left(\delta_{ik}\delta_{jl}+\delta_{il}\delta_{jk}-\frac{2}{3}\delta_{ij}\delta_{kl}\right)\delta\left(\mathbf{r}-\mathbf{r}'\right)\delta\left(t-t'\right).$$

B.2.4.2. Correlation function for the energy.

In this paragraph, we compute the correlation function $\mathbb{E}\left(J_{i}^{\theta}\left(\mathbf{r},t\right)J_{j}^{\theta}\left(\mathbf{r}',t'\right)\right)$ of the temperature noise flux of the fluctuating compressible Navier-Stokes equation (B.17). As previously, we will use the relation (B.19) to compute correlations. Using (B.18), we have

$$\begin{aligned}\mathbb{E}\left(J_{i}^{\theta}\left(\mathbf{r},t\right)J_{j}^{\theta}\left(\mathbf{r}',t'\right)\right)=\mathbb{E}\Bigg(&\theta^{3}\int\mathrm{d}\mathbf{V}\mathrm{d}\mathbf{V}'\,\left(\theta^{3/2}a\left(V\right)A_{i}\left(\mathbf{V}\right)+\theta u_{i}b\left(V\right)B_{ik}(\mathbf{V})\right)\\&\times\left(\theta^{3/2}a\left(V'\right)A_{j}\left(\mathbf{V}'\right)+\theta u_{l}b\left(V'\right)B_{jl}(\mathbf{V}')\right)\eta\left(\sqrt{\theta}\mathbf{V}'+\mathbf{u}'\right)\Bigg).\end{aligned}$$

Then, if we apply (B.19), the correlations can be recast as following

$$\mathbb{E}\left(J_i^\theta\left(\mathbf{r},t\right)J_j^\theta\left(\mathbf{r}',t'\right)\right)=-2\delta\left(\mathbf{r}-\mathbf{r}'\right)\delta\left(t-t'\right)\theta^{3/2}$$
$$\times\int\mathrm{d}\mathbf{V}\,\left(\theta^{3/2}a\left(V\right)A_i\left(\mathbf{V}\right)+\theta u_k b\left(V\right)B_{ik}(\mathbf{V})\right)\left(\theta^{3/2}A_j\left(\mathbf{V}\right)+\theta u_l B_{jl}(\mathbf{V})\right)M_h\left(\mathbf{V}\right).$$

We recall that

$$\frac{-\rho}{\left(2\pi\right)^{3/2}}\int\mathrm{d}\mathbf{V}\,4\theta^3 a\left(V\right)A_i\left(\mathbf{V}\right)A_j\left(\mathbf{V}\right)\mathrm{e}^{-V^2/2}=4\theta^2\kappa\delta_{ij},$$

and

$$\frac{-\rho\theta}{\left(2\pi\right)^{3/2}}\int\mathrm{d}\mathbf{V}\,b\left(V\right)B_{ij}\left(\mathbf{V}\right)B_{kl}\left(\mathbf{V}\right)\mathrm{e}^{-V^2/2}=\nu\left(\delta_{ik}\delta_{jl}+\delta_{il}\delta_{jk}-\frac{2}{3}\delta_{ij}\delta_{kl}\right).$$

Then we obtain

$$\mathbb{E}\left(J_i^\theta\left(\mathbf{r},t\right)J_j^\theta\left(\mathbf{r}',t'\right)\right)=2\left(\theta^2\kappa\delta_{ij}+\theta\nu B_{ij}\left(\mathbf{u}\right)\right)\delta\left(\mathbf{r}-\mathbf{r}'\right)\delta\left(t-t'\right).$$

B.3. Derivation of the gradient-flow structure for the Navier-Stokes equations

In section 7.5.1, we explained how to compute the transverse gradient-flow decomposition for a PDE whose the relaxation path for the large deviations of a macroscopic field, describing a time-reversible microscopic dynamics. Once the quadratic part of the Hamiltonian is computed, the transverse gradient-flow decomposition can be directly obtained. This appendix is dedicated to the computation of the quadratic large deviation Hamiltonian associated with the SPDEs we derived: the compressible and the incompressible fluctuating Navier-Stokes equaions.

B.3.1. Gradient-flow structure for the incompressible Navier-Stokes equations

For the case of the incompressible Navier–Stokes equation, the large deviation rate is $\lambda=\epsilon\alpha$, E is the space of divergence free vector fields, and F is the space of tensor fields. η is $\mathbf{J}/2$, a random Gaussian tensor field with correlations given in (7.62). We have $\mathbf{\Sigma}\cdot\mathbf{T}=\mathbb{P}\nabla\cdot\mathbf{T}$, where $\mathbf{T}$ is a second order tensor, and ∇ the linear operator that corresponds to the divergence of a tensor. By definition of the noise cross correlation (7.62), and by analogy with 7.5.1, the operator $\mathcal{C}$ is a fourth order tensor

$$\mathcal{C}_{ijkl}\left(\mathbf{r},\mathbf{r}'\right)=\nu\left[\delta_{ik}\delta_{jl}+\delta_{il}\delta_{jk}-\frac{2}{3}\delta_{ij}\delta_{kl}\right]\delta(\mathbf{r}-\mathbf{r}').$$

The operator $\mathcal{A}$ from vector fields to vector fields is thus

$$\mathcal{A}=-\mathbb{P}\nabla\mathcal{C}\nabla\mathbb{P},$$

where we have used that the adjoint of the divergence of a tensor field, for the L^2 norms, is the opposite of the gradient of a vector field (the second ∇ in the formula takes a vector as an argument and gives back a tensor), and we have used that $\mathbb{P}$ is self adjoint with respect to the L^2 norm.

We denote $\mathbf{p}(\mathbf{r})$ the conjugated momentum associated to $\mathbf{u}(\mathbf{r})$. The quadratic term in the large deviation Hamiltonian is then,

$$H^{(2)}[\mathbf{u},\mathbf{p}] = (\mathbf{p},\mathbf{p}),$$

with $(\mathbf{p},\mathbf{p}) = \nu \int \mathrm{d}\mathbf{r}\ \langle \nabla\mathbb{P}\mathbf{p}, \nabla\mathbb{P}\mathbf{p}\rangle$ and where

$$\langle \mathbf{T},\mathbf{R}\rangle = \left[\delta_{ik}\delta_{jl} + \delta_{il}\delta_{jk} - \frac{2}{3}\delta_{ij}\delta_{kl}\right] T_{ij}T_{kl}, \tag{B.20}$$

where we sum over repeated indices. As $\left[\delta_{ik}\delta_{jl} + \delta_{il}\delta_{jk} - \frac{2}{3}\delta_{ij}\delta_{kl}\right]$ is the covariance of a Gaussian field, it is a positive operator, and $\langle .,. \rangle$ is positive. We now check this more directly. We see that the first term for the local contribution of $\langle \mathbf{T},\mathbf{T}\rangle$ is $\delta_{ik}\delta_{jl}T_{ij}T_{kl} = T_{ij}T_{ij} = \mathrm{Tr}\left(\mathbf{T}^2\right)$ (where the product is contraction of two tensors, and Tr is the trace). The second term is $\delta_{il}\delta_{jk}T_{ij}T_{kl} = \mathbf{T} : \mathbf{T}^\top = \mathrm{Tr}\left(\mathbf{T}\cdot\mathbf{T}^\top\right)$. This suggests to decompose the tensors into their symmetric and antisymmetric parts: $\mathbf{T} = \mathbf{T}_s + \mathbf{T}_a$, with $2\mathbf{T}_s = \mathbf{T} + \mathbf{T}^\top$. Then the sum of the two first terms is $\mathrm{Tr}\left(\mathbf{T}^2\right) + \mathrm{Tr}\left(\mathbf{T}\cdot\mathbf{T}^\top\right) = 2\mathrm{Tr}\left(\mathbf{T}_s^2\right)$. Finally we note that $\delta_{ij}\delta_{kl}T_{ij}T_{kl} = (\mathrm{Tr}\mathbf{T})^2$. Hence

$$\langle \mathbf{T},\mathbf{R}\rangle = 2\mathrm{Tr}\left(\mathbf{T}_s\mathbf{R}_s\right) - \frac{2}{3}\left(\mathrm{Tr}\mathbf{T}_a\right)\left(\mathrm{Tr}\mathbf{R}_a\right).$$

We note that the bilinear form is positive definite on the set of symmetric tensors, and equal to zero on the set of antisymmetric tensors, and that the set of symmetric tensor is orthogonal to the set of antisymmetric tensors for this bilinear form. We also note that $\mathrm{Tr}\left(\nabla\mathbf{v}\right) = 0$ for divergence free vector fields $\mathbf{v}$. Then the quadratic term in the Hamiltonian is

$$(\mathbf{p},\mathbf{p})_i = \nu\int \mathrm{d}\mathbf{r}\ \langle \nabla\mathbb{P}\mathbf{p}, \nabla\mathbb{P}\mathbf{p}\rangle_i \quad \text{with} \quad \langle \mathbf{T},\mathbf{R}\rangle_i = \frac{1}{2}\mathrm{Tr}\left(\left(\mathbf{T}+\mathbf{T}^\top\right)\left(\mathbf{R}+\mathbf{R}^\top\right)\right)$$

The Hamiltonian that describes the large deviations for the incompressible Navier-Stokes equation is then

$$H[\mathbf{u},\mathbf{p}] = \int \mathrm{d}\mathbf{r}\ \left[\nu\langle \nabla\mathbb{P}\mathbf{p}, \nabla\mathbb{P}\mathbf{p}\rangle_i + \mathbf{p}.\left(-\mathbb{P}\left(\mathbf{u}\cdot\nabla\mathbf{u}\right) + \nu\Delta\mathbf{u}\right)\right].$$

If we now restrict $\mathbf{p}$ to the set of divergence free vector fields, we can write more simply

$$H[\mathbf{u},\mathbf{p}] = \int \mathrm{d}\mathbf{r}\ \left[\frac{\nu}{2}\mathrm{Tr}\left(\nabla\mathbf{p} + \nabla\mathbf{p}^\top\right)^2 - \mathbf{p}.\left(\mathbf{u}\cdot\nabla\mathbf{u}\right) + \nu\mathbf{p}.\Delta\mathbf{u}\right].$$

Moreover, denoting $\mathbf{S} = \frac{1}{2}\left(\nabla\mathbf{p} + \nabla\mathbf{p}^\top\right)$, we have $2\mathrm{Tr}\left(\mathbf{S}\right)^2 = 2\mathbf{S} : \nabla\mathbf{p} = 2\nabla : \left(\mathbf{S}\mathbf{p}\right) - 2\mathbf{p} : \nabla\mathbf{S} = 2\nabla.\left(\mathbf{S}\mathbf{p}\right) - \mathbf{p}.\nabla\mathbf{p}$, where for the last equality we have used that $\nabla\cdot\mathbf{p} = 0$. Hence a simpler expression for H is

$$H[\mathbf{u},\mathbf{p}] = \int \mathrm{d}\mathbf{r}\ \left[-\mathbf{p}.\left(\mathbf{u}\cdot\nabla\mathbf{u}\right) + \nu\mathbf{p}.\left(\Delta\mathbf{u} - \Delta\mathbf{p}\right)\right].$$

We expect the kinetic energy

$$K\left[\mathbf{u}\right] = \frac{1}{2}\int \mathrm{d}\mathbf{r}\, \mathbf{u}^2$$

to be the quasipotential for the large deviations. This is easily proved by checking that $\frac{\delta K}{\delta \mathbf{u}} = \mathbf{u}$ solves the stationary Hamilton–Jacobi equation: $H\left[\mathbf{u}, \frac{\delta K}{\delta \mathbf{u}}\right] = 0$, and using that the deterministic Navier–Stokes equation has a single attractor $\mathbf{u} = 0$. $H\left[\mathbf{u}, \frac{\delta K}{\delta \mathbf{u}}\right] = 0$ is easily proved using that

$$\int \mathrm{d}\mathbf{r}\, \frac{\delta K}{\delta \mathbf{u}}.\left(\mathbf{u}\cdot\nabla\mathbf{u}\right) = 0,$$

which is at the same time the classical energy conservation result and the transversality condition for the reversible part of the deterministic dynamics, with respect to the quasipotential. Moreover, we also note that for any divergence free field $\mathbf{p}$

$$\left(\mathbf{p}, \frac{\delta U}{\delta \mathbf{u}}\right)_i = -\nu \int \mathrm{d}\mathbf{r}\, \mathbf{p}\cdot\Delta\mathbf{u},$$

which proves that $\Delta\mathbf{u}$ is the opposite of the gradient of K with respect to the noise scalar product $(.,.)_i$.

B.3.2. Gradient-flow structure for the compressible Navier-Stokes equations

For the case of the compressible Navier–Stokes equations, we independently consider the evolution equation for ρ, which is deterministic, and the ones for the fields $(\mathbf{u}, s)$, which are stochastic. With the notations of section 7.5.1, E is the vector space of the fields $(\mathbf{u}, s)$, while F is the space of fields $(\mathbf{J}, \mathbf{q})$. The large deviation rate is $\lambda = \epsilon\alpha^4$. The linear operator $\mathbf{\Sigma}$ is defined by

$$\mathbf{\Sigma}\left(\mathbf{J}, \mathbf{q}\right) = \frac{1}{2}\left(\frac{\nabla\cdot\mathbf{J}}{\rho}, \frac{m\nabla\cdot\left(\mathbf{u}\cdot\mathbf{J}\right) - \nabla\cdot\mathbf{q}}{\rho\theta}\right),$$

and the covariance operator $\mathbf{C}$ is block diagonal: $\mathbf{C} = \mathbf{C}^t + \mathbf{C}^v$, where $\mathbf{C}^t$ acts only of the tensor part of the space F, while $\mathbf{C}^v$ acts only on the vector part, and with

$$C^t_{ijkl}\left(\mathbf{r}, \mathbf{r}'\right) = \nu\theta\left[\left(\delta_{ik}\delta_{jl} + \delta_{il}\delta_{jk}\right) + \left(\gamma - \frac{2}{3}\right)\delta_{ij}\delta_{kl}\right]\delta(\mathbf{r} - \mathbf{r}')$$

and

$$\mathbf{C}^v = \kappa\theta^2 \mathrm{Id}\delta(\mathbf{r} - \mathbf{r}').$$

Then, we have

$$\mathbf{\Sigma}^\top\left(\mathbf{p}_\mathbf{u}, p_s\right) = \left(-\nabla\left(\frac{\mathbf{p}_\mathbf{u}}{\rho}\right) + \frac{p_s\nabla\mathbf{u}}{\rho\theta}, \nabla\left(\frac{p_s}{\rho\theta}\right)\right)$$

For a rank 2 tensor $\mathbf{T}$, we have $\mathbf{C}^t \cdot \mathbf{T} = \nu\theta\left[\left(\mathbf{T}+\mathbf{T}^\top\right)+\left(\gamma-\frac{2}{3}\right)\mathrm{Tr}\left(\mathbf{T}\right)\mathrm{Id}\right]\delta(\mathbf{r}-\mathbf{r}')$, and for a vector $\mathbf{q}$, we have $\mathbf{C}^v \cdot \mathbf{q} = \kappa\theta^2\mathbf{q}\delta(\mathbf{r}-\mathbf{r}')$. Hence

$$\mathbf{C}\boldsymbol{\Sigma}^\top\left(\mathbf{p}_\mathbf{u}, p_s\right) = \left(\nu\theta\left[-\nabla\left(\frac{\mathbf{p}_\mathbf{u}}{\rho}\right)+\frac{p_s\nabla\mathbf{u}}{\rho\theta}-\nabla\left(\frac{\mathbf{p}_\mathbf{u}}{\rho}\right)^\top+\left(\frac{p_s\nabla\mathbf{u}}{\rho\theta}\right)^\top+\left(\gamma-\frac{2}{3}\right)\left(-\nabla.\left(\frac{\mathbf{p}_\mathbf{u}}{\rho}\right)+\frac{p\nabla.\mathbf{u}}{\rho\theta}\right)\mathrm{Id}\right], \kappa\theta^2\nabla\left(\frac{p_s}{\rho\theta}\right)\right)\delta(\mathbf{r}-\mathbf{r}')$$

from which we can write the Hamiltonian $H = H_r + H_i + H_q$, with H_r time symmetric linear part in p (reversible deterministic evolution), H_i the time antisymmetric linear part in p (irreversible deterministic evolution) and H_q the quadratic one (stochastic evolution). H_r and H_i are chosen so that

$$\partial_t\begin{pmatrix}\rho\\ \mathbf{u}\\ s\end{pmatrix} = \begin{pmatrix}\frac{\delta H_r}{\delta p_\rho}\\ \frac{\delta H_r}{\delta p_\mathbf{u}}\\ \frac{\delta H_r}{\delta p_s}\end{pmatrix} + \begin{pmatrix}\frac{\delta H_i}{\delta p_\rho}\\ \frac{\delta H_i}{\delta p_\mathbf{u}}\\ \frac{\delta H_i}{\delta p_s}\end{pmatrix}.$$

is the deterministic compressible Navier–Stokes system, where the first term on the r.h.s. is the transport term, and the second term on the r.h.s. is the diffusive term. As discussed above, the quadratic part of the Hamiltonian should read

$$H_q\left[\rho,\mathbf{u},s,p_\rho,\mathbf{p}_\mathbf{u},p_s\right] = \int \mathrm{d}\mathbf{r}\ \left(\mathbf{p}_\mathbf{u},p_s\right)^\top\cdot\mathbf{A}\left(\mathbf{p}_\mathbf{u},p_s\right)$$

where $\mathbf{A} = \boldsymbol{\Sigma}\mathbf{C}\boldsymbol{\Sigma}^\top$. The final result reads

$$H_r\left[\rho,\mathbf{u},s,p_\rho,\mathbf{p}_\mathbf{u},p_s\right] = -\int \mathrm{d}\mathbf{r}\ \left[p_\rho\nabla\cdot(\rho\mathbf{u})+\mathbf{p}_\mathbf{u}\cdot\left(\mathbf{u}\cdot\nabla\mathbf{u}+\frac{\nabla P}{\rho}\right)+p_s\mathbf{u}\cdot\nabla s\right],$$

$$H_i\left[\rho,\mathbf{u},s,p_\rho,\mathbf{p}_\mathbf{u},p_s\right] = \alpha\int \mathrm{d}\mathbf{r}\ \left\{\frac{\nu\mathbf{p}_\mathbf{u}}{\rho}\cdot\nabla\cdot\left[\left(\nabla\mathbf{u}+(\nabla\mathbf{u})^\top\right)+\left(\gamma-\frac{2}{3}\right)(\nabla\cdot\mathbf{u})\,\mathrm{Id}\right],\right.$$
$$\left.+\frac{p_s\nu}{\rho\theta}\left[\frac{1}{2}\left(\nabla\mathbf{u}+(\nabla\mathbf{u})^\top\right)^2+\left(\gamma-\frac{2}{3}\right)(\nabla\cdot\mathbf{u})^2\right]+\frac{p_s}{\rho\theta}\nabla.(\kappa\nabla\theta)\right\}.$$

and

$$H_q\left[\rho,\mathbf{u},s,p_\rho,\mathbf{p}_\mathbf{u},p_s\right] = \alpha\int \mathrm{d}\mathbf{r}\left\{\nu\theta\left(\left[\nabla\left(\frac{\mathbf{p}_\mathbf{u}}{\rho}\right)-\frac{p_s\nabla\mathbf{u}}{\rho\theta}+\nabla\left(\frac{\mathbf{p}_\mathbf{u}}{\rho}\right)^\top-\left(\frac{p_s\nabla\mathbf{u}}{\rho\theta}\right)^\top\right]^2\right.\right.$$
$$\left.\left.+\left(\gamma-\frac{2}{3}\right)\left[\nabla\cdot\left(\frac{\mathbf{p}_\mathbf{u}}{\rho}\right)-\frac{p_s\nabla\cdot\mathbf{u}}{\rho\theta}\right]^2\right)+\kappa\theta^2\left[\nabla\left(\frac{p_s}{\rho\theta}\right)\right]^2\right\}.$$

Quasipotential for the fluctuating compressible Navier-Stokes equations. We expect the quasipotential to be negative of the total entropy up to conservation laws

$$U = -S = \begin{cases} -\int \mathrm{d}\mathbf{r}\,\rho s \ \text{ if } \ \int \mathrm{d}\mathbf{r}\,\rho = M \ \text{ and } \ \int \mathrm{d}\mathbf{r}\ \left(\frac{1}{2}\mathbf{u}^2+\frac{3}{2}\theta\right) = E. \\ +\infty \ \text{ otherwise}\end{cases} \tag{B.21}$$

This is easily checked by verifying the Hamilton–Jacobi equation $H\left[\rho,\mathbf{u},s,\frac{\delta U}{\delta\rho},\frac{\delta U}{\delta\mathbf{u}},\frac{\delta U}{\delta s}\right] = 0$, using that H has the conservation law symmetries, and taking for granted that for any initial condition with mass M and energy E, the deterministic hydrodynamic equation

converges to the equilibrium state with mass M and energy E. In order to check the Hamilton–Jacobi equation, we use that $\frac{\delta U}{\delta \rho} = -s$, $\frac{\delta U}{\delta \mathbf{u}} = 0$, and $\frac{\delta U}{\delta s} = -\rho$. By identification and by performing part integrations, it is easily checked that

$$H_r\left[\rho, \mathbf{u}, s, -s, 0, -\rho\right] = 0$$

and that

$$H_i\left[\rho, \mathbf{u}, s, -s, 0, -\rho\right] + H_q\left[\rho, \mathbf{u}, s, -s, 0, -\rho\right] = 0.$$

We can thus conclude that U (B.21) is the quasipotential.

We also check the time reversal symmetry of the Hamiltonian. We expect the reversible part of the Hamiltonian H_r to be time reversible. Defining the time reversal involution by $I\left[\rho, \mathbf{u}, s\right] = \left[\rho, -\mathbf{u}, s\right]$ and $I\left[p_\rho, \mathbf{p_u}, p_s\right] = \left[p_\rho, -\mathbf{p_u}, p_s\right]$ (we also note that $I\left[P\right] = P$, where P is the pressure), this requires

$$H_r\left[I\left[\rho, \mathbf{u}, s\right], -\left[p_\rho, \mathbf{p_u}, p_s\right]\right] = H_r\left[\rho, \mathbf{u}, s, p_\rho + \frac{\delta U}{\delta \rho}, \mathbf{p_u} + \frac{\delta U}{\delta \mathbf{u}}, p_s + \frac{\delta U}{\delta s}\right],$$

or equivalently

$$H_r\left[\rho, -\mathbf{u}, s, -p_\rho, \mathbf{p_u}, -p_s\right] = H_r\left[\rho, \mathbf{u}, s, p_\rho - s, \mathbf{p_u}, p_s - \rho\right].$$

This can be checked by direct computations. We expect the irreversible and stochastic parts of the Hamiltonian $H_i + H_q$ to have the symmetry

$$\left(H_i + H_s\right)\left[\rho, \mathbf{u}, s, p_\rho, \mathbf{p_u}, p_s\right] = \left(H_i + H_s\right)\left[\rho, -\mathbf{u}, s, p_\rho + \frac{\delta U}{\delta \rho}, -\mathbf{p_u} + \frac{\delta U}{\delta \mathbf{u}}, p_s + \frac{\delta U}{\delta s}\right] = \left(H_i + H_s\right)\left[\rho, -\mathbf{u}, s, p_\rho - s, \mathbf{p_u}, p_s - \rho\right].$$

This is also easily checked.

Transverse-gradient-flow structure. For any given $\left[\rho, \mathbf{u}, s\right]$, the quadratic part of the Hamiltonian considered as functional over the fields $\left[p_\rho, \mathbf{p_u}, p_s\right]$ defines a semi-norm (it is positive but not definite positive has the action on p_ρ is zero, and it conserves the energy). We have

$$H_q\left[\rho, \mathbf{u}, s, p_\rho, \mathbf{p_u}, p_s\right] = < \left[p_\rho, \mathbf{p_u}, p_s\right], B_{(\rho,\mathbf{u},s)}\left[p_\rho, \mathbf{p_u}, p_s\right] >$$

where $< \left[a, \mathbf{b}, c\right], \left[c, \mathbf{d}, e\right] > = \int \mathbf{dr}\ \left(ac + \mathbf{b}\cdot\mathbf{d} + ce\right)$ is the L^2 scalar product and $B_{(\rho,\mathbf{u},s)}$ is the non negative symmetric operator $B_{(\rho,\mathbf{u},s)} = \alpha\left(0, B^{p_\mathbf{u}}_{(\rho,\mathbf{u},s)}, B^{p_s}_{(\rho,\mathbf{u},s)}\right)$ with

$$B^{p_\mathbf{u}}_{(\rho,\mathbf{u},s)}\left[p_\rho, \mathbf{p_u}, p_s\right] = -\frac{1}{\rho}\nabla.\left\{\nu\theta\left[\nabla\left(\frac{\mathbf{p_u}}{\rho}\right) + \left(\nabla\left(\frac{\mathbf{p_u}}{\rho}\right)\right)^\top\right] + \frac{\eta\nu p}{\rho}\left[\nabla\mathbf{u} + \left(\nabla\mathbf{u}\right)^\top\right]\right\} + \frac{1}{\rho}\nabla\left\{\left(\zeta - \frac{2}{3}\nu\right)\left[-\theta\nabla.\left(\frac{\mathbf{p_u}}{\rho}\right) + \frac{p_s}{\rho}\nabla.\mathbf{u}\right]\right\}, \tag{B.22}$$

and

$$B^{p_s}_{(\rho,\mathbf{u},s)}\left[p_\rho, \mathbf{p_u}, p_s\right] = -\frac{\nu}{\rho}\nabla\mathbf{u}.\left[\nabla\left(\frac{\mathbf{p_u}}{\rho}\right) + \left(\nabla\left(\frac{\mathbf{p_u}}{\rho}\right)\right)^\top\right] + \frac{\nu p_s}{\rho^2\theta}\nabla\mathbf{u}.\left[\nabla\mathbf{u} + \left(\nabla\mathbf{u}\right)^\top\right] - \frac{1}{\rho}\left(\zeta - \frac{2}{3}\nu\right)\nabla.\left(\frac{\mathbf{p_u}}{\rho}\right)\nabla.\mathbf{u} + \frac{p_s}{\rho^2\theta}\left(\zeta - \frac{2}{3}\nu\right)\left(\nabla.\mathbf{u}\right)^2 - \nabla.\left[\kappa\theta^2\nabla\left(\frac{p_s}{\rho\theta}\right)\right]. \tag{B.23}$$

This defines the gradient structure. Indeed, it is easily checked that the dissipative operator

$$D = \left[0, \frac{\nabla.\left(\mathbf{\Pi}_d(\mathbf{u})\right)}{\rho}, \nabla\mathbf{u}.\mathbf{\Pi}_d(\mathbf{u}) + \frac{\nabla.\left(\kappa\nabla\theta\right)}{\rho\theta}\right]$$

is the gradient of the quasipotential (minus the entropy) with respect to the norm defined by H_q:

$$D\left(\rho, \mathbf{u}, s\right) = -\mathrm{Grad}_{H_{q,(\rho,\mathbf{u},s)}}(-S) = -B_{(\rho,\mathbf{u},s)}\left(-\frac{\delta S}{\delta\rho}, -\frac{\delta S}{\delta\mathbf{u}}, -\frac{\delta S}{\delta s}\right) = -B_{(\rho,\mathbf{u},s)}\left(s, 0, \rho\right).$$

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Ouassim FELIACHI

Grandes déviations dans les limites cinétiques et hydrodynamiques

Résumé :
Comprendre comment décrire un système avec des équations macroscopiques, qui sont généralement déterministes, en partant d'une description microscopique, qui peut être stochastique est le problème fondamental de la physique statistique. Souvent, cette tâche implique au moins deux limites : une limite "grand N" et une limite "d'équilibre local". La première permet de décrire un système de N particules par une fonction de distribution dans l'espace des phases, tandis que la seconde reflète la séparation des échelles de temps entre l'approche rapide de l'équilibre local et l'évolution lente des modes hydrodynamiques. En supposant ces deux limites, on obtient une description macroscopique déterministe. Pour des raisons à la fois théoriques et de modélisation (N est grand mais pas infini, la séparation des échelles de temps n'est pas parfaite), il est parfois important de comprendre les fluctuations autour de cette description macroscopique. L'hydrodynamique fluctuante fournit un cadre pour décrire l'évolution des champs macroscopiques tout en prenant en compte les fluctuations induites par le nombre fini de particules dans la limite hydrodynamique.
Cette thèse traite de la dérivation de l'hydrodynamique fluctuante à partir de la description microscopique de la dynamique des particules. La dérivation de l'hydrodynamique fluctuante se fait en deux étapes. Premièrement, la limite "grand N" doit être affinée pour prendre en compte les fluctuations au-delà du comportement moyen du système. Pour ce faire, nous utilisons la théorie des grandes déviations pour établir des principes de grandes déviations qui décrivent la probabilité de tout chemin d'évolution pour le système de particule au-delà du chemin le plus probable décrit par l'équation cinétique. Ensuite, nous dérivons la l'hydrodynamique fluctuante en étudiant la limite hydrodynamique du principe de grande déviation cinétique, ou l'équation cinétique fluctuante associée. Ce manuscrit contient l'explication de ce programme et son application à divers systèmes physiques allant du gaz dilué aux particules actives.

Mots clés : Grandes déviations, Théorie cinétique, Limites hydrodynamiques, Hydrodynamique fluctuante, Matière active

From Particles to Fluids: A Large Deviation Theory Approach to Kinetic and Hydrodynamical Limits

Abstract:
The central problem of statistical physics is to understand how to describe a system with macroscopic equations, which are usually deterministic, starting from a microscopic description, which may be stochastic. This task requires taking at least two limits: a "large N" limit and a "local equilibrium" limit. The former allows a system of N particles to be described by a phase-space distribution function, while the latter reflects the separation of time scales between the fast approach to local equilibrium and the slow evolution of hydrodynamic modes. When these two limits are taken, a deterministic macroscopic description is obtained. For both theoretical and modeling reasons (N is large but not infinite, the time-scale separation is not perfect), it is sometimes important to understand the fluctuations around this macroscopic description. Fluctuating hydrodynamics provides a framework for describing the evolution of macroscopic, coarse-grained fields while taking into account finite-particle-number induced fluctuations in the hydrodynamic limit.
This thesis discusses the derivation of fluctuating hydrodynamics from the microscopic description of particle dynamics. The derivation of the fluctuating hydrodynamics is twofold. First, the "large N" limit must be refined to account for fluctuations beyond the average behavior of the system. This is done by using large deviation theory to establish kinetic large deviation principles that describe the probability of any evolution path for the empirical measure beyond the most probable path described by the kinetic equation. Then, the fluctuating hydrodynamics is derived by studying the hydrodynamical limit of the kinetic large deviation principle, or the associated fluctuating kinetic equation. This dissertation discusses this program and its application to several physical systems ranging from the dilute gas to active particles.

Keywords : Large deviation theory, Kinetic theory, Hydrodynamical limits, Fluctuating hydrodynamics, Active matter

Université d'ORLÉANS

Institut Denis Poisson
Rue de Chartres B.P. 6759
45067 ORLEANS CEDEX 2

INSTITUT ORLÉANS - TOURS Mathématiques & Physique Théorique DENIS POISSON