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Cesare Nardini

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Energy landscapes, equilibrium and out of equilibrium physics of long and short range interacting systems

Cesare Nardini

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Contents

General overview	1
I Energy landscape approach to equilibrium phase transitions	3
Overview of Part I	5
1 Introduction	9
1.1 Preliminaries: Morse theory	9
1.2 Topological conjecture	11
1.3 Microcanonical singularities in finite systems	13
1.3.1 Singularities in the configurational entropy	13
1.3.2 Role of the kinetic energy	15
1.4 KSS Theorems	17
1.5 Controversy on the Franzosi-Pettini theorem	19
2 The self-gravitating ring model	23
2.1 KSS criterion	24
2.2 Application of the KSS criterion to the SGR model	25
2.2.1 The model	25
2.2.2 Saddles of the landscape and phase transitions in the SGR model	26
2.3 An effective model obtained from SGR	30
2.3.1 Effective model	31
2.3.2 Microcanonical thermodynamics	33
2.4 Conclusions	37
3 $O(n)$ spin models	39
3.1 $O(n)$ spin models and Ising stationary configurations	40
3.2 Application of the KSS criterion to short range systems	42
3.3 On a microcanonical relation between continuous and discrete spin models	44
3.3.1 A striking similarity between critical energy densities	45
3.4 The one-dimensional and mean-field XY models	48
3.4.1 The mean-field XY model	48
3.4.2 The one-dimensional XY model	53
3.5 Conclusions	56
Conclusions and perspectives of Part I	60

CONTENTS

II	Perturbed long-range interacting systems	65
	Overview of Part II	67
4	Isolated long-range interacting systems	73
4.1	Long-range interacting particle systems	74
4.2	Phenomenology: Quasi-Stationary-States	77
4.3	Kinetic approach	78
4.3.1	BBGKY hierarchy	79
4.3.2	Closures of the BBGKY hierarchy	80
4.4	Vlasov equation	81
4.4.1	Linear Vlasov equation and Landau Damping	83
4.5	Lyapunov equations	90
4.5.1	Definition of the Ornstein–Uhlenbeck process	91
4.5.2	Formal solutions in real time	92
4.5.3	Formal solution in frequency space	93
4.6	Lenard-Balescu equation	94
4.6.1	Explicit derivation of the Lenard-Balescu equation	97
4.6.2	About the Lenard-Balescu equation	99
4.7	Conclusions	100
5	Deterministic perturbations: linear response theory on the Vlasov equation	103
5.1	Linear response theory for QSS	104
5.2	Homogeneous QSS	107
5.3	Application to the Hamiltonian mean-field model	109
5.3.1	Model	109
5.3.2	Linear response of homogeneous QSS	110
5.3.3	Linear response of the homogeneous equilibrium state	114
5.4	Comparison with N -particle simulations	115
5.4.1	Linear response of homogeneous QSS: Single realization	116
5.4.2	Linear response of the homogeneous equilibrium state: Single realization	116
5.4.3	Average over initial realizations	116
5.4.4	Relaxation of QSS to equilibrium	119
5.5	Conclusions	119
6	Stochastic forcing on particle systems	123
6.1	Long-range interacting systems driven by stochastic fields	125
6.2	Methods of analysis	126
6.2.1	Kinetic theory for homogeneous stationary states	126

6.2.2 Numerical simulations	131
6.3 Predictions of the kinetic theory and comparison with simulations	132
6.4 Nonequilibrium phase transition and collapse	136
6.5 Conclusions and perspectives	142
7 Stochastic forcing on fluid models	145
7.1 Quasi-linear approximation	146
7.2 The linearized two-dimensional Euler equation	151
7.2.1 Spectral stability	151
7.2.2 Asymptotic stability: the Orr mechanism	152
7.3 Stochastic Orr mechanism	153
7.4 How to obtain explicit results?	155
7.5 Conclusions and perspectives	158
Conclusions and perspectives of Part II	160
A Appendix to Chapter 2	165
A.1 Density of states of the effective model	165
B Appendix to Chapter 3	169
B.1 Specific heat critical exponent from Eq. (3.14)	169
C Appendix to Chapter 5	171
C.1 Normalization, energy density, and stability criterion for the Fermi-Dirac distribution	171
D Appendices to Chapter 6	173
D.1 Condition of detailed balance for the dynamics (6.2)	173
D.2 Closure of the BBGKY hierarchy	174
D.3 Evolution of the kinetic energy for the dynamics	176
D.4 Proof that the kinetic equation admits non-Gaussian stationary distribution with Gaussian tails	177
Bibliography	179

Journal publications

Parts of this thesis are based on material published in the following papers. Their order reflects the one in which the results are presented in the thesis:

- **Energy landscape and phase transitions in the self-gravitating ring models**
C. Nardini and L. Casetti,
Phys. Rev. E 80, 060103(R), 2009.
- **A solvable model of a self-gravitating system**
L. Casetti and C. Nardini,
J. Stat. Mech., P05006, 2010.
- **Microcanonical Relation between Continuous and Discrete Spin Models**
L. Casetti, C. Nardini and R. Nerattini,
Phys. Rev. Lett., 106, 057208, 2011.
- **Density of states of continuous and discrete spin models: a case study**
C. Nardini, R. Nerattini and L. Casetti,
J. Stat. Mech., P02007, 2012.
- **Linear response theory for long-range interacting systems in quasistationary states**
A. Patelli, S. Gupta, C. Nardini and S. Ruffo,
Phys. Rev. E, 85, 021133, 2012.
- **Kinetic theory for non-equilibrium stationary states in long-range interacting systems**
C. Nardini, S. Gupta, S. Ruffo, T. Dauxois and F. Bouchet,
J. Stat. Mech., L01002, 2012.
- **Kinetic theory of non-equilibrium stochastic long-range systems: Phase transition and bistability**
C. Nardini, S. Gupta, S. Ruffo, T. Dauxois and F. Bouchet,
arXiv preprint arXiv:1210.0492, accepted for publication in J. Stat. Mech.

Other papers not covered in this thesis to which the author contributed:

- **Caloric curve of star clusters**
L. Casetti and C. Nardini,
Phys. Rev. E, 85, 061105, 2012.
- **Hot gets hotter through long-range contact with a cold bath**
P. De Buyl, G. De Ninno, D. Fanelli, C. Nardini, A. Patelli, F. Piazza, Y.Y. Yamaguchi,
arXiv preprint arXiv:1211.2528, submitted to Phys. Rev. Lett.

CONTENTS

A paper whose content forms a part of this Thesis is in preparation:

- **Lyapunov equation in kinetic theories of plasmas and fluid models**
F. Bouchet and C. Nardini, in preparation

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General overview

This thesis is divided in two parts, corresponding to the two main subjects on which I have worked during my Ph.D. The two parts do not belong to a common project, even if both of them fit in the field of statistical mechanics.

Part I is an extension of my Master thesis and my work has been supervised by L. Casetti; it is devoted to equilibrium statistical mechanics of long and short range interacting systems and in particular, to the application of techniques coming from energy landscape theory to some specific models.

Part II has been mainly developed in Lyon under the supervision of T. Dauxois. It is devoted to the study of forced long-range interacting systems and mainly deals with problems of non-equilibrium statistical physics.

We refer the reader to the introductory Sections of Part I and Part II for a detailed overview of both the research fields and of my contribution.

Part I

Energy landscape approach to equilibrium phase transitions

Overview

This part of the Thesis is devoted to the study of equilibrium phase transitions in classical Hamiltonian systems from an energy landscape point of view. In principle, both the Newtonian dynamics and the thermodynamical behavior are determined by the potential energy function V so that one may ask which are the characteristic features of V that are crucial for the dynamics and/or for thermodynamics of the system.

In the literature, one refers to energy landscape methods [1], or more precisely to potential energy landscape methods, when the properties of the potential energy V are studied in connection with the thermodynamical or dynamical behavior. From a mathematical point of view the stationary points, that is those points q of the phase space Γ such that

$$\nabla V(q) = 0, \tag{1}$$

yield important informations on V . For example, if the temperature of a system is very low, and V has only one minimum, it is well known that the thermodynamics can be obtained replacing V by its harmonic expansion around it. On the other hand, in the case in which the system is frustrated, the Stillinger and Weber thermodynamical formalism takes care of the contribution of every minimum of the landscape [2, 3]. Examples of applications include clusters [1], disordered systems and glasses [4, 5], biomolecules, protein folding [6]. In most of the studies only minimum or first order saddles are taken into account. An example of this second kind is the instanton theory, in which the transition probability and the transition path of a thermally activated system between two minimum, through a first order saddle, can be computed via field-theoretical methods.

In some later works, stationary points with an arbitrary number of negative directions have been considered, for instance to characterize glassy behavior [7, 8]. Most of the works in energy landscapes, however, deal only with minimum and first order saddles.

The potential relevance of energy landscape techniques to the study of equilibrium phase transitions was suggested after it was realized that stationary points of the Hamiltonian are connected with topology changes of the phase space accessible to the system. It was conjectured that some of these topology changes, and therefore some of the stationary points, are at the origin of thermodynamic phase transitions [9–13]; quite some research activity followed [14–34], some focused on specific models, others trying to shed light on the general mechanisms (see [35, 36] for reviews).

The main difference with respect to classical studies in energy landscapes is that to apply the techniques and the ideas developed in this field, all the stationary points of the system are needed. However, finding all the stationary points of a given Hamiltonian is an essentially impossible task both analytically and numerically, except in some very simple (usually mean-field or one-dimensional) examples. For this reason, the ideas and the results

emerged have not been tested if not on very simple models. One of the scope of the work presented here is to study models whose energy landscape is much more complicated than what was previously done developing techniques and approximations which do not need the knowledge of all stationary points to be applied. The drawback is that, often, the approximations used are not under control, so that it is not simple to understand which is the degree of approximations in the results. This notwithstanding, we will see that some interesting predictions will be obtained, both in negative (on the applicability of the so-called KSS criterion) and in positive (especially about $O(n)$ models).

This part of the Thesis is structured as follows:

Chapter 1 In the first Chapter, we review the general results connecting the energy landscape properties with equilibrium phase transitions. In particular, we review a recently proved theorem by Kastner et al. [37, 38], the KSS theorem, which gives some necessary conditions such that the stationary points of V can induce a phase transition in the thermodynamic limit. We will also review some of the previous results, such as the Franzosi and Pettini theorem which proves a weak version of the topological conjecture and a recent debate which arose around its validity.

Chapter 2 presents the content of [28] and [39] and, in part, of my Master thesis [40]. The KSS theorem is not of simple applicability to non mean-field systems. In this second Chapter we reformulate it as a criterion, the KSS criterion, to single out phase transitions. The advantage of the the KSS criterion with respect to the original theorem stays in the fact that it is not necessary to know all the critical points of V to apply it. This gave us the possibility to study a non-exactly solvable model of self-gravitating particles, the SGR model. We will show that the KSS criterion singles out the phase transition between a homogeneous and a clustered phase. We shall also show that the criterion indicates the possible presence of another phase transition, not previously known, and we conjecture on its nature thanks to an effective model constructed for this purpose.

Chapter 3 presents the content of [41] and [42]. The reformulation of the KSS theorem in the form of the KSS criterion has given the possibility of applying this technique to models in which not all stationary points are known. Thanks to this, Nerattini et al. [43, 44] have applied the criterion to the two and three dimensional nearest-neighbors ferromagnetic XY models, in which a special class of stationary points is known. We review their analysis which clearly shows that the KSS criterion is not useful in these cases. Indeed, the KSS does not single out any peculiar energy in which the phase transition should be located.

To understand the mechanism by which the phase transition emerges in these mod-

els, we derive an approximate expression of the density of states. The approximation we do is rather crude, but led us to the following conjecture: if a $O(n)$ model with ferromagnetic interactions on a hypercubic lattice has a phase transition, its critical energy density is equal to that of the $n = 1$ case, i.e., a system of Ising spins with the same interactions. We will see that this conjecture gives extremely good estimates for the critical energy densities of short-range ferromagnetic $O(n)$ models.

Finally we show that our derivation, which is rather crude for general short-range $O(n)$ models, can be followed rigorously in the simple cases of mean-field and 1-dimensional XY models. The difficulties in generalizing such results to the case of short-range $O(n)$ models are also discussed.

Conclusions and perspectives We discuss the the general results we obtained and the future perspectives opened by our work.

1

Introduction

We describe here some results on the connections between energy landscape properties and equilibrium phase transitions in Hamiltonian systems of the form

$$\mathcal{H}(p, q) = \sum_{i=1}^N \frac{p_i^2}{2} + V(q) , \quad (1.1)$$

where V is a Morse function. The theory is naturally developed in the microcanonical formalism, at variance with the usual formulation of the theory of phase transitions. In this Chapter, we mainly concentrate on general results and address the reader to [35, 36] for recent reviews on the subject both for the details and for a resume of the works dealing with specific model systems.

The Chapter is organized as follows. In Section 1.1 we recall some basic concepts about finite dimensional Morse theory. In Section 1.2 we briefly discuss the topological conjecture, according to which phase transitions should be connected to sufficiently strong topology changes of the accessible phase space; a theorem by Franzosi and Pettini proves a weak version of it. In Section 1.3 we review the work by Kastner et al. showing a correspondence between stationary points and singularities in the microcanonical entropy of finite systems. The entropy is however $N/2$ times differentiable so that this singularities are very weak. It is natural to ask if there is a mechanism which permits this singularities to survive in the $N \rightarrow \infty$ limit. This is the content of the KSS theorem, which we review in Section 1.4. Finally, in Section 1.5 we present the discussion recently emerged about the actual validity of the Franzosi and Pettini theorem.

1.1 Preliminaries: Morse theory

We briefly review here the basic concepts of finite dimensional Morse theory, to set the notations and the definitions useful for the following. We address the reader to [45] for a complete exposition and the proofs of the quoted results.

CHAPTER 1. INTRODUCTION

Let us consider a smooth function $V : M \subseteq \mathbb{R}^N \rightarrow \mathbb{R}$, where M is a manifold. The points $q_c \in M$ such that $dV(q_c) = 0$ are called critical points or stationary points or saddles of V . We denote by \mathbb{H}_V or simply by \mathbb{H} the Hessian of V .

V is called a Morse function if

$$\det[\mathbb{H}_V(q_c)] \neq 0 \quad (1.2)$$

for every stationary point of V . A critical point q_c for which Eq. (1.2) holds is called non-degenerate. Moreover, the values $v_c \in \mathbb{R}$ which are image under V of critical points are called critical values or stationary values. Given a critical point, the number of negative eigenvalues of the Hessian matrix evaluated at that critical point is called index.

It can be shown that, for Morse functions, all critical points are isolated. This can be deduced by the Morse lemma:

Theorem 1.1.1 (Morse Lemma). *Let us consider a non-degenerate critical point q_c of V with index k . It exists a local coordinate system (x_1, \dots, x_N) in a neighborhood of q_c such that*

$$V = V(q_c) - x_1^2 - \dots - x_k^2 + x_{k+1}^2 + \dots + x_N^2 \quad (1.3)$$

is exact in the above defined neighborhood.

In the following of this Chapter, we will mainly consider Morse potentials. However, this is not so restrictive. Indeed, it can be shown that the Morse functions are an open and dense subset of all C^∞ functions [46]. This means that, even if the potential is not a Morse function, one can add an arbitrarily small perturbation such that the perturbed potential is a Morse function. For example, from the theorem 1.1.1 we have that any potential with a continuous symmetry is not a Morse function. In this case, perturbing the potential breaks explicitly the symmetry. A trick sometimes more useful is to consider the same system fixing a finite number of coordinates. This method will be used in the following of the Thesis.

The following theorem explains the connection between Morse functions and the topology of the set

$$M_v = \left\{ q \in M \mid \frac{V(q)}{N} \leq v \right\}. \quad (1.4)$$

Indeed, it can be proven the following:

Theorem 1.1.2. *Let us consider a smooth Morse function $V : M \subseteq \mathbb{R}^N \rightarrow \mathbb{R}$. Suppose that $[a, b] \in \mathbb{R}$ contains a single critical value v_c which corresponds to a single critical point q_c with index k ; if M_a and M_b are compact, then M_b is homeomorphic to the manifold obtained attaching¹ a k -handle to M_a , where a k -handle is the direct product of a k -disc with a $(N-k)$ -disc.*

¹For a precise definition of this operation, we address the reader to [45].

Thanks to this theorem, one can study the topology of the accessible phase space M_ν “only” studying the critical points of V . Observe, however, that for many-body systems M_ν is a high dimensional object and its topology very complicated. A topological invariant of M_ν is the Euler characteristic, defined as

$$\chi(M_\nu) = \sum_{i=0}^N (-1)^i \mu_i. \quad (1.5)$$

where μ_i is the i -th Morse number, defined as the number of critical points of V with index i and critical values smaller than ν ; to evaluate the Euler characteristic it is necessary to know all the critical points of V and their index.

1.2 Topological conjecture

The study of a series of simple models (see [35, 36] for reviews on this subject), has shown that strong changes in the topology² of

$$M_\nu = \left\{ q \in M \mid \frac{V(q)}{N} \leq \nu \right\} \quad (1.6)$$

at a given value of the potential energy ν_c are often associated to a singular behavior of thermodynamic quantities at the same value of the potential energy. This led the authors of [9] to propose that phase transitions are due to sufficiently strong topology changes in M_ν , and this proposal has been indicated as the “topological conjecture” in [11]. At this level, what exactly means “sufficiently strong” is a completely open question. Quite some research activity followed [14–34], some focused on specific models, others trying to shed light on the general mechanisms (see [35, 36] for reviews).

In this Chapter we mainly review the general results that have been obtained through this approach. We do not review the works in which specific models have been studied, but we highlight that most of these works concentrate on exactly-solvable mean-field models. The reason for this is that it is necessary to know all critical points to evaluate topological invariants such as the Euler characteristic (1.5). On the other hand, finding all the critical points of a generic many-body potential is a very hard, or impossible, task both analytically and numerically.

Franzosi and Pettini has announced in [47–49] the proof of a theorem³ proving a weaker version of the the above conjecture.

²In these early studies, the topological invariant which was usually used to characterize topology changes was the Euler characteristic, or quantities connected to it.

³The validity of this theorem has been recently questioned. We will discuss in Section 1.5 such an issue.

CHAPTER 1. INTRODUCTION

Theorem 1.2.1 (Franzosi-Pettini theorem). *Let us consider a smooth, confining, short-range and limited from below potential V in the form*

$$V_N(q) = \sum_{i=1}^N \phi(q_i) + \sum_{i,j=1}^N c_{ij} \psi(|q_i - q_j|).$$

If there exists N_0 and an interval $[v_1, v_2]$ such that $\forall N > N_0$ the hypersurfaces $(M_v)_{v \in [v_1, v_2]}$ do not change topology, then in the thermodynamic limit the free energy is at least $C^2[\beta(v_1), \beta(v_2)]$, where $\beta(v)$ is the value of the inverse temperature corresponding to the potential energy v .

The authors state that the extension of such a theorem to take into account higher derivatives of the free energy is, even if laborious, affordable with similar techniques. On the other hand, it is known that none of the hypotheses of the theorem is merely technical; counterexamples are indeed known for long-range, non-confining or singular potentials [35].

Thanks to Morse theory, this theorem can be clearly stated using stationary points. Indeed, if V is a Morse function, topological changes of the manifolds $(M_v)_{v \in [v_1, v_2]}$ correspond to the existence of stationary points of the potential V whose energy density value are belong to $[v_1, v_2]$.

At qualitative level, the connection between stationary points of the Hamiltonian and equilibrium statistical properties can be inferred in the microcanonical formalism. This can be understood by observing that, for a system with N degrees of freedom, the entropy density is defined as ⁴

$$s(\varepsilon) = \frac{1}{N} \log \omega(\varepsilon), \quad (1.7)$$

where $\varepsilon = E/N$ is the energy density and ω is the density of states. For a system described by continuous variables, ω can be written as

$$\omega(\varepsilon) = \int_{\Gamma} \delta(\mathcal{H} - N\varepsilon) d\Gamma = \int_{\Gamma \cap \Sigma_\varepsilon} \frac{d\Sigma}{|\nabla \mathcal{H}|}, \quad (1.8)$$

where Γ denotes the phase space and $d\Gamma$ its volume measure, Σ_ε is the hypersurface of constant energy $E = N\varepsilon$, and $d\Sigma$ stands for the $N - 1$ -dimensional Hausdorff measure on Σ_ε . The rightmost integral stems from a co-area formula [50]. At a stationary point q_c , the gradient $\nabla \mathcal{H}(q_c)$ vanishes and the integrand diverges; at the same time, the measure Σ_ε shrinks, such that ω in general remains finite for finite systems. In next Section, we will see that, although the integral on the right hand side of Eq. (1.8) remains finite in the vicinity of a stationary point, the density of states is non-analytic in correspondence of all the stationary values $\varepsilon_c = H(q_c)/N$ of the energy density for any finite N .

⁴Throughout the Thesis we set Boltzmann's constant k_B to unity.

1.3 Microcanonical singularities in finite systems

At variance with the canonical and grand-canonical ensemble, in which the free energies of finite systems are smooth functions [51], the microcanonical entropy shows singularities. From a conceptual point of view, this should be known since long time because even one-dimensional systems, such as the pendulum, present this feature. Surprisingly, for many-body systems, such a property of the entropy has been realized only recently [52–55].

Here, we review the results due to Kastner, Schreiber and Schnetz [37, 56] which completely characterize, for finite systems, the singularities of the configurational entropy and their strength. They found a one-to-one correspondence between the stationary values of the potential energy and the singularities of the configurational entropy. The kind of singular behavior is also characterized; in particular, the entropy presents a discontinuity only in a derivative whose order grows linearly with N .

We then discuss the results of [57], in which the role of the kinetic energy is analyzed: the kinetic energy increases the regularity of the entropy, which remains anyway a singular function.

1.3.1 Singularities in the configurational entropy

Let us consider a Hamiltonian system of the form (1.1), where V is a smooth and confining potential. We review here the work presented in [37, 56], where the authors have analyzed the singularities of the configurational density of states⁵, defined as

$$\omega_N^c(v) = \int_{\Gamma_N} \delta(V(q) - Nv) dq \quad (1.10)$$

or, equivalently of the configurational entropy

$$s_N^c(v) = \frac{1}{N} \log \omega_N^c(v). \quad (1.11)$$

First of all, the singularities of $\omega_N^c(v)$ are strictly connected to the critical values of V . Indeed, it is possible to prove [48] that if there are not critical values of V/N in $[v_1, v_2]$, then ω_N^c and s_N^c are smooth in the same interval.

Let us consider a given value of the potential energy density v and the set

$$V^{-1}(v) = \left\{ q \in \Gamma_N \mid \frac{V(q)}{N} = v \right\}; \quad (1.12)$$

⁵Very similar results are valid considering the integrated density of states $\Omega_N^c(v) = \int_{\Gamma_N} \Theta(V(q) - Nv) dq$ and the corresponding entropy $\sigma_N^c(v) = \frac{1}{N} \log \Omega_N^c(v)$, which is connected to the previous definitions via

$$\omega_N^c(v) = \frac{d\Omega_N^c(v)}{dv}. \quad (1.9)$$

CHAPTER 1. INTRODUCTION

if $V^{-1}(v)$ does not contain critical points of V , then ω_N^c is smooth in v . Otherwise, if $V^{-1}(v)$ contains critical points, the Morse property guarantees that they are isolated; for every critical point q_c^i , we can thus choose a neighborhood $U_{q_c^i}$ which does not contain any other critical point but q_c^i . We can thus suppose that only one critical point q_c is present: the generalization to the case of many only corresponds to add up the various contributions. The density of states can be written as

$$\omega_N^c(v) = \int_{U_{q_c}} \delta(V(q) - Nv) dq + \int_{\Gamma_N - U_{q_c}} \delta(V(q) - Nv) dq; \quad (1.13)$$

where the second term gives a smooth contribution.

Without any loss of generality, we can choose $V(q_c) = 0$. Thanks to the Morse lemma, the neighborhood U_{q_c} of the critical point and the coordinate system (x_1, \dots, x_N) can be chosen such that

$$V(q(x)) = - \sum_{i=1}^k x_i^2 + \sum_{i=k+1}^N x_i^2 \quad (1.14)$$

is valid in the whole neighborhood U_{q_c} ; in the above expression, k is the index of the critical point q_c . Denoting by $J(x)$ the determinant of the Jacobian of the coordinate transformation, let us consider the following expansion around $x = 0$:

$$J(x) = \sum_{I=\{i_1, \dots, i_N\}} a_I x^I, \quad (1.15)$$

where a multi-index notation $x^I = x_1^{i_1} \dots x_N^{i_N}$ has been used. The 0-th order is linked to the second derivatives of the potential at the critical point, that is:

$$J(0) = a_0 = \left| \det \left[\frac{\mathbb{H}_V(0)}{2} \right] \right|^{-\frac{1}{2}}. \quad (1.16)$$

Using these facts and choosing as U_{q_c} a small enough ball around q_c , the authors of [37] evaluated the non-analytic contribution to the configurational density of states due to the first term of (1.13) at all the orders in the expansion of the determinant of the Jacobian. To our scope, the 0-th order⁶ will be sufficient; in this case the theorem has the form:

Theorem 1.3.1 (Singularities of the configurational entropy for finite systems). *Let us consider a Morse function $V : G \subseteq \mathbb{R}^N \rightarrow \mathbb{R}$ with a single critical point q_c with index k in an open set G ; we denote by $\frac{V(q_c)}{N} = v_c$ the critical value corresponding to q_c . The configurational density of states can be written as the sum of an analytic plus a singular part, that is:*

$$\omega_N^c = \omega_N^a + \omega_N^{na}. \quad (1.17)$$

⁶For the proof and the general statement of the theorem at any order in the expansion of the Jacobian, we address the reader to [37].

1.3. MICROCANONICAL SINGULARITIES IN FINITE SYSTEMS

The leading order of the singular part is given by

$$\omega_N^{na}(v) = \frac{(N\pi)^{N/2}}{N\Gamma(\frac{N}{2})\sqrt{\left|\det\left[\frac{\mathbb{H}_V(q_c)}{2}\right]\right|}} h_{N,k(\bmod 4)}^{na}(v) \quad (1.18)$$

where the singularity is given by

$$h_{N,k(\bmod 4)}^{na}(v) = \begin{cases} (-1)^{k/2} v^{(N-2)/2} \Theta(v) & k \text{ even,} \\ (-1)^{(k+1)/2} v^{(N-2)/2} \pi^{-1} \log|v| & N \text{ even, } k \text{ odd,} \\ (-1)^{(N-k)/2} (-v)^{(N-2)/2} \Theta(-v) & N, k \text{ odd.} \end{cases} \quad (1.19)$$

$h_{N,k(\bmod 4)}^{na}(v)$ is universal in the sense that it is independent of V . In the case in which there are more than one critical points of V , their contributions sum up. Finally, the contribution of the singularities due to higher order in the expansion of the determinant (1.15) only changes the pre-factor in Eq. (1.18) and not the universal function $h_{N,k(\bmod 4)}^{na}(v)$.

It can be verified that in any of the three cases in Eq. (1.19), ω_N^c is $\lfloor(N-3)/2\rfloor$ times differentiable⁷, where we denote by $\lfloor x \rfloor$ the largest natural number smaller than x . Let us observe that asking that the potential is a Morse function is actually a stronger hypothesis with respect to what is needed. Indeed, if V is a function with non-degenerate critical points on $\Gamma_N - U$, where U is a given set, the previous analysis is still valid for all those values of potential energy except for those included in $V(U)$.

In short, Theorem 1.3.1 says that the singularities of the configurational entropy of a Hamiltonian system with a Morse potential are in one-to-one correspondence with the critical values of the potential. Moreover, the entropy becomes smoother and smoother by increasing N . This could lead us to the conclusion that, in the $N \rightarrow \infty$ limit, such singularities disappear. We will see in the next Section, however, that this is not necessarily the case.

1.3.2 Role of the kinetic energy

A standard kinetic energy term, of the form in Eq. (1.1), gives a trivial contribution to the canonical partition function both for finite systems and in the thermodynamic limit; it just translates by a constant the thermodynamical functions. In the microcanonical ensemble, the effect of such a term is more subtle and has been analyzed in [57]. The results are the following:

- (i) for finite systems: the entropy density is singular in $\varepsilon = v_c$ if and only if the configurational entropy density is singular at v_c . Moreover, if the configurational entropy density is m times differentiable, then the entropy density is $m + \lfloor N/2 \rfloor$ times differentiable.

⁷Considering the integrated density of states, defined in Eq. (1.9), one obtains a slightly higher regularity; indeed, Ω_N^c is $\lfloor(N-1)/2\rfloor$ differentiable.

CHAPTER 1. INTRODUCTION

(ii) in the thermodynamic limit: if the configurational entropy density is singular in ν_c , then the entropy density is singular in ε such that $\langle \nu \rangle(\varepsilon) = \nu_c$, where $\langle \nu \rangle$ denotes the average of the potential energy per particle. Thus the two values ε and ν_c coincide only if the average kinetic energy is zero.

Let us give a hint of how these results can be obtained; we address the reader to [57] for the complete proofs. First of all, let us observe that q_c is a critical point of V if and only if $(0, q_c)$ is a critical point of the Hamiltonian (1.1). Moreover, for a system as (1.1), the density of states can be written as a convolution product [58]. Indeed, defining a kinetic density of states

$$\omega_N^k(\gamma) = \int_{\mathbb{R}^N} \delta \left(\frac{1}{2} \sum_{i=1}^N p_i^2 - N\gamma \right) dp = \frac{2\pi^{N/2}}{\Gamma(\frac{N}{2})} (2N^{\frac{N}{2}-1}) \gamma^{\frac{N}{2}-1}, \quad (1.20)$$

we have

$$\omega_N(\varepsilon) = \int_0^\infty \omega_N^k(\varepsilon - \gamma) \omega_N^c(\gamma) d\gamma. \quad (1.21)$$

From Theorem 1.3.1, all the singularities of $\omega_N^c(\nu)$ are algebraic; the results for finite systems can be obtained by directly evaluating the convolution product.

For what concerns infinite systems, assuming the $N \rightarrow \infty$ limit of s_N^c exists, it can be proven [58] that also the $N \rightarrow \infty$ limit of s_N exists and is given by

$$s_\infty(\varepsilon) = \lim_{N \rightarrow \infty} \frac{1}{N} \log \left\{ \max_{\gamma \geq 0} [\omega_N^k(\gamma) \omega_N^c(\varepsilon - \gamma)] \right\} = s_\infty^k[\tilde{\gamma}(\varepsilon)] + s_\infty^c[\varepsilon - \tilde{\gamma}(\varepsilon)], \quad (1.22)$$

where $\tilde{\gamma}(\varepsilon)$ is the value of γ which maximizes the previous expression. Thus, $\tilde{\gamma}(\varepsilon)$ coincides with the average kinetic energy density; the final results is obtained writing the entropy as

$$s_\infty(\varepsilon) = s_\infty^k[\varepsilon - \langle \nu \rangle(\varepsilon)] + s_\infty^c[\langle \nu \rangle(\varepsilon)]. \quad (1.23)$$

Let us observe that the the only property needed in the proof, ensured by Theorem 1.3.1, is that there are only algebraic singularities. Considering a potential which is not a Morse function but such that singularities in the configurational entropy density are algebraic, the conclusions above are not altered. A model with these properties has actually been studied in [57].

Let us conclude with some comments. The classical definition of phase transitions, valid in the canonical and grand-canonical ensembles, for which a phase transition is a singular point of the thermodynamical functions, cannot be translated without modifications to the microcanonical ensemble: typically, the number of critical points of the potential energy is $\mathcal{O}(e^N)$. For finite systems, the number of points in which the entropy is singular is thus of this order; however, they are essentially irrelevant for the thermodynamics, as the singularity is on a derivative of order $N/2$ of the entropy. Is there any way for a singularity of the entropy of a finite system to survive in the thermodynamic limit, giving rise to a phase transition? The next Section addresses this point.

1.4 KSS Theorems

It is natural to ask if some of the singularities of the microcanonical entropy of a finite system can survive in the $N \rightarrow \infty$ limit, giving thus rise to a phase transition. Here we discuss a Theorem due to Kastner, Schreiber and Schnetz [37, 38] which gives a necessary condition for this to happen, at least from a theoretical point of view. However, the applicability of such result for non-trivial systems is not completely straightforward. In Chapter 2, we will see how this problem can be handled. For the moment, however, we give a sketch of the argument which leads to Theorem 1.4.1 and we state precisely the results.

Let us consider the configurational density of states in a small interval $(\nu_0 - \epsilon, \nu_0 + \epsilon)$ around a given value of the potential energy density ν_0 ; to lighten the notation, we denote here by $\omega_N(\nu)$ the configurational density of states, omitting the apex c . We write

$$\omega_N^{\nu_0, \epsilon}(\nu) = A_N^{\nu_0, \epsilon}(\nu) + B_N^{\nu_0, \epsilon}(\nu), \quad (1.24)$$

where $B_N^{\nu_0, \epsilon}(\nu)$ contains the singular contribution due to all the critical points whose energies are in the interval $(\nu_0 - \epsilon, \nu_0 + \epsilon)$, as specified in Theorem 1.3.1:

$$B_N^{\nu_0, \epsilon}(\nu) = \sum_{\{v_c \mid |v_c - \nu_0| < \epsilon\}} \sum_{\{q_c \mid \frac{v(q_c)}{N} = v_c\}} \omega_{N, q_c}^{n_a}(\nu). \quad (1.25)$$

Using Theorem 1.3.1, we can add to $B_N^{\nu_0, \epsilon}(\nu)$ a smooth function $A_N^{\nu_0, \epsilon}(\nu)$ such that Eq. (1.24) coincides with the configurational density of states in the set $(\nu_0 - \epsilon, \nu_0 + \epsilon)$.

We are interested to the regularity properties of the entropy density; the latter can be written, in the set $(\nu_0 - \epsilon, \nu_0 + \epsilon)$:

$$s^{\nu_0, \epsilon}(\nu) = \lim_{N \rightarrow \infty} \frac{1}{N} \log[\omega_N^{\nu_0, \epsilon}(\nu)] = \lim_{N \rightarrow \infty} \frac{1}{N} \log[A_N^{\nu_0, \epsilon}(\nu) + B_N^{\nu_0, \epsilon}(\nu)]. \quad (1.26)$$

We observe that we can also write

$$s^{\nu_0, \epsilon}(\nu) = \max\{a^{\nu_0, \epsilon}(\nu), b^{\nu_0, \epsilon}(\nu)\}, \quad (1.27)$$

where

$$\begin{aligned} a^{\nu_0, \epsilon}(\nu) &= \lim_{N \rightarrow \infty} \frac{1}{N} \log[A_N^{\nu_0, \epsilon}(\nu)], \\ b^{\nu_0, \epsilon}(\nu) &= \lim_{N \rightarrow \infty} \frac{1}{N} \log[B_N^{\nu_0, \epsilon}(\nu)], \end{aligned} \quad (1.28)$$

unless

$$\lim_{N \rightarrow \infty} \frac{B_N^{\nu_0, \epsilon}(\nu)}{A_N^{\nu_0, \epsilon}(\nu)} = -1, \quad (1.29)$$

which is a very peculiar situation and therefore not considered here.

CHAPTER 1. INTRODUCTION

It is clear from Eq. (1.27) that it is impossible to find (necessary or sufficient) conditions for the regularity of $s^{\nu_0, \epsilon}(\nu)$ without the knowledge of both the terms $a^{\nu_0, \epsilon}(\nu)$ and $b^{\nu_0, \epsilon}(\nu)$. For example, a mechanism by which it is possible to generate a singularity in $s^{\nu_0, \epsilon}(\nu)$ is a *crossover* between the two terms in the maximization: in general they will not match analytically. Moreover, even if $A_N^{\nu_0, \epsilon}(\nu)$ is smooth, there are no results ensuring its uniform convergence in the $N \rightarrow \infty$ limit, and hence the smoothness of $a^{\nu_0, \epsilon}(\nu)$.

In [37, 38], necessary conditions have been found such that the singular term $B_N^{\nu_0, \epsilon}(\nu)$ gives a non vanishing contribution for every small neighbourhood of ν_0 in the $N \rightarrow \infty$ limit. We report the reasoning followed in [37, 38] without entering in the details.

The analytic pre-factor of Eq. (1.18)

$$\frac{(N\pi)^{N/2}}{N\Gamma(N/2)} \quad (1.30)$$

is exponential in N . Then, $B_N^{\nu_0, \epsilon}(\nu)$ contributes to $\omega_N^{\nu_0, \epsilon}(\nu)$ with a term which goes to zero when ϵ goes to zero. On the other hand, we want that $b^{\nu_0, \epsilon}(\nu)$ dominates on $a^{\nu_0, \epsilon}(\nu)$ independently on ϵ and thus, the only possibility is that

$$\lim_{N \rightarrow \infty} \left| \det [\mathbb{H}_V(q_c)] \right|^{\frac{1}{N}} = 0. \quad (1.31)$$

The quantity (1.31) will be called normalized determinant of the Hessian evaluated in q_c . The argument presented here is not rigorous because it is not clear in which order we perform the limits $N \rightarrow \infty$ and $\epsilon \rightarrow 0$. The final Theorem takes the form:

Theorem 1.4.1 (KSS Theorem). *Let us consider $V : \Gamma_N \subseteq \mathbb{R}^N \rightarrow \mathbb{R}$ a confining potential. Denoting by q_c the critical points of V and their index by $k(q_c)$, we call ‘‘Jacobian densities’’ the following quantities:*

$$j_l(\nu_0) = \limsup_{N \rightarrow \infty} \frac{1}{N} \log \left[\frac{\sum_{q_c \in Q_l([\nu_0, \nu_0 + \epsilon])} J(q_c)}{\sum_{q_c \in Q_l([\nu_0, \nu_0 + \epsilon])} 1} \right], \quad (1.32)$$

where

$$J(q_c) = \frac{1}{\sqrt{\left| \det \left[\frac{\mathbb{H}_V(q_c)}{2} \right] \right|}} \quad (1.33)$$

and

$$Q_l(\nu_0) = \left\{ q_c \mid \left(\frac{V(q_c)}{N} = \nu_0 \right) \wedge [k(q_c) = l \pmod{4}] \right\}. \quad (1.34)$$

Then, the contribution $b^{\nu_0, \epsilon}(\nu_0)$ defined in Eq. (1.28) cannot induce a phase transition in the limit $N \rightarrow \infty$ at the potential energy ν_0 if

1. the total number of critical points is limited by $\exp(CN)$ for a given constant $C > 0$;
2. $\forall \epsilon$ small enough the Jacobian densities satisfy $j_l(\nu_0) < \infty$, $\forall l \in \{0, 1, 2, 3\}$.

1.5. CONTROVERSY ON THE FRANZOSI-PETTINI THEOREM

The proof consists in finding an estimate from above of $b^{v_0, \epsilon}(v)$ which depends only on ϵ and not on V . The estimate is:

$$b^{v_0, \epsilon}(v) \leq \frac{1}{2} \log \epsilon + \sqrt{2\pi e} + \max_{\{l \in \{0,1,2,3\}, |v-v'| < \epsilon\}} [n_l + j_l(v')], \quad (1.35)$$

where

$$n_l = \lim_{N \rightarrow \infty} \frac{1}{N} \log \sum_{q_c \in Q_l(\mathbb{R})} 1 \quad (1.36)$$

is the total density of critical points. If the hypotheses of the Theorem are satisfied, the last term in Eq. (1.35) is finite and we can choose ϵ small enough such that $a^{v_0, \epsilon}(v)$ dominates over $b^{v_0, \epsilon}(v)$; in this case the contribution of critical points of V is negligible in the limit $N \rightarrow \infty$.

In the literature, the KSS Theorem has been applied to three models [37]:

1. the XY mean field model
2. the k -trigonometric model
3. the spherical model with nearest-neighbor interactions. In this case, a singularity of the Euler characteristic in a value of potential energy v_t does not correspond to a phase transition [22]; this is consistent with the fact that the KSS criterion is not satisfied.

In these cases the evaluation of $j_l(v)$ is possible inverting the relation between the critical points and the critical values, that is finding the relation $q_c = q_c(v_c)$. For a general model this operation can be essentially impossible and thus the application of the KSS Theorem is extremely difficult. As we will see in Section 2.1, this problem can be essentially avoided; this fact will give the possibility to apply the KSS criterion to non-trivial models, and also to the case in which only a subset of all the critical points is known.

1.5 Controversy on the Franzosi-Pettini theorem

We conclude this introductory part discussing a recent debate on the validity of the Franzosi-Pettini theorem. The content of this Section contains very recent (and partially not published) results, so that it has to be considered as a very preliminary discussion on the subject: most of the questions raised here are still open.

In [59] the authors claimed that a counterexample to the Franzosi-Pettini Theorem is provided by the φ^4 model

$$V_\varphi = \sum_{i \in \Lambda} \left[\frac{\lambda}{4!} \varphi_i^4 - \frac{\mu^2}{2} \varphi_i^2 + \frac{J}{4} \sum_{j \in \mathcal{N}(i)} (\varphi_i - \varphi_j)^2 \right], \quad (1.37)$$

CHAPTER 1. INTRODUCTION

where $J, \lambda, \mu > 0$, $\Lambda \subset \mathbb{Z}^2$ is a finite square lattice and by $\mathcal{N}(i)$ we denote the four nearest-neighbor sites of i .

After the claim, in a second paper [60], they proved that the Hamiltonian in Eq. (1.37) satisfies the hypotheses of the Franzosi-Pettini theorem. The most difficult hypothesis to prove is the Morse property, which is not valid for all the values of λ, μ, J and N . However (see appendix of [60]), the hypotheses of the theorem are still satisfied.

Now, with a very simple calculation [59], it is possible to show that, for every N , there are no critical points at energy density greater than zero.

However, it is well known that the φ^4 model undergoes to a phase transition; performing Monte-Carlo simulations [59, 60], they showed that it occurs at energy density well separated from zero for a wide range of parameters. This result is thus in evident contradiction with the Franzosi-Pettini theorem, as stated in [48].

From private communications with Franzosi, Pettini and Kastner, it looks that the flaw in the theorem is the absence of an hypothesis in its statement. It looks like that the authors used for the proof the following additional hypothesis:

there must be no sequences $q_N \in \Gamma_N$ such that $V(q_N) \rightarrow v_0$ with $v_0 \in [v_1, v_2]$ and $\|\nabla V(q_N)\| \rightarrow 0$ in the $N \rightarrow \infty$ limit.

This hypothesis is clearly much stronger than, as originally asked in Theorem 1.2.1, the absence of critical points with critical values in $[v_1, v_2]$ for N large enough. From a qualitative point of view, the new request corresponds to ask that “changes in the topology of $(M_\nu)_{\nu \in [v_1, v_2]}$ cannot happen neither asymptotically”. Let us however observe that the infinite-dimensional Morse theory is not a direct generalization of its finite-dimensional counterpart, so that our interpretation is just qualitative.

We observe that such a scenario is actually natural. Indeed, stationary points of the potential can be very easily transformed in non-stationary points with the application of external fields or fixing different boundary conditions, even in the case in which one expect no differences in the thermodynamical behavior. However, a property like the one stated above should not be altered unless the external fields or the changes in the boundary conditions are so strong that even the thermodynamical behavior changes.

Anyway, the fact that these results are very recent (and in part not published) makes mandatory to revisit them with care before drawing any conclusion. We want to underline that these results have not influenced our work because they have been obtained after ours.

Observe that results from [48] have been used to prove the Theorem 1.3.1 on singularities in the microcanonical entropy of finite systems. However, we have not used the Franzosi-Pettini theorem for this scope but only a much weaker result, on the smoothness of ω_N^a for

1.5. CONTROVERSY ON THE FRANZOSI-PETTINI THEOREM

fixed N ; the φ^4 model is not a counterexample for this result and its validity is not under debate. We thus think that the results presented in this Chapter (with the exception, of course, of the Franzosi-Pettini theorem) should be free of errors; however, all the discussion here has to be analyzed with care in the future. Also the fact that the counterexample proposed by Kastner et al. actually satisfies all the hypotheses of the Franzosi-Pettini theorem, and in particular the Morse property, should be carefully checked.

2

The self-gravitating ring model

The applicability of the KSS theorem to non mean-field systems seems very difficult, if not impossible. To apply it directly, one has indeed to know not only all the critical points of the potential but also their index; moreover, one should be able to invert the relation between the critical points q_c and the critical energies $V(q_c)$. Each of these steps can be extremely difficult, or even impossible, for generic Hamiltonian systems.

In Section 2.1, we show how this problem can be handled. It turns out that, from a practical point of view, the KSS Theorem can be reformulated in terms of a criterion to find phase transitions. We will call it the “KSS criterion”.

The most interesting fact coming out from this analysis is that the KSS criterion can be applied even if we do not know all the saddles of the potential V and without any knowledge of their index. In Section 2.2, we apply the KSS criterion to the Self-Gravitating Ring (SGR) model, which is the first not exactly solvable model to which the criterion has been applied. We show analytically that the criterion correctly singles out the phase transition between a homogeneous and a clustered phase and also suggests the presence of another phase transition, not previously known.

To analyze the nature of such possible phase transition, we construct in Section 2.3 an effective model of the SGR whose thermodynamics is analytically solvable. It turns out that this effective model has an interest in itself: despite the rather crude approximations involved in its derivation, it compares quite well with the SGR model. In [39] the similarities between our effective model and another model introduced by Thirring¹ forty years ago are discussed. The two models are very similar and can be considered as examples of a class of minimal models of self-gravitating systems.

The material presented in Sections 2.1 and 2.2 is part of the Master Thesis of the author [40] and is only briefly sketched here; we address the reader to [40] and [28] for further

¹The Thirring model, first introduced in [61], is defined in the following way. N particles are confined in a box of volume V and two particles interact with a constant potential if both of them finds inside a smaller volume V_0 ; otherwise, they do not interact.

details.

2.1 KSS criterion

It is commonly believed [1, 62] that the total number of critical points in a generic Hamiltonian system does grow exponentially with the number of degrees of freedom. A proof of this property is not available and, actually, there are examples in which this is not the case: for example, in the mean-field spherical model [37] the total number of critical points does not increase with N . Anyway, the exponential behavior is the most common one. The first hypothesis of Theorem 1.4.1 is probably only technical and we proceed assuming that it is satisfied.

It is natural to reformulate the KSS theorem under the form of a criterion to find phase transitions:

In the limit $N \rightarrow \infty$, there can be a singularity in the configurational entropy induced by saddles of V in a value ν_0 of potential energy density only if at least one of the Jacobian densities $j_l(\nu_0)$ diverges.

In this spirit, let us suppose that we want to verify the condition of the above criterion at a given value of energy density ν_0 . Suppose also that we know only a class of critical points of V which not necessarily contains all of them. This is the most common situation considering a non-trivial system, as we will see in the following of this Thesis. We thus have to prove that $l \in \{0, 1, 2, 3\}$ exists such that, in the limit $N \rightarrow \infty$, the quantity

$$\frac{1}{N} \log \left[\frac{\sum_{q_c \in Q_l([\nu_0, \nu_0 + \epsilon])} J(q_c)}{\sum_{q_c \in Q_l([\nu_0, \nu_0 + \epsilon])} 1} \right] \quad (2.1)$$

is not definitely bounded. The first interesting fact is that the index does not play any role: indeed, if we prove that the quantity in Eq. (2.1) is not bounded, at least one of the four subsequences is not. Because $J(q_c) > 0$, the quantity in Eq. (2.1) can be estimated from above restricting the sums to a subset of the critical points:

$$\frac{1}{N} \log \left[\frac{\sum_{q_c \in Q_l([\nu_0, \nu_0 + \epsilon])} J(q_c)}{\sum_{q_c \in Q_l([\nu_0, \nu_0 + \epsilon])} 1} \right] \geq \frac{1}{N} \log \left[\sum_{q_c \in \tilde{Q}} J(q_c) \right] - \text{constant}. \quad (2.2)$$

Here we have assumed the first hypothesis of the KSS theorem to be valid to neglect the denominator. Recalling the results in Section 1.3.2, we thus arrive to state the following criterion:

KSS criterion: Consider a classical Hamiltonian system of the form (1.1) and assume that the stationary points of V are isolated and their overall number grows at most exponentially

2.2. APPLICATION OF THE KSS CRITERION TO THE SGR MODEL

with N . Then, in the $N \rightarrow \infty$ limit, a singularity in the microcanonical entropy $s(\varepsilon)$ at energy density ε_c induced by saddles of V can be present only if the following two conditions are met. First, there must be a sequence of critical points $\{q_c^N\}_{N=1}^\infty$ whose corresponding stationary values converge to $v_0 = \langle v \rangle(\varepsilon_c)$, where the brackets denote the statistical average. This means:

$$\lim_{N \rightarrow \infty} v(q_c^N) = v_0. \quad (2.3)$$

Second, the Hessian matrix \mathbb{H}_V of the potential V computed on the stationary configurations q_c^N is such that

$$\lim_{N \rightarrow \infty} \left| \det [\mathbb{H}_V(q_c^N)] \right|^{1/N} = 0. \quad (2.4)$$

Since the eigenvalues of \mathbb{H}_V can be seen as curvatures of the potential energy landscape, Eq. (2.4) means that the saddles become asymptotically “flat”.

Note that to check whether Eqs. (2.3) and (2.4) are satisfied one does not need to know all the saddles of the potential V ; it is sufficient to determine the “right” ones. This is a big difference with respect to other criteria previously proposed, which made use of topological invariants like the Euler characteristic [11, 35, 36]. It is however important to underline that without a complete knowledge of the critical points of V , it is impossible to prove the validity of the second hypothesis of the KSS theorem.

2.2 Application of the KSS criterion to the SGR model

We review in this Section the application of the KSS criterion to the SGR model. The details can be found in [40].

2.2.1 The model

The model we studied is the Self-Gravitating Ring (SGR) model, first introduced in [63] as a simplified model of a self-gravitating system. It is a model of N points of unitary mass moving on a circle of unitary radius and mutually interacting via gravitational forces, regularized at short distances. Its Hamiltonian is of the form (1.1) with potential

$$V = -\frac{1}{2N\sqrt{2}} \sum_{i,j=1}^N \frac{1}{\sqrt{1 - \cos(q_i - q_j) + \alpha}}, \quad (2.5)$$

where $q_i \in (-\pi, \pi]$, $i = 1, \dots, N$, are the angles giving the position of the i -th particle on the ring and $\alpha > 0$ is the softening parameter regularizing the potential for $(q_i - q_j) \rightarrow 0$. The $\frac{1}{N}$ factor in Eq. (2.5) ensures extensivity according to the Kac prescription. Observe that the quantity $1/\left[1 - \cos(q_i - q_j)\right]$ is the length of the chord connecting q_i and q_j , see Fig. 2.1.

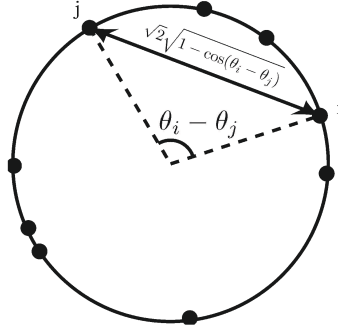


Figure 2.1 – SGR model with unitary radius. The particles are visualized on the circle and their position is specified by the angles q_i , measured with respect to a given direction. The distance between two particles is given by the length of the chord show in the Figure.

Numerical results (N -body simulations [63] as well as variational calculations in the $N \rightarrow \infty$ limit [64]) for the microcanonical thermodynamics show that the system has a phase transition separating a homogeneous high-energy phase from a clustered phase where the rotational symmetry of the potential is spontaneously broken. If the softening parameter α is sufficiently small the clustered phase contains an energy interval with negative specific heat, there is nonequivalence between the microcanonical and the canonical ensemble and the qualitative behavior of the system is very similar to that of three-dimensional self-gravitating models. In the opposite limit $\alpha \rightarrow \infty$ SGR becomes equivalent to the ferromagnetic HMF model [65].

Assuming that in the high-energy phase the particles are homogeneously distributed on the ring, as suggested by the numerical results, one can calculate the expectation value of the potential energy density at the transition in the limit $N \rightarrow \infty$, obtaining

$$v_c = \langle v \rangle(\epsilon_c) = \frac{1}{\pi \sqrt{2(2+\alpha)}} \mathcal{K} \left(\frac{2}{2+\alpha} \right), \quad (2.6)$$

where $\mathcal{K}(x) = \int_0^{\pi/2} d\vartheta / \sqrt{1 - x \sin^2 \vartheta}$ is the complete elliptic integral of the first kind.

2.2.2 Saddles of the landscape and phase transitions in the SGR model

Let us now study the potential energy landscape of the SGR model. First of all let us note that the stationary points of the potential (2.5) are not isolated, due to its rotational invariance. However, this difficulty can be circumvented by fixing the value of one of the q 's, which has an irrelevant effect on the thermodynamic functions as $N \rightarrow \infty$ and only fixes the position of the center of the cluster in the broken-symmetry phase: from now on we assume $q_1 \equiv 0$.

The stationary points of V are the solutions of the form $(\bar{q}_1 \equiv 0, \bar{q}_2, \dots, \bar{q}_N)$ of the N cou-

2.2. APPLICATION OF THE KSS CRITERION TO THE SGR MODEL

pled nonlinear equations $\nabla V = 0$, i.e.,

$$\nabla V = \frac{1}{2N\sqrt{2}} \sum_{i=1}^N \frac{\sin(q_i - q_k)}{[1 - \cos(q_i - q_k) + \alpha]^{3/2}} = 0, \quad (2.7)$$

with $k = 1, \dots, N$. Physically the above equations mean that the force acting on each particle is radial. There are at least two classes of solutions that can be easily found.

- First of all there are the solutions we shall refer to as $0-\pi$ *saddles*, where N_π particles are in $q = \pi$ and the others are in $q = 0$, with $0 \leq N_\pi \leq N - 1$. We shall denote such configurations as q_{n_π} , where $n_\pi = N_\pi/N$.
- The other class of solutions of Eqs. (2.7) that is easily found is that of configurations where the particles are in the p vertices of a regular polygon, with the same number r of particles in each vertex; from symmetry considerations one sees that the force can be only radial. We shall refer to the latter solutions as *polygonal saddles* and we shall denote them as $q_{p,r}$, with $N = pr$.

There are also many other saddles of the SGR potential that do not belong to any of these two classes. For instance, consider three angles 0 , γ and δ , and put N_0 particles in 0 , N_γ in γ and N_δ in δ . It can be shown that for almost any value of γ and δ such that $0 < \gamma < \pi$, $-\pi < \delta < 0$ and $0 < \delta - \gamma < \pi$ one can choose sufficiently large N , N_0 , N_γ and N_δ such that this configuration is stationary; moreover, one can find arguments suggesting that also more complex stationary configurations exist [40]. The polygonal and $0-\pi$ saddles, then, are not the only saddles of the potential energy landscape of the SGR model.

The fact that we do not know all the saddles of the potential energy landscape, does not prevent the KSS criterion to be effectively applied to this model. Let us calculate the stationary values $v = V/N$ corresponding to the $0-\pi$ and polygonal saddles, respectively. For q_{n_π} we have

$$v(n_\pi) = -\frac{1}{2\sqrt{2}} \left[\frac{(1 - n_\pi)^2 + n_\pi^2}{\sqrt{\alpha}} + \frac{2n_\pi(1 - n_\pi)}{\sqrt{2 + \alpha}} \right]. \quad (2.8)$$

The maximum of $v(n_\pi)$ is attained for $n_\pi = 1/2$ and the minimum, corresponding to $n_\pi = 0$, is also the absolute minimum of the potential. Hence

$$-\frac{1}{2\sqrt{2\alpha}} \leq v(n_\pi) \leq -\frac{1}{4\sqrt{2}} \left[\frac{1}{\sqrt{\alpha}} + \frac{1}{\sqrt{2 + \alpha}} \right], \quad (2.9)$$

and the values of $v(n_\pi)$ become dense in the above interval as $N \rightarrow \infty$.

For polygonal saddles $q_{p,r}$ we have that the stationary values depend only on the number of vertices p :

$$v(p) = -\frac{1}{2p\sqrt{2}} \sum_{j=0}^{p-1} \frac{1}{\sqrt{1 - \cos\left(\frac{2\pi j}{p}\right) + \alpha}}. \quad (2.10)$$

CHAPTER 2. THE SELF-GRAVITATING RING MODEL

The function $v(p)$ is monotonously increasing with p and

$$v(p) \geq -\frac{1}{4\sqrt{2}} \left[\frac{1}{\sqrt{\alpha}} + \frac{1}{\sqrt{2+\alpha}} \right], \quad (2.11)$$

so that $v(p) > v(n_\pi) \forall p, n_\pi$. Moreover, a simple calculation shows that $\lim_{p \rightarrow \infty} v(p) = v_c$, where v_c is given by Eq. (2.6) and is also the upper bound of the potential energy per particle. We have thus two nontrivial results:

- (i) since as $N \rightarrow \infty$ the distance between two successive stationary values tends to zero in both cases of $v(n_\pi)$ and $v(p)$, although $0-\pi$ and polygonal saddles are not the only stationary values of V , their stationary values do encompass all the available values of the potential energy of the model;
- (ii) the sequence of stationary values $v(p)$ converges to the critical potential energy v_c of the phase transition between the homogeneous and the clustered phase as $p \rightarrow \infty$.

The last result suggests to investigate whether the KSS criterion is satisfied for $v = v_c$, i.e., whether a sequence of saddles satisfying Eqs. (2.3) and (2.4) exists, with v_c given by Eq. (2.6). To this end, consider the sequence of polygonal saddles with one particle in each vertex, $q_{N,1}$, where N is prime; Eq. (2.3) is satisfied—see item (ii) above.

It remains to show that also Eq. (2.4) is satisfied. Define

$$f_k = \frac{1}{4N\sqrt{2}} \frac{2 - (2 + 2\alpha) \cos \frac{2\pi k}{N} + \sin^2 \frac{2\pi k}{N}}{\left(1 - \cos \frac{2\pi k}{N} + \alpha\right)^{5/2}}; \quad (2.12)$$

then the diagonal elements of the Hessian matrix are

$$[\mathbb{H}_V(q_{N,1})]_{kk} = -\sum_{i=1}^{N-1} f_i \quad (2.13)$$

and the off-diagonal ones are

$$[\mathbb{H}_V(q_{N,1})]_{lk} = f_{k-l}, \quad (2.14)$$

so that the Hessian calculated in $q_{N,1}$ is a circulant matrix. Since we fixed the position of the first particle, in Eq. (2.4) the Hessian \mathbb{H}_V must be replaced by \mathbb{H}'_V which is obtained from \mathbb{H}_V by deleting the first row and the first column. Using the Hadamard inequality [66] to obtain an upper bound to the absolute value of the determinant of a matrix as the product of the Euclidean norms of its rows and observing that in a circulant matrix all the rows have the same norm, after some algebra we can write

$$\lim_{N \rightarrow \infty} \left| \det [\mathbb{H}'_V(q_{N,1})] \right|^{1/N} \leq \lim_{N \rightarrow \infty} \left| \sum_{k=1}^{N-1} f_k \right|. \quad (2.15)$$

2.2. APPLICATION OF THE KSS CRITERION TO THE SGR MODEL

The r.h.s. of the above equation can be written as an integral, so that Eq. (2.4) is satisfied if

$$\int_0^{2\pi} dx \frac{2 - (2 + 2\alpha) \cos x + \sin^2 x}{(1 - \cos x + \alpha)^{5/2}} = 0; \quad (2.16)$$

the above result can be proved by explicit integration, so that the KSS criterion is satisfied for $v = v_c$.

The properties of the circulant matrices [67] can also be used to prove that Eq. (2.4) is *not* satisfied for all the stationary values $v(p) \neq v_c$ (details may be found in [40]). Hence, as far as the stationary values of V associated to polygonal saddles are concerned, we have shown analytically that the KSS criterion is satisfied if and only if $v = v_c$. Since the system is not exactly solvable, this is, to the best of our knowledge, the only analytical indication of the presence of a phase transition between a homogeneous and a clustered phase in the SGR model.

To complete the analysis of the whole range of potential energy values we now turn to the $0-\pi$ saddles. Since the stationary values (2.8) depend only on $n_\pi = N_\pi/N$, let us consider sequences of saddles q_{n_π} with varying N at fixed n_π . The Hessian calculated on such saddles can be written as

$$\mathbb{H}_V(q_{n_\pi}) = \mathbb{D} + \mathbb{A}, \quad (2.17)$$

where \mathbb{A} has rank 2 and $\mathbb{D} = \text{diag}(d_1, \dots, d_k)$ with

$$d_k = \begin{cases} \frac{N_\pi}{N\lambda_1} - \frac{N-N_\pi}{N\lambda_2} & \text{if } 1 \leq k \leq N_\pi, \\ \frac{N-N_\pi}{N\lambda_1} - \frac{N_\pi}{N\lambda_2} & \text{if } N_\pi + 1 \leq k \leq N; \end{cases} \quad (2.18)$$

here $\lambda_1 = 2\sqrt{2\alpha^3}$ and $\lambda_2 = 2\sqrt{2(2+\alpha)^3}$. Using such decomposition one can prove that only the elements of \mathbb{D} contribute to $|\det[\mathbb{H}'_V(q_{n_\pi})]|^{1/N}$ when $N \rightarrow \infty$:

$$\lim_{N \rightarrow \infty} |\det[\mathbb{H}'_V(q_{n_\pi})]|^{1/N} = [a(n_\pi)]^{n_\pi} [b(n_\pi)]^{1-n_\pi}, \quad (2.19)$$

where

$$a(n_\pi) = \frac{n_\pi}{\lambda_1} - \frac{(1-n_\pi)}{\lambda_2} \quad (2.20)$$

and

$$b(n_\pi) = \frac{(1-n_\pi)\lambda_2}{\lambda_1\lambda_2 - n_\pi}. \quad (2.21)$$

The quantity in Eq. (2.19) vanishes if and only if $n_\pi = n_\pi^c$ or $n_\pi = 1 - n_\pi^c$, where

$$n_\pi^c = \frac{\alpha^{3/2}}{(2+\alpha)^{3/2} + \alpha^{3/2}} \quad (2.22)$$

and $v(n_\pi^c) = v(1 - n_\pi^c) = v'_c$, with

$$v'_c = -\frac{4 + \alpha[6 + \alpha(5 + 2\alpha)]}{\sqrt{2\alpha} [(2 + \alpha)^{3/2} + \alpha^{3/2}]}. \quad (2.23)$$

The KSS criterion is then satisfied not only at v_c given by Eq. (2.6) but also at v'_c given by Eq. (2.23).

Is there a phase transition in the SGR model at ε'_c such that $\langle v \rangle(\varepsilon'_c) = v'_c$, as suggested by the KSS criterion? We do not have a final answer. Previous numerical studies of the SGR model [63, 64] have not detected such a phase transition. However, we note that v'_c is extremely close to the absolute minimum of the potential for small values of α , where the SGR model is close to a “true” self-gravitating system. Conversely, $v'_c \simeq v_c$ for large values of α , where it behaves like a mean-field ferromagnet. Only for $\alpha \simeq 1$ one has that v'_c is clearly separated from both the minimum and v_c , but these values of α have not been thoroughly studied in [63, 64].

Moreover, the analysis that we will carry on the next Section suggest that such a phase transition may indeed exist but its effect on the thermodynamic quantities may be weak, so that it may not be easy to detect numerically.

If such a phase transition exists, which phases does it separate? An answer may be suggested again by an analysis of the potential energy landscape. Computing the number of negative eigenvalues of the Hessian one can show that saddles q_{n_π} with $n_\pi < n_\pi^c$ are proper saddles, i.e., their index is greater than zero, while saddles with $n_\pi > n_\pi^c$ are minimum. Minima are visited with high probability, at variance with higher-order saddles. One is thus lead to the conjecture that for $\langle v \rangle < v'_c$ the equilibrium phase is such that the fraction of particles that may cross $q = \pi$, i.e., visit the whole circle, is zero, while it becomes nonzero as $\langle v \rangle > v'_c$, i.e., at $\varepsilon > \varepsilon'_c$.

2.3 An effective model obtained from SGR

In this Section, we introduce and discuss an effective model of SGR whose equilibrium thermodynamics can be solved in the microcanonical ensemble, up to a maximization with respect to a single variable. Such a model can be derived from the SGR model, allowing a quantitative comparison between the thermodynamics of the two. Originally, our main motivation for this study was to understand the possible presence (and in case the nature) of a second phase transition suggested by the KSS criterion in the SGR model at potential energy density v'_c given by Eq. (2.23).

Even if the effective model we present here does not give a definitive answer to this question, a crossover and not a phase transition is indeed found in the effective model in the very low energy region. This suggest that something similar could actually happen in the SGR model and this is in accord with recent numerical works [68].

Apart from this, it turns out that the effective model has some interest in itself. Indeed, despite the rather crude approximations involved in its derivation, it compares quite well with the SGR model not only qualitatively but also quantitatively.

In [39], we have also discussed the relation between the effective model presented here and another model introduced by Thirring forty years ago. The two are indeed very similar, although the latter was not aimed at approximating any particular explicit model. We do not report here this analysis, because it would lead us a bit too far from the central theme of this part of the Thesis, that is, the energy landscape approach to equilibrium phase transitions.

2.3.1 Effective model

We now want to approximate the SGR Hamiltonian in order to make it solvable, i.e., such that the density of states can be explicitly computed.

Numerical simulations of the dynamics of the SGR model reported in [63] have shown that, at a given energy, particles can be roughly divided into three classes according to their dynamical behavior: *cluster* particles, *gas* particles, and *halo* particles. Cluster particles are tightly bound in a cluster and never get far from it; gas particles move almost freely around the ring; halo particles have a complicated dynamics that is somehow intermediate between the other two. The relative population of particles in the three classes depends on the energy (or temperature): at low energy almost all the particles are cluster particles, while at high energy all the particles are gas particles.

The strategy we are going to implement in order to define an effective model is to consider only the first two classes of particles (cluster and gas) and to assume that each particle belongs to one of the two classes. This allows a simplification of the potential energy which makes the model solvable.

Let us then assume that N_g particles, with $1 \leq N_g \leq N$, are gas particles. We can split the potential energy V into three parts:

$$V(q_1, \dots, q_N) = V_{\text{gas}}(q_1, \dots, q_{N_g}) + V_{\text{cluster}}(q_{N_g+1}, \dots, q_N) + V_{\text{int}}(q_1, \dots, q_N), \quad (2.24)$$

where

$$V_{\text{gas}}(q_1, \dots, q_{N_g}) = -\frac{1}{2N\sqrt{2}} \sum_{i,j=1}^{N_g} v(q_i - q_j), \quad (2.25)$$

$$V_{\text{cluster}}(q_{N_g+1}, \dots, q_N) = -\frac{1}{2N\sqrt{2}} \sum_{i,j=N_g+1}^N v(q_i - q_j), \quad (2.26)$$

$$V_{\text{int}}(q_1, \dots, q_N) = -\frac{1}{N\sqrt{2}} \sum_{i=1}^{N_g} \sum_{j=N_g+1}^N v(q_i - q_j), \quad (2.27)$$

where

$$v(x) = \frac{1}{\sqrt{1 - \cos x + \alpha}}. \quad (2.28)$$

Up to this point we have only rewritten the potential energy in a different form. However, this form naturally allows to introduce the approximations which make the model soluble. Let us now discuss the approximations.

CHAPTER 2. THE SELF-GRAVITATING RING MODEL

- (i) Since the N_g gas particles are essentially free particles, as far as their interaction V_{gas} is concerned, we consider them as uniformly distributed on the circle. The interaction energy (2.25) between these particles is then a constant:

$$V_{\text{gas}} = -\gamma \frac{N_g^2}{2N\sqrt{2}} \quad (2.29)$$

where

$$\gamma = \frac{1}{2\pi} \int_{-\pi}^{\pi} v(x) dx = \frac{2}{\pi\sqrt{2+\alpha}} \mathcal{K} \left(\frac{2}{2+\alpha} \right) \quad (2.30)$$

and $\mathcal{K}(x)$ is the complete elliptic integral of the first kind.

- (ii) We consider the $N - N_g$ remaining particles as confined in a cluster. We assume the cluster is tight, i.e., the particles are all close to each other:

$$q_i - q_j \ll 1 \quad \forall i, j = N_g + 1, \dots, N. \quad (2.31)$$

We can thus expand the interaction energy (2.26) among these particles up to the harmonic order, and write

$$V_{\text{cluster}} = -\frac{(N - N_g)^2}{2N\sqrt{2\alpha}} + \frac{1}{8\alpha N\sqrt{2\alpha}} \sum_{i,j=N_g+1}^N (q_i - q_j)^2; \quad (2.32)$$

such an approximation is reliable if an assumption stronger than (2.31) holds, i.e.,

$$\frac{(q_i - q_j)^2}{\alpha} \ll 1 \quad \forall i, j = N_g + 1, \dots, N. \quad (2.33)$$

Moreover, since the particles in the cluster do not “feel” the \mathbb{S}^1 topology of the circle, we assume that

$$-\infty < q_i < +\infty, \quad \forall i = N_g + 1, \dots, N; \quad (2.34)$$

this will allow the analytical computation of the configurational integrals in the density of states.

- (iii) As far as the interaction (2.27) between cluster and gas particles is concerned, we note that as long as the assumption (2.31) holds, the typical distance between a gas particle and a cluster particle is much larger than typical interparticle distances in the cluster, so that we may assume that all the cluster particles are in the same location, i.e., $q = 0$. Being the gas particles uniformly distributed on the circle, this yields a constant for V_{int} , i.e.,

$$V_{\text{int}} = -\gamma \frac{N_g(N - N_g)}{N\sqrt{2}}, \quad (2.35)$$

where γ is given by (2.30).

The Hamiltonian of our effective model is then

$$\mathcal{H}_{\text{eff}} = \frac{1}{2} \sum_{i=1}^N p_i^2 + V_{\text{eff}}, \quad (2.36)$$

where

$$V_{\text{eff}} = -V_0(N, N_g, \alpha) + \frac{\mu}{2} \sum_{i,j=N_g+1}^N (q_i - q_j)^2, \quad (2.37)$$

and where we have set

$$V_0(N, N_g, \alpha) = \frac{(N - N_g)^2}{2N\sqrt{2\alpha}} + \gamma \left[\frac{N_g(N - N_g)}{N\sqrt{2}} + \frac{N_g^2}{2N\sqrt{2}} \right] \quad (2.38)$$

and

$$\mu = \frac{1}{2N(2\alpha)^{3/2}}. \quad (2.39)$$

2.3.2 Microcanonical thermodynamics

Let us now discuss the solution of the effective model in the microcanonical ensemble; also the canonical ensemble has been considered in [39] but we will not report the results here. In the limit $N \rightarrow \infty$, at fixed N_g the model is exactly solvable in both ensembles. However, N_g is not *a priori* assigned and must be fixed in a self-consistent way. The simplest way to do so is to take into account all possible values of N_g ; as we shall show in the following, in the limit $N \rightarrow \infty$ the model is still solvable up to a maximization in a single variable which must be performed numerically, whose physical meaning is just to determine the value of N_g that maximizes the entropy.

To solve the model in the microcanonical ensemble we need to calculate the entropy density

$$s(\varepsilon) = \lim_{N \rightarrow \infty} \frac{1}{N} \log \omega_N(\varepsilon), \quad (2.40)$$

where ω_N is the density of states calculated for the Hamiltonian \mathcal{H}_{eff} :

$$\begin{aligned} \omega_N(\varepsilon) &= \int_{-\infty}^{\infty} dp_1 \cdots dp_N \int_{-\pi}^{\pi} dq_1 \cdots dq_{N_g} \int_{-\infty}^{\infty} dq_{N_g+1} \cdots dq_N \delta(\mathcal{H}_{\text{eff}} - N\varepsilon) \\ &= \sum_{N_g=0}^N \frac{N!}{N_g!(N - N_g)!} \int_{-\infty}^{\infty} dp_1 \cdots dp_N \int_{-\pi}^{\pi} dq_1 \cdots dq_{N_g} \\ &\quad \times \int_{-\infty}^{\infty} dq_{N_g+1} \cdots dq_N \delta \left[\frac{1}{2} \sum_{i=1}^N p_i^2 + \frac{\mu}{2} \sum_{i,j=N_g+1}^N (q_i - q_j)^2 - V_0 - N\varepsilon \right]. \end{aligned} \quad (2.41)$$

In the above expression we have summed over all the possible choices of N_g , properly counted by the degeneracy factor $\binom{N}{N_g}$.

CHAPTER 2. THE SELF-GRAVITATING RING MODEL

The calculation of the above integral is straightforward, albeit a bit involved, and can be performed following a procedure similar to that used in [55, 69]. The details are reported in Appendix A.1. It turns out that the entropy density in the thermodynamic limit is given by

$$s(\varepsilon) = \sup_{n_g \in [0, n_g^{\max}(\varepsilon)]} s(\varepsilon, n_g). \quad (2.42)$$

where we have introduced the fraction of gas particles $n_g = \frac{N_g}{N}$ and $n_g^{\max}(\varepsilon)$ is the maximum fraction of gas particles allowed at a given energy density ε , given by Eq. (A.15). The explicit expression of $s(\varepsilon, n_g)$ is

$$\begin{aligned} s(\varepsilon, n_g) &= \frac{1 - n_g}{2} \log \left[\frac{4\pi(2\alpha)^{3/2}}{(1 - n_g)(2 - n_g)} \right] + \frac{1}{2} \log \left(\frac{2\pi\sqrt{2}}{2 - n_g} \right) \\ &+ \frac{2 - n_g}{2} [1 + \log a(n_g, \alpha, \varepsilon)] + n_g \log(2\pi) \\ &- n_g \log n_g - (1 - n_g) \log(1 - n_g), \end{aligned} \quad (2.43)$$

with

$$a(n_g, \alpha, \varepsilon) = \frac{\gamma}{2\sqrt{2}} n_g (2 - n_g) + \frac{(1 - n_g)^2}{2\sqrt{2}\alpha} + \varepsilon; \quad (2.44)$$

one can check that $a(n_g, \alpha, \varepsilon) > 0$ if $n_g \in [0, n_g^{\max}(\varepsilon)]$ and $\varepsilon > \varepsilon_{\min}$, where $\varepsilon_{\min} = -\frac{1}{2\sqrt{2}\alpha}$ is the absolute minimum of the potential energy per degree of freedom.

As anticipated, the solution of the effective model in the microcanonical ensemble amounts to finding the value $\bar{n}_g(\varepsilon)$ of n_g realizing the extremum in (2.42). This can be easily done numerically, since the explicit form (2.43) of $s(\varepsilon, n_g)$ is available.

Results for the thermodynamic quantities

In the following we report the results for the fraction of gas particles $\bar{n}_g(\varepsilon)$ and for the caloric curve, i.e., the temperature $T(\varepsilon) = \left(\frac{ds}{d\varepsilon}\right)^{-1}$, as a function of ε . We also compare the latter quantity with that computed for the SGR model via the numerical method introduced in [64]; for $\bar{n}_g(\varepsilon)$ such a comparison is impossible, because no such quantity is easily defined for the SGR model. In Fig. 2.2 we report $\bar{n}_g(\varepsilon)$ and $T(\varepsilon)$ computed for a softening parameter $\alpha = 10^{-2}$, as well as a comparison with $T(\varepsilon)$ for the SGR model; in Fig. 2.3 we report the same quantities for $\alpha = 3 \times 10^{-5}$. The agreement with the SGR model is reasonably good already at $\alpha = 10^{-2}$ and becomes very good at $\alpha = 3 \times 10^{-5}$. In both cases we find a phase transition from a homogeneous phase (characterized by $\bar{n}_g \simeq 1$) to a clustered phase while lowering ε below a critical value ε_c ; the critical energy is $\varepsilon_c \simeq -0.46$ for $\alpha = 10^{-2}$ and $\varepsilon_c \simeq -0.8$ for $\alpha = 3 \times 10^{-5}$. These values should be compared with those found for the SGR model, i.e., $\varepsilon_c \simeq -0.32$ for $\alpha = 10^{-2}$ and $\varepsilon_c \simeq -0.5$ for $\alpha = 3 \times 10^{-5}$. The agreement is good, especially for the lower value of α . In the case $\alpha = 10^{-2}$ the phase transition is continuous, while it is discontinuous (the temperature T jumps between two different values at ε_c) at $\alpha = 3 \times 10^{-5}$.

2.3. AN EFFECTIVE MODEL OBTAINED FROM SGR

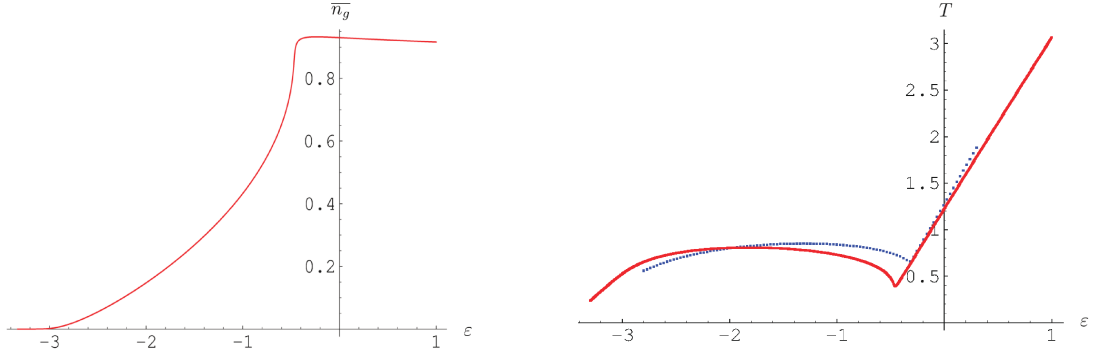


Figure 2.2 – Effective model in the microcanonical ensemble, $\alpha = 10^{-2}$. (left) Fraction of gas particles $\overline{n}_g(\varepsilon)$ (red line); (right) temperature $T(\varepsilon)$ computed for the effective model (red line) and for the SGR model (blue symbols).

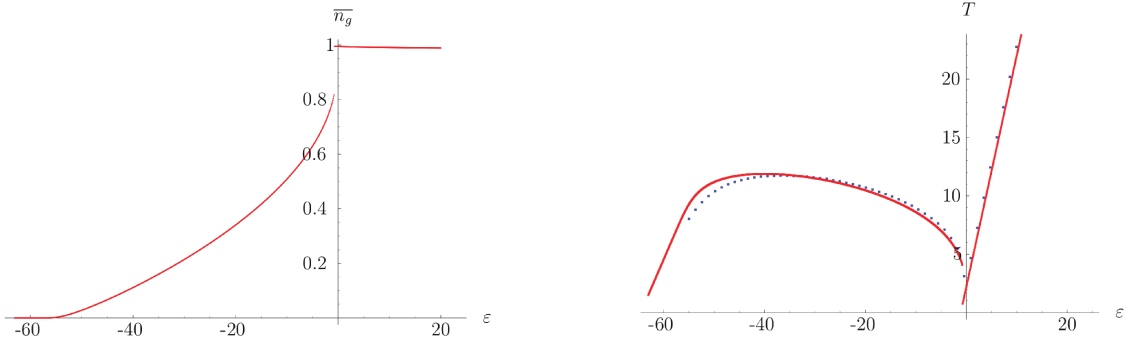


Figure 2.3 – As in Fig. 2.2 for $\alpha = 3 \times 10^{-5}$.

We find indeed a microcanonical tricritical point which is located at $\alpha \simeq 5 \times 10^{-3}$; in the case of the SGR model this point is located at $\alpha \simeq 10^{-4}$, so that also in this respect the two models are very similar. We stress that the above results come from a numerical maximization so that we have no rigorous proof of the existence of true singularities in the microcanonical ensemble for the effective model. However, the same holds for the SGR model too, as long as the softening parameter α is finite.

In the SGR model, the high-energy phase ($\varepsilon > \varepsilon_c$) is a perfect gas phase, as shown by the numerical calculations² reported in [64]. We should thus expect $\overline{n}_g \equiv 1$ for $\varepsilon > \varepsilon_c$. This does not happen, although \overline{n}_g is very close to 1 ($\overline{n}_g \simeq 0.93$ for $\varepsilon \gtrsim \varepsilon_c$ when $\alpha = 10^{-2}$ and $\overline{n}_g \simeq 0.995$ for $\varepsilon \gtrsim \varepsilon_c$ when $\alpha = 3 \times 10^{-5}$). This is due to the presence of the degeneracy term $\binom{N}{N_g}$ in the density of states, which makes the slope of the entropy to diverge for $n_g = 1$ and $n_g = 0$, so that the extremum of the entropy (2.43) can never be realized in the boundaries of the domain of n_g when the energy density is strictly larger than its absolute minimum ε_{\min} . For the latter value of ε , however, we have $\overline{n}_g \equiv 0$, and there is a whole region of energy

²In the limit $\alpha \rightarrow \infty$, when the SGR model becomes equivalent to the ferromagnetic HMF model [70], this can be shown analytically; however, for large values of α our effective model is not a good approximation.

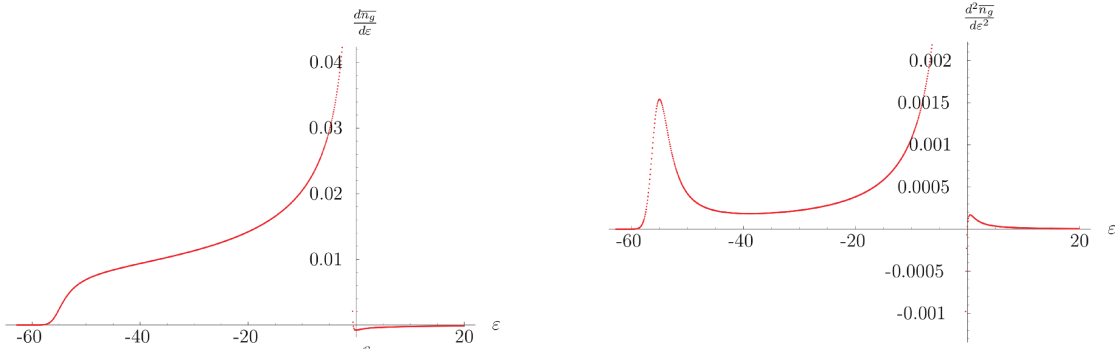


Figure 2.4 – Effective model in the microcanonical ensemble, $\alpha = 3 \times 10^{-5}$. (left) First derivative of the fraction of gas particles, $\frac{d\bar{n}_g}{d\varepsilon}$; (right) Second derivative $\frac{d^2\bar{n}_g}{d\varepsilon^2}$.

densities where $\bar{n}_g \simeq 0$. This can already be seen in the top panels of Figs. 2.2 and 2.3; however, it is more evident if we look at the first and second derivatives of $\bar{n}_g(\varepsilon)$, reported in Fig. 2.4 in the case $\alpha = 3 \times 10^{-5}$. The peak in the second derivative of $\bar{n}_g(\varepsilon)$ can be effectively taken as the upper limit of a “highly clustered phase” (which is not a “true” phase because there is no singularity). The existence of such a region is a very interesting feature of this model: it reminds what has been observed in simulations of confined and regularized three-dimensional self-gravitating systems [71–73], where one finds a low-energy clustered phase, an intermediate-energy “core-halo” phase (which would be mimicked by the coexistence of gas and cluster particles in the effective model) and a high-energy perfect gas phase.

An unphysical feature of the model is that when ε is very large the number of gas particles starts to decrease and eventually $\bar{n}_g \rightarrow 0$ for $\varepsilon \rightarrow \infty$. This happens for any value of α and is due to the fact that the coordinates of the cluster particles are allowed to take values in \mathbb{R} instead of in $(-\pi, \pi]$, so that at very high energy it is always convenient to make a “loose” cluster whose effective size is larger than the circle. However, this happens at values of ε which get larger and larger as α gets smaller, so that one can safely ignore this fact in practice: in Fig. 2.2 one can see a first hint of this phenomenon, which is instead invisible in the energy range of Fig. 2.3.

A feature of the model that does not compare well with the SGR model is that for any value of α there is a region of nonconcave entropy: there is always ensemble inequivalence, so that, there is no canonical tricritical point and the phase transition in the canonical ensemble is always discontinuous [39]. In the SGR model, on the contrary, the ensemble inequivalence is present only for $\alpha < \alpha_{CT}$ with $\alpha_{CT} \simeq 0.1$. On the other hand, the approximations made to derive the effective model are only reasonable for small values of α , so that this is not a big surprise.

2.4 Conclusions

The interpretation of the KSS theorem in the form of the KSS criterion gave us the opportunity to study more complicated models than what done previously. Indeed, it is not necessary to know all the critical points of the potential to apply the KSS criterion and it is not necessary to invert the relation between critical points and critical energies.

We have discussed in this Chapter the application of the KSS criterion to the SGR model which, at variance with the few models the criterion had previously been applied to, is not exactly solvable. The KSS criterion, as formulated by us, has been applied to other models later on [30, 31, 44, 74]. In particular, we will review the case of the short-range ferromagnetic XY models in the next Chapter. We stress that such applications would not have been possible using directly the KSS theorem instead of the KSS criterion.

In the case of the SGR model, the KSS criterion correctly singles out the phase transition between a homogeneous and a clustered phase. We have also shown that the criterion indicates the possible presence of another phase transition, not previously known, and we have conjectured on its nature.

To understand the possible presence of such a second phase transition, we have constructed a solvable effective model; unfortunately, this has not given a final answer to the question. Indeed, the effective model does not present a phase transition at very low energies; however, there is a low-energy region where the fraction of gas particles n_g is very small and stays very small up to a certain energy where it starts rising rapidly. Just after our work, T. Tatekawa [75] has performed precise numerical computations with the variational method proposed in [64] without finding any evidence of the presence of a phase transition.

One could thus think that a weaker transition or a transitional phenomenon without a true singularity of the thermodynamic functions occurs in the SGR model. According to the effective model, such transitional phenomenon should separate two phases, one in which all the particles are bound in the cluster and the other one in which a finite fraction of particles is not bounded. The authors of [68] have performed very precise N -body simulations and mean-field calculations with the method of [64] showing that such a crossover phenomena actually happens in the SGR model in a similar way as in our effective model. The energy value at which this phenomena occurs, however, does not quantitatively match with ν'_c . Analogously, the authors of [76] have performed a geometrical study of the energy landscape of the SGR model and found analogous results for geometric observables, known to be very sensitive order parameters.

The effective model introduced here possesses an interest in itself: on the one hand it is very similar to the Thiring model³ and, on the other hand, it provides a very accurate ap-

³The thermodynamical behavior of the Thiring model is qualitatively similar to our effective model; moreover, the the fraction of particles belonging to \mathbb{V}_0 plays the same role as $(1 - n_g)$ in our effective model. We

CHAPTER 2. THE SELF-GRAVITATING RING MODEL

proximation of the thermodynamics of the SGR model for values of the softening parameter such that the potential is very close to the gravitational one. It was not previously known that such toy models can give a quantitative, and not only qualitative, description of the thermodynamics of self-gravitating systems.

address the reader to [39] for further details.

3

$O(n)$ spin models

This Chapter is devoted to the study of ferromagnetic short-range and long-range $O(n)$ models on hypercubic lattices from an energy landscape perspective.

In Section 3.1, we discuss a very simple class of critical points of these models: all the configurations of the Ising model defined on the same graph with the same interaction matrix as the $O(n)$ model are stationary points. In Section 3.2, we review the application of the KSS criterion to two and three-dimensional XY models with nearest-neighbor interactions, which was been analyzed by Nerattini et al. in [43, 44]: the criterion does not single out the energy at which the phase transitions are located.

To understand the mechanism by which the phase transition emerges, we thus construct in Section 3.3 an approximate relation between the density of states of the $O(n)$ models and the one of the Ising model, which ends with Eq. (3.14). By means of it we are lead to the following conclusion: if a $O(n)$ model with ferromagnetic interactions on a lattice has a phase transition, its critical energy density is equal to that of the $n = 1$ case, i.e., a system of Ising spins with the same interactions.

We will see from numerical data that this conclusion is verified at least with an extremely good accuracy, except for the case of two dimensions and $n = 2$, in which the agreement is less good. Surprisingly, such a striking similarity between critical energies was not known before.

The approximations needed to obtain Eq. (3.14) are not easily controlled. In Section 3.4, we show that the same derivation can be followed rigorously in the cases of the one-dimensional and mean-field XY models.

The content of this Chapter is mainly based on the results presented in [41, 42], except for Section 3.2 in which the analysis performed by Nerattini et al. in [43, 44] is resumed.

3.1 $O(n)$ spin models and Ising stationary configurations

We consider in this Chapter classical isotropic spin models defined on a lattice (or more generally on a graph) with Hamiltonian

$$\mathcal{H}^{(n)} = - \sum_{i,j=1}^N J_{ij} S_i \cdot S_j = - \sum_{i,j=1}^N J_{ij} \sum_{a=1}^n S_i^a S_j^a, \quad (3.1)$$

where i and j run over the N lattice sites and the classical spin vectors $S_i = (S_i^1, \dots, S_i^n)$ have unitary norm, i.e.,

$$\sum_{a=1}^n (S_i^a)^2 = 1 \quad (3.2)$$

$\forall i = 1, \dots, N$. The real matrix J_{ij} dictates the interactions; in case they are long-ranged a normalization is understood such as to obtain an extensive energy, using e.g. the Kac prescription.

The Hamiltonian (3.1) is globally invariant under the $O(n)$ group. In the special cases $n = 1$, $n = 2$, and $n = 3$, one obtains the Ising, XY, and Heisenberg models, respectively. The case $n = 1$ is even more special because $O(1) \equiv \mathbb{Z}_2$ is a discrete symmetry group. In this special case the Hamiltonian (3.1) becomes the Ising Hamiltonian

$$\mathcal{H}^{(1)} = - \sum_{i,j=1}^N J_{ij} \sigma_i \sigma_j, \quad (3.3)$$

where $\sigma_i = \pm 1 \forall i$. In all other cases $n \geq 2$ the $O(n)$ group is continuous; each spin vector S_i lives on an $n - 1$ unit sphere \mathbb{S}^{n-1} .

In this Chapter, we will mainly consider $O(n)$ models defined on hypercubic lattices and ferromagnetic interactions non-vanishing only among nearest-neighbors. Their thermodynamical behavior is a very classical topic in statistical mechanics: we only recall here that all of them have a continuous phase transition in dimension greater than two and belong to different universality classes. The case of two dimensions is peculiar: the Ising model was solved exactly by Onsager and has a second order phase transition; the XY model has a Berezinskij-Kosterlitz-Thouless transition and it is believed that no transition is present for $n > 2$.

Let us now consider the stationary configurations of $\mathcal{H}^{(n)}$ for $n \geq 2$, i.e., the solutions $\bar{S} = (\bar{S}_1, \dots, \bar{S}_N)$ of the N vector equations $\nabla \mathcal{H}^{(n)} = 0$. The latter can be written as nN scalar equations,

$$- \sum_{j=1}^N J_{kj} S_j^a + \lambda_k S_k^a = 0, \quad a = 1, \dots, n, \quad k = 1, \dots, N, \quad (3.4)$$

3.1. $O(N)$ SPIN MODELS AND ISING STATIONARY CONFIGURATIONS

where the λ 's are N Lagrange multipliers, plus the N nonlinear constraints in Eq. (3.2), which prevent the above equations from being easily solved. However, a particular class of solutions can be found by assuming that all the spins are parallel or antiparallel to a given direction (here the n -th direction of the spins):

$$S_i^1 = \dots = S_i^{n-1} = 0 \quad \forall i. \quad (3.5)$$

In this case, the $N(n-1)$ equations (3.4) with $a = 1, \dots, n-1$, corresponding to the first $n-1$ components of the spins, are trivially satisfied. As to the n -th component, the constraints $(S_i^n)^2 = 1$ imply $S_i^n = \sigma_i \forall i$, so that the remaining N equations read as

$$-\sum_{j=1}^N J_{kj} \sigma_j + \lambda_k \sigma_k = 0, \quad k = 1, \dots, N. \quad (3.6)$$

The above equations are satisfied by any of the 2^N possible choices of the σ 's provided one puts

$$\lambda_k = \frac{1}{\sigma_k} \sum_{j=1}^N J_{kj} \sigma_j, \quad k = 1, \dots, N. \quad (3.7)$$

The Hamiltonian (3.1) becomes the Ising Hamiltonian (3.3) when the spins belong to this class of stationary configurations.

Therefore we have a one-to-one correspondence between a class of stationary configurations of the Hamiltonian (3.1) of a $O(n)$ spin model and all the configurations of the Ising model (3.3), i.e., the Ising model defined on the same graph with the same interaction matrix J_{ij} ; the corresponding stationary values are just the energy levels of this Ising Hamiltonian. We shall refer to the class of stationary configurations $\bar{S}_i = (0, \dots, 0, \sigma_i) \forall i = 1, \dots, N$ as "Ising stationary configurations".

We stress anyway that there are other stationary configurations [44] in these models and, generically, not all of them are known except for the special cases of one dimension [31] and mean-field interactions [13]. Nonetheless, we believe that the 2^N Ising ones are a non-negligible fraction of the whole, especially at large N because the number of stationary points of a short-range potential is expected to be¹ $\mathcal{O}(e^N)$ [77].

The above results hold for $O(n)$ and Ising models defined on any graph. From now on we shall restrict to regular d -dimensional hypercubic lattices and to ferromagnetic interactions $J_{ij} > 0$. In this case, in the thermodynamic limit $N \rightarrow \infty$ the energy density levels of the Ising Hamiltonian (3.3),

$$\frac{1}{N} \mathcal{H}^{(1)}(\sigma_1, \dots, \sigma_N), \quad \forall \sigma_i = \pm 1, \quad (3.8)$$

become dense and cover the whole energy density range of all the $O(n)$ models.

¹We use here the imprecise notation $\mathcal{O}(e^N)$ to indicate an exponential law of the form a^N where a is a positive constant.

Finally, we want to highlight a property of the Ising configurations. If we perturb the Hamiltonian (3.1) with external fields $h_i = (0, \dots, h_i^n)$ parallel to a given direction (here the n -th direction of the spins) but with a strength which can be different from site to site, that is

$$\mathcal{H}_p^{(n)} = - \sum_{i,j=1}^N J_{ij} \sum_{a=1}^n S_i^a S_j^a + \sum_{i=1}^N h_i^n S_i^n, \quad (3.9)$$

still the Ising configurations are stationary points of the perturbed Hamiltonian. This is of course not true generically for other stationary points.

All these facts made us suppose that the Ising configurations are not merely a subclass of the stationary points of the $O(n)$ models but are actually the most important class. In the following of this Chapter we will take seriously this statement to understand if some prediction can be obtained from it.

3.2 Application of the KSS criterion to short range systems

Nerattini et al. [44] have applied the KSS criterion to the two and three-dimensional XY models, defined by the Hamiltonian

$$\mathcal{H}^{(2)} = -\frac{1}{2} \sum_{i=1}^N \sum_{j \in \mathcal{N}(i)} \cos(q_i - q_j), \quad (3.10)$$

where $\mathcal{N}(i)$ denotes the set of nearest neighbors and the lattice is an hypercubic lattice. We review here the aspects of their work which are relevant for the following of this Thesis. In their analysis, the authors have not only considered Ising stationary configurations but also other classes of critical points. However, we will restrict here only to Ising stationary configurations, because no much information is added by the others.

Even restricting only to Ising stationary configurations, the application of the KSS criterion for these models is not trivial. The main problem is the following: given an Ising stationary configuration it is simple to calculate its energy. However, the converse is not true: given an energy at which we want to check if the KSS criterion holds, it is not straightforward to construct Ising configurations at that energy.

The authors of [44] used MonteCarlo simulations on the Ising model to solve this problem and, once a large number of configurations with a given energy had been obtained, they calculated the normalized determinant of the Hessian of the Hamiltonian and its index divided by N . The results are shown in Fig. 3.1 and 3.2 for the two and three dimensional cases. Of course this procedure does not fully sample the Ising stationary configurations. However, we see that both the normalized determinant and the index divided by N show a thermodynamical behavior, in the sense that they seem to converge to a single curve in the

3.2. APPLICATION OF THE KSS CRITERION TO SHORT RANGE SYSTEMS

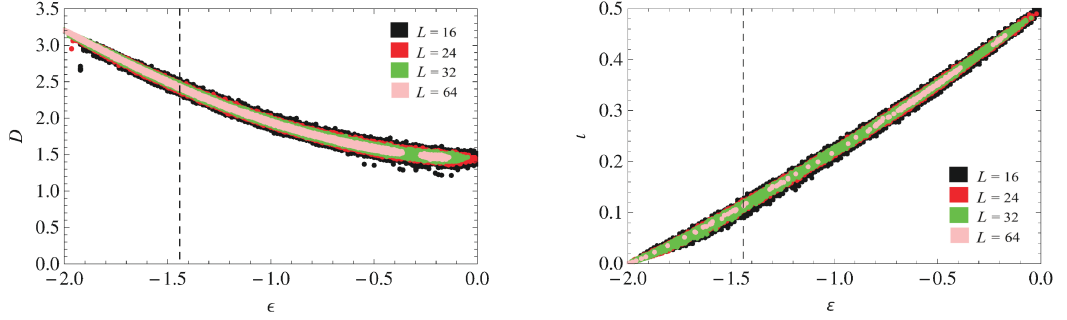


Figure 3.1 – Rescaled Hessian determinant D (left) and rescaled index (right) of Ising stationary configurations for the two-dimensional XY model, plotted as a function of the energy density ε . Data symbols correspond to lattices of side lengths $L = 16$ (black), 24 (red), 32 (green) and 64 (lighter red). The critical energy density $\varepsilon_c^{2d} \approx -1.446$ of the BKT transition is marked by a vertical dashed line. The Ising configurations are obtained with a canonical MonteCarlo simulations.

$N \rightarrow \infty$ limit.

This means the following: the energy landscape in a small neighborhood around most of the Ising stationary configurations with the same energy density is very similar.

On the other hand, it is clear that no sign of a vanishing determinant is found at the critical energy density, the curve of the normalized determinant as a function of the energy being well separated from zero at every energy. This result clearly does not exclude the possibility that there exists a sequence of stationary points of the XY models that makes the normalized determinant vanish, because only a MonteCarlo sampling has been used to construct Fig. 3.1 and 3.2.

Actually, it can be analytically shown [44] that Ising stationary configurations which make the normalized determinant exactly vanish do exist. Moreover, the energy levels of these “singular configurations” become dense in the whole energy interval of the XY models. This is possible because a change of an Ising configuration which involves only \sqrt{N} spins does not alter its energy density but can cause a row of zeros in the Hessian matrix. According to the KSS criterion, there thus may be a phase transition in XY models at every value of the energy density².

Concluding, even if the KSS criterion as stated in Chapter 2 can be applied to XY models, it does not single out the energy at which the phase transition is located. The analysis in [44] is restricted to two and three dimensional ferromagnetic nearest-neighbors XY mod-

²The situation is a bit more involved than how it is presented here. Indeed, it is shown in [44] that “singular configurations” are not isolated; this imply that the Hamiltonian of the XY models is not a Morse function (as supposed in the KSS Theorem) neither once that the rotational invariance has been broken by fixing one spin. This difficulty can be overcome using a perturbed Hamiltonian as in Eq. (refeq:H-On-perturbed) for vanishingly external fields h_i . We address the reader to [44] for further details, which do not significantly modify the general picture we give here.

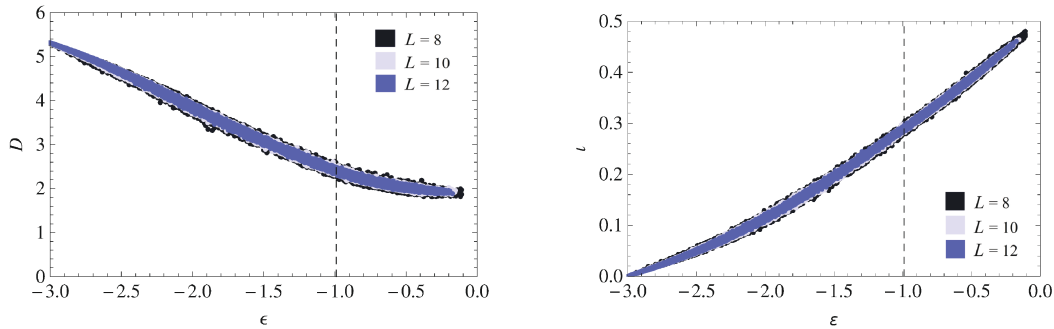


Figure 3.2 – Rescaled Hessian determinant D (left) and rescaled index (right) as a function of the energy density ε for the three-dimensional XY model. Data symbols correspond to lattices of side lengths $L = 8$ (darker blue), 10 (lighter blue) and 12 (blue). The critical energy density $\varepsilon_c^{3d} \approx -0.99$ of the ferromagnetic transition is marked by a vertical dashed line.

els. Despite the very different nature of the phase transition present in these two models, the results obtained are very similar, different only at quantitative level. This makes us suppose that similar results hold for a general ferromagnetic short-range $O(n)$ model.

3.3 On a microcanonical relation between continuous and discrete spin models

Because the KSS criterion does not single out the phase transition in short-range $O(n)$ models, it is natural to ask which is the mechanism which induce the phase transition in these cases. Roughly speaking, in the present Section we take seriously the idea that the stationary points contribution to the density of states is the most important one; by considering Ising stationary configurations, we construct an approximate form of the density of states which suggests a relation between the phase transitions occurring in these models. We compare the predictions obtained with numerical data already known in literature.

We have seen in Section 3.1 that every configuration of the Ising model is a stationary configuration of the $O(n)$ model defined by the Hamiltonian 3.1, on the same graph with the same interaction matrix. We restrict here to regular d -dimensional hypercubic lattices and to ferromagnetic interactions $J_{ij} > 0$. In this case, in the thermodynamic limit $N \rightarrow \infty$ the energy density levels of the Ising Hamiltonian (3.3) become dense and cover the whole energy density range of all the $O(n)$ models. Moreover, Ising stationary configurations are not destroyed by replacing the Hamiltonian with the perturbed one in Eq. (3.9).

This suggests that Ising stationary configurations are the most important ones, so that we may approximate the density of states $\omega^{(n)}(\varepsilon)$ of an $O(n)$ model in terms of these configura-

3.3. ON A MICROCANONICAL RELATION BETWEEN CONTINUOUS AND DISCRETE SPIN MODELS

tions. To this end, let us first rewrite Eq. (1.8) as

$$\omega^{(n)}(\varepsilon) = \sum_p \int_{U_p \cap \Sigma_\varepsilon} \frac{d\Sigma}{|\nabla \mathcal{H}^{(n)}|} \quad (3.11)$$

where p runs over the 2^N Ising stationary configurations and U_p is a neighborhood of the p -th Ising configuration such that $\{U_p\}_{p=1}^{2^N}$ is a proper partition of the configuration space $\Gamma = (\mathbb{S}^{n-1})^N$, that coincides with phase space for spin models (3.1). Since Ising configurations are isolated points in the configuration space of a $O(n)$ model, such a partition always exists. Let us now introduce two assumptions allowing to write Eq. (3.11) in a more transparent, albeit approximate, way:

(i) We assume that the integrals in Eq. (3.11) depend only on ε , i.e., the neighborhoods U can be chosen, or deformed, such as

$$\int_{U_p} \delta(\mathcal{H}^{(n)} - N\varepsilon) d\Gamma = \int_{U_q} \delta(\mathcal{H}^{(n)} - N\varepsilon) d\Gamma = g^{(n)}(\varepsilon) \quad (3.12)$$

for any p, q such that $\mathcal{H}^{(n)}(p) = \mathcal{H}^{(n)}(q) = N\varepsilon$.

(ii) At a given value of ε , the largest contribution to $\omega^{(n)}(\varepsilon)$ in Eq. (3.11) is likely to come from those U_p such that $\mathcal{H}^{(n)}(p) = N\varepsilon$, because if $\mathcal{H}^{(n)}(q) \neq N\varepsilon$ then $|\nabla \mathcal{H}^{(n)}(x)| \neq 0 \forall x \in U_q \cap \Sigma_\varepsilon$, unless a zero in $|\nabla \mathcal{H}^{(n)}(x)|$ comes from a stationary configuration which does not belong to the Ising class. Since it was assumed that non-Ising stationary configurations could be neglected, only neighborhoods centered around stationary configurations at energy density ε have been retained in the sum (3.11).

Hence, using assumptions (i) and (ii), Eq. (3.11) becomes

$$\omega^{(n)}(\varepsilon) \simeq g^{(n)}(\varepsilon) \sum_p \delta[\mathcal{H}^{(n)}(p) - N\varepsilon]. \quad (3.13)$$

The sum in the r.h.s. of Eq. (3.13) is over Ising configurations, so that it equals the density of states of the corresponding Ising model, that we shall denote by $\omega^{(1)}(\varepsilon)$. We can thus write

$$\omega^{(n)}(\varepsilon) \simeq \omega^{(1)}(\varepsilon) g^{(n)}(\varepsilon). \quad (3.14)$$

We do not expect such relation to be exact for a general $O(n)$ model. We will discuss in the following of this thesis the validity of these hypotheses. For the moment, let us see which predictions can be obtained from Eq. (3.14).

3.3.1 A striking similarity between critical energy densities

Were exact, Eq. (3.14) would imply that if $\omega^{(1)}(\varepsilon)$ is nonanalytic at $\varepsilon = \varepsilon_c$, then also $\omega^{(n)}(\varepsilon)$ is nonanalytic at $\varepsilon = \varepsilon_c$ for any n , unless the function $g^{(n)}(\varepsilon)$ precisely cancels this nonanalyticity, which seems a rather special case.

CHAPTER 3. $O(N)$ SPIN MODELS

Table 3.1 – Comparison of critical energy densities ε_c and critical temperatures T_c for ferromagnetic models with long-range (LR) interactions (first row) and nearest-neighbor interactions on a d -dimensional hypercubic lattice (all the other rows). LR interactions means here $J_{i,j} \propto |i - j|^\alpha$ with $0 \leq \alpha \leq d$ and the exact values for the two-dimensional Ising model are given by $\varepsilon_c = -\sqrt{2}$ and $T_c = 2/\log(1 + \sqrt{2})$

	model	ε_c	T_c	derivation method
LR	Ising	0	1	exact solution
	$O(n)$	0	$1/n$	exact solution [79]
$d = 1$	Ising	-1	0	exact solution
	$O(n)$	-1	0	exact solution
$d = 2$	Ising	-1.414...	2.269...	exact solution
	$O(2)$	-1.4457(4)	0.8929(1)	numerical [80, 81]
$d = 3$	Ising	-0.991(1)	4.5112(3)	numerical [82]
	$O(2)$	-0.99184(6)	2.20167(9)	numerical [83]
	$O(3)$	-0.9896(1)	1.44298(2)	numerical [84]

There are very simple arguments that imply, or at least suggest, that Eq. (3.14) is not exact, even in the thermodynamic limit $N \rightarrow \infty$, unless, again, $g(\varepsilon)$ has some very special features: with a generic $g(\varepsilon)$ a density of states of the form (3.14) would not reproduce the known critical exponents of the $O(n)$ universality classes [78]; However, with a generic $g(\varepsilon)$ Eq. (3.14) correctly implies a negative value for the specific heat critical exponent of $O(n)$ spin models (i.e., the specific heat of continuous models does not diverge at criticality, but rather has a cusp-like behavior), see Appendix B.1 and the conclusions of this Chapter. This is a common feature of $O(n)$ models [78] and reinforces the belief that the approximation (3.14), although rather crude, may properly capture the main features of the nonanalyticities of the density of states when $N \rightarrow \infty$, as the location of such nonanalyticities. Therefore we put forward the following

Conjecture. *If a $O(n)$ spin model defined on a d -dimensional hypercubic lattice with Hamiltonian (3.1) and ferromagnetic interaction matrix $J_{ij} > 0$ has a phase transition, its critical energy density $\varepsilon_c = E_c/N$ is equal to that of the $n = 1$ case, i.e., a system of Ising spins with the same interactions.*

We stress that the above conjecture concerns the critical value of the control parameter of the microcanonical ensemble, the energy density, and says nothing about critical temperatures, which may well be different—and typically are— at different n .

We now discuss known results, both analytical and numerical, in order to assess the validity of this conjecture in some particular cases. The results we were able to collect are

3.3. ON A MICROCANONICAL RELATION BETWEEN CONTINUOUS AND DISCRETE SPIN MODELS

reported in Table 3.1. The conjecture is true for systems with long-range interactions on d -dimensional lattices, $J_{ij} = N^{(\alpha/d)-1}|i-j|^{-\alpha}$ with $0 \leq \alpha < d$; $\alpha = 0$ is the mean-field case of models defined on complete graphs with the same interaction strength between any two sites, $J_{ij} = 1/N$. All these systems have a mean-field-like phase transition at the maximum value of ε ($\varepsilon_c = 0$ with our choice of units), with critical temperatures $T_c = 1/n$ [79]. We stress again that critical energy densities are equal but critical temperatures are not and depend on n . As to systems with nearest-neighbor interactions, $\varepsilon \in [-d, d]$ and the conjecture is true for $d = 1$ at any n , although this case is somehow trivial because there is no transition at finite temperature.

For $d = 2$, the Mermin-Wagner theorem rules out a long-range-ordered phase for any $n > 1$. However, a remarkable transition between a disordered and a quasi-ordered phase occurs for $n = 2$ (XY model), usually referred to as the Berezinskij-Kosterlitz-Thouless (BKT) transition [85]. In Table 3.1 we report the best recent estimate of the critical temperature obtained by Hasenbusch [81] and the corresponding critical energy density (estimated from a MonteCarlo simulation of a system with 256×256 spins [80]). The difference between this value and the exact value of the critical energy density of the Ising model on a square lattice is around 2%. This difference, though small, appears significant since it is orders of magnitude larger than the statistical error on the numerical estimate of the energy. Based on this result one should conclude that the conjecture is not verified in the case of the XY model in $d = 2$. However, we are comparing an exact result in the thermodynamic limit with a numerical estimate of the energy on a finite lattice, whose statistical accuracy does not consider the systematic error due to the finite size effects, which could be quite large in this particular case [86, 87].

Moreover, also the precise determination of the critical temperature of the BKT transition is a subtle and difficult task due to its elusive nature. This is witnessed by the remarkable spread of values of T_c reported in different papers: the summary given in Ref. [87] shows that estimated critical temperatures vary in the interval $[0.88, 0.99]$ while Ref. [88] gave $[0.85, 0.95]$ as confidence interval for T_c . The energy values given in Ref. [80] corresponding to both these temperature intervals do contain the Ising value $\varepsilon_c = -\sqrt{2}$; for instance, the temperature interval $[0.85, 0.95]$ corresponds to $\varepsilon_c \in [-1.48, -1.38]$. We thus believe that the available data are not conclusive as far as a confirmation of the conjecture is concerned in this particular case.

For $d = 3$ the comparison is entirely between simulation outcomes, since no exact solution exists even for the Ising case. Results in Table 3.1 show that the critical energy measured for a $O(2)$ spin system (XY model) [83] is clearly consistent with that measured for the Ising case [82]. The difference between the estimated ε_c of the $O(3)$ case (Heisenberg model) [84] and that of the Ising model is less than 1.5 times the error on the latter. Therefore the two estimates are consistent if one considers quoted errors as standard statistical errors.

Concluding, it would be very surprising if the conjecture proposed, being deduced from the very approximate Eq. (3.14), would hold exactly. Preliminary numerical results we obtained with a cluster MonteCarlo provided in the ALPS package [89], indeed indicate a very small difference between critical energy densities also in the cases of $d = 3$; more work is however needed to fully clarify this point.

Anyway, the striking similarities between critical energy densities, as well as the prediction of a negative exponent for the specific heat suggests that some physics is actually captured by the argument presented here. In order to better understand this point, we will now concentrate on the simpler possible system in the class of Hamiltonians (3.1).

3.4 The one-dimensional and mean-field XY models

The approximations which led us to the Eq. (3.14) are not under control, the argument we presented being only qualitative. It is thus natural to ask if the argument of the previous Section can be derived with controlled approximations, or even exactly, in those cases in which the equality between critical energy densities holds. This is the scope of the present Section.

We consider here the mean-field XY model and the 1-dimensional nearest-neighbor XY model, i.e., two $n = 2$ representatives of the two classes of $O(n)$ models where the critical energies are known to be exactly equal to that of the corresponding Ising model. We will show that for these two models the following expression holds for any energy:

$$\omega^{(n)}(\varepsilon) = \omega^{(1)}(\tilde{\varepsilon})G^{(n)}(\varepsilon, \tilde{\varepsilon}), \quad (3.15)$$

where $\tilde{\varepsilon}$ is a suitable function of ε . The function $\tilde{\varepsilon}$ has the property that $\tilde{\varepsilon} \rightarrow \varepsilon_c$ when $\varepsilon \rightarrow \varepsilon_c$; we thus recover Eq. (3.14) for $\varepsilon \rightarrow \varepsilon_c$.

The technical aspects of the derivation strongly rely on the peculiarities of the two models so that we do not see an immediate possibility of generalization of the results derived in this Section to generic $O(n)$ models. This notwithstanding, we are convinced that our derivation and results may help in understanding more deeply the relation between $O(n)$ and Ising models, as we shall argue in the conclusions.

Sections 3.4.1 and 3.4.2 are devoted to the explicit derivation of the relation between the Ising model density of states and the density of states of the mean-field XY and 1-dimensional XY models, respectively. In Sec. 3.5 the results are discussed in a more general perspective, with emphasis on generalization to general d dimensional lattices.

3.4.1 The mean-field XY model

We shall now show that the density of states of the mean-field XY model can be written in the form (3.15), with $\tilde{\varepsilon} \rightarrow \varepsilon$ when $\varepsilon \rightarrow \varepsilon_c$.

3.4. THE ONE-DIMENSIONAL AND MEAN-FIELD XY MODELS

The mean-field XY model is a system of N globally coupled planar spins (or alternatively of N globally interacting particles constrained on a ring), with Hamiltonian

$$\mathcal{H}_{\text{MF}} = -\frac{1}{2N} \sum_{i,j=1}^N \cos(q_i - q_j), \quad (3.16)$$

where $q_i \in [0, 2\pi)$, so that the configuration (or phase) space of the system is the torus \mathbb{T}^N . This model has a mean-field phase transition from a ferromagnetic (or clustered, if one thinks of particles) to a paramagnetic (or uniform) phase at $\varepsilon_c = \varepsilon_{\text{max}} = 0$ and has been thoroughly studied being one of the simplest models of systems with long-range interactions [90]; it belongs to the class (3.1) with $n = 2$ and $J_{ij} = 1/N$. By introducing the magnetization density vector $\mathbf{m} = (m_x, m_y)$, where

$$m_x = \frac{1}{N} \sum_{i=1}^N \cos q_i, \quad (3.17)$$

$$m_y = \frac{1}{N} \sum_{i=1}^N \sin q_i, \quad (3.18)$$

$$(3.19)$$

we can write the total energy of the system as a function of the modulus $m = |\mathbf{m}|$ of the magnetization density:

$$\mathcal{H}_{\text{MF}} = -\frac{Nm^2}{2}. \quad (3.20)$$

For XY models, Ising stationary points are configurations where the angles q_i differ from each other by either 0 or π . Due to the $O(2)$ invariance of the Hamiltonian, these stationary solutions are not isolated but belong to a manifold. We make them isolated by fixing³ $q_N = 0$, so that the Ising stationary configurations are all the configurations $\bar{q} = \{\bar{q}_i\}_{i=1}^N$ where the angles are either 0 or π , and can be parametrized by the number N_π of angles equal to π . The configurations with given N_π are

$$\bar{q}_i = \pi \quad \forall i = 1, \dots, N_\pi \quad (3.21)$$

$$\bar{q}_i = 0 \quad \forall i = N_\pi + 1, \dots, N \quad (3.22)$$

and all the others obtained by permutations of the indices i . The number $\nu(N_\pi)$ of such configurations is given by the binomial coefficient

$$\nu(N_\pi) = \frac{N!}{N_\pi!(N - N_\pi)!}, \quad (3.23)$$

³This does not affect the thermodynamics of the system in the $N \rightarrow \infty$ limit but for the fact that it chooses the direction of the breaking of the $O(2)$ symmetry below the critical energy density in such a way that $\langle m_y \rangle \equiv 0$ also in the broken symmetry phase.

CHAPTER 3. $O(N)$ SPIN MODELS

while their magnetization and energy density depend only on N_π and are given by

$$m(N_\pi) = m_x(N_\pi) = \frac{N - 2N_\pi}{N} = 1 - 2n_\pi, \quad (3.24)$$

$$\varepsilon(N_\pi) = -\frac{m^2(N_\pi)}{2} = -\frac{(N - 2N_\pi)^2}{2N^2} = -\frac{(1 - 2n_\pi)^2}{2}, \quad (3.25)$$

where we have introduced the fraction of angles equal to π , $n_\pi = N_\pi/N$.

Given a stationary configuration $p = \{\bar{q}_1, \dots, \bar{q}_N\}$, let us define the neighborhood

$$U_p = \begin{cases} q_i \in \left[\frac{\pi}{2}, \frac{3\pi}{2} \right] & \text{if } \bar{q}_i = \pi \\ q_i \in \left[\frac{3\pi}{2}, \frac{\pi}{2} \right] & \text{if } \bar{q}_i = 0 \end{cases} \quad (3.26)$$

so that $\{U_p\}_{p=1}^{2^N}$ is a partition of the phase space \mathbb{T}^N . The density of states ω_{MF} of the mean-field XY model can thus be written as

$$\omega_{\text{MF}}(\varepsilon) = \sum_{N_\pi=0}^N \nu(N_\pi) G_{\text{MF}}(\varepsilon, N_\pi) \quad (3.27)$$

where

$$G_{\text{MF}}(\varepsilon, N_\pi) = \int_{\pi/2}^{3\pi/2} dq_1 \cdots dq_{N_\pi} \int_{3\pi/2}^{\pi/2} dq_{N_\pi+1} \cdots dq_N \delta[\mathcal{H}_{\text{MF}}(q_1, \dots, q_N) - N\varepsilon]. \quad (3.28)$$

We note that $\nu(N_\pi)$ given by Eq. (3.23) is nothing but the density of states $\omega_{\text{MF}}^{(1)}$ of the mean-field Ising model

$$\mathcal{H}_{\text{MF}}^{(1)} = -\frac{1}{2N} \sum_{i,j=1}^N \sigma_i \sigma_j, \quad (3.29)$$

as a function of the number of “up” spins $\sigma = 1$; using the relation (3.25) to obtain the energy density ε' of the Ising stationary configuration as a function of N_π , Eq. (3.27) can be written as

$$\omega_{\text{MF}}(\varepsilon) = \sum_{\varepsilon'} \omega_{\text{MF}}^{(1)}(\varepsilon') G_{\text{MF}}(\varepsilon, \varepsilon'), \quad (3.30)$$

where the sum runs over the energy density levels of the Ising mean-field Hamiltonian (3.29). It is important to stress that this result is a consequence of the fact that the energy of a Ising stationary configuration depends only on N_π and that all the neighborhoods U_p with the same N_π contribute equally to the sum (3.27).

Let us now compute the function G_{MF} defined in Eq. (3.28). To make the calculation simpler it is useful to express G_{MF} as a function of m instead of ε ; one then gets back to ε using Eq. (3.20). Since we fixed the magnetization to be along the x axis, the function

3.4. THE ONE-DIMENSIONAL AND MEAN-FIELD XY MODELS

$G_{\text{MF}}(m, N_\pi)$ is given by

$$G_{\text{MF}}(m, N_\pi) = \int_{\pi/2}^{3\pi/2} dq_1 \dots dq_{N_\pi} \int_{3\pi/2}^{\pi/2} dq_{N_\pi+1} \dots dq_N \delta \left(\sum_{i=1}^N \cos q_i - Nm \right) \delta \left(\sum_{i=1}^N \sin q_i \right). \quad (3.31)$$

Using the integral representation of the Dirac delta distribution, Eq. (3.31) becomes

$$G_{\text{MF}}(m, N_\pi) = \left(\frac{1}{2\pi} \right)^2 \int_{\pi/2}^{3\pi/2} dq_1 \dots dq_{N_\pi} \int_{3\pi/2}^{\pi/2} dq_{N_\pi+1} \dots dq_N \int_{-\infty}^{\infty} dq_1 \int_{-\infty}^{\infty} dq_2 \exp \left[i q_1 \left(\sum_{i=1}^N \cos q_i - Nm \right) \right] \exp \left[i q_2 \left(\sum_{i=1}^N \sin q_i \right) \right]; \quad (3.32)$$

by writing

$$A(q_1, q_2) = \int_{\pi/2}^{3\pi/2} dq e^{i q_1 \cos q + i q_2 \sin q}, \quad (3.33)$$

$$B(q_1, q_2) = \int_{3\pi/2}^{\pi/2} dq e^{i q_1 \cos q + i q_2 \sin q} = \int_{\pi/2}^{3\pi/2} dq e^{i q_1 \cos(q-\pi) + i q_2 \sin(q-\pi)}, \quad (3.34)$$

we get

$$G_{\text{MF}}(m, N_\pi) = \left(\frac{1}{2\pi} \right)^2 \int_{-\infty}^{\infty} dq_1 \int_{-\infty}^{\infty} dq_2 e^{N(-imq_1 + n_\pi \log A(q_1, q_2) + (1-n_\pi) \log B(q_1, q_2))}. \quad (3.35)$$

The integrals in Eq. (3.35) can be computed with the saddle-point method [91] in the limit $N \rightarrow \infty$. The saddle point is given by $q_2 = 0$ e $q_1 = -i\gamma$, where $\gamma \in \mathbb{R}$ satisfies the self-consistency equation

$$m = n_\pi \frac{I_1(\gamma) - L_{-1}(\gamma)}{I_0(\gamma) - L_0(\gamma)} + (1 - n_\pi) \frac{I_1(\gamma) + L_{-1}(\gamma)}{I_0(\gamma) + L_0(\gamma)}; \quad (3.36)$$

in Eq. (3.36), $I_k(\gamma)$ are modified Bessel functions of order k and $L_k(\gamma)$ are modified Struve functions of order k [92]. We can thus write, in the thermodynamic limit $N \rightarrow \infty$,

$$G_{\text{MF}}(m, n_\pi) = \left(\frac{1}{2\pi} \right)^2 \exp \left\{ N \left[-m\gamma + n_\pi \log \tilde{A}(\gamma, 0) + (1 - n_\pi) \log \tilde{B}(\gamma, 0) \right] \right\}, \quad (3.37)$$

where we have written n_π instead of N_π since we are in the $N \rightarrow \infty$ limit, γ must be numerically determined solving Eq. (3.36), and the functions \tilde{A} and \tilde{B} are

$$\tilde{A}(\gamma, 0) = \pi [I_0(\gamma) - L_0(\gamma)], \quad (3.38)$$

$$\tilde{B}(\gamma, 0) = \pi [I_0(\gamma) + L_0(\gamma)]. \quad (3.39)$$

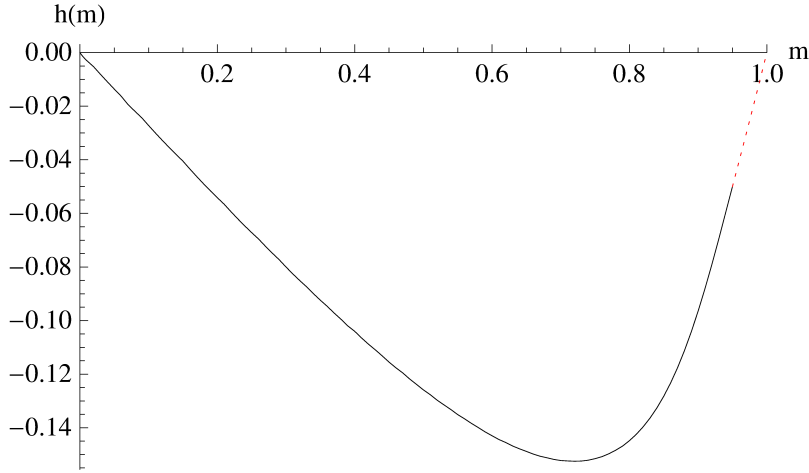


Figure 3.3 – Numerical results for the function $h(m)$ defined in Eq. (3.42) for the mean-field XY model. The red (dotted) part of the curve is obtained by interpolation (see text).

We can thus write, in the large N limit, the density of states (3.27) as a function of m as

$$\omega_{\text{MF}}(m) = \int_0^1 dn_\pi \exp \left[N(-m\gamma + n_\pi \log \tilde{A}(\gamma, 0) + (1 - n_\pi) \log \tilde{B}(\gamma, 0) - n_\pi \log n_\pi - (1 - n_\pi) \log(1 - n_\pi)) \right], \quad (3.40)$$

where we have neglected the subleading contributions in N . Again, the integral (3.40) can be computed with the saddle-point method as $N \rightarrow \infty$, so that, given m and thus ε , only a particular value of n_π (and thus of m' and, in turn, of ε') is singled out and the density of states ω_{MF} assumes the product form (3.15). The particular value of n_π which is singled out is the one such that the exponent in Eq. (3.40) is maximum; it has to be computed numerically.

The saddle point on Eq. (3.40) singles out a value \tilde{m} of the magnetization such that

$$\omega_{\text{MF}}(m) = \omega^{(1)}(\tilde{m}) G_{\text{MF}}(m, \tilde{m}). \quad (3.41)$$

In order to show that the value of \tilde{m} as a function of m converges to m as $m \rightarrow m_c$, where $m_c = 0$ is the critical value of the magnetization, in Fig. 3.3 we plot the function

$$h(m) = m - \tilde{m}. \quad (3.42)$$

Figure 3.3 shows that $h \rightarrow 0$ as $m \rightarrow 0$, so that the density of states $\omega_{\text{MF}}(m)$ is such that

$$\omega_{\text{MF}}(m) \rightarrow \omega^{(1)}(m) g_{\text{MF}}(m), \quad (3.43)$$

where $g_{\text{MF}}(m) = G_{\text{MF}}(m, m)$, for $m \rightarrow m_c$. More precisely, h appears to be a linear function of m as $m \rightarrow 0$, $h(m) \propto -m$. When $m \rightarrow 1$ the numerical procedure we used to compute $h(m)$ had some convergence problems. Since $m = 1$ implies $h(m) = 0$ and $n_\pi = 1$, to avoid these numerical problems the curve plotted in Fig. 3.3 in the range $m \in [0.97, 1]$ has been evaluated interpolating the numerical results obtained for $m < 0.97$ with the constraint $h(1) = 0$.

3.4. THE ONE-DIMENSIONAL AND MEAN-FIELD XY MODELS

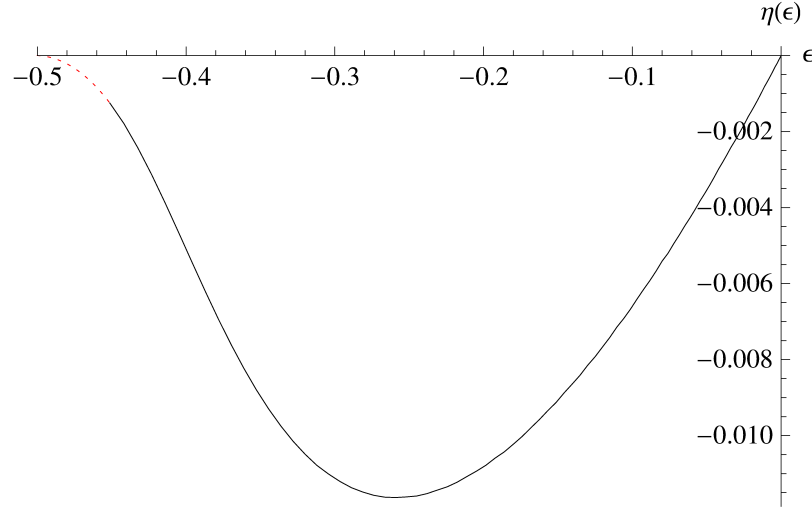


Figure 3.4 – Numerical results for the function $\eta(\varepsilon) = h(-\sqrt{2\varepsilon})$ defined in Eq. (3.46) for the mean-field XY model. The red (dotted) part is obtained by interpolation (see Fig. 3.3 and text).

The interpolating curve is drawn in red and in dotted style in Figure 3.3. We stress that the part of the curve relevant to the phase transition is that in the opposite limit, $m \rightarrow 0$, where the numerical procedure easily converges.

We can now go back to the energy, using $\varepsilon = -m^2/2$, and write

$$\omega_{\text{MF}}(\varepsilon) = \omega^{(1)}(\tilde{\varepsilon}) G_{\text{MF}}(\varepsilon, \tilde{\varepsilon}), \quad (3.44)$$

where $\tilde{\varepsilon} \rightarrow \varepsilon$ as $\varepsilon \rightarrow \varepsilon_c = 0$. One can thus write, as $\varepsilon \rightarrow \varepsilon_c$,

$$\omega_{\text{MF}}(\varepsilon) \rightarrow \omega^{(1)}(\varepsilon) g_{\text{MF}}(\varepsilon), \quad (3.45)$$

where $g_{\text{MF}}(\varepsilon) = G_{\text{MF}}(\varepsilon, \varepsilon)$, for $\varepsilon \rightarrow \varepsilon_c$. Figure 3.4 shows the function

$$\eta(\varepsilon) = h(\sqrt{-2\varepsilon}) = \varepsilon - \tilde{\varepsilon}; \quad (3.46)$$

as $\varepsilon \rightarrow \varepsilon_c = 0$, $\eta(\varepsilon) \propto -\sqrt{-\varepsilon}$. Since $|\eta(\varepsilon)|$ is the difference between the energy $\tilde{\varepsilon}$ singled out by the saddle point and the energy ε at which the density of states is calculated, it somehow measures also the “distance” between the function $G_{\text{MF}}(\varepsilon, \tilde{\varepsilon})$ and the function $g_{\text{MF}}(\varepsilon) = G_{\text{MF}}(\varepsilon, \varepsilon)$. From Fig. 3.4 we see that this difference reaches its maximum (roughly equal to 1.2×10^{-2}) around the center of the energy density range. Comparing this value to the width of the energy range itself we see that this difference is at most of the order of 2%.

3.4.2 The one-dimensional XY model

Let us now consider the one-dimensional XY model, which is a system of N planar spins with nearest-neighbor coupling, described by the Hamiltonian

$$\mathcal{H}_{1d} = - \sum_{i=1}^{N-1} \cos(q_{i+1} - q_i), \quad (3.47)$$

CHAPTER 3. $O(N)$ SPIN MODELS

where, as in the mean-field XY model, $q_i \in [0, 2\pi)$, so that the configuration (or phase) space of the system is the torus \mathbb{T}^N . This model does not have a bulk broken symmetry phase; it is ordered only in its state of minimum energy. Hence, the phase transition from a ferromagnetic to a paramagnetic phase occurs at $\varepsilon_c = \varepsilon_{\min} = -1$, and at zero temperature. It belongs to the class (3.1) with $n = 2$ and $J_{ij} = 1$ for i and j nearest-neighbors and zero otherwise.

As we shall see in the following, also for this model the density of states can be written as

$$\omega_{1d}(\varepsilon) = \omega^{(1)}(\tilde{\varepsilon}) G_{1d}(\varepsilon, \tilde{\varepsilon}), \quad (3.48)$$

where, in this case, $\omega^{(1)}$ is the density of states of the one-dimensional Ising model

$$\mathcal{H}_{1d}^{(1)} = - \sum_{i=1}^{N-1} \sigma_i \sigma_{i+1}, \quad (3.49)$$

and $\tilde{\varepsilon} \rightarrow \varepsilon$ as $\varepsilon \rightarrow \varepsilon_c = \varepsilon_{\min}$. One can thus write, as $\varepsilon \rightarrow \varepsilon_c$,

$$\omega_{1d}(\varepsilon) \rightarrow \omega^{(1)}(\varepsilon) g_{1d}(\varepsilon), \quad (3.50)$$

where $g_{1d}(\varepsilon) = G_{1d}(\varepsilon, \varepsilon)$, for $\varepsilon \rightarrow \varepsilon_c$. The derivation follows very closely that of the mean-field model, with a few differences that will be underlined.

Let us fix $q_N = 0$, and leave open the boundary condition at the other side of the chain. As in the mean-field case, the Ising stationary configurations are those where the angles \bar{q} are either 0 or π . However, their energy is no longer parametrized by N_π . On an Ising stationary configuration, the energy can be written as

$$\mathcal{H}_{1d}(\bar{q}_1, \dots, \bar{q}_{N-1}) = \mathcal{H}_{1d}^{(1)} = 2N_d - N + 1, \quad (3.51)$$

where N_d is the number of the domain walls in the configuration, i.e., the number of flips between $\bar{q} = 0$ and $\bar{q} = \pi$ (and viceversa) along the chain. This implies that one can no longer use the definition (3.26) of the neighborhoods U_p to build the partition of the configuration space, because this would imply that stationary points with the same energy would give different contributions.

Let us then change variables from (q_1, \dots, q_N) to (x_1, \dots, x_N) as follows:

$$\begin{cases} x_k &= q_{k+1} - q_k \quad \text{if } k = 1, \dots, N-1, \\ x_N &= q_N = 0. \end{cases} \quad (3.52)$$

In the new variables the Ising stationary points are still such that $\bar{x}_k = 0$ or $\bar{x}_k = \pi$, but now the energy is given in terms of the number of x 's equal to π , because the number of domain walls N_d is precisely that number. One can thus define the partition of the configuration

3.4. THE ONE-DIMENSIONAL AND MEAN-FIELD XY MODELS

space using the neighborhoods U_p defined as

$$U_p = \begin{cases} x_i \in \left[\frac{\pi}{2}, \frac{3\pi}{2} \right] & \text{if } \bar{x}_i = \pi \\ x_i \in \left[\frac{3\pi}{2}, \frac{\pi}{2} \right] & \text{if } \bar{x}_i = 0 \end{cases} \quad (3.53)$$

and write the density of states of the 1- d XY model as

$$\omega_{1d}(\varepsilon) = \sum_{N_d=0}^{N-1} v(N_d) G_{1d}(\varepsilon, N_d) \quad (3.54)$$

where

$$v(N_d) = \frac{(N-1)!}{N_d!(N-N_d-1)!} \quad (3.55)$$

is the number of Ising configurations with N_d domain walls, i.e., the density of states $\omega^{(1)}(\varepsilon')$ of the one-dimensional Ising model with energy density

$$\varepsilon' = \frac{2N_d - N + 1}{N}, \quad (3.56)$$

and

$$G_{1d}(\varepsilon, N_d) = \int_{\pi/2}^{3\pi/2} dx_1 \cdots dx_{N_d} \int_{3\pi/2}^{\pi/2} dx_{N_d+1} \cdots dx_{N-1} \delta \left(- \sum_{k=1}^{N-1} \cos x_k - N\varepsilon \right). \quad (3.57)$$

The computation then proceeds following very closely what already done for the mean-field case. The 1- d case is even simpler, because one can directly compute G_{1d} as a function of the energy density, without the need to consider it as a function of the magnetization. Using the integral representation of the δ and integrating on the x variables we can write in the large N limit

$$G_{1d}(\varepsilon, n_d) = \frac{1}{2\pi} \int_{-\infty}^{\infty} dq \exp \{ N [-iq\varepsilon + n_d \log b(q) + (1-n_d) \log a(q)] \}, \quad (3.58)$$

where $n_d = N_d/N$ and the functions a and b are given by

$$a(q) = \int_{3\pi/2}^{\pi/2} dx \exp(-iq \cos x), \quad (3.59)$$

$$b(q) = \int_{\pi/2}^{3\pi/2} dx \exp(-iq \cos x). \quad (3.60)$$

Performing again a saddle point with $q = -i\gamma$ we get, in the $N \rightarrow \infty$ limit,

$$G_{1d}(\varepsilon, n_d) = \frac{1}{\pi} \exp \{ N [-\gamma\varepsilon + n_d \log \tilde{b}(\gamma) + (1-n_d) \log \tilde{a}(\gamma)] \}, \quad (3.61)$$

where

$$\bar{a}(\gamma) = \tilde{A}(\gamma, 0), \quad (3.62)$$

$$\bar{b}(\gamma) = \tilde{B}(\gamma, 0), \quad (3.63)$$

with \tilde{A} and \tilde{B} given by Eqs. (3.38) and (3.39), respectively, and where γ satisfies the self-consistency equation

$$\varepsilon = (1 - n_d) \frac{I_1(\gamma) - L_{-1}(\gamma)}{I_0(\gamma) - L_0(\gamma)} + n_d \frac{I_1(\gamma) + L_{-1}(\gamma)}{I_0(\gamma) + L_0(\gamma)}. \quad (3.64)$$

We can thus realize that Eqs. (3.61) and (3.64) coincide with the same equations derived for the mean-field case, i.e., Eqs. (3.37) and (3.36), provided

$$\begin{cases} m & \rightarrow \varepsilon \\ n_\pi & \rightarrow 1 - n_d \end{cases} \quad (3.65)$$

The latter reflect the fact that in the $1-d$ case the transition occurs at the minimum value of ε instead of at the maximum.

From now on, the calculation of $\omega_{1d}(\varepsilon)$ is exactly the same as that of $\omega_{\text{MF}}(m)$, with the substitutions (3.65). A given value of \tilde{n}_d of n_d will be singled out, which corresponds to an energy density $\tilde{\varepsilon}$ via Eq. (3.56). We thus obtain

$$\omega_{1d}(\varepsilon) = \omega^{(1)}(\tilde{\varepsilon}) G_{1d}(\varepsilon, \tilde{\varepsilon}), \quad (3.66)$$

where $\tilde{\varepsilon} \rightarrow \varepsilon$ as $\varepsilon \rightarrow \varepsilon_c = \varepsilon_{\min}$; more precisely, defining the function

$$\zeta(\varepsilon) = \varepsilon - \tilde{\varepsilon} = h(m = \varepsilon + 1), \quad (3.67)$$

where $h(m)$ is the function (3.42) defined for the mean-field XY model, we have that $\zeta \rightarrow 0$ when $\varepsilon \rightarrow \varepsilon_c = \varepsilon_{\min} = -1$, and in particular $\zeta \propto -(1 + \varepsilon)$ for ε close to $\varepsilon_c = -1$. If one plots ζ as a function of ε one thus obtains exactly the same curve reported in Fig. 3.3, with the horizontal axis shifted so that $\varepsilon \in [-1, 0]$. Since $|h(m)|$ is maximum for $m \simeq 0.75$, the function $|\zeta(\varepsilon)|$ reaches its maximum value (roughly equal to 0.15) around $\varepsilon \simeq -0.25$; the maximum difference between ε and $\tilde{\varepsilon}$ in this case is around 15% of the full energy density range, larger than in the mean-field case.

3.5 Conclusions

In this Chapter we have analyzed the energy landscape of ferromagnetic $O(n)$ models with short and long range interactions. We have shown that every configuration of the Ising model defined on the same graph and with the same interaction matrix as the $O(n)$ model is a stationary configuration of the $O(n)$ model with $n > 2$.

The KSS criterion, thanks to the formulation given in Chapter 2, has been applied by Nerattini et al. [44] in the cases of two and three dimensional ferromagnetic nearest-neighbors XY models. However the criterion is not predictive because it does not single out any energy value at which the phase transition should be located. We do not expect differences considering short-range $O(n)$ models.

Analyzing, from an energy landscape perspective, the mechanism by which the phase transition in $O(n)$ models should emerge, we arrived to an approximate relation between the density of states of $O(n)$ models and the one of the Ising model defined on the same lattice with same interactions. This approximate relation is given in Eq. (3.14). Even if we do not expect this relation to be exact, it led us to the conjecture on a striking relation between the critical energy densities of $O(n)$ models.

Available analytical and numerical data are consistent with the conjecture, with the exception of the $O(2)$ case in $d = 2$. Preliminary numerical results for $O(n)$ models with power-law decaying interactions $1/|i - j|^\alpha$ with $\alpha > d$ as well for short-range $O(n)$ models in dimension greater than three and/or $n > 3$, show that the conjecture is still well verified.

In the case of $d = 2$ and $n = 2$, i.e. the Berežinskij-Kosterlitz-Thouless transition, the conjecture does not hold but available data seem not conclusive. In our opinion, more precise numerical estimates of the critical energy of the BKT transition would be very interesting, as well as estimates of other critical parameters made using the conjectured value of ε_c . Besides yielding an exact value for the critical energy of the BKT transition, a confirmation of the conjecture for the XY model in two dimensions might hint at a stronger version of the conjecture. Such a stronger conjecture would be that any $O(n)$ spin model on a d -dimensional hypercubic lattice has a phase transition at the critical energy density of the d -dimensional Ising model, even for $n > 2$ in $d = 2$. We note that the presence of a phase transition in $O(n)$ models at any n in two dimensions has already been suggested by Patrascioiu et al. [93,94]. Although, to the best of our knowledge, no direct evidence of such a transition has been found yet and the scenario is believed to be unlikely on the basis of numerical simulations [95–97], the possibility remains that the transition exists but is weak and elusive: our conjecture might help in finding it, suggesting where to look at.

Equation (3.14) has been derived with approximations which are not under control. For this reason, we have shown that the argument leading to Eq. (3.14) can be followed rigorously in the cases of 1-d and mean-field XY models. The relation between their density of states and the one of the Ising model is given by Eq. (3.15), which reduces to Eq. (3.14) for $\varepsilon \rightarrow \varepsilon_c$. These two models are very special and both of them are exactly solvable in the microcanonical ensemble. This feature is crucial for the derivation we have presented. As a consequence, a generalization of these results to $O(n)$ models with short-range interactions on a d -dimensional lattice is not straightforward at all, the difficulties being similar to exactly solving their thermodynamics in the microcanonical ensemble.

CHAPTER 3. $O(N)$ SPIN MODELS

Our work on 1-d and mean-field XY models confirms that Eq. (3.14) cannot be exact for a generic value of the energy density; at most, it could be valid for $\varepsilon = \varepsilon_c$. Indeed, we already pointed out that the relation (3.14) could not hold with an equality for a generic $O(n)$ model, since the specific heat critical exponent α of a $O(n)$ model would then have the correct sign, but the wrong absolute value. More precisely, Eq. (3.14) implies that if α_I is the microcanonical specific heat exponent of the Ising model on a given lattice, then the microcanonical specific heat exponent of the $O(n)$ model on the same lattice and with the same interactions is $\alpha = -\alpha_I$, regardless of n . In $d = 3$, for instance, this yields the correct sign of the $O(n)$ exponents, because $\alpha_I > 0$ so that $\alpha < 0$; the $O(n)$ specific heat is not divergent, but cuspy at the transition. However, the absolute value of the exponent is wrong, because it should depend on n , as shown by well-established results for the $O(n)$ universality classes [78].

In principle, our results could apply to more general models, like those with competing interactions or frustration; however, in this case the overlap of the energy ranges between Ising and $O(n)$ models is no longer guaranteed so that further work is needed to understand whether such generalization may be possible.

Following the argument that led us to Eq. (3.14) with approximations that can be taken under control, is a completely open issue for the moment. Some results in this direction would be of interest: they would help, for example, in a deeper understanding of the striking similarity between critical energy densities of ferromagnetic models on hypercubic lattices and would shed light on the generality of the phenomena for different models. We are currently working in collaboration with L. Casetti and R. Nerattini in this direction.

As a starting point, we write the density of states as a sum over Ising configurations

$$\omega^{(n)}(\varepsilon) = \sum_p \tilde{C}(p, U_p, \varepsilon), \quad (3.68)$$

where \tilde{C} are given by

$$\tilde{C}(p, U_p, \varepsilon) = \int_{U_p} d\Gamma \delta(\mathcal{H}^{(n)} - N\varepsilon); \quad (3.69)$$

the variable dependence of \tilde{C} means here that, in general, it depends both on the Ising configuration p and on the choice of the set U_p . The exact evaluation of Eq. (3.69) is a task as difficult as the exact solution of the density of states of the $O(n)$ model and thus it is, in the case of short-range systems and $d > 1$, not achievable.

We believe that some results can be obtained by approximating the continuous weights \tilde{C} . Possible techniques may be a harmonic expansion of $\mathcal{H}^{(n)}$ around every Ising configuration and a local mean-field approximation, as developed in [43].

Once that the $\tilde{C}(p, U_p)$ are approximated, they will generically depend on some parameters, instead of depending on p and U_p :

$$\tilde{C}(p, U_p, \varepsilon) \simeq C(\mathbf{z}(p), \varepsilon), \quad (3.70)$$

where $\mathbf{z}(p)$ is a vector of intensive parameters whose value is given by the Ising configuration p . For example, using a harmonic expansion of $\mathcal{H}^{(n)}$, these parameters are the index (divided by N), the determinant (raised to $1/N$) of the Hessian of $\mathcal{H}^{(n)}$ evaluated on p and the energy density of the stationary configuration $\varepsilon_p = \mathcal{H}^{(n)}(p)$.

We can thus approximate the full density of states in the following way:

$$\omega^{(n)}(\varepsilon) \simeq \sum_{\mathbf{z}} \Omega(\mathbf{z}) C(\mathbf{z}, \varepsilon), \quad (3.71)$$

where $\Omega(\mathbf{z})$ is a degeneracy factor, due to the fact that many distinct Ising configurations can give the same continuous weight. In general, both $\Omega(\mathbf{z})$ and $C(\mathbf{z}, \varepsilon)$ satisfy a large deviations law:

$$\Omega(\mathbf{z}) \simeq_{N \gg 1} \exp [Ns(\mathbf{z})] \quad (3.72)$$

$$C(\mathbf{z}) \simeq_{N \gg 1} \exp [Nc(\mathbf{z})]. \quad (3.73)$$

If one is able to evaluate (analytically or numerically) the large deviation functions s and c , Eq. (3.71) can be obtained with a saddle point procedure. If the computation of c usually does not pose much problems, because the approximations to evaluate the continuous weights can be chosen appropriately, s is usually harder to be obtained. For example, in the case of the harmonic approximation, $\Omega(\mathbf{z})$ gives the number of Ising configurations at energy density ε_p with a given index and a given value of the determinant: the evaluation of this quantity with numerical techniques (such as MonteCarlo simulations) is not a trivial task and we are currently working to understand how to handle such a problem.

Conclusions and perspectives

A number of results, some focused on specific models, others trying to shed light on the general mechanisms, appeared in last years trying to connect equilibrium phase transitions and energy landscape properties [35, 36] of classical Hamiltonian systems. However, a general picture is still lacking; one of the main obstacles is that only very simple systems, mean-field and one-dimensional, could be studied, being necessary to know all the saddles of the potential energy to apply these techniques or to verify the proposed ideas and conjectures.

The main scope of our work was to study models whose energy landscape is much more complicated than what previously done, developing techniques and approximations which do not need the knowledge of all the stationary points to be applied. The drawback is that, often, the approximations we used are not under control. This notwithstanding, we have obtained some interesting result, mainly on the applicability of the so-called KSS criterion and on the critical behavior of ferromagnetic $O(n)$ models on hypercubic lattices.

In parallel to our work, Kastner et al. [59, 60] have found a counterexample to the Franzosi and Pettini theorem, see Section 1.5. The implications of such results have still to be explored. In particular, it seems that the flaw in the theorem 1.2.1 stands in a forgotten hypothesis, used in the proof but not stated.

From a qualitative point of view, this additional hypothesis corresponds to the request that “topology changes cannot happen neither asymptotically”. If this is true, not only stationary points at finite N but also points that become stationary only in the $N \rightarrow \infty$ limit may be at the origin of phase transitions. We observed that such scenario is actually natural, because it is very simple to destroy stationary points without altering the thermodynamics of a system; on the other hand, a property like the one stated above should not be altered unless the external fields or change in the boundary conditions are so strong that even the thermodynamical behavior changes. The fact that this results are very recent (and in part not published) makes mandatory to revisit them with care before drawing any conclusion. We want to underline that these observations have not influenced the works presented in this thesis mainly because they have been obtained after ours.

In [37,38] a theorem which gives necessary conditions such that the saddles of the potential energy of finite systems can induce a phase transition in the thermodynamic limit has been proven. Our reformulation of the KSS theorem as a criterion for searching phase transitions, the KSS criterion, gave the possibility to study systems in which not all the stationary points are known. We have applied the KSS criterion to the SGR model and we have shown that it correctly singles out the phase transition between a homogeneous and a clustered phase. We have also shown that the criterion indicates the possible presence of another phase transition, not previously known, and we have conjectured on its nature constructing

an effective model of the SGR. We have also seen that the effective model possess an interest in itself, providing a very accurate approximation of the thermodynamics of the SGR model for values of the softening parameter such that the potential is very close to the gravitational one. It was not previously known that such toy models can give a quantitative, and not only qualitative, description of the thermodynamics of self-gravitating systems.

Initially we had the impression that the KSS criterion may be a useful instrument for the search of phase transitions in non-exactly solvable models. However, we rapidly realized with the results in [30, 31, 74] and in particular with those concerning the short-range XY models [44] reviewed in Chapter 3, that this is not the case. The KSS criterion is not able to single out the phase transition in short-range ferromagnetic XY models and it is quite safe to say that the same thing should happen for any short-range ferromagnetic $O(n)$ model.

We thus asked, from an energy landscape point of view, if it is a different mechanism that causes the presence of the phase transition in $O(n)$ models. This led us to an approximate relation, given in Eq. (3.14), between the density of states of $O(n)$ models and the one of the Ising model defined on the same lattice with same interactions. Even if we do not expect this relation to be exact, it led us to our conjecture on a striking relation between the critical energy densities of $O(n)$ models.

We thus compared the conjecture with analytical and numerical data available in literature, finding a very good agreement with the exception of the $O(2)$ case in $d = 2$, in which the difference between critical energies is around 2%. Preliminary numerical results for $O(n)$ models with power-law decaying interactions $1/|i - j|^\alpha$ with $\alpha > d$ as well for short-range $O(n)$ models in dimension greater than three and/or $n > 3$, show that the conjecture is still well verified in these cases. It would be very surprising if the conjecture proposed, being deduced from the very approximate Eq. (3.14), would hold exactly. Anyway, the striking similarities between critical energy densities, as well as the prediction of a negative exponent for the specific heat suggests that some physics is actually captured by our argument. Besides yielding an exact value for the critical energy of the BKT transition, the conjecture for the XY model in two dimensions might hint that any $O(n)$ spin model on a d -dimensional hypercubic lattice has a phase transition at the critical energy density of the d -dimensional Ising model, even for $n > 2$ in $d = 2$. The presence of a phase transition in $O(n)$ models at any n in two dimensions has already been suggested in literature [93, 94] and believed to be unlikely on the basis of numerical simulations [95–97]. However, the possibility remains that the transition exists but is weak and elusive: our conjecture might help in finding it, suggesting (at least approximately) where to look at.

The approximations leading to Eq. (3.14) are not under control, but it seems from the arguments above that some physics is actually captured. As a first step in understanding with more rigor the argument which led us to Eq. (3.14), we concentrated on the simplest

cases possible, the 1-d and mean-field XY models, showing that the argument leading to Eq. (3.14) can be followed rigorously. The relation between their density of states and the one of the Ising model is slightly more general, see Eq. (3.15), but reduces to Eq. (3.14) for ε that tends to ε_c . Unfortunately, these results have been obtained using the fact that these models are exactly solvable and we see no direct generalization for short-range systems. We are currently working in collaboration with L. Casetti and R. Nerattini to try to develop some approximation that may enable to follow the argument leading to Eq. (3.15) with approximations that can be taken under control.

Part II

Perturbed long-range interacting systems

Overview

A wide range of problems in physics concern systems with long-range interactions; one finds examples of long-range interacting systems in astrophysics [98–100], plasma physics [101, 102], hydrodynamics [103–105] and other physical systems [90, 106, 107]. However, their statistical and dynamical properties are much less understood than those of short-range interacting systems.

Let us define which is the property of the interaction that makes it short or long-ranged. We consider systems where the interaction potential is given by the sum, over pairs of the elementary constituents, of a two-body translationally invariant potential. For sufficiently large distances r , the absolute value of the two-body potential is bounded by $r^{-\alpha}$. If $\alpha < d$ we define the system to be long-range. In Fig. 3.5 is shown the (α, d) plane with the location of some long-range physical systems. In this thesis we will mainly consider particle systems; however, also models of two-dimensional and quasi two-dimensional turbulence, relevant for the study of geophysical flows [104, 108], do belong to the class of long-range interacting systems.

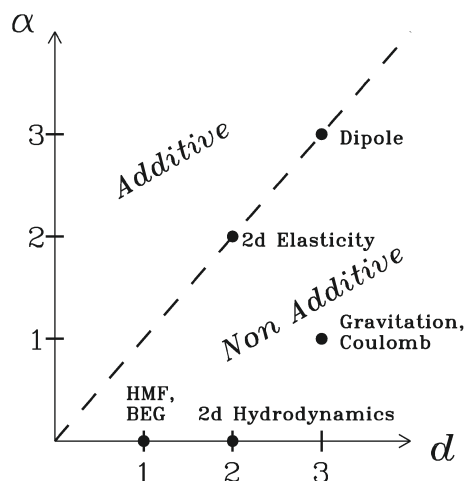


Figure 3.5 – Location of some physical systems in the plane where the abscissa is the spatial dimension d and the ordinate is the exponent α characterizing the spatial decay at large distances of the pair potential. The figure has been taken from [90].

Both the equilibrium and the out-of-equilibrium properties of long-range interacting systems show peculiarities [90] from a statistical physics perspective. At equilibrium, the most striking difference with short-range interacting systems is the possibility that the microcanonical and the canonical descriptions are not equivalent [109], and the possible presence of negative microcanonical specific heat.

As far as out-of-equilibrium dynamical properties are concerned, many-body long-range systems again show peculiar behaviors. The approach to equilibrium of short-range sys-

tems is usually characterized by the time scales that govern the equations of motion of the elementary constituents [110]. For systems without disorder, these time scales are typically small when compared to the observational time scales. Sometimes these systems can be trapped in metastable states that last for long times. These states are local extrema of thermodynamic potentials and, in practical cases, their realization requires a very careful preparation of the system (e.g. undercooled liquids and superheated solids). If perturbed, the system rapidly converges towards the equilibrium state.

For long-range systems, dynamics can be very slow and the approach to equilibrium can take a very long time, that increases with the number N of elementary constituents [98, 102, 111]. This feature is induced by the long-range nature of the interaction itself and is not a consequence of the existence of a collective phenomenon. The state of the system during this long transient is usually quasi-stationary [112, 113], since its very slow time evolution allows us to define slowly varying macroscopic observables, like for local equilibrium or quasi-static transformations. It should be however remarked that Quasi-Stationary states (QSSs) are not thermodynamic metastable states, since they do not lie on local extrema of equilibrium thermodynamic potentials.

The emergence of Quasi-Stationary states is nowadays well understood in terms of kinetic theory which is, as well as the Boltzmann kinetic theory, a perturbative approach to the macroscopic evolution of the system. However, at variance to the case of perfect gases, the small parameter here is $1/N$. At leading order one obtains the Vlasov equation, which is simply the mean-field approximation of the dynamics of the system. Stationary and stable solutions of the Vlasov equation are the QSS of the N -body system. At next order in $1/N$, one obtained the Lenard-Balescu equation, first obtained independently in [114] and in [115], which describes the slow evolution of a particle system with long-range interactions from the initial condition to the final Maxwell-Boltzmann equilibrium through a sequence of Quasi-Stationary States.

Most of these features are well known in plasma physics and astrophysical community since a long time [98, 102, 111]. They have attracted some attention in last years, in which much study has been devoted to simplified systems with long-range interactions, where numerical simulations can be performed with high precision: we address the reader to [90, 106, 107] for recent reviews and for broad discussions on the study of simplified models with long-range interactions. Still, some important questions remain open, among which: the possible selection of periodic solutions of the Vlasov equation instead of a QSS; the complete understanding of the timescales for the relaxation to equilibrium, especially when the system remains trapped in a non-homogeneous QSS; the rigorous derivation of the equations of the kinetic theory (especially the Lenard-Balescu equation); the construction of controllable laboratory experiments in which the peculiarities of long-range interacting systems may be studied [116]. However, the general setting on which studying these

features is well settled.

On the other hand, much less is known on the behavior of long-range interacting systems under the effect of external driving. In this thesis we start to work in this direction, considering perturbations which evolves both deterministically and stochastically in time. We think this second case to be of particular interest and most of our work has been devoted to the of study long-range interacting systems driven away from equilibrium by external stochastic forces.

Our work stands at the edge between the study of long-range interacting systems and the study of non-equilibrium systems [117–120], where stationary states are sustained by fluxes of conserved quantities. The main difference with most of the studies in non-equilibrium statistical mechanics, is that short-range interacting systems are naturally coupled locally to the driving forces: for example, thermostats act at the boundary of a short-range interacting system or independently on each degree of freedom (such as in the case of mesoscopic particles in water). On the other hand, long-range interacting systems are naturally acted upon by fields that couple coherently to all the degrees of freedom.

This situation is classical in geophysical flows, in which large scale structures are often observed [104, 105, 108], such as strong jet streams, atmospheric cyclones or ocean currents which stands for very long times with respect to the internal dynamical time-scales. Such large scale structures emerge from a balance between energy injection provided by the environment and dissipation due to boundaries effects.

Also long-range interacting particle systems are often acted upon by external stochastic forces, which can be due to the effect of the environment, such as in self-gravitating systems [121, 122] or to imposed external electric or magnetic fields [123].

In this part of the thesis, we present a generalization of the theoretical and numerical techniques, well developed for isolated long-range interacting systems, to study the behavior of systems driven away of equilibrium. Because of technical reasons, the analysis of particle systems is simpler than for fluid models; we thus concentrated mainly in the first case, the generalization of our results to turbulence models being one of the most interesting perspectives of our work. This part of the thesis is structured as follows:

Chapter 4 In this first Chapter, we mainly review the kinetic theory description of isolated long-range interacting particle systems. We present phenomenologically their intriguing slow relaxation to the Maxwell-Boltzmann equilibrium and the presence of QSSs in which the system remains trapped for a time-scale diverging with the system size. This behavior can be understood using kinetic theory, which is a perturbation theory in the small parameter $1/N$. At leading order in kinetic theory, one obtains the Vlasov equation and at next order the Lenard-Balescu equation. Developing the kinetic theory, we also present the phenomena of the Landau damping for homogeneous states.

The results in this Chapter are very classical in plasma physics and astrophysics; however, the derivation of the Lenard-Balescu equation as presented here is in some way original. The generality with which we derive the Lenard-Balescu equation will be useful in the following of the thesis for the derivation of kinetic theories for stochastically forced systems, in Chapter 6 and 7, and will be contained in [124].

Chapter 5 presents the content of [125]. For short-range interacting systems, Kubo linear response theory is a very classical and fundamental result which describes how a system prepared in equilibrium responds to a small external perturbation. Long-range interacting systems, however, are often found trapped in QSS; Kubo theory is of little utility here.

As a first step in understanding the effect of perturbations on systems with long-range interactions, we consider here the following situation: we prepare a long-range interacting system in a QSS and we apply a (small) external field which evolves deterministically in time. We show that a formula similar to the Kubo formula holds, where the differences arise from the non-linearity of the Vlasov equation in contrast to the Liouville equation. Explicit predictions can be simply obtained for systems homogeneous in coordinates, using techniques very similar to those presented in Chapter 4 to obtain the Landau damping. Theoretical predictions are successfully compared with N -body simulations. Our results have been recently generalized to some case of non-homogeneous initial states by Ogawa et al. [126] and by Patelli et al. [127].

Chapter 6 presents the content of [128] and [129]. We consider here a long-range interacting particle system stochastically forced by external fields which act coherently on all particles: one should think to these fields as electric fields, gravitational fields, etc. In situations of stochastic driving, the systems at long times often reach a nonequilibrium stationary state that violates detailed balance. In such a state, the power injected by the external random fields balances on average the dissipation, and there is a steady flux of conserved quantities through the system.

Beside the fact that we are dealing with long-range interacting systems, the study of nonequilibrium stationary states (NESS) is an active area of research of modern day statistical mechanics. Our work provides, to the best of our knowledge, the first study of NESS in long-range systems with statistical mechanical perspectives.

The main theoretical results of this Chapter is a detailed development of a generalization of the kinetic theory for isolated long-range systems to describe nonequilibrium stationary states in systems with long-range interactions driven by external stochastic forces, valid in the limit of small external stochastic fields and for homogeneous systems. Our kinetic theory is quite general, being applicable to any long-range interacting system composed by particles. In the limit of small external forcing. The

predictions of our kinetic equation for spatially homogeneous stationary states compare very well with results of our extensive N -particle numerical simulations on the stochastically forced HMF model.

Moreover, we study numerically how the phase transition at equilibrium is altered when the detailed balance is broken. We demonstrate the occurrence of bistability between homogeneous and non-homogeneous states, with a mean residence time that diverges as an exponential in the inverse of the strength of the external stochastic forces. Similar bistable behavior has recently been observed in two-dimensional turbulence with stochastic forcing and thus look as a quite general phenomena for stochastically driven long-range interacting systems.

Chapter 7 contains preliminary results. A very interesting situation in which a long-range interacting system is acted upon by random fields comes from geophysics, in which two-dimensional and quasi two-dimensional turbulence models are often used to explain the emergence of large scale structures with very long life times. In these cases, the effect of the environment resulting in turbulent fluctuation acting at small spatial scales, is not negligible, and some friction is present at large spatial scales due to boundary effects. Again, the system reach stationary states in which fluxes of energy and other conserved quantities break the detailed balance.

The situation is very analogous to the one studied in Chapter 6, so that one can hope that the theory there developed for particle systems is generalizable to the present case. From a phenomenological point of view, there are some efforts in this direction in literature, see for example [130–134], going under the name of second order closure expansion or stochastic structural stability theory. In this Chapter, we start the study of the problem from a theoretical point of view, identifying the forcing amplitude as the small parameter in which the kinetic theory is a perturbation theory. It is of interest to develop a theoretical framework at least for two reasons: to clarify when the kinetic theory gives reliable predictions and to find the simplest possible way to obtain explicit results on the stationary state attained and on the evolution of the mean flow. We show that the theory is well posed and we describe how to obtain explicit predictions. However, we do not discuss explicit numerical results, being only partial for the moment.

Conclusions and perspectives We resume the work presented and we discuss the perspectives of this part of the thesis.

4

Isolated long-range interacting systems

In this introductory Chapter we present a brief review of isolated long-range interacting systems in which the degrees of freedom are particles. Even if these systems show a peculiar behavior both for what concern the equilibrium and the relaxation to equilibrium [90], we only concentrate here on this second aspect, discussing the kinetic theory [98, 102, 111, 135, 136].

Isolated long-range interacting particle systems show an intriguing slow relaxation to the Maxwell-Boltzmann equilibrium. Starting from an arbitrary initial condition, they often remain trapped in out of equilibrium states, called Quasi-Stationary State (QSSs), whose lifetime diverge with the system size; the QSS in which the system remains trapped depends on the initial condition. Only after a time diverging algebraically with the system size, the system relaxes to the Maxwell-Boltzmann equilibrium. Such behavior can be understood using kinetic theory, which is a perturbation theory in the small parameter $1/N$, where N is the number of particles.

At leading order in kinetic theory, one obtains the Vlasov equation, which is the mean-field approximation of the dynamics of the system. Vlasov equation is an infinite dimensional dynamical system and posses an infinite number of stationary states. If a given stationary states of the Vlasov equation is stable with respect to small perturbations, starting close to it the N -body system remains close for long times, until when corrections to the Vlasov equation have to be taken into account. Stationary and stable states of the Vlasov equation are the QSS of the N -body system.

At next order in the parameter $1/N$, one can take into account two particles correlations while discarding three-particle and higher-order correlations. This is the analogous in the Boltzmann theory of taking into account two-body encounters while discarding three body and higher order encounters. We will show that this is a self-consistent procedure (even if not rigorously founded) for long-range interacting systems in the large N limit. One thus arrives to the Lenard-Balescu equation, independently obtained in [114] and [115]. The Lenard-Balescu equation describes the slow evolution of a particle system with long-range interactions from the initial condition to the final Maxwell-Boltzmann equilibrium through a sequence of Quasi-Stationary States.

CHAPTER 4. ISOLATED LONG-RANGE INTERACTING SYSTEMS

The Chapter is organized as follow: in Section 4.1 we introduce isolated particle systems with long-range interactions and we set some notations; we also introduce the Hamiltonian Mean Field (HMF) model, a simplified system with long-range interactions. In Section 4.2 we discuss numerical simulations showing the existence of QSSs and the relaxation to equilibrium in the HMF model. Then, we introduce the kinetic theory. In Section 4.3, we discuss the BBGKY hierarchy of a long-range interacting system and its closures. We derive at leading order in $1/N$, in Section 4.4, the Vlasov equation; we also discuss the notion of linear stability of a stationary state of the Vlasov equation, which leads us to discuss the phenomena of the Landau damping.

We then consider the problem of going beyond the mean field approximation. In Section 4.5 we develop some technique useful to solve Lyapunov equations; this is useful because the second equation of the BBGKY hierarchy, which describes the evolution of two-particle correlations, is a Lyapunov equation. Finally, we apply in Section 4.6 the techniques of the previous Section to obtain the Lenard-Balescu equation.

This Chapter mainly contains results which are known since long time in plasma physics [102, 111, 135, 136]. However, for what concern the derivation of the Lenard-Balescu equation, we follow a non-standard way, through the BBGKY hierarchy; this is not the usual approach followed in many books and reviews, in which usually the Klimontovich approach or some diagrammatic technique is preferred. As far as the author know, only in the book of Nicholson [102] the theory is fully developed using the BBGKY hierarchy. However a number of obscure points in this reference, forced us in carefully reviewing its derivation. The way in which the results are presented here, in particular the results in Section 4.5 and their application to obtain the Lenard-Balescu equation, are thus original and form a part of [124]. The general results of Section 4.5 will be useful in the following of the Thesis for the derivation of kinetic theories for stochastically forced systems, in Chapter 6 and 7.

4.1 Long-range interacting particle systems

In this Part of the Thesis, we mainly consider systems composed of N particles interacting through a pair potential, and described by the Hamiltonian

$$H = \sum_{i=1}^N \frac{p_i^2}{2} + \frac{1}{2} \sum_{i,j=1}^N v(q_i - q_j). \quad (4.1)$$

Here, q_i and p_i are, respectively, the coordinate and the momentum of the i -th particle, and $v(q)$ is the two-body interaction pair potential. For the sake of simplicity in the notations, we take the particles to be of unit mass and we regard the variables q_i as scalar periodic variables of period 2π . We will also suppose that the particles in the system belong to only one

4.1. LONG-RANGE INTERACTING PARTICLE SYSTEMS

species excluding thus the case, for example, of a plasma of electrons and protons. Anyway, all the theoretical discussions present in this thesis are very easily generalizable to $q_i \in \mathbb{R}^n$, with arbitrary n and to systems composed by more than one species of particles. In the few cases in which differences arise, they will be underlined.

This Part of the Thesis is about systems with long-range interactions, which means that the pair potential v has a slow decay at infinity; in particular we say that a system of the form (4.3) is a long-range interacting system is bounded by

$$v(q) \sim \frac{1}{q^\alpha} \quad \alpha < d \quad (4.2)$$

for large distances, where d is the spatial dimension of the system¹. Systems with long-range interactions do not only include particle systems but also models from two dimensional and quasi two dimensional turbulence, such as the Euler equation, the quasi-geostrophic equation and the shallow-water equation. We will only deal with turbulence models in Section 7; we address the reader to [104, 105, 108] for broad reviews on this subject.

In plasma physics, the typical number of particles interacting with one particle is given by the coupling parameter $\Gamma = n\lambda_D^3$, where n is the number density, and λ_D is the Debye length. It is then usual to rescale time such that the inverse of Γ multiplies the interaction term [102]. Analogously, in self-gravitating systems, the dynamics is dominated by collective effects, so that it is natural to rescale time in such a way that the parameter $1/N$ multiplies the interaction potential [139]. Rescaling time with N in such a way that a factor $1/N$ appears in front of the potential energy is called the Kac prescription [140]. From now on, we will consider Hamiltonian system of the form

$$H = \sum_{i=1}^N \frac{p_i^2}{2} + \frac{1}{2N} \sum_{i,j=1}^N v(q_i - q_j). \quad (4.3)$$

where we emphasize that no generality is lost in adopting the Kac prescription

If considering one dimensional systems or higher dimensional system, as well as the form of the potential $v(q)$, is not so important from a theoretical point of view², it makes an huge difference in numerical simulations. Indeed, due to the long-range character of the forces, the cost of N -body simulations using codes such as symplecting integrators

¹For systems in $d > 1$, with attractive potentials with strong (but finite) variations in v , recent results suggest [137, 138] that the bound $\alpha < d$ is not sufficient to ensure the typical dynamical properties of long-range interacting systems, such as the existence of Quasi-Stationary States. In this cases the bound $\alpha < (d - 1)$ seem to be more appropriate.

²We observe anyway that rigorous mathematical results, such as for example the Braun-Hepp theorem [141] (see the Section 4.7), usually strongly rely on the hypothesis of a smooth interparticle potential.

CHAPTER 4. ISOLATED LONG-RANGE INTERACTING SYSTEMS

scales as N^2 and hence becomes prohibitively heavy already for moderate N . For this reason, simplified models with long-range interactions have attracted some attention in last years [90, 106]. Among them, the most famous is the so called Hamiltonian Mean Field model introduced in [70], in which the particles are confined on a circle of unit radius and we take the potential to be the one of the mean-field XY model:

$$v(q) = 1 - \cos q. \quad (4.4)$$

Because the HMF model is a mean-field model, the potential energy can be written as a function of a single collective variable, that is the magnetization $m = (m_x, m_y)$, where

$$m_x = \frac{1}{N} \sum_{i=1}^N \cos q_i \quad \text{and} \quad m_y = \frac{1}{N} \sum_{i=1}^N \sin q_i. \quad (4.5)$$

It is thus easy to realize that the cost of the numerical integration of the motion equations of the HMF models scales only linearly with N .

From what concern the equilibrium behavior, it is known from exact results both in the canonical [70] and microcanonical [142] ensemble, that the HMF model at equilibrium shows a continuous phase transition from a low-energy clustered phase, in which the particles are close together on the circle ($|m| \neq 0$), to a high-energy homogeneous phase corresponding to a uniform distribution of particles on the circle ($|m| = 0$). The caloric curve, i.e. temperature as a function of the energy density, is reported in Fig. 4.1.

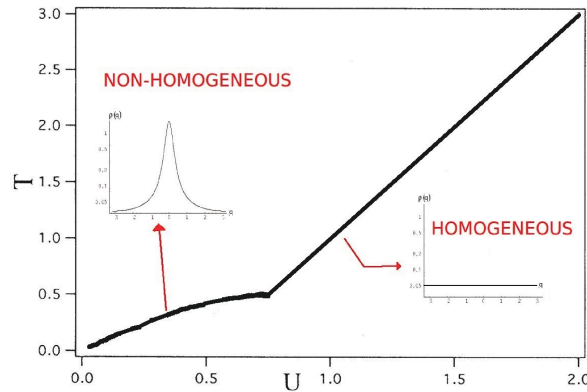


Figure 4.1 – Equilibrium caloric curve, i.e. microcanonical temperature as a function of the energy per particle, of the HMF model. At high energies the system is homogeneous ($|m| = 0$) and at low energy it is not ($|m| \neq 0$). $\rho(q)$ is the spatial density of particles at the point q in the equilibrium configuration at the energy indicated by the arrow.

Beside its simplicity, the HMF model has a relevance as a simplified model of the free electron laser [143–145] and shows many important features of long-range interacting systems, especially for what concern the presence of Quasi-Stationary states. We discuss this latter point in the next Section.

4.2 Phenomenology: Quasi-Stationary-States

Systems with long-range interactions (4.3) can get trapped in Quasi-Stationary States for times which diverge algebraically with the system size³ before relaxing to the Maxwell-Boltzmann equilibrium. We do not want to report on the many numerical results on this subject but only to give a qualitative idea of the phenomena that we will try to explain with kinetic theory. We thus consider the very simple example of the HMF model defined above.

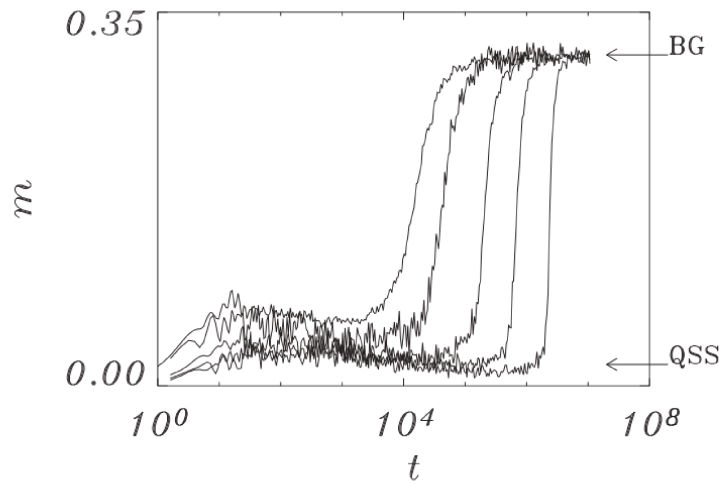


Figure 4.2 – Time evolution of $|m|$ for different particle numbers $N = 10^3, 2 \times 10^3, 5 \times 10^3, 10^4, 2 \times 10^4$ from left to right and energy slightly below the equilibrium phase transition. Two values of the magnetization, indicated by horizontal arrows, can be identified in this figure; the upper one (labeled BG) corresponds to the Maxwell-Boltzmann equilibrium, while the lower one, labeled QSS, represent the value of the magnetization in the QSS. The Figure has been taken from [90].

Let us thus consider the following experiment [113]. We prepare the system in an homogeneous, i.e. $|m| = 0$, state sampling the initial velocities of the N particles from the distribution

$$f_0(p) = \frac{1}{2\pi} \frac{1}{2p_0} \left[\Theta(p + p_0) - \Theta(p - p_0) \right]; \quad p \in [-p_0, p_0], \quad (4.6)$$

which is usually called a water-bag initial condition; p_0 is an external parameter connected to the initial kinetic energy of the system. If p_0 is set such that the initial energy is slightly below the energy where is located the phase transition at equilibrium, one observes the behavior of Fig. 4.2. First of all (at time-scales of order between 1 and 20 in the Figure) the system experiences some kind of relaxation which does not look to depend on N : the presence of this phenomena was supposed by Lynden-Bell in [148] and it is usually called violent relaxation in astrophysical context [98, 149]. After this transient, the system gets trapped in a very slowly evolving state, called Quasi-Stationary state. The larger is the system, the more

³In [146], the authors state that exponentially long QSS can be found in the HMF model for some particular initial condition. However, some recent analysis [147] seems to be in contraddiction with this conclusion.

is the time it needs to relax to the Maxwell-Boltzmann equilibrium, that is, longer it is the life-time of the Quasi-Stationary State. The relaxation time diverges algebraically with N and, in the HMF model for the initial condition (4.6), it behaves as $N^{1.7}$; other relaxation scalings are possible depending on the dimensionality of the system and on the fact that the system is homogeneous or not. We will see developing the kinetic theory that, in general, the relaxation time is expected to be of order N .

The qualitative behavior observed here has been observed also in other models with long-range interactions and starting with different initial conditions, see for example [150–152]. This kind of behavior is pictorially represented in Fig. 4.3.

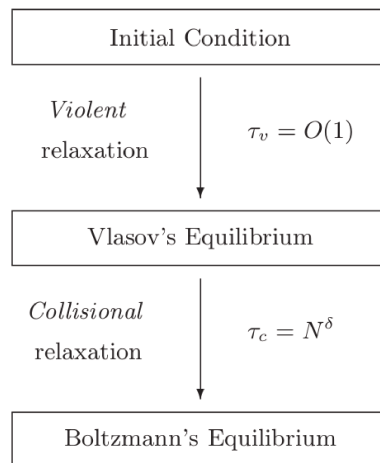


Figure 4.3 – Schematic description of the typical dynamical evolution of systems with long-range interactions. The Figure has been taken from [90].

We start now to develop the kinetic theory that, as we will see, explains the strange phenomenology presented above, gives insight on how to characterize the QSSs, on which role is played by the initial condition and on how to explain the scaling with N of the relaxation time.

4.3 Kinetic approach

The starting point of the kinetic approach we will follow here is to derive the BBGKY hierarchy for systems with Hamiltonian (4.3). It is well known that the BBGKY hierarchy is exact and fully equivalent to the motion equations; thus, the important point is to understand how to close the hierarchy in a self-consistent way for the description we want to obtain. Discarding three particle and higher order correlations while taking into account two particle correlations is a self-consistent procedure, as we will see; however, it is not rigorously founded and it is actually the main obstacle to put on rigorous basis the kinetic theory approach [153, 154].

4.3.1 BBGKY hierarchy

The BBGKY hierarchy corresponding to the Hamiltonian in Eq. (4.3) can be obtained with standard techniques [51, 102]. The starting point is to write the corresponding Liouville equation, obtaining:

$$\frac{\partial f_N}{\partial t} = \sum_{i=1}^N -p_i \cdot \frac{\partial}{\partial q_i} f_N + \frac{1}{2N} \sum_{i,j=1}^N \frac{\partial}{\partial q_i} v(q_i - q_j) \cdot \left(\frac{\partial}{\partial p_i} - \frac{\partial}{\partial p_j} \right) f_N, \quad (4.7)$$

where $f_N(q_1, \dots, q_N, p_1, \dots, p_N, t)$ is normalized to unity. We observe here that everywhere in the Thesis we will use both the notation $\frac{\partial g}{\partial x}$ or $g'(x)$ when no confusion is possible to indicate the derivative of a function. The Liouville equation for Hamiltonian systems is a very detailed description of the system. Using kinetic theory, we want to describe the evolution of the one-particle distribution function

$$f(z_1, t) = \int \prod_{i=2}^N dz_i f_N(z_1, \dots, z_N, t), \quad (4.8)$$

where we have used the notation $z_i \equiv (q_i, p_i)$. We note that with this definition, the normalization is $\int dz f(z, t) = 1$. Substituting in the Liouville equation (4.7) the reduced distribution functions⁴ ($f_1 = f$)

$$f_s(z_1, \dots, z_s, t) = \frac{N!}{(N-s)!N^s} \int \prod_{i=s+1}^N dz_i f_N(z_1, \dots, z_N, t), \quad (4.9)$$

and using standard techniques, we get the BBGKY hierarchy, as follows:

$$\begin{aligned} \frac{\partial f_s}{\partial t} + \sum_{i=1}^s p_i \cdot \frac{\partial}{\partial q_i} f_s - \frac{1}{N} \sum_{i,j=1}^s \frac{\partial}{\partial q_i} v(q_i - q_j) \cdot \frac{\partial}{\partial p_i} f_s &= \\ = \sum_{i=1}^s \int dz_{s+1} \frac{\partial}{\partial q_i} v(q_i - q_{s+1}) \cdot \frac{\partial}{\partial p_i} f_{s+1} & \end{aligned} \quad (4.10)$$

for $s = 1, \dots, N-1$. Observe moreover that we will always suppose that f_N , and thus also f_s , is invariant for permutations of its arguments z_i 's, which corresponds to suppose that the system is composed only by one species of particles and no correlations are present in the initial state:

$$f_N(z_1, \dots, z_N, t=0) = \prod_{i=1}^N f(z_i, t=0), \quad (4.11)$$

which is called a product state.

⁴One could be tempted to use reduced distribution functions defined without the normalization factor $\frac{N!}{(N-s)!N^s}$. This procedure, however, gives a hierarchy of equations which is not useful to define self-consistent closures.

The BBGKY hierarchy, as well as the Liouville equation, is an exact description of the dynamics of the system and thus an unnecessarily complicated to describe its macroscopic behavior. The first important step is then to understand how to close the BBGKY hierarchy, depending on the time-scale at which we want to describe the dynamics.

4.3.2 Closures of the BBGKY hierarchy

As is usual in kinetic theory, we split the reduced distribution functions into connected and non-connected parts, e.g.,

$$f_2(z_1, z_2, t) = f(z_1, t)f(z_2, t) + \tilde{g}(z_1, z_2, t), \quad (4.12)$$

$$\begin{aligned} f_3(z_1, z_2, z_3, t) &= f(z_1, t)f(z_2, t)f(z_3, t) + f(z_1, t)\tilde{g}(z_2, z_3, t) \\ &+ f(z_2, t)\tilde{g}(z_1, z_3, t) + f(z_3, t)\tilde{g}(z_1, z_2, t) + h(z_1, z_2, z_3, t), \end{aligned} \quad (4.13)$$

and similarly, for other f_s 's for $s \geq 4$.

Introducing such definitions in the BBGKY hierarchy (4.10), we get for the first equation

$$\frac{\partial f}{\partial t} + p \frac{\partial f}{\partial q} - \frac{\partial f}{\partial p} \frac{\partial \Phi[f]}{\partial q} = \frac{\partial}{\partial p} \int dq_1 dp_1 v'(q - q_1) \tilde{g}(z, z_1, t), \quad (4.14)$$

where

$$\Phi[f](q, t) = \int dq_1 dp_1 v(q - q_1) f(q_1, p_1, t) \quad (4.15)$$

is the mean-field potential. For the second equation of the hierarchy, we obtain

$$\begin{aligned} \frac{\partial \tilde{g}(z_1, z_2, t)}{\partial t} &= \left[-p_1 \frac{\partial \tilde{g}}{\partial q_1} + \frac{\partial \tilde{g}}{\partial p_1} \frac{\partial \Phi[f]}{\partial q_1} + \frac{f(z_2)}{N} \frac{\partial v(q_1 - q_2)}{\partial q_1} \frac{\partial f}{\partial p_1} + \frac{1}{N} \frac{\partial v(q_1 - q_2)}{\partial q_1} \frac{\partial \tilde{g}}{\partial p_1} \right. \\ &\left. + \frac{\partial f}{\partial p_1} \int dz_3 \frac{\partial v(q_1 - q_3)}{\partial q_1} \tilde{g}(z_2, z_3) + \int dz_3 \frac{\partial v(q_1 - q_3)}{\partial q_1} \frac{\partial h}{\partial p_1} \right] + \{1 \leftrightarrow 2\}, \end{aligned} \quad (4.16)$$

where the symbol $\{1 \leftrightarrow 2\}$ stands for an expression obtained from the bracketed one on the right hand side by exchanging the subscripts 1 and 2.

Let us analyze the order of magnitude of the terms in Eq. (4.16). First of all, we have $f \sim 1$, as it is normalized to unity. However, we do not know a priori the order of magnitude of \tilde{g} and h . Thus, the order of magnitude of all but the term $\frac{f(z_2)}{N} \frac{\partial v(q_1 - q_2)}{\partial q_1} \frac{\partial f}{\partial p_1}$ is unknown; we have

$$\frac{f(z_2)}{N} \frac{\partial v(q_1 - q_2)}{\partial q_1} \frac{\partial f}{\partial p_1} \sim \frac{1}{N} \ll 1. \quad (4.17)$$

If we suppose h of higher order in $1/N$ with respect to g , we thus obtain that $\tilde{g} \sim 1/N$. Observe that to have $\tilde{g} \sim 1/N$, we have supposed that there are no correlations in the initial condition for f_N , that is Eq. (4.11); otherwise, $\tilde{g} \sim 1/N$ is already false at $t = 0$ and, in general, false at every time.

Once we have established that $\tilde{g} \sim 1/N$, one can write down the equation of the hierarchy for h and, with a similar reasoning as above, one then finds that h is of order $1/N^2$, so that the term

$$\int dz_3 \frac{\partial v(q_1 - q_3)}{\partial q_1} \frac{\partial h}{\partial p_1} \quad (4.18)$$

is of order $1/N^2$ and thus negligible in Eq. (4.16). The iterative procedure can be repeated at any order of the hierarchy. Discarding three-particle and higher-order correlations is thus a self-consistent procedure.

Moreover, we note that in Eq. (4.16), also the term

$$\frac{1}{N} \frac{\partial v(q_1 - q_2)}{\partial q_1} \frac{\partial \tilde{g}}{\partial p_1} \quad (4.19)$$

is of order $1/N^2$ and thus can be discarded.

Because we have concluded that $\tilde{g} \sim 1/N$, it is convenient to rescale \tilde{g} with the small parameter $1/N$. In the following, we will then use the expansion in the connected and non-connected parts of the reduced distribution functions, once discarded three-particle and higher order correlations, as follows:

$$f_2(z_1, z_2, t) = f(z_1, t)f(z_2, t) + \frac{1}{N}g(z_1, z_2, t), \quad (4.20)$$

$$f_3(z_1, z_2, z_3, t) = f(z_1, t)f(z_2, t)f(z_3, t) + \frac{1}{N}f(z_1, t)g(z_2, z_3, t) \quad (4.21)$$

$$+ \frac{1}{N}f(z_2, t)g(z_1, z_3, t) + \frac{1}{N}f(z_3, t)g(z_1, z_2, t) \quad (4.22)$$

so that the final form of the first two equations of the hierarchy is:

$$\frac{\partial f}{\partial t} + p \frac{\partial f}{\partial q} - \frac{\partial f}{\partial p} \frac{\partial \Phi[f]}{\partial q} = \frac{1}{N} \frac{\partial}{\partial p} \int dq_1 dp_1 v'(q - q_1) g(z, z_1, t), \quad (4.23)$$

and

$$\begin{aligned} \frac{\partial g(z_1, z_2, t)}{\partial t} = & \left[-p_1 \frac{\partial g}{\partial q_1} + \frac{\partial g}{\partial p_1} \frac{\partial \Phi[f]}{\partial q_1} + f(z_2) \frac{\partial v(q_1 - q_2)}{\partial q_1} \frac{\partial f}{\partial p_1} \right. \\ & \left. + \frac{\partial f}{\partial p_1} \int dz_3 \frac{\partial v(q_1 - q_3)}{\partial q_1} g(z_2, z_3) \right] + \{1 \leftrightarrow 2\}. \end{aligned} \quad (4.24)$$

4.4 Vlasov equation

We have seen that the connected part of the two-particle correlations is of order $1/N$. This imply that the right hand side of the first equation of the BBGKY hierarchy (4.14) is of order $1/N$ and thus negligible in the large N limit, because all the other terms are of order 1.

CHAPTER 4. ISOLATED LONG-RANGE INTERACTING SYSTEMS

This is the mean-field approximation of the dynamics of the system and leads to the Vlasov equation (or collisionless Boltzmann equation, in astrophysical community)

$$\frac{\partial f}{\partial t} + p \frac{\partial f}{\partial q} - \frac{\partial f}{\partial p} \frac{\partial \Phi[f]}{\partial q} = 0, \quad (4.25)$$

where

$$\Phi[f](q, t) = \int dq_1 v(q - q_1) \rho(q_1, t) \quad (4.26)$$

is the mean-field potential and the spatial density ρ is given by

$$\rho(q, t) = \int dp f(q, p, t). \quad (4.27)$$

The Vlasov equation is an infinite dimensional Hamiltonian⁵ system [155] describing the evolution of the density of particles in the μ -space, that is the single particle phase space. Many of the interesting properties of the Vlasov equation are connected to the fact that there are an infinite number of integrals of motion. Indeed, for any smooth function s , the quantity

$$\mathcal{C}[s] = \int dp dq s(f(q, p, t)) \quad (4.28)$$

is an invariant of the Vlasov dynamics; $\mathcal{C}[s]$ are called Casimirs. Observe, that, among all the Casimirs, there is the mean-field entropy

$$S[f] = - \int dp dq f \log f. \quad (4.29)$$

The other invariants of the Vlasov equation are the single particle Hamiltonian

$$h[f](q, p) = \frac{p^2}{2} + \Phi[f] \quad (4.30)$$

and, if present, the other single particle quantities associated to the invariants of the N -body dynamics, such as the momentum, angular momentum etc.

Vlasov equation possess an infinite number of stationary solutions. For example, if we suppose the system to be homogeneous at all times,

$$f(q, p, t) = f(p, t), \quad (4.31)$$

then we directly obtain $\partial_t f = 0$.

As usual for dynamical systems, not all stationary solutions are stable. In the following, we study the stability of stationary solutions of the Vlasov equation. Stable stationary solutions of the Vlasov equations are the Quasi-Stationary states of the N -body dynamics.

⁵The formal definition of the Hamiltonian structure is slightly more involved than usual due to the infinite dimensionality of the system and this fact lead to non-canonical Poisson parenthesis. We address the reader to [155] on this topic.

4.4.1 Linear Vlasov equation and Landau Damping

Vlasov equation conserves the mean-field entropy and is a time-reversible equation. A natural question is to understand what happens if we slightly perturb a stationary state. The microscopic evolution never ends leading to a finer and finer structure of the distribution function; this process is called filamentation and it is due to the time-reversibility of the Vlasov equation. However, if the initial state is stable (we will carefully define what does it mean) the system remains in some norm close to the original state. Indeed, from a macroscopic point of view, the system relaxes: looking at averages over the μ -space, they decay in time to a stationary value. This is what happens, for example, to the spatial density defined by Eq. (4.27) and to the mean field potential (4.26).

This phenomena, first discovered by Landau [156], is a very well-known phenomena both in plasma physics and astrophysics and goes under the name of Landau damping. In Fig. 4.4 it is pictorially represented for the free evolution case. The technique used is the linear stability analysis which strongly resembles the one used in dynamical system, the only difference with the standard case being the fact that the Vlasov equation is infinite dimensional.

To introduce the problem, we start considering the evolution of free particles in a box: this simple system shows Landau damping, and is technically simpler to handle. This will permit us to introduce some notations for the following.

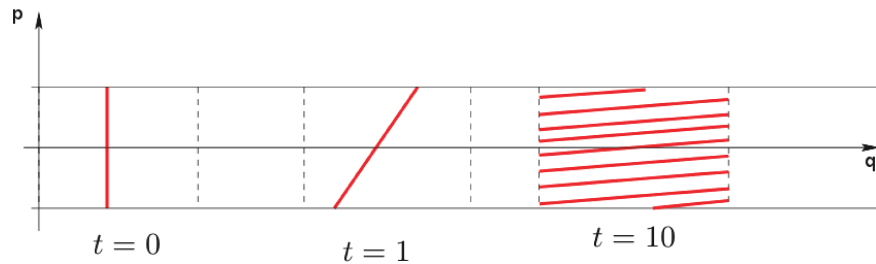


Figure 4.4 – Free transport evolution in a box at three different times. The structure becomes finer and finer in the μ -space; once averaged over p , however, the system becomes homogeneous very rapidly. This is the mechanism of Landau damping.

Landau Damping for the free transport

Let us consider the Vlasov equation associated to the Hamiltonian (4.3) with $v(q) = 0$

$$\frac{\partial f}{\partial t} + p \frac{\partial f}{\partial q} = 0, \tag{4.32}$$

this is nothing else than the free transport equation. We consider Eq. (4.32) with initial datum $f(q, p, t = 0) = r(q, p)$, which we suppose to be a real analytic function of the velocities

CHAPTER 4. ISOLATED LONG-RANGE INTERACTING SYSTEMS

p : this will be important for the following. Moreover, we suppose r to be normalizable, so that it decays sufficiently fast at infinity.

Of course Eq. (4.32) can be solved explicitly: $f(q, p, t) = r(q - pt, p)$. The simplicity of this formula is deceptive, and the free transport equation displays much trickier behavior than one would imagine at first sight.

To study the properties of Eq. (4.32) it is useful to use the Fourier transform in space and Laplace transform in time. Here and in the following, our conventions for the Fourier transform of a given function h are

$$h_k = \int_0^{2\pi} \frac{dq}{2\pi} h(q) e^{-ikq}, \quad h(q) = \sum_{k=-\infty}^{\infty} h_k e^{ikq}. \quad (4.33)$$

For the Laplace transform in time of a function h we have:

$$\tilde{h}(\omega) = \int_0^{\infty} dt h(t) e^{i\omega t}, \quad \text{Im}(\omega) > 0; \quad (4.34)$$

if no confusion is possible, we will use the notation $h(\omega) = \tilde{h}(\omega)$ omitting the tilde symbol. The inverse Laplace transform, reads:

$$h(t) = \int_{\Gamma} \frac{d\omega}{2\pi} \tilde{h}(\omega) e^{-i\omega t}, \quad (4.35)$$

where Γ is a contour which passes above all the singularities of the integrand. Observe that, for the latter definition to be valid, we have to suppose that the integral does not depend on the choice of Γ . This can be proved, for example, for integrands $h(\omega) e^{-i\omega t}$ that decay sufficiently fast at $-i\infty$ so that the contour Γ can be appropriately chosen, or for integrands which decay sufficiently fast at infinity in a stripe around the real axis. We will not comment further this point, which is sometimes a bit tricky, when using the inverse Laplace transform⁶.

Applying the Fourier transform to Eq. (4.32), we get:

$$\frac{\partial f_k}{\partial t} + ikp f_k(p, t) = 0. \quad (4.36)$$

We already see that the 0-th mode does not evolve

$$f_0(p, t) = r_0(p). \quad (4.37)$$

For the other modes, applying the Laplace transform, we have:

$$f_k(p, \omega) = \frac{r_k(p)}{-i\omega + ikp}, \quad \text{Im}(\omega) > 0, \quad (4.38)$$

⁶The careful inversion of the Laplace transform is the most tricky point in the rigorous proof of the Landau damping [157, 158].

and thus for the spatial density:

$$\rho_k(\omega) = \int_{-\infty}^{+\infty} dp \frac{r_k(p)}{-i\omega + ikp}, \quad \text{Im}(\omega) > 0. \quad (4.39)$$

To perform the inverse Laplace transform, as to obtain $\rho_k(t)$, we need to analytically continue the above expression to $\omega \in \mathbb{R}$. The expression for $\rho_k(\omega)$ can be analytically continued because the integrand posses a single pole on the real axis, located at $\omega = kp$. All along the thesis we will not change notation for a function and its analytic continuation; we get for the spatial density:

$$\rho_k(\omega) = \int dp \frac{r_k(p)}{-i\omega + ikp} + \pi l(\omega) \frac{\text{sgn}(k)}{k} r_k\left(\frac{\omega}{k}\right) \quad (4.40)$$

where

$$l(\omega) = \begin{cases} 0 & \text{Im}(\omega) > 0 \\ 1 & \text{Im}(\omega) = 0 \\ 2 & \text{Im}(\omega) < 0. \end{cases} \quad (4.41)$$

In Eq. (4.40), $\text{sgn}(k)$ denotes the sign of k and the integral has to be considered as a Cauchy (or Principal Value) integral when $\text{Im}(\omega) = 0$.

From Eq. (4.40) one sees $\rho_k(\omega)$ can have a singularity in $\bar{\omega}$ only if $\text{Im}(\bar{\omega}) < 0$. This can be deduced by the fact that we are supposing the initial datum $r_k(p)$ to be a real analytic function of the p variable. Indeed, any real analytic function is a complex analytic function on a sufficiently small stripe around the real axis.

We can now perform the inverse Laplace transform; recalling that $\rho_k(\omega)$ is analytic for $\omega \in \mathbb{R}$, we can choose Γ to be below the real axis. The integral term in Eq. (4.40) vanishes closing the contour at $-i\infty$ because it has no singularities in the lower half plane. We thus get

$$\rho_k(t) = \pi \frac{\text{sgn}(k)}{k} \int_{\Gamma} \frac{d\omega}{2\pi} l(\omega) r_k\left(\frac{\omega}{k}\right) e^{-i\omega t} \quad (4.42)$$

where Γ passes above all the singularities of r_k . With a change of variables, we have

$$\rho_k(t) = \int_{\Gamma} d\omega r_k(\omega \text{sgn}(k)) e^{-i|k|\omega t}, \quad (4.43)$$

where Γ is below the real axis. In the large time limit, we thus obtain that $\rho_k(t)$ goes to zero (at least) exponentially for all $k \neq 0$. The rate at which $\rho_k(t)$ goes to zero depends on two things: the spatial mode k we are considering (higher modes decay faster) and how far from the real axis the contour Γ can be deformed. For example if the only singularities of f_k are single poles and the integrand decays sufficiently fast at $-i\infty$, $\rho_k(t)$ can be explicitly computed with the Residue theorem. We observe that this argument does not hold if r_k is

CHAPTER 4. ISOLATED LONG-RANGE INTERACTING SYSTEMS

Gaussian, because in this case the contour cannot be closed at $-i\infty$; in this case a different closure of Γ leads to a super-exponential decay.

This is the mechanism of the Landau damping: from a macroscopic point of view, the system loose memory of its initial state and relaxes to an homogeneous state. This behavior is, of course, not in contradiction with the time-reversibility of the free transport equation. Indeed, the relaxation happens only in quantities which are average of the distribution function over the space. The behavior of the distribution function f never ends leading to a finer and finer structure; this is the process of filamentation, see Fig. 4.4. To see it explicitly, it suffice to apply the inverse Laplace transform to Eq. (4.38), considered as a function defined on the whole complex plane. We get

$$f_k(p, t) = 2\pi r_k(p) e^{-ikpt}; \quad (4.44)$$

the velocity structure of the k -th mode of the distribution f at time \bar{t} is on a velocity scale of order $1/(k\bar{t})$.

Observe that for the Landau damping to take place it is necessary that the system is confined in a box. Otherwise, there are modes with arbitrary small k that are damped at slower and slower rate. Moreover the request that the initial datum r is analytic is important; if this is not the case, the above argument does not hold and the decay can be much slower than exponential or there could be no decay at all: more regular is the initial datum, faster is the decay [157].

Landau Damping for homogeneous states

Let us now describe the Landau damping mechanism for homogeneous systems described by the Vlasov equation. We will also introduce some very important quantities for the following of this Thesis: the resolvent operator and the dielectric function. The procedure presented here is exactly the analogous of what we have done for the free transport, except that the solution in Fourier and Laplace transform of the linear Vlasov equation is a bit more involved.

Let us consider an homogeneous long-range interacting system in a box whose initial condition is $f(p)$. As for the free transport, it is important that the system is confined in a box and that $f(p)$ is analytic.

We want to understand the evolution of a perturbation $h(q, p, t)$ to the state $f(p)$; for easiness in the notation, we call r the initial value of the perturbation $h(q, p, t = 0) = r(q, p)$. We suppose the perturbation r to be small with respect to f and to be a real analytic function. It is thus natural to guess that the evolution is well described by the linearized Vlasov equation around f , that is

$$\frac{\partial h}{\partial t} + p \frac{\partial h}{\partial q} - \frac{\partial f}{\partial p} \frac{\partial \Phi[h]}{\partial q} = 0 \quad h(q, p, t = 0) = r(q, p), \quad (4.45)$$

where we have neglected the non-linear contribution in h ; moreover, we have used that the system is homogeneous, that is f is a steady state of the Vlasov equation and the mean field force vanishes. In this case, the Vlasov operator linearized around f and acting on a function $h(q, p)$ is given by

$$(L_f h)(q, p) = p \frac{\partial h}{\partial q} - \frac{\partial f}{\partial p} \frac{\partial \Phi[h]}{\partial q}. \quad (4.46)$$

Because the system is homogeneous, it is useful to use the Fourier transform with respect to the spatial variable, obtaining

$$\frac{\partial h}{\partial t} + (L_{f,k} h_k)(p, t) = 0 \quad (4.47)$$

where $L_{f,k}$ is the k -th component of the linear Vlasov operator and its action on a given function $h(p)$ is

$$(L_{f,k} h)(p) = ik p h(p) - 2\pi i k v_k f'(p) \int dp' h(p'). \quad (4.48)$$

Let us observe a very important property: because of the homogeneity of the system, the evolution of every Fourier mode is independent on the others. Moreover, we get

$$\frac{\partial h_0}{\partial t} = 0, \quad (4.49)$$

that is $h_0(p, t) = r_0(p)$: again, the 0-th mode does not evolve.

We can now use the Laplace transform on Eq. (4.47), to obtain for $\text{Im}(\omega) > 0$

$$h_k(p, \omega) = \frac{1}{-i\omega + ikp} \left[r_k(p) + 2\pi i k v_k f'(p) \int dp' h_k(p', \omega) \right]. \quad (4.50)$$

Integrating such expression to obtain $\int dp' h_k(p', \omega)$ and substituting the result in the last term of the previous one, we have

$$h_k(p, \omega) = (R_{f,k}(\omega) r_k)(p), \quad (4.51)$$

where $R_{f,k}(\omega)$ is the resolvent operator associated with $L_{f,k}$ in frequency space defined as

$$R_{f,k}(\omega) \equiv \frac{1}{-i\omega + L_{f,k}}. \quad (4.52)$$

Explicitly, we have

$$(R_{f,k}(\omega) h)(p) = \frac{1}{-i\omega + ikp} \left[h(p) + \frac{2\pi i k v_k}{\epsilon(k, \omega)} f'(p) \int dp' \frac{h(p')}{-i\omega + ikp'} \right], \quad (4.53)$$

where $\epsilon(k, \omega)$ is the dielectric function, defined for $\text{Im}(\omega) > 0$ as

$$\epsilon(k, \omega) = \left[1 - 2\pi i v_k k \int dp \frac{f'(p)}{-i\omega + ikp} \right]. \quad (4.54)$$

CHAPTER 4. ISOLATED LONG-RANGE INTERACTING SYSTEMS

From Eq. (4.51) we also obtain for the k -th mode of the spatial density

$$\rho_k(\omega) = \int dp (R_{f,k}(\omega)r_k)(p) = \frac{1}{\epsilon(k, \omega)} \int dp \frac{r_k(p)}{-i\omega + ikp} \quad (4.55)$$

from which is simple to evaluate the mean field potential. One should recall that all the expressions above are valid for $\text{Im}(\omega) > 0$.

To obtain the time behavior of the spatial density $\rho_k(t)$ and of $h_k(p, t)$ we have to invert the Laplace transform; to do it, it is necessary, exactly as in the free transport case, to give a meaning to the expressions presented above for $\text{Im}(\omega) \leq 0$. We thus perform, whenever possible, an analytic continuation to $\omega \in \mathbb{R}$. This corresponds to replace the terms of the form

$$\int dp \frac{g(p)}{-i\omega + ikp} \quad (4.56)$$

where g is an analytic function, with

$$\int dp \frac{g(p)}{-i\omega + ikp} + \pi l(\omega) \frac{\text{sng}(k)}{k} g(\omega/k). \quad (4.57)$$

For example, for the dielectric function, we obtain

$$\epsilon(k, \omega) = 1 - 2\pi i v_k k \int dp \frac{f'(p)}{-i\omega + ikp} - 2\pi^2 i l(\omega) \text{sng}(k) v_k f' \left(\frac{\omega}{k} \right) \quad (4.58)$$

where $l(\omega)$ is given by Eq. (4.41) and the integral has to be interpreted as a Cauchy integral for $\text{Im}(\omega) = 0$.

Suppose now that the roots $\bar{\omega}$ of $\epsilon(k, \bar{\omega}) = 0$ are only such that $\text{Im}(\bar{\omega}) < 0$. In this case, it is possible to perform the analytic continuation of the integral of the resolvent operator (4.55). Indeed, interpreting ϵ as in Eq. (4.58), it is a real analytic function. Thus, it is a complex analytic function on a small enough stripe around the real line. From the identity theorem we thus get that the set in which ϵ vanishes cannot contain an accumulation point in a stripe around the real line. Because we are also supposing r to be an analytic function, the integral of the resolvent operator is free of singularities around the real axis. This proves that Eq. (4.55) can be analytically continued to $\omega \in \mathbb{R}$ and the procedure to do it is the one sketched above. We get

$$\rho_k(\omega) = \frac{1}{\epsilon(k, \omega)} \left[\int dp \frac{r_k(p)}{-i\omega + ikp} + \pi l(\omega) \frac{\text{sng}(k)}{k} r_k \left(\frac{\omega}{k} \right) \right], \quad (4.59)$$

where, as usual, the integral has to be interpreted as a Cauchy integral for $\text{Im}(\omega) = 0$.

We can now perform the inverse Laplace transform to get $\rho_k(t)$. We have

$$\rho_k(t) = \int_{\Gamma} \frac{d\omega}{2\pi} \frac{e^{-i\omega t}}{\epsilon(k, \omega)} \left[\int dp \frac{r_k(p)}{-i\omega + ikp} + \pi l(\omega) \frac{\text{sng}(k)}{k} r_k \left(\frac{\omega}{k} \right) \right] \quad (4.60)$$

where Γ can be chosen to stay below the real axis. Observe that the singularities of the first term in Eq. (4.60) are given only by the zeros of the dielectric function whereas, in the second one, singularities can be given also by the initial datum r_k . The rate of the damping is again given by how far from the real axis the contour Γ can be deformed and this depends both on where the zeros of the dielectric function are located and where are the possible singularities of r_k seen as a complex function of its argument.

The case we have treated is the one in which the zeros of the dielectric function are present only in the lower half plane. In this case, the state f is called a stable state; the spatial density or the mean field potential of any small perturbation to the base state decays exponentially to zero in time. On the other hand, if zeros of the dielectric function are present for $\text{Im}(\omega) > 0$, $\rho_k(t)$ diverges exponentially in time. The state f will be thus called unstable. Finally, if zeros of ϵ are found only for $\text{Im}(\omega) \leq 0$, $\rho_k(t)$ present undamped oscillations and in this case f is called marginally stable.

The time evolution of h itself is very different to the one of ρ or of the mean field potential. To see this, we have first to give a meaning to Eq. (4.51) for $\text{Im}(\omega) \leq 0$; this can be done replacing the integral in Eq. (4.53) with Eq. (4.57). Then, applying the inverse Laplace transform, we see that the contribution of the pole $\omega = kp$ give an undamped oscillation. This term is only due to the free transport in the Vlasov equation, i.e. it is exactly the same effect we have already seen for the free transport equation.

Stability is a very important property of a stationary states because only stable (and marginally stable) states can be observed for not very small times: in a numerical or real experiment it is impossible to exactly prepare the system in a given state. Quasi-Stationary States we talked about phenomenologically in Section 4.2 are nothing else than stationary and stable solution of the Vlasov equation.

However, in practice, it is quite hard to explicitly compute the zeros of the dielectric function (as it is generically hard to compute the zeros of a general complex-valued function). Among the many available criteria to determine it, we highlight the one proposed by Penrose in [159]: f is a stable distribution if and only if for every $\omega \in \mathbb{R}$ such that $f'(\omega) = 0$,

$$\int^* dp \frac{f'(p)}{p - \omega} < 1, \quad (4.61)$$

where \int^* stands for a Cauchy integral.

The analysis carried here for the Landau damping is not rigorous, mainly due to our use of the inverse Laplace transform. The first completely rigorous treatment of the linear Landau damping is due to Backus [158] who checked carefully the invertibility of the Laplace transform of the solution. Around the same time Penrose [159] proposed an alternative reasoning based on the general theory of the Laplace transform, and more importantly derived

the stability criterion now called Penrose criterion.

Recently Villani and Mouhot proved that Landau damping persist considering the non-linear Vlasov equation instead of the linearized one [160] in the perturbative regime. We refer the reader to [157] for further references on the (broad) mathematical literature on Landau damping.

Landau Damping for non-homogeneous states

We have presented the Landau damping in the case in which f is an homogeneous state. However, in many physical situations such as in astrophysical systems, the relevant states are not homogeneous: a galaxy, for example, shows a very high density contrast between the central and the outer parts. One of the main difficulties of proving Landau damping for non-homogeneous states is that the evolution of different spatial modes do not decouple, as in the homogeneous case. Very few works [161, 162] are present, especially at theoretical level, to deal with this situation, due to the much more involved mathematical analysis which is needed.

We highlight [163, 164] in which the problem is solved for states in which the one-particle dynamics is integrable, such that one can use action-angle variables. The main difference with the homogeneous states is that the dispersion relation analogous to the dielectric function in Eq. (4.58) presents branch cuts which can touch the real axis. This impose a much more refined analysis to perform the analytic continuation. This branch cuts in the dispersion relation give rise to algebraic Landau damping after an exponential transient. The situation is analogous to what has been found before in the 2d Euler equation for shear flows that we will briefly discussed in Chapter 7.

4.5 Lyapunov equations

In this section we study the Ornstein–Uhlenbeck process and Lyapunov equations in a general setting, which will turn out to be useful both in the derivation of the Lenard-Balescu equation and in kinetic theories presented in Chapters 6 and 7. Indeed it will turn out in all this cases, that the equation describing the evolution of the connected part of two-particle correlations is a Lyapunov equation.

The standard solution of the finite dimensional Ornstein–Uhlenbeck process can be generalized to the infinite dimensional case. However, for what concern the long-time limit, different techniques have to be used. We will describe how this problem can be handled: in particular, if the solution to the Lyapunov equation converges exponentially in time, a simplified expression for the stationary solution can be given working in the frequency space.

4.5.1 Definition of the Ornstein–Uhlenbeck process

The Ornstein–Uhlenbeck process [165] is a Gaussian process defined by the following stochastic differential equation:

$$\partial_t h(\mathbf{r}, t) + (Lh)(\mathbf{r}, t) = \sqrt{2}F(\mathbf{r}, t) \quad (4.62)$$

where $\mathbf{r} \in \mathcal{D} \subseteq \mathbb{R}^n$ and $h \in \mathcal{H}$ is a complex function belonging to some Hilbert space \mathcal{H} ; L is a linear operator acting on \mathcal{H} and generically infinite dimensional. $F(\mathbf{r}, t)$ is a complex Gaussian random process with variance:

$$\langle F(\mathbf{r}, t)F^*(\mathbf{r}', t') \rangle = C(\mathbf{r} - \mathbf{r}')\delta(t - t'), \quad (4.63)$$

where $*$ denotes the adjoint operation (or the complex conjugate, depending on the case in hand).

We will consider here the Ornstein–Uhlenbeck process with initial condition $h(\mathbf{r}, t = 0) = 0$, because this is the relevant case for kinetic theories: the generalization of all the results presented below to general initial conditions is straightforward.

The Ornstein–Uhlenbeck process is characterized by the two point correlations functions. We will consider in the following the single-time correlation function $\phi(\mathbf{r}, \mathbf{r}', t) = \langle h(\mathbf{r}, t)h^*(\mathbf{r}', t) \rangle$. The equation for the time evolution of ϕ is easily obtained using the Ito formula and averaging:

$$\partial_t \phi + L^{(1)}\phi + L^{*(2)}\phi = C(\mathbf{r} - \mathbf{r}'), \quad (4.64)$$

where $L^{(1)}$ (respectively $L^{(2)}$) is the linear operator L acting on the first (the second) variable of ϕ and C is the average effect of the stochastic force. Eq. (4.64) is called the Lyapunov equation associated to the Ornstein–Uhlenbeck process (4.62).

Introducing the Fourier basis $\{e_{\mathbf{k}}(\mathbf{r}) = e^{i\mathbf{k}\mathbf{r}}\}_k$, we write the correlation function in Fourier transform

$$C(\mathbf{r} - \mathbf{r}') = \sum_{\mathbf{k}} f_{\mathbf{k}} e_{\mathbf{k}}(\mathbf{r}) e_{\mathbf{k}}^*(\mathbf{r}'). \quad (4.65)$$

Because of the linearity of the Lyapunov equation, the solution to Eq. (4.64) can be written as

$$\phi(\mathbf{r}, \mathbf{r}', t) = \sum_{\mathbf{k}} f_{\mathbf{k}} \phi_{\mathbf{k}}(\mathbf{r}, \mathbf{r}', t), \quad (4.66)$$

where $\phi_{\mathbf{k}}$ is the solutions of

$$\partial_t \phi_{\mathbf{k}} + L^{(1)}\phi_{\mathbf{k}} + L^{*(2)}\phi_{\mathbf{k}} = b_{\mathbf{k}}(\mathbf{r})b_{\mathbf{k}}^*(\mathbf{r}'), \quad (4.67)$$

with $b_{\mathbf{k}} = e_{\mathbf{k}}$. We introduce the Ornstein–Uhlenbeck processes

$$\partial_t h_{\mathbf{k}}(\mathbf{r}, t) + (Lh_{\mathbf{k}})(\mathbf{r}, t) = \sqrt{2}b_{\mathbf{k}}(\mathbf{r})W(t), \quad (4.68)$$

where $W_{\mathbf{k}}$ are independent complex Gaussian processes:

$$\langle W_{\mathbf{k}}(t)W_{\mathbf{k}'}^*(t') \rangle = \delta_{\mathbf{k},\mathbf{k}'}\delta(t - t'). \quad (4.69)$$

We thus recover Eq. (4.70) as the evolution equation for $\phi_{\mathbf{k}}(\mathbf{r}, \mathbf{r}', t) = \langle h_{\mathbf{k}}(\mathbf{r}, t)h_{\mathbf{k}}^*(\mathbf{r}', t) \rangle$.

We consider in the following of this section Lyapunov equations of the form

$$\partial_t \phi_{\mathbf{k}} + L^{(1)}\phi_{\mathbf{k}} + L^{*(2)}\phi_{\mathbf{k}} = b(\mathbf{r})c(\mathbf{r}'), \quad (4.70)$$

for generic functions b and c .

4.5.2 Formal solutions in real time

The solution to the Lyapunov equation (4.70) can be found using the formal solution of the Ornstein–Uhlenbeck process, as in the case in which the operator L is finite dimensional; we refer to [165] for standard results in the finite dimensional case.

The solution of the Ornstein–Uhlenbeck process is given by the following stochastic integral

$$h(\mathbf{r}, t) = \sqrt{2} \int_0^t \left(e^{-(t-u)L}b \right)(\mathbf{r}) dW(u), \quad (4.71)$$

as can be proven differentiating Eq. (4.71). Observe that $e^{-(t-u)L}b$ is the solution at time t of the deterministic equation

$$\partial_t h(\mathbf{r}, t) + (Lh)(\mathbf{r}, t) = 0 \quad (4.72)$$

with initial condition $h(\mathbf{r}, t = 0) = b(\mathbf{r})$.

By direct computation, we then obtain the solution to the Lyapunov equation (4.70)

$$\phi(\mathbf{r}, \mathbf{r}', t) = 2 \int_0^t \left(e^{-uL}b \right)(\mathbf{r}) \left(e^{-uL^*}c \right)(\mathbf{r}') du. \quad (4.73)$$

Let us observe that we can also easily obtain the evolution for linear transforms of ϕ . If S is a linear operator acting on \mathcal{H} , we have $(S^{(2)}\phi)(\mathbf{r}, \mathbf{r}', t) = \langle h(\mathbf{r}, t)(Sh^*)(\mathbf{r}', t) \rangle$ and, explicitly:

$$(S^{(2)}\phi)(\mathbf{r}, \mathbf{r}', t) = 2 \int_0^t \left(e^{-uL}b \right)(\mathbf{r}) \left(Se^{-uL^*}c \right)(\mathbf{r}') du, \quad (4.74)$$

where $S^{(2)}$ is the linear operator S acting on the first variable of ϕ and Se^{-uL^*} denotes the composition of the operator S with the operator e^{-uL^*} ; an analogous expression holds for $S^{(1)}\phi$ or for more general linear transforms of ϕ .

For what concern kinetic theories, we are mainly interested in stationary values of expressions like Eq. (4.74). In the finite dimensional case, when L is a normal operator, the time-asymptotics of Eq. (4.74) can be explicitly computed in terms of the eigenvalues of L , see [165]. In kinetic theories, however, L is infinite-dimensional and usually not normal. Thus we are not able to find an explicit expression.

Equation (4.73) and (4.74) express the fact that, if we are able to compute the solution to the deterministic equation (4.72), we can compute the solution to the Lyapunov equation (4.70) or its linear transforms.

4.5.3 Formal solution in frequency space

If the deterministic evolution $e^{-tL}b$ is bounded and $Se^{-tL^*}c$ decrease exponentially in time, then we can simplify the expression for the long time limit of Eq. (4.74) working in the frequency space. This is expressed below in Theorem 4.5.1.

In this section, we do not take a different notation for the function $h(t)$ its Laplace transform $h(\omega)$ except for their variable dependence.

The solution of the Lyapunov equation in frequency space is easily obtained taking the Laplace transform of the Ornstein–Uhlenbeck process and following the same step of the previous section to compute $\phi(\mathbf{r}, \mathbf{r}', \omega)$; we then write $\phi(\mathbf{r}, \mathbf{r}', t)$ by means of the inverse Laplace transform. Introducing the Resolvent operators $R_L(\omega) = (-i\omega + L)^{-1}$ and $R_{L^*}(\omega) = (-i\omega + L^*)^{-1}$, and with some simple manipulations, we get

$$(S^{(2)}\phi)(\mathbf{r}, \mathbf{r}', t) = \frac{i}{2\pi^2} \int_{\Gamma_1} d\omega_1 \int_{\Gamma_2} d\omega_2 \frac{e^{-i(\omega_1 + \omega_2)t}}{\omega_1 + \omega_2} (R_L(\omega_1)b)(\mathbf{r}) (SR_{L^*}(\omega_2)c)(\mathbf{r}'), \quad (4.75)$$

where Γ_1 and Γ_2 are contours in the complex plane passing above all the poles of the respective integrands; observe that $R_L(\omega)$ is the Laplace transform of the operator e^{-tL} and analogously for $R_{L^*}(\omega)$.

The following theorem, whose proof is a simple manipulation of Eq. (4.75), permits to evaluate the time asymptotics of $(S^{(2)}\phi)(\mathbf{r}, \mathbf{r}', t)$ under certain hypothesis.

Theorem 4.5.1. *Let us suppose that $(R_L(\omega)b)(\mathbf{r})$ is an analytic function of ω for ω such that $\text{Im}(\omega) > 0$ and that $[SR_{L^*}(\omega_2)c](\mathbf{r}')$, can be analytically continued to $\omega \in \mathbb{R}$. Then, without changing notation for the analytic continuation, we have*

$$\lim_{t \rightarrow \infty} (S^{(2)}\phi)(\mathbf{r}, \mathbf{r}', t) = \frac{1}{\pi} \int_{\Gamma} d\omega (R_L(\omega)b)(\mathbf{r}) (SR_{L^*}(-\omega)c)(\mathbf{r}'), \quad (4.76)$$

where Γ is a contour which passes above all the poles of $[R_L(\omega)b](\mathbf{r})$.

CHAPTER 4. ISOLATED LONG-RANGE INTERACTING SYSTEMS

Proof. Let us consider the Eq. (4.75): Γ_1 passes above all the poles of $(R_L(\omega_1)b)(\mathbf{r})$, where Γ_2 passes above all the poles of $(SR_{L^*}(\omega_2)c)(\mathbf{r}')$ and above $-\omega_1$ for every $\omega_1 \in \Gamma_1$.

Now, because $(R_L(\omega_1)b)(\mathbf{r})$ is an analytic function of ω_1 for $Im \omega_1 > 0$ and $(SR_{L^*}(\omega_2)c)(\mathbf{r}')$ is an analytic function of ω_2 for $Im \omega_2 \geq 0$, we can choose Γ_1 and Γ_2 such that $-\Gamma_1$ is above all the poles of $(SR_{L^*}(\omega_2)c)(\mathbf{r}')$.

Consider then the integral over ω_2 . We can make Γ_2 passes below ω_1 for every ω_1 using the Residue theorem. We get

$$\left(S^{(2)}\phi\right)(\mathbf{r}, \mathbf{r}', t) = \frac{i}{2\pi^2} \int_{\Gamma_1} d\omega_1 \int_{\Gamma_2'} d\omega_2 \frac{e^{-i(\omega_1+\omega_2)t}}{\omega_1 + \omega_2} \left(R_L(\omega_1)b\right)(\mathbf{r}) \left(SR_{L^*}(\omega_2)c\right)(\mathbf{r}') + \quad (4.77)$$

$$+ \frac{1}{\pi} \int_{\Gamma_1} d\omega_1 \left(R_L(\omega_1)b\right)(\mathbf{r}) \left(SR_{L^*}(\omega_2)c\right)(\mathbf{r}'), \quad (4.78)$$

where the contour Γ_2' appearing in the first term on the right hand side passes below $-\omega_1$ and above all the poles of $(SR_{L^*}(\omega_2)c)(\mathbf{r}')$.

The proof is completed using the fact that the real part of $-i(\omega_1 + \omega_2)$ is negative so that the first ingral in Eq. (4.77) vanishes in the limit $t \rightarrow \infty$. \square

As anticipated above, the hypothesis of the theorem are equivalent to require that $(e^{-tL}b)$ is bounded and $(Se^{-tL^*}c)$ decreases exponentially in time. In kinetic theory of particles systems with long-range interactions, and for homogeneous states, the exponential decay is given by the mechanism of the Landau damping (see Section 4.4.1).

4.6 Lenard-Balescu equation

In terms of the linearized Vlasov operator, the first two equations of the BBGKY hierarchy (4.23) and (4.24) can be rewritten as

$$\frac{\partial f}{\partial t} + p \frac{\partial f}{\partial q} - \frac{\partial f}{\partial p} \frac{\partial \Phi[f]}{\partial q} = \frac{1}{N} \frac{\partial}{\partial p} \int dq_1 dp_1 v'(q - q_1) g(z, z_1, t), \quad (4.79)$$

and

$$\frac{\partial g(z_1, z_2, t)}{\partial t} + L_f^{(1)} g + L_f^{(2)} g = \frac{\partial v(q_1 - q_2)}{\partial q_1} \left[\frac{\partial}{\partial p_1} - \frac{\partial}{\partial p_2} \right] f(z_1) f(z_2) \quad (4.80)$$

where $L_f^{(1)}$ (resp. $L_f^{(2)}$) is the linearized Vlasov operator around f acting on the first variable of $g(z_1, z_2, t)$ (resp. the second variable).

It is now straightforward to realize that the Eq. (4.80) is a Lyapunov equation; however, the two equations of the BBGKY hierarchy are coupled and hence, difficult to solve even numerically.

We thus assume that the distribution function f is a stationary solution of the Vlasov equation at all times. This correspond to

$$p \frac{\partial f}{\partial q} - \frac{\partial f}{\partial p} \frac{\partial \Phi[f]}{\partial q} = 0 \quad (4.81)$$

for every time t . With this assumption, we readily see that the two-particle correlation g evolves over a timescale of order one, whereas the one-particle distribution function $f(p, t)$ evolves over a timescale of order N . We may then use this timescale separation and compute the long-time limit of g from Eq. (4.80) by assuming f to be steady in time; this is the so called Bogoliubov's hypothesis or the Markovianization procedure. Note that for this timescale separation to be valid, we must also suppose that the one-particle distribution function $f(p, t)$ is a stable solution of the Vlasov equation at all times. Indeed, if this is not the case, one sees from Eq. (4.74) that g diverges in the limit $t \rightarrow \infty$. The physical content of this hypothesis is that the system slowly evolves from the initial condition through a sequence of Quasi Stationary states.

In principle, to obtain the long time limit of g with f fixed in time, one can use the machinery presented in Section 4.5 and in particular the Eq. (4.74). However, as we have seen in Section 4.4, the solution to the linear Vlasov equation analytically achievable with simple techniques only if the state f around which the Vlasov operator is linearized is homogeneous. We thus suppose that f is homogeneous in space at all times, that is $f(q, p, t) = f(p, t)$ and g depends only on $q_1 - q_2$ and not on q_1 and q_2 separately. With this hypothesis, the linearized Vlasov operator becomes the one in Eq. (4.46) so that we have for $L_f^{(1)} g$,

$$\left(L_f^{(1)} g \right) (q_1 - q_2, p_1, p_2, t) = p_1 \frac{\partial g}{\partial q_1} - f'(p_1, t) \int dq_3 dp_3 v'(q_1 - q_3) g(q_3 - q_2, p_3, p_2, t). \quad (4.82)$$

$L_f^{(2)} g$ is obtained from Eq. (4.46) by exchanging the subscripts 1 and 2.

Because we assume the system to be homogeneous in space, it is useful to Fourier transform Eqs. (4.79) and (4.80) with respect to the spatial variable; we get

$$\frac{\partial f}{\partial t} = -\frac{2\pi i}{N} \sum_{k=-\infty}^{\infty} k v_k \frac{\partial}{\partial p} \int dp' g_k(p, p', t), \quad (4.83)$$

and

$$\left(\frac{\partial g_k}{\partial t} + L_{f,k}^{(1)} g_k + L_{f,-k}^{(2)} g_k \right) (p_1, p_2, t) = i v_k k \left[\frac{\partial}{\partial p_1} - \frac{\partial}{\partial p_2} \right] f(p_1) f(p_2), \quad (4.84)$$

where $g_k(p_1, p_2, t)$ is the Fourier transform of $g(q, p_1, p_2, t)$ with respect to the spatial variable, and v_k is the k -th Fourier coefficient of the pair potential $v(q)$. We recall here the explicit expression, already given in Eq. (4.48), for the k -th Fourier component of the linear

CHAPTER 4. ISOLATED LONG-RANGE INTERACTING SYSTEMS

Vlasov operator $L_{f,k}$ acting on a function $h(p)$

$$(L_{f,k}h)(p) = ikph(p) - 2\pi ikv_k f'(p) \int dp' h(p'). \quad (4.85)$$

One has analogous expressions for $L_{f,k}^{(1)}$ and for $L_{f,-k}^{(2)}$. We readily see that $L_{f,k}^* = L_{f,-k}$.

From the right hand side of Eq. (4.83), we see that to obtain a single kinetic equation, we only need the Fourier transform $g_k(p, p', t)$ and more specifically, thanks to the time-scales separations, we want to compute

$$\int dp' g_k^\infty(p, p', t) = \lim_{t \rightarrow \infty} \int dp' g_k(p, p', t). \quad (4.86)$$

The integral with respect to the second momentum variable p' is the linear operator S appearing in the Theorem 4.5.1. From Section 4.4.1 and Section 4.5.2, we know that $g_k(p, p', t)$ is an oscillating quantity, it is bounded in time but it does not have a well-defined time-asymptotic (it converges only in weak sense). However, its integral with respect to p' does have.

To apply the Theorem 4.5.1 and obtain the Lenard-Balescu equation, we need the Resolvent operator $R_{f,k}(\omega)$ associated with the linearized Vlasov operator $L_{f,k}$ defined in Eq. (4.46). As we have seen in Section 4.4.1, this is connected to the mechanism of the Landau Damping and it is given by Eq. (4.53).

As we have seen, the linear stability of stationary states of the Vlasov equation is defined through the properties of the dielectric function [90, 113, 159]: f is a stable stationary state if zeros of the dielectric functions are present only for ω such that $\text{Im}\omega < 0$; in the case in which zeros are present for ω such that $\text{Im}\omega = 0$, we have a marginally stable state; finally, we have an unstable state if zeros are present for ω such that $\text{Im}\omega > 0$. We then see that the hypothesis that the one-particle distribution function f is a stable solution of the Vlasov equation is equivalent to require that the Resolvent operator is an analytic function for $\text{Im}\omega > 0$, as asked in the hypothesis of the Theorem 4.5.1.

Moreover, it can be readily seen that the integral with respect to p of $(R_{f,-k}(\omega)h)(p)$

$$\int dp (R_{f,-k}(\omega)h)(p) = \frac{1}{\epsilon(-k, \omega)} \int dp \frac{h(p)}{-i\omega - ikp} \quad (4.87)$$

admits an analytic continuation to $\omega \in \mathbb{R}$. We thus conclude that the hypothesis of the Theorem 4.5.1 are satisfied. We can then compute

$$\int dp' g_k^\infty(p, p', t) \quad (4.88)$$

using Eq. (4.76).

The derivation of the Lenard-Balescu equation is then obtained applying the Theorem 4.5.1 and it is just a long exercise in complex analysis. We report the details in the next section.

4.6.1 Explicit derivation of the Lenard-Balescu equation

To perform the computation explicitly, it is useful to split g_k in two parts

$$g_k = g_k^A + g_k^B \quad (4.89)$$

such that

$$\left(\frac{\partial g_k^A}{\partial t} + L_{f,k}^{(1)} g_k^A + L_{f,-k}^{(2)} g_k^A \right) (p_1, p_2, t) = i v_k k \frac{\partial}{\partial p_1} f(p_1) f(p_2), \quad (4.90)$$

and

$$\left(\frac{\partial g_k^B}{\partial t} + L_{f,k}^{(1)} g_k^B + L_{f,-k}^{(2)} g_k^B \right) (p_1, p_2, t) = -i v_k k \frac{\partial}{\partial p_2} f(p_1) f(p_2). \quad (4.91)$$

We start computing

$$\lim_{t \rightarrow \infty} \int dp' g_k^A(p, p', t) \quad (4.92)$$

by setting

$$b(p) = i k v_k f'(p) \quad \text{and} \quad c(p) = f(p) \quad (4.93)$$

in the Theorem (4.5.1).

Using Eq. (4.53), the definition of the dielectric function and recalling that $\omega \in \Gamma$ and Γ passes above all the poles of $(R_{f,k}(\omega)b)$, we obtain

$$(R_{f,k}(\omega)b)(p) = \frac{i k v_k f'(p)}{-i\omega + i k p} \frac{1}{\epsilon(k, \omega)}, \quad (4.94)$$

which is valid for all ω once that $\epsilon(k, \omega)$ is the analytic continuation of the Eq. (4.54).

With a similar reasoning, we obtain for the quantity in Eq. (4.87)

$$\int dp (R_{f,-k}(\omega)c)(p) = \frac{i}{\epsilon(-k, \omega)} \int dp' \frac{f(p')}{k p' + \omega}, \quad (4.95)$$

valid for $\text{Im}(\omega) > 0$. For the analytic continuation of such function we have

$$\int dp (R_{f,-k}(\omega)c)(p) = \frac{i}{\epsilon(-k, \omega)} \int dp' \frac{f(p')}{k p' + \omega} + \frac{\pi l(\omega)}{\epsilon(-k, \omega)} \int dp' f(p') \delta(k p' + \omega) \quad (4.96)$$

where $l(\omega)$ is defined in Eq. (4.41).

Recall now that Γ passes above the poles of $(R_{f,k}(\omega)b)(p)$, so that $\text{Im}(\omega) > 0$ for all $\omega \in \Gamma$. Using Theorem 4.5.1, Eq. (4.94) and Eq. (4.96), we obtain

$$\lim_{t \rightarrow \infty} \int dp' g_k^A(p, p', t) = \quad (4.97)$$

$$\begin{aligned} &= \frac{1}{\pi} \int_{\Gamma} d\omega \frac{1}{-i\omega + i k p} \frac{i k v_k f'(p)}{\epsilon(k, \omega) \epsilon(-k, -\omega)} \int dp' \frac{f(p')}{i\omega - i k p'} + \\ &+ \int_{\Gamma} d\omega \int dp' \frac{1}{-i\omega + i k p} \frac{i k v_k f'(p)}{\epsilon(k, \omega) \epsilon(-k, -\omega)} l(\omega) f(p') \delta(\omega - k p') \end{aligned} \quad (4.98)$$

CHAPTER 4. ISOLATED LONG-RANGE INTERACTING SYSTEMS

Let us now consider the second term

$$\lim_{t \rightarrow \infty} \int dp' g_k^B(p, p', t) \quad (4.99)$$

which again can be computed from Theorem 4.5.1 by setting

$$b(p) = f(p) \quad \text{and} \quad c(p) = -ikv_k f'(p). \quad (4.100)$$

The reasoning goes as in the previous case. We obtain

$$(R_{f,k}(\omega)b)(p) = \frac{1}{-i\omega + ikp} \left[f(p) + \frac{2\pi ikv_k}{\epsilon(k, \omega)} f'(p) \int dp' \frac{f(p')}{-i\omega + ikp'} \right] \quad (4.101)$$

which is valid for all ω once that $\epsilon(k, \omega)$ is the analytic continuation of the Eq. (4.54).

We also have

$$\int dp (R_{f,-k}(\omega)c)(p) = \frac{1}{2\pi} \left[\frac{1}{\epsilon(-k, \omega)} - 1 \right], \quad (4.102)$$

which again is valid for all ω once that $\epsilon(k, \omega)$ is the analytic continuation of the Eq. (4.54).

We thus obtain for Eq. (4.99)

$$\begin{aligned} \lim_{t \rightarrow \infty} \int dp' g_k^B(p, p', t) &= \quad (4.103) \\ &= \frac{1}{2\pi^2} \int_{\Gamma} d\omega \frac{1}{-i\omega + ikp} \left[\frac{1}{\epsilon(-k, -\omega)} - 1 \right] f(p) + \\ &+ \frac{1}{2\pi^2} \int_{\Gamma} d\omega \frac{1}{-i\omega + ikp} \frac{2\pi ikv_k}{\epsilon(k, \omega)\epsilon(-k, -\omega)} f'(p) \int dp' \frac{f(p')}{-i\omega + ikp'} - \\ &- \frac{1}{2\pi^2} \int_{\Gamma} d\omega \frac{1}{-i\omega + ikp} \frac{2\pi ikv_k}{\epsilon(k, \omega)} f'(p) \int dp' \frac{f(p')}{-i\omega + ikp'}. \end{aligned}$$

Closing the integration contour at $-i\infty$ in the first integral in the right hand side of Eq. (4.103) and observing that f is supposed to be a linearly stable distribution, the only enclosed pole is at $\omega = kp$; we thus get for this term:

$$\frac{f(p)}{2\pi} \left[\frac{1}{\epsilon^*(k, kp)} - 1 \right], \quad (4.104)$$

where we have used that $\epsilon(-k, -\omega) = \epsilon^*(k, \omega)$ for $\omega \in \mathbb{R}$.

On the other hand, the third integral in the right hand side of Eq. (4.103) vanishes closing the contour Γ at $+i\infty$. With this results, summing up the Eq. (4.97) and (4.103), we obtain

$$\lim_{t \rightarrow \infty} \int dp' g_k(p, p', t) = \frac{f(p)}{2\pi} \left[\frac{1}{\epsilon^*(k, kp)} - 1 \right] + \quad (4.105)$$

$$+ \int_{\Gamma} d\omega \int dp' \frac{1}{-i\omega + ikp} \frac{ikv_k f'(p)}{\epsilon(k, \omega)\epsilon(-k, -\omega)} l(\omega) f(p') \delta(\omega - kp'). \quad (4.106)$$

From Eq. (4.83), we observe that we need only the Imaginary part of Eq. (4.105); we thus get

$$\text{Im} \left(\lim_{t \rightarrow \infty} \int dp' g_k(p, p', t) \right) = \frac{i\pi k v_k}{|\epsilon(k, kp)|^2} \int dp' \delta(k(p - p')) \left[\frac{\partial}{\partial p} - \frac{\partial}{\partial p'} \right] f(p)f(p'). \quad (4.107)$$

Inserting Eq. (4.107) in the right hand side of Eq. (4.83) we finally obtain the Lenard-Balescu equation:

$$\frac{\partial f}{\partial t} = \frac{2\pi^2}{N} \int_{-\infty}^{\infty} dk (k v_k)^2 \frac{\partial}{\partial p} \int dp' \frac{1}{|\epsilon(k, kp)|^2} \delta(k(p - p')) \left[\frac{\partial}{\partial p} - \frac{\partial}{\partial p'} \right] f(p)f(p'). \quad (4.108)$$

As it is known since long time in plasma physics [166], and it can be easily checked from Eq. (4.108) using the Dirac delta, the Lenard-Balescu operator vanishes⁷. This is due to the fact that we are dealing with one-dimensional systems and it is consistent with the fact that the relaxation time in Fig. 4.2 scales as N^δ with $\delta > 1$.

The derivation presented here could be done in any dimension without any difference. The result is

$$\frac{\partial f}{\partial t} = \frac{\pi(2\pi)^d}{N} \int d\mathbf{k} v^2(\mathbf{k}) \mathbf{k} \cdot \nabla_{\mathbf{p}} \int d\mathbf{p}' \frac{1}{|\epsilon(\mathbf{k}, \mathbf{k} \cdot \mathbf{p})|^2} \delta(\mathbf{k} \cdot (\mathbf{p} - \mathbf{p}')) [\mathbf{k} \cdot (\nabla_{\mathbf{p}} - \nabla_{\mathbf{p}'})] f(\mathbf{p})f(\mathbf{p}'), \quad (4.109)$$

for a d -dimensional system [102, 111, 135] in which $q_i \in [0, 2\pi]^d$; it is straightforward to observe that in dimension greater than one, the Lenard-Balescu operator does not vanishes.

4.6.2 About the Lenard-Balescu equation

Lenard-Balescu equation has a number of properties analogous to the Boltzmann equation [135]: if f is positive at the initial time, it remains positive at all times; the mass of the system, the momentum and its kinetic energy is conserved. Besides these facts which are not more than consistency checks, however, any Maxwellian is a stationary solution of the Lenard-Balescu equation and it is possible to prove a version of the H theorem. Thus, from a physicist perspective, any solution approaches to a Maxwellian in the $t \rightarrow \infty$ limit.

The dielectric function ϵ entering in the Lenard-Balescu operator, describes collective effects. For ionized plasmas, this term takes into account the effect of the Debye screening, which cuts off the interaction at large enough distances [111, 168]. The Landau equation [111], does not describes collective effects and can be recovered from the previous one replacing ϵ by the unity.

In dimension greater than one, Lenard-Balescu equation explains the relaxation to the Maxwell-Boltzmann equilibrium of a long-range interacting system previously settled in a QSS after a time-scale of order N . Observe that to derive this equation, it is necessary to

⁷This is also due to the fact that we are dealing with a one-component systems; for more components systems, the Lenard-Balescu operator does not vanish [167]

suppose that the system is in a stationary stable solution of the Vlasov equation at all times. The Lenard-Balescu equation does not describe the evolution of unstable initial states.

We have presented the derivation of the Lenard-Balescu equation when the system is homogeneous. Heyvaerts [169], see also [170] for a previous and more abstract work, has recently generalized the Lenard-Balescu equation to non-homogeneous systems using action-angle variables. His equation, technically much more complicated than the one presented here, is valid under the hypothesis that the system stays at all times in a state f in which the single-particle Vlasov dynamics is integrable; the technique used are analogous to those developed in [163, 164] to obtain the Landau damping for non-homogeneous states under the same assumptions. However, due to the high complexity of the Heyvaerts kinetic equation, the kind of informations that can be obtained from it is at the moment not clear to the author; some result in this direction would have some interest.

On the other hand, we recall here that the Landau equation, albeit approximate, is very simply generalizable to non-homogeneous states [111] and predicts that even for one-dimensional systems the relaxation time-scale of non-homogeneous QSS is of order N . This seems in agreement with recent numerical simulations performed on simplified models [150].

We conclude observing that, due to its high non-linear character, the Lenard-Balescu equation has not been extensively used in plasma community, for which it mainly represents a theoretical motivation to derive the Landau equation. Very few works, for example, perform extensive numerical comparisons between the predictions of the Lenard-Balescu equation and results from N -body dynamics: we are only aware of [167, 171, 172] in this respect.

4.7 Conclusions

We have presented in this Chapter the kinetic theory for Hamiltonian long-range interacting systems (4.3), describing the derivation of the Vlasov and of the Lenard-Balescu equation. Vlasov equation is the mean field approximation of the dynamics of the system, where Lenard-Balescu equation, which takes into account two-particle correlations while discarding three-particle and higher order correlations, is the analogous of the Boltzmann equation for long-range interacting systems: it gives the first order correction in the small parameter $1/N$ to the mean-field dynamics.

Stationary and stable states of the Vlasov equation are the QSSs in which the N -body system get trapped starting from arbitrary out of equilibrium initial conditions. We want to stress here that instead to converging to a QSS, the system may be also converge to a time-dependent solution of the Vlasov equation, see for example [173, 174]. The life-time

of QSS, except for the special case of one dimensional homogeneous systems, is expected to be of order N according to kinetic theory. At this time scale, correlations have to be taken into account and the Lenard-Balescu equation describes the slow relaxation to the Maxwell-Boltzmann equilibrium. However, because the truncation of the BBGKY hierarchy (and hence the kinetic theory) is not a rigorous procedure, one may wonder if such conclusions are correct.

Braun and Hepp [141] have rigorously proven that two solutions (in weak sense) of the Vlasov equation diverge at most exponentially in time, under the hypothesis that the inter-particle potential is a smooth function. From here it is simple to prove that, for uncorrelated initial states, the solution to the Vlasov equation approximate well the trajectory of the N -body system at least for a time of order $\log N$. On the basis of numerical results [175] it is believed that this estimate is actually optimal when the system starts from an unstable initial state. As far as we know, there are no results aiming to understand if the first two equations of the hierarchy (4.79) and (4.80), without any further assumption, can describe the emergence of this time-scale. In practice, it is not simple to handle this problem because the two equations (4.79) and (4.80) are coupled. A study of this kind could be probably done on simple quantum systems like those considered in [176], because in these cases the equations of the hierarchy are ordinary, instead of partial, differential equations and thus much easier to handle.

Caglioti and Rousset [177] proved that if the N -body system starts close to a stationary and stable solution of the Vlasov equation and for smooth two-body potentials, the N -body dynamics remains close to the Vlasov one at least for times of order $N^{1/8}$. This seems to go in the direction of the prediction of the kinetic theory, but we are not aware of further rigorous results.

From numerical experiments on one-dimensional systems, it emerges that the relaxation time-scale of a long-range interacting system does scale as N when the system is not homogeneous [150] and as N^2 when the system is homogeneous at all times [178]. The first fact is consistent with the fact that the Landau kinetic equation for non-homogeneous systems is not trivial already in dimension one [111] and the second one with the fact that the Lenard-Balescu operator vanishes in dimension one, for one component systems [167]. The scaling $N^{1.7}$ found in the HMF model when going from an homogeneous initial state from a non-homogeneous Maxwell-Boltzmann equilibrium can be quite reasonably interpreted as mixed situation between the precedent two [179].

The content of this Chapter form the basis for the following Chapters. In particular, the structure of kinetic theory and the general results of Section 4.5 will be useful in Chapters 6 and 7 for the derivation of kinetic theories for stochastically forced systems.

5

Deterministic perturbations: linear response theory on the Vlasov equation

For short-range interacting systems, Kubo linear response theory [180,181] is a very classical and fundamental result which describes how a system prepared in equilibrium responds to a small external perturbation. Long-range interacting systems, however, are often found trapped in QSSs; Kubo theory is of little utility here.

As a first step in understanding the effect of perturbations on systems with long-range interactions, we consider the following situation: we prepare a long-range interacting system in a QSS and we apply a (small) external field which evolves deterministically in time. Working in the limit $N \rightarrow \infty$, we show that a formula similar to the Kubo formula holds, where differences arise due to the non-linearity of the Vlasov equation in contrast to the Liouville equation. Explicit results can be obtained reformulating the techniques we used to derive the Landau Damping in Section 4.4.1.

The Chapter is organized as follows. In Section 5.1, we obtain the analogous to the Kubo formula for the Vlasov equation whose initial condition is a generic stationary and stable state of the unperturbed system. In Section 5.2, we specialize to QSSs homogeneous in the coordinate, and derive a closed form expression for the change induced by the external perturbation in a single-particle dynamical quantity. Section 5.3 is devoted to the application of the theory to study the response of three representative homogeneous QSSs in the HMF model, namely, the widely studied water-bag QSS, the Fermi-Dirac QSS and the homogeneous equilibrium state. In the following Section, we compare results from N -particle numerical simulations of the HMF dynamics with those from the linear response theory, and obtain good agreement. We also discuss the long-time relaxation of the water-bag QSS to Boltzmann-Gibbs equilibrium under the action of the perturbation. We draw our conclusions in Section 5.5.

Our results, reported in [125], have been recently generalized to some non-homogeneous states by Ogawa et al. [126] and by Patelli et al. in [127].

5.1 Linear response theory for QSS

Consider a system of N particles interacting through a long-ranged pair potential (4.3). The system evolves under deterministic Hamiltonian dynamics: the equations of motion for the i -th particle are

$$\dot{q}_i = p_i, \quad (5.1)$$

$$\dot{p}_i = -\frac{\partial}{\partial q_i} \frac{1}{N} \sum_{i < j}^N v(q_i - q_j), \quad (5.2)$$

where dots denote differentiation with respect to time. As usual, we regard q_i variables on a unit circle, even if the formalism can be easily extended to \mathbb{R}^n with a generic n .

We start with the system in a QSS at time $t = 0$ and apply an external field $K(t)$. Assuming the field $K(t)$ to couple to the coordinates of the individual particles, the perturbed Hamiltonian is

$$H(t) = H_0 + H_{\text{ext}} = H_0 - K(t) \sum_{i=1}^N b(q_i). \quad (5.3)$$

Here, $b(q_i)$ denotes the dynamical quantity for the i th particle that is conjugate to $K(t)$. The equations of motion are modified from Eq. (5.2) to

$$\dot{q}_i = p_i, \quad (5.4)$$

$$\dot{p}_i = -\frac{\partial}{\partial q_i} \frac{1}{N} \sum_{i < j}^N v(q_i - q_j) + K(t) \frac{\partial b(q_i)}{\partial q_i}. \quad (5.5)$$

In this work, we study the temporal response of the initial QSS to the field $K(t)$, in particular, the linear response. We ask: How does a single-particle dynamical quantity $a(q)$, that starts from a value corresponding to the QSS, evolve in time under the action of $K(t)$? We seek answers to this question by considering the system in the limit $N \rightarrow \infty$, so that size effects are negligible and the evolution of the QSS is due to the field $K(t)$ alone. Because a QSS is represented by a stable stationary solution of the dynamics (5.2), we will work at the level of Vlasov equation instead than at the level of N -body dynamics. We also regard $K(t)$ to satisfy the following conditions: $K(t)$ is a monotonically increasing function of t and has a value $\ll 1$ at all times, $K(t = 0) = 0$, and $K(t \rightarrow \infty)$ equals to a constant much smaller than 1. While discussing the time-asymptotic response, we will mean the ordering of limits $N \rightarrow \infty$ first, followed by $t \rightarrow \infty$. The Vlasov equation associated to the Hamiltonian (5.3) is¹

$$\frac{\partial f}{\partial t} - \mathcal{L}(q, p, t)[f]f = 0, \quad (5.6)$$

¹Observe that in this Chapter, we use a slightly different notation for the operators acting on a function and thus we write them in calligraphic style. The reason for this is that here we have in mind that $\mathcal{L}(q, p, t)[f]$ is the analogous to the Liouville operator.

where the operator $\mathcal{L}(q, p, t)[f]$ is just the Vlasov operator given by

$$\mathcal{L}(q, p, t)[f] = -p \frac{\partial}{\partial q} + \frac{\partial \Phi[f](q, t)}{\partial q} \frac{\partial}{\partial p} - K(t) \frac{\partial b}{\partial q} \frac{\partial}{\partial p}, \quad (5.7)$$

while $\Phi[f](q, t)$ is the mean-field potential in Eq. (4.15).

We investigate the response of the system to the external field by monitoring the observable

$$\langle a(q) \rangle(t) \equiv \int dq dp a(q) f(q, p, t). \quad (5.8)$$

To obtain its time dependence, we need to solve Eq. (5.6) for $f(q, p, t)$, with the initial condition

$$\overline{f}(q, p, 0) = f_0(q, p). \quad (5.9)$$

Here, $f_0(q, p)$ characterizes a QSS, i.e., a stable stationary solution of the Vlasov equation for the unperturbed dynamics (5.2). Thus, $f_0(q, p)$ satisfies

$$\mathcal{L}_0(q, p)[f_0]f_0 = 0, \quad (5.10)$$

where

$$\mathcal{L}_0(q, p)[f_0] = -p \frac{\partial}{\partial q} + \frac{\partial \Phi[f_0](q)}{\partial q} \frac{\partial}{\partial p}. \quad (5.11)$$

To solve Eq. (5.6) for $K(t) \ll 1$, we expand $f(q, p, t)$ to linear order in $K(t)$ as

$$f(q, p, t) = f_0(q, p) + \Delta f(q, p, t), \quad (5.12)$$

with the initial condition

$$\Delta f(q, p, 0) = 0. \quad (5.13)$$

Substituting Eq. (5.12) in Eq. (5.6), and separating terms to order 1 and $K(t)$, we get, respectively,

$$\frac{\partial f_0}{\partial t} - \mathcal{L}_0(q, p)[f_0]f_0 = 0, \quad (5.14)$$

and

$$\frac{\partial \Delta f}{\partial t} - \mathcal{L}_0(q, p)[f_0]\Delta f = \mathcal{L}_{\text{ext}}(q, p, t)[\Delta f]f_0. \quad (5.15)$$

Here, the operator

$$\mathcal{L}_{\text{ext}}(q, p, t)[\Delta f] = \frac{\partial \Phi[\Delta f](q, t)}{\partial q} \frac{\partial}{\partial p} - K(t) \frac{\partial b}{\partial q} \frac{\partial}{\partial p} \quad (5.16)$$

describes the effects of the external field, which are two-fold: (i) to generate a potential due to its direct coupling with the particles, and (ii) to modify the mean-field potential from its value $\Phi[f_0](q)$ in the absence of the field. Clearly, this second effect is only due to the

CHAPTER 5. DETERMINISTIC PERTURBATIONS: LINEAR RESPONSE THEORY ON THE VLASOV EQUATION

non-linear character of the Vlasov equation and is absent in Kubo linear response theory. Defining an effective single-particle potential,

$$v_{\text{eff}}[\Delta f](q, t) = \Phi[\Delta f](q, t) - K(t)b(q), \quad (5.17)$$

Eq. (5.15) may be written as

$$\frac{\partial \Delta f}{\partial t} - \mathcal{L}_0(q, p)[f_0]\Delta f = \frac{\partial v_{\text{eff}}(q, t)[\Delta f]}{\partial q} \frac{\partial f_0}{\partial p}. \quad (5.18)$$

Equation (5.14) is satisfied by virtue of the definition of $f_0(q, p)$. We thus solve Eq. (5.18) for $\Delta f(q, p, t)$ in order to determine $f(q, p, t)$ from Eq. (5.12). With the condition (5.13), the formal solution is

$$\Delta f(q, p, t) = \int_0^t d\tau e^{(t-\tau)\mathcal{L}_0(q, p)[f_0]} \frac{\partial v_{\text{eff}}[\Delta f](q, \tau)}{\partial q} \frac{\partial f_0(q, p)}{\partial p}. \quad (5.19)$$

Using Eq. (5.19) in Eqs. (5.8) and (5.12) gives the change in the value of $\langle a(q) \rangle(t)$ due to the external field

$$\begin{aligned} \langle \Delta a(q) \rangle(t) &\equiv \int dq dp a(q) (f(q, p, t) - f_0(q, p)) \\ &= \int_0^t d\tau \int dq dp a(q) e^{(t-\tau)\mathcal{L}_0(q, p)[f_0]} \times \frac{\partial v_{\text{eff}}[\Delta f](q, \tau)}{\partial q} \frac{\partial f_0(q, p)}{\partial p} \\ &= - \int_0^t d\tau \left\langle \frac{\partial a(t-\tau)}{\partial p} \frac{\partial v_{\text{eff}}[\Delta f](q, \tau)}{\partial q} \right\rangle_{f_0}. \end{aligned} \quad (5.20)$$

Here, angular brackets with f_0 in the subscript denote averaging with respect to $f_0(q, p)$, e.g.,

$$\langle a(q) \rangle_{f_0} \equiv \int dq dp a(q) f_0(q, p), \quad (5.21)$$

while

$$a(t-\tau) = e^{-(t-\tau)\mathcal{L}_0(q, p)[f_0]} a(q) \quad (5.22)$$

is the time-evolved $a(q)$ under the dynamics of the unperturbed system. In obtaining the last equality in Eq. (5.20), we have used the definition of \mathcal{L}_0 , have performed integration with respect to q , and have assumed the boundary terms involving $f_0(q, p)$ to vanish.

Defining the Poisson bracket between two dynamical variables $g(q, p)$ and $g'(q, p)$ in the single-particle phase space as

$$\{g(q, p), g'(q, p)\} \equiv \frac{\partial g}{\partial q} \frac{\partial g'}{\partial p} - \frac{\partial g'}{\partial q} \frac{\partial g}{\partial p}, \quad (5.23)$$

Eq. (5.20) may be rewritten as

$$\langle \Delta a(q) \rangle(t) = \int_0^t d\tau \left\langle \{ a(t-\tau), v_{\text{eff}}[\Delta f](q, \tau) \} \right\rangle_{f_0}. \quad (5.24)$$

This is the central result of this Chapter. The above equation is the analogous to the Kubo formula for the response of a dynamical quantity defined in the full $2N$ -dimensional phase space to an external perturbation [180, 181]. The difference between the two is that in Eq. (5.24) we have an effective potential v_{eff} , defined in Eq. (5.17), and not the external field alone. This is due to the non-linearity of the Vlasov equation in contrast to the linearity of the Liouville equation. The external field not only generates a potential due to its direct coupling with the particles, but it also modify the mean-field potential from its value $\Phi[f_0](q)$ in the absence of the field. The relation of formula (5.24) with more general ones derived by Ruelle [182] in the context of dynamical system theory remains to be investigated. In the following section, we discuss the special case of a homogeneous QSS, i.e., $f_0(q, p) = f_0(p)$ is a function solely of the momentum, to obtain an explicit form of the formal solution (5.19).

5.2 Homogeneous QSS

We consider a homogeneous QSS with $f_0(q, p) = f_0(p)$, where $f_0(p)$ is any distribution of the momentum, with the normalization

$$\int dq dp f_0(p) = 1, \quad \int dp f_0(p) = \frac{1}{2\pi}, \quad (5.25)$$

where 2π is the total volume of the coordinate space.

For a homogeneous QSS, Eq. (5.11) gives

$$\mathcal{L}_0(q, p)[f_0] = -p \frac{\partial}{\partial q}, \quad (5.26)$$

so that Eq. (5.19) becomes

$$\Delta f(q, p, t) = \int_0^t d\tau e^{-(t-\tau)p \frac{\partial}{\partial q}} \frac{\partial v_{\text{eff}}[\Delta f](q, \tau)}{\partial q} \frac{\partial f_0(p)}{\partial p}, \quad (5.27)$$

which implies that the spatial Fourier and temporal Laplace transform of $\Delta f(q, p, t)$ satisfies

$$\Delta f_k(p, \omega) = \frac{\partial f_0(p)}{\partial p} ik \frac{1}{-i\omega + ikp} \left[2\pi v_k \int dp' \Delta f_k(p', \omega) - K(\omega) b_k \right]. \quad (5.28)$$

assuming $\text{Im}(\omega)$ to be positive. Integrating both sides of Eq. (5.28) with respect to p gives

$$\int dp \Delta f_k(p, \omega) = \frac{K(\omega) b_k}{2\pi v_k} \left(\frac{\epsilon(k, \omega) - 1}{\epsilon(k, \omega)} \right). \quad (5.29)$$

CHAPTER 5. DETERMINISTIC PERTURBATIONS: LINEAR RESPONSE THEORY ON THE VLASOV EQUATION

Here, $\epsilon(k, \omega)$ is the dielectric function given, for $\text{Im}(\omega) > 0$, by Eq. (4.54). As discussed in Section 4.4.1, to obtain the time behavior of Δf_k , we need to give a meaning to Eq. (5.29) in the whole complex plane. This can be done just interpreting $\epsilon(k, \omega)$ as in Eq. (4.58). For the integral of the distribution function, we have

$$\int dp f(q, p, t) = \frac{1}{2\pi} + \frac{1}{2\pi} \int_{\Gamma} d\omega e^{-i\omega t} \int dk e^{ikq} \left[\frac{K(\omega)b_k}{2\pi v_k} \left(\frac{\epsilon(k, \omega) - 1}{\epsilon(k, \omega)} \right) \right], \quad (5.30)$$

where Γ is the Laplace contour. Let us suppose that the expression enclosed by square brackets has singularities which are isolated poles of any order. Let $\{\omega_p(k)\}$ be the set of poles, while $\{r_p(k)\}$ is the set of residues at these poles. Then, by the theorem of residues, we get

$$\int dp f(q, p, t) = \frac{1}{2\pi} + \frac{1}{2\pi} \int dk e^{ikq} \sum_p (2\pi i) r_p(k) e^{-i\omega_p(k)t}. \quad (5.31)$$

From Eq. (5.30), we see that the poles correspond either to poles of $K(\omega)$ or to the zeros of the dielectric function, i.e., values $\omega_p(k)$ (complex in general) that satisfy

$$\epsilon(k, \omega_p(k)) = 0. \quad (5.32)$$

Equation (5.31) implies that these poles determine the growth or decay of $\int dp \Delta f_k$ in time depending on the location of the poles in the complex- ω plane, as we have already seen discussing the Landau damping in Section 4.4.1. For example, when there are poles in the upper-half complex ω -plane, the difference grows in time. If, on the other hand, the poles lie either on or below the real- ω axis, the difference does not grow in time, but oscillates or decays in time, respectively.

We have to ensure that our analysis leading to Eq. (5.31) is consistent with the decomposition in Eq. (5.12) for perturbations about a *stable* stationary state $f_0(q, p) = f_0(p)$. It is thus required that $\int dp \Delta f_k$ does not grow in time, which means that the aforementioned poles cannot lie in the upper-half ω -plane. Now, since $K(t)$ was chosen to satisfy the conditions $K(t=0) = 0$ and $K(t \rightarrow \infty) = \text{a constant much smaller than 1}$, it follows that $K(\omega)$ cannot have poles in the upper-half ω -plane. We therefore conclude that Eq. (5.31) is valid when the poles $\omega_p(k)$ that come from the zeros of $\epsilon(k, \omega)$ satisfy

$$\epsilon(k, \omega_p(k)) = 0; \quad \text{Im}(\omega_p(k)) \leq 0, \quad (5.33)$$

corresponding to linear stability of the stationary state $f_0(p)$. The condition $\text{Im}(\omega_p(k)) = 0$ corresponds to marginal stability of $f_0(p)$. In this case, the zeros of the dielectric function lie on the real- ω axis so that $\omega_p(k) = \omega_{pr}(k)$ is real. From Eqs. (5.32) and (4.58), we find that $\omega_{pr}(k)$ satisfies

$$1 - 2\pi k v_k \int^* \frac{dp}{kp - \omega_{pr}(k)} \frac{\partial f_0(p)}{\partial p} - i 2\pi^2 v_k \left. \frac{\partial f_0(p)}{\partial p} \right|_{\omega_{pr}(k)/k} = 0, \quad (5.34)$$

5.3. APPLICATION TO THE HAMILTONIAN MEAN-FIELD MODEL

where \int^* stands for the Cauchy integral. Equating the real and the imaginary parts to zero, we get

$$1 - 2\pi k v_k \int^* \frac{dp}{kp - \omega_{\text{pr}}(k)} \frac{\partial f_0(p)}{\partial p} = 0, \quad (5.35)$$

$$\left. \frac{\partial f_0(p)}{\partial p} \right|_{\omega_{\text{pr}}(k)/k} = 0. \quad (5.36)$$

We now move on to apply our analysis to the Hamiltonian mean-field model, a paradigmatic model of long-range interactions.

5.3 Application to the Hamiltonian mean-field model

5.3.1 Model

In the following, we apply the previous formalism to the HMF model, defined in Section 4.1. Let us recall some useful facts.

The model in the equilibrium state shows a continuous transition from a low-energy clustered phase, in which the particles are close together on the circle, to a high-energy homogeneous phase corresponding to a uniform distribution of particles on the circle. The clustering of the particles is measured by the magnetization vector $\langle \mathbf{m} \rangle(t)$ with components

$$(\langle m_x \rangle(t), \langle m_y \rangle(t)) = \int dq dp (\cos q, \sin q) f(q, p, t), \quad (5.37)$$

and magnitude $\langle m \rangle(t) = \sqrt{\langle m_x \rangle^2(t) + \langle m_y \rangle^2(t)}$. In terms of $\langle m \rangle(t)$, the energy density is

$$e = \left\langle \frac{p^2}{2} \right\rangle(t) + \frac{1}{2} [1 - \langle m \rangle^2(t)], \quad (5.38)$$

where the kinetic energy defines the temperature T of the system:

$$\left\langle \frac{p^2}{2} \right\rangle(t) = \int dq dp \frac{p^2}{2} f(q, p, t) = \frac{T}{2}. \quad (5.39)$$

Note that e is conserved under the dynamics.

In equilibrium, the single-particle distribution assumes the canonical form, $f_{\text{eq}}(q, p)$, which is Gaussian in p with a non-uniform distribution for q below the transition energy density e_c and a uniform one above [183]:

$$f_{\text{eq}}(q, p) = \frac{\sqrt{\beta} \exp \left[-\beta \left(\frac{p^2}{2} - m_x^{eq} \cos(q - \phi) \right) \right]}{(2\pi)^{3/2} I_0(\beta m_x^{eq})}. \quad (5.40)$$

Here, I_0 is the modified Bessel function of zero order, β is the inverse temperature, while m_x^{eq} is the equilibrium magnetization that decreases continuously from unity at zero energy

CHAPTER 5. DETERMINISTIC PERTURBATIONS: LINEAR RESPONSE THEORY ON THE VLASOV EQUATION

density to zero at e_c and remains zero at higher energies. The arbitrary phase ϕ in Eq. (5.40) is a result of the rotational invariance of the HMF Hamiltonian. The energy at equilibrium is

$$e = \frac{1}{2\beta} + \frac{1 - (m_x^{eq})^2}{2}. \quad (5.41)$$

The phase transition in the HMF model occurs within both microcanonical and canonical ensembles [65, 184]. Thus, ensemble equivalence, though not guaranteed for long-range interacting systems [109], holds for the HMF model [90]. The microcanonical transition energy is $e_c = 3/4$, which corresponds to a transition temperature $T_c = 1/2$ in the canonical ensemble.

5.3.2 Linear response of homogeneous QSS

Consider the QSS distribution $f_0(q, p) = f_0(p)$ which is homogeneous in coordinate (thus, $\langle m_x \rangle_{f_0} = \langle m_y \rangle_{f_0} = 0$), but has an arbitrary normalized distribution for the momentum. Here, we study the response of this QSS to the external perturbation

$$H_{\text{ext}} = -K(t) \sum_{i=1}^N \cos q_i, \quad (5.42)$$

which corresponds to the choice

$$b(q) = \cos q. \quad (5.43)$$

in Eq. (5.3). The specific $K(t)$ we choose is a step function:

$$K(t) = \begin{cases} 0 & \text{for } t < 0, \\ h & \text{for } t \geq 0; \quad h \ll 1. \end{cases} \quad (5.44)$$

The changes in the magnetization components due to the field are

$$\begin{aligned} \langle \Delta m_x \rangle(t) &= \int dq dp \left(f(q, p, t) - f_0(p) \right) \cos q \\ &= \frac{1}{2} \int_{\Gamma} d\omega e^{-i\omega t} \int dp \left(\Delta f_1(p, \omega) + \Delta f_{-1}(p, \omega) \right), \end{aligned} \quad (5.45)$$

and

$$\begin{aligned} \langle \Delta m_y \rangle(t) &= \int dq dp \left(f(q, p, t) - f_0(p) \right) \sin q \\ &= \frac{1}{2i} \int_{\Gamma} d\omega e^{-i\omega t} \int dp \left(\Delta f_{-1}(p, \omega) - \Delta f_1(p, \omega) \right). \end{aligned} \quad (5.46)$$

Using

$$v_k = \left[\delta_{k,0} - \frac{\delta_{k,-1} + \delta_{k,1}}{2} \right], \quad (5.47)$$

5.3. APPLICATION TO THE HAMILTONIAN MEAN-FIELD MODEL

$$b_k = \frac{\delta_{k,-1} + \delta_{k,1}}{2}, \quad (5.48)$$

$$K(\omega) = -\frac{h}{i\omega}, \quad (5.49)$$

and Eq. (5.29) in Eqs. (5.45) and (5.46) gives

$$\langle \Delta m_x \rangle(t) = \frac{h}{2\pi} \int_{\Gamma} d\omega e^{-i\omega t} \frac{1}{i\omega} \left(\frac{\epsilon(1, \omega) - 1}{\epsilon(1, \omega)} \right), \quad (5.50)$$

and

$$\langle \Delta m_y \rangle(t) = 0. \quad (5.51)$$

Here, we have used the fact that for the HMF model,

$$\epsilon(1, \omega) = \epsilon(-1, \omega). \quad (5.52)$$

It may also be seen that

$$\epsilon(k, \omega) = 1 \text{ for } k \neq \pm 1. \quad (5.53)$$

Now, using the fact that $\langle m_x \rangle_{f_0} = \langle m_y \rangle_{f_0} = 0$, Eqs. (5.50) and (5.51) imply that

$$\langle m_x \rangle(t) = \frac{h}{2\pi} \int_{\Gamma} d\omega e^{-i\omega t} \frac{1}{i\omega} \left(\frac{\epsilon(1, \omega) - 1}{\epsilon(1, \omega)} \right), \quad (5.54)$$

and

$$\langle m_y \rangle(t) = 0. \quad (5.55)$$

It can be proven straightforwardly from the Vlasov equation (5.6) that Eq. (5.55) holds also in the non-linear response regime ($K(t)$ not necessarily small) for all homogeneous $f_0(p)$ which are even in p .

When the zeros of $\epsilon(1, \omega)$ lie only in the lower-half complex- ω plane, Eq. (5.54) gives the time-asymptotic response

$$\overline{m}_x \equiv \lim_{t \rightarrow \infty} \langle m_x \rangle(t) = h \left(\frac{1 - \epsilon(1, 0)}{\epsilon(1, 0)} \right). \quad (5.56)$$

Note that $K(\omega)$, given in Eq. (5.49), has a pole only at $\omega = 0$. Following the discussions in Section 5.2, we thus conclude that the conditions (5.35) and (5.36) solely determine the parameters characterizing the distribution $f_0(p)$ such that it is marginally stable. For the HMF model, we need to consider only $k = \pm 1$ in these conditions. Since $\epsilon(1, \omega) = \epsilon(-1, \omega)$, we write $\omega_{\text{pr}}(1) = \omega_{\text{pr}}(-1) = \omega_{\text{pr}}$, so that these conditions become

$$1 + \pi \int^* \frac{dp}{p \mp \omega_{\text{pr}}} \frac{\partial f_0(p)}{\partial p} = 0, \quad (5.57)$$

$$\left. \frac{\partial f_0(p)}{\partial p} \right|_{\omega_{\text{pr}}} = 0. \quad (5.58)$$

CHAPTER 5. DETERMINISTIC PERTURBATIONS: LINEAR RESPONSE THEORY ON THE VLASOV EQUATION

Observe that the quantity \overline{m}_x/h is the susceptibility of the system, which clearly depends on $f_0(p)$. For distributions $f_0(p)$ with a simple bump in $p = 0$, the above formula implies that the susceptibility diverges when the state loses its stability. This is a generalization of the divergence of the susceptibility at equilibrium when the system is close to a second order phase transition. For what concerns the explicit prediction of \overline{m}_x , Eq. (5.56) has a meaning only if $\overline{m}_x < 1$: the closer we are to the situation of marginal stability, the smaller is the region of values of the external field h such that the predictions of the linear response theory are reliable.

We now consider two representative $f_0(p)$ and obtain the linear response of the corresponding QSS by using Eq. (5.54). For the first case, we obtain the full temporal behavior of the response, while in the second case, we discuss only the time-asymptotic response.

Water-bag QSS

The water-bag state corresponds to coordinates uniformly distributed in $[0, 2\pi]$ and momenta uniformly distributed in $[-p_0, p_0]$:

$$f_0(p) = \frac{1}{2\pi} \frac{1}{2p_0} \left[\Theta(p + p_0) - \Theta(p - p_0) \right]; \quad p \in [-p_0, p_0]. \quad (5.59)$$

Here, $\Theta(x)$ denotes the unit step function. The energy density is obtained from Eq. (5.38) as

$$e = \frac{p_0^2}{6} + \frac{1}{2}. \quad (5.60)$$

We get

$$\epsilon(1, \omega) = 1 - \frac{1}{2(p_0^2 - \omega^2)}, \quad (5.61)$$

which, a priori, should be considered only for $\text{Im}(\omega) > 0$. However, the previous expression does not admit an analytic continuation for $\omega \in \mathbb{R}$ and it is univocally determined by Eq. (5.61) on the whole complex plane. We observe that Eq. (5.61) is analytic in the whole of the ω -plane, except at the two points $\omega = \pm p_0$.

As discussed in Section 5.2, the zeros of the dielectric function determine the temporal behavior of $\int dp \Delta f(q, p, t)$. The zeros of Eq. (5.61) occur at $\omega_p = \pm \sqrt{p_0^2 - 1/2}$. For $p_0 < p_0^* = 1/\sqrt{2}$, (correspondingly, $e < e^* = 7/12$), the pair of zeros lies on the imaginary- ω axis, one in the upper half-plane and one in the lower. The one in the upper half-plane makes the water-bag state linearly unstable for $e < e^*$. As e approaches e^* from below, the zeros move along the imaginary- ω axis and hit the origin when $e = e^*$. At higher energies, the zeros start moving on the real- ω axis away from the origin in opposite directions. The fact that the zeros of the dielectric function are strictly real for $e \geq e^*$ implies that the water-bag state is marginally stable at these energies.

From the discussions in Section 5.2 and those following Eq. (5.56), it follows that the result of the linear Vlasov theory, Eq. (5.54), is valid and physically meaningful only when

5.3. APPLICATION TO THE HAMILTONIAN MEAN-FIELD MODEL

$p_0^2 > 1/2$. Using Eq. (5.61) in Eq. (5.54) and performing the integral by the residue theorem gives

$$\langle m_x \rangle(t) = \frac{2h}{2p_0^2 - 1} \sin^2 \left(\frac{t}{2} \sqrt{p_0^2 - \frac{1}{2}} \right); \quad p_0^2 > \frac{1}{2}. \quad (5.62)$$

Thus, the linear Vlasov theory predicts that in the presence of an external field along x , the corresponding magnetization exhibits oscillations for all times and does not approach any time-asymptotic constant value. This prediction is verified in numerical simulations discussed in Section 5.4.1. The average of $\langle m_x \rangle(t)$ over a period of oscillation is

$$\langle m_x \rangle_{\text{Time average}} \equiv \frac{1}{T} \int_0^T dt \langle m_x \rangle(t) = \frac{h}{2p_0^2 - 1}; \quad p_0^2 > \frac{1}{2}, \quad (5.63)$$

where T is the period of oscillation. In Section 5.4, we will compare this average with numerical results.

Fermi-Dirac QSS

We now consider a Fermi-Dirac state in which the coordinate is uniformly distributed in $[0, 2\pi]$, while the momentum has the usual Fermi-Dirac distribution:

$$f_0(p) = A \frac{1}{2\pi} \frac{1}{1 + e^{\beta(p^2 - \mu)}}; \quad p \in [-\infty, \infty]. \quad (5.64)$$

Here, $\beta \geq 0$ and $\mu \geq 0$ are parameters characterizing the distribution, while A is the normalization constant. We consider the state (5.64) in the limit of large β in which analytic computations of various physical quantities is possible. As $\beta \rightarrow \infty$ the Fermi-Dirac state converges to the water-bag state (5.59) with $p_0 = \sqrt{\mu}$.

As shown in Appendix C.1, to leading order in $1/\beta^2$, the normalization is given by

$$A = \frac{1}{2\sqrt{\mu}} \left(1 + \frac{\pi^2}{24\beta^2\mu^2} \right), \quad (5.65)$$

while the energy density is

$$e = \frac{\mu}{6} \left(1 + \frac{\pi^2}{6\beta^2\mu^2} \right) + \frac{1}{2}. \quad (5.66)$$

Let us now investigate the conditions (5.57) and (5.58) for the marginal stability of the state (5.64). Since $f_0(p)$ satisfies $\left. \frac{\partial f_0(p)}{\partial p} \right|_{p=0} = 0$, the condition (5.58) implies that $\omega_{\text{pr}} = 0$, which on substituting in condition (5.57) gives

$$\epsilon(1, 0) = 0, \quad (5.67)$$

where, as shown in the Appendix, to order $1/\beta^2$, we have

$$\epsilon(1, 0) = 1 - \frac{1}{2\mu} \left(1 + \frac{\pi^2}{6\beta^2\mu^2} \right). \quad (5.68)$$

CHAPTER 5. DETERMINISTIC PERTURBATIONS: LINEAR RESPONSE THEORY ON THE VLASOV EQUATION

Solving Eq. (5.67) gives μ^* , the value of μ at the marginal stability of the state (5.64). To order $1/\beta^2$, we get

$$\mu^* = \frac{1}{2} + \frac{2\pi^2}{3\beta^2}, \quad (5.69)$$

which gives the corresponding energy density

$$e^* = \frac{7}{12} + \frac{\pi^2}{6\beta^2}, \quad (5.70)$$

such that at higher energies, the state (5.64) is a QSS.

Following our earlier discussions on the regime of validity of the linear Vlasov theory, and using Eq. (5.68) in Eq. (5.56), we get

$$\bar{m}_x = \frac{h \left(1 + \frac{\pi^2}{6\beta^2\mu^2} \right)}{2\mu - 1 - \frac{\pi^2}{6\beta^2\mu^2}}; \quad \mu > \mu^*. \quad (5.71)$$

5.3.3 Linear response of the homogeneous equilibrium state

It is interesting to consider the response of the distribution (5.40) with magnetization $m_x^{eq} = 0$, which is the equilibrium state of the HMF model for energies $e > e_c$. We thus consider the choice

$$f_0(p) = \sqrt{\frac{\beta}{2\pi}} \exp \left[-\frac{\beta p^2}{2} \right]. \quad (5.72)$$

The stability condition (5.58) gives $\omega_{pr} = 0$, so that Eq. (5.57) gives

$$\epsilon(1, 0) = 0, \quad (5.73)$$

where $\epsilon(1, 0)$ is given by

$$\epsilon(1, 0) = 1 - \frac{\beta}{2}. \quad (5.74)$$

Thus, the state (5.40) is marginally stable at $\beta = 2$, and correspondingly, $e = e^* = 3/4 = e_c$. For $e > e^*$, the state is a QSS and also the Boltzmann-Gibbs equilibrium state.

Using Eqs. (5.74) and (5.56), one gets

$$\bar{m}_x = \frac{h}{2/\beta - 1}; \quad \beta < 2. \quad (5.75)$$

Therefore, under the perturbation, Eqs. (5.42) and (5.44), the equilibrium state evolves to an inhomogeneous QSS predicted by our linear response theory. Let us compare the value of \bar{m}_x in Eq. (5.75) with the one predicted by equilibrium statistical mechanics, $m_x^{eq}(\beta, h)$, at the same values of the energy and h . This latter quantity is obtained by solving the implicit equation

$$\frac{X}{\beta} - h = \frac{I_1(X)}{I_0(X)}, \quad (5.76)$$

5.4. COMPARISON WITH N -PARTICLE SIMULATIONS

with $I_1(X)$ the modified Bessel function of first order, and using the solution $\bar{X}(\beta, h)$ to get

$$m_x^{eq}(\beta, h) = \frac{I_1(\bar{X})}{I_0(\bar{X})}. \quad (5.77)$$

The corresponding energy is

$$e = \frac{1}{2\beta} + \frac{1 - (m_x^{eq}(\beta, h))^2}{2} - h m_x^{eq}(\beta, h). \quad (5.78)$$

The two values given in Eqs. (5.75) and (5.77) are in general different. However, in the high-energy regime, one can solve Eq. (5.76) for small X to obtain for the equilibrium magnetization the same formula as the one obtained by the linear response theory, Eq. (5.75). While comparing the two magnetization values with numerical results at high energies in Section 5.4.2, we are thus not able to distinguish between equilibrium and QSS magnetization in the presence of the field.

5.4 Comparison with N -particle simulations

To verify the analysis presented in Section 5.3, we performed extensive numerical simulations of the N -particle dynamics (5.5) for the HMF model for large N . The equations of motion were integrated using a fourth-order symplectic scheme [185], with a time step varying from 0.01 to 0.1. In simulations, we prepare the HMF system at time $t = 0$ in an initial state by sampling independently for every particle the coordinate q uniformly in $[0, 2\pi]$ and the momentum according to either the water-bag, the Fermi-Dirac, or the Gaussian distribution. Thus, the probability distribution of the initial state is

$$f_N(q_1, p_1, q_2, p_2, \dots, q_N, p_N) = \prod_{i=1}^N f_0(p_i) \quad (5.79)$$

where $f_0(p)$ is given by either Eq. (5.59), (5.64), or (5.72). The energy of the initial state is chosen to be such that it is a QSS. Then, at time $t_0 > 0$, we switch on the external perturbation, Eqs. (5.42) and (5.44), and follow the time evolution of the x -magnetization.

In obtaining numerical results, two different approaches were adopted. In one approach, we followed in time the evolution of a single realization of the initial state. These simulations are intended to check if our predictions based on the Vlasov equation for the smooth distribution $f(q, p, t)$ for infinite N are also valid for a typical time-evolution trajectory of the system. As discussed in Chapter 4, when $f_0(p)$ is a stable stationary solution of the Vlasov equation, it is known numerically and analytically that these times diverge as a power of N , and are therefore sufficiently long to allow us to check even for moderate values of N the predictions of our linear Vlasov theory for perturbations about Vlasov-stable stationary solution $f_0(p)$.

CHAPTER 5. DETERMINISTIC PERTURBATIONS: LINEAR RESPONSE THEORY ON THE VLASOV EQUATION

In a second approach, we obtained numerical results by averaging over an ensemble of realizations of the initial state. The time evolution that we get using this second method is different from the first one. This approach allows us to reach the average and/or asymptotic value of an observable, here $\langle m_x \rangle(t)$, on a faster time scale because of a mechanism of convergence in time, as we describe below.

5.4.1 Linear response of homogeneous QSS: Single realization

The oscillatory behavior of $\langle m_x \rangle(t)$ predicted for the water-bag state, see formula (5.62), is checked in Fig. 5.1(a). Oscillations around a well-defined average persist indefinitely with no damping, as predicted by the theory. In the inset of the same panel, the theoretical prediction is compared with the numerical result for a few oscillations. While the agreement is quite good for the first two periods of the oscillations, the numerical data display a small frequency shift with respect to the theoretical prediction. Moreover, an amplitude modulation may also be observed. We have checked in our N -particle simulations that different initial realizations produce different frequency shifts, which has a consequence when averaging over an ensemble of initial realizations, as discussed below.

In Fig. 5.1(b), we show $\langle m_x \rangle(t)$ for the Fermi-Dirac QSS. In this case, we have the theoretical prediction only for the asymptotic value \overline{m}_x given in Eq. (5.71). The time evolution of $\langle m_x \rangle(t)$ displays beatings and revivals of oscillations around this theoretical value, shown by the dashed horizontal line in the figure. There is no sign of asymptotic convergence, even running for longer times. For this high value of β , which makes the Fermi-Dirac distribution very close to the water-bag one, we cannot conclude that there will be damping in time. We have observed a damping for smaller values of β when the Fermi-Dirac distribution comes closer to a Gaussian.

5.4.2 Linear response of the homogeneous equilibrium state: Single realization

In Fig. 5.2, we show $\langle m_x \rangle(t)$ for the Gaussian QSS. After the application of the external field, the magnetization sharply increases and fluctuates around a value which is slightly below the theoretical prediction, Eq. (5.75). Convergence to this latter value is observed on longer times.

5.4.3 Average over initial realizations

In this section, we present numerical results for the three initial QSSs (water-bag, Fermi-Dirac, Gaussian), obtained after averaging the time evolution of $\langle m_x \rangle(t)$ over a set of realiza-

5.4. COMPARISON WITH N -PARTICLE SIMULATIONS

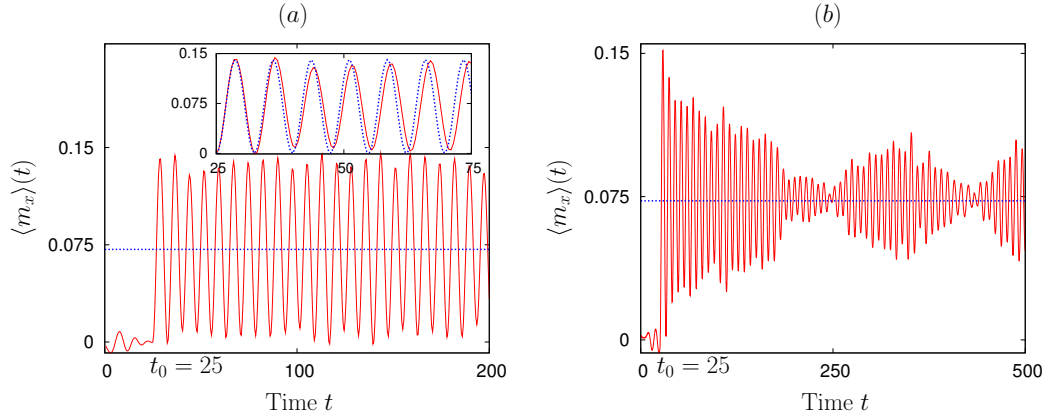


Figure 5.1 – $\langle m_x \rangle(t)$ vs. time t for the (a) water-bag QSS, and (b) Fermi-Dirac QSS, in the HMF model under the action of the perturbation, Eqs. (5.42) and (5.44), with $h = 0.1$ switched on at time $t_0 = 25$. (a) The full line in the main plot shows the result of N -particle simulation, while the dashed horizontal line is the theoretical time-averaged value of $\langle m_x \rangle(t)$ given in Eq. (5.63). The system size is $N = 10^5$, while the parameter p_0 , corresponding to energy $e = 0.7$, is approximately 1.095. In the inset, the numerical result (full line) is compared with the theoretical prediction (5.62) (dashed line). (b) The full line represents simulation results, while the horizontal dashed line is the theoretical asymptotic value given in Eq. (5.71). The system size is $N = 10^5$, while $\beta = 10$ and $\mu = 1.2$, giving energy $e \approx 0.7$.

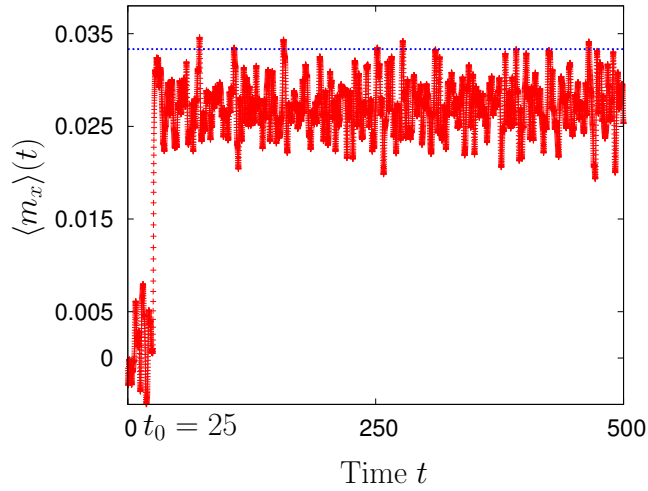


Figure 5.2 – $\langle m_x \rangle(t)$ vs. time t for the Gaussian QSS in the HMF model under the action of the perturbation, Eqs. (5.42) and (5.44), with $h = 0.1$ switched on at time $t_0 = 25$. The line made of pluses represents the result of N -particle simulation, while the dashed horizontal line is the theoretical asymptotic value given in Eq. (5.75). The system size is $N = 10^5$, while $\beta = 0.5$, so that the energy $e = 1.5$.

tions (typically a thousand) of the initial state. We define the average

$$\langle m_x \rangle_{\text{Ensemble average}}(t) = \frac{1}{N_s} \sum_{n=1}^{N_s} \langle m_x \rangle_n(t), \quad (5.80)$$

CHAPTER 5. DETERMINISTIC PERTURBATIONS: LINEAR RESPONSE THEORY ON THE VLASOV EQUATION

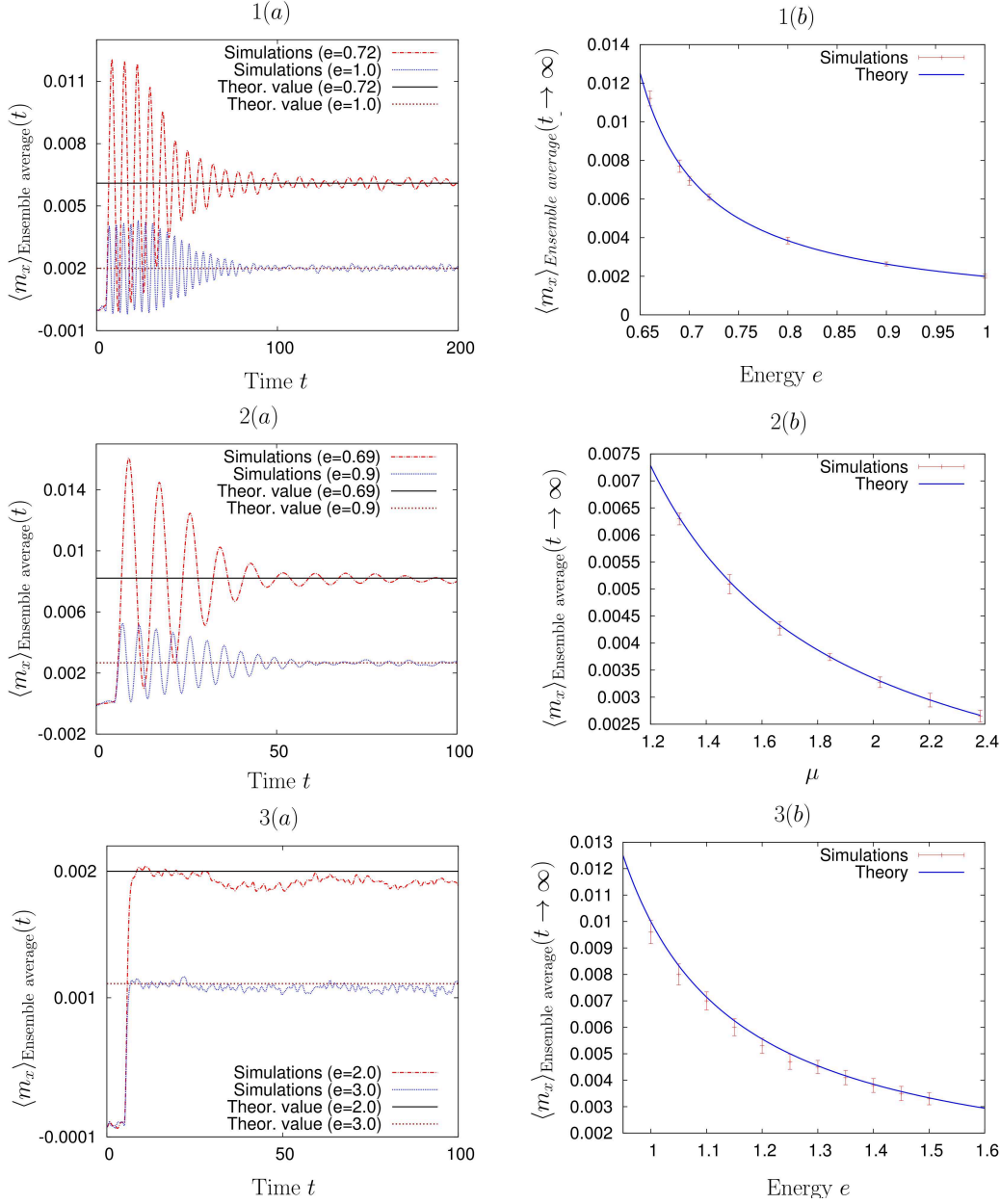


Figure 5.3 – Linear response of a water-bag QSS (panels 1(a), 1(b)), a Fermi-Dirac QSS with $\beta = 10$ (panels 2(a), 2(b)), and the homogeneous equilibrium state (panels 3(a), 3(b)) for the HMF model under the perturbation, Eqs. (5.42) and (5.44), with $h = 0.01$. All simulation data have been averaged over several thousand realizations of the initial state. In each case, panel (a) shows the time evolution of the $\langle m_x \rangle_{\text{Ensemble average}}(t)$ as obtained from N -particle simulations, and its asymptotic approach either to the time average in Eq. (5.63) for the water-bag initial state or to \bar{m}_x given in Eq. (5.71) for the Fermi-Dirac QSS, or to \bar{m}_x given in Eq. (5.75) for the Gaussian QSS. In panel (b), we show the N -particle simulation results for the asymptotic magnetization as a function of energy (the parameter μ in the Fermi-Dirac case). The error bars denote the standard deviation of fluctuations around the asymptotic value. The results compare well with the theoretical predictions. The system size N is 16,000 for panels 1(a), 1(b) and panels 2(a), 2(b), and 10,000 for panels 3(a), 3(b).

where $\langle \cdot \rangle_n$ labels the sample and N_s is the total number of different realizations.

In all cases, we observe a relaxation to an asymptotic value. For the water-bag distribution, this value compares quite well with the time-averaged magnetization given in formula (5.63), see Fig. 5.3 panels (a) and (b). The mechanism by which the relaxation to the asymptotic value occurs in the water-bag case, in the absence of a true relaxation of a single initial realization, is the frequency shift present in the different initial realizations. This leads at a given time to an incoherent superposition of the oscillations of the magnetization. For other distributions, the numerically determined asymptotic value is compared with the theoretical value for the single realization \overline{m}_x , given in Eq. (5.71) and Fig. 5.3 panels 2(a) and 2(b), and formula (5.75) and Fig. 5.3 panels 3(a) and 3(b). The agreement is quite good.

5.4.4 Relaxation of QSS to equilibrium

For finite values of N , the perturbed HMF system finally relaxes to the Boltzmann-Gibbs equilibrium state. The presence of a two-step relaxation of the initial water-bag QSS with energy $e = 0.65$, first to the perturbed Vlasov state and then to equilibrium, is shown in Fig. 5.4 for increasing system sizes for perturbation, Eqs. (5.42) and (5.44), with $h = 0.01$. The relaxation to the first magnetization plateau with value ≈ 0.125 predicted by the linear response theory takes place on a time of $O(1)$. The final relaxation to the equilibrium value of the magnetization ≈ 0.42 occurs on a timescale that increases with system size, presumably with a power law that remains to be investigated further.

5.5 Conclusions

In this Chapter, we studied the response of a Hamiltonian long-range system in a QSS to a deterministic external perturbation. The perturbation couples to the canonical coordinates of the individual constituents. We pursued our study by analyzing the Vlasov equation for the time evolution of the single-particle phase space distribution. We linearized the perturbed Vlasov equation about the QSS for weak enough external perturbation to obtain a formal expression for the response observed in a single-particle dynamical quantity. From a theoretical point of view, we obtained a formula (5.24) which is the analogous of the Kubo formula. The difference between the two is that it enters an effective potential ν_{eff} , defined in Eq. (5.17), and not the external field alone. This is due to the non-linearity of the Vlasov equation in contrast to the linearity of the Liouville equation. The external field not only generates a potential due to its direct coupling with the particles, but it also modify the mean-field potential from its value $\Phi[f_0](q)$ in the absence of the field.

The explicit use of Eq. (5.24) relies on techniques very similar to those presented to obtain the Landau Damping in the previous Chapter and it is thus easily feasible when the QSS is

CHAPTER 5. DETERMINISTIC PERTURBATIONS: LINEAR RESPONSE THEORY ON THE VLASOV EQUATION

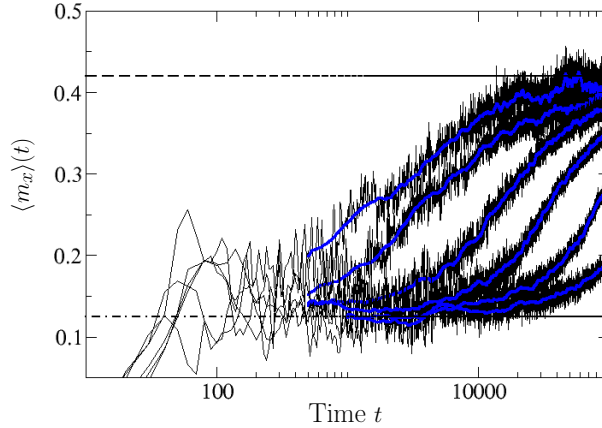


Figure 5.4 – Two-step relaxation of the water-bag QSS toward the Boltzmann-Gibbs equilibrium: $\langle m_x \rangle(t)$ vs. time t for increasing system size from $N = 2000$ to $N = 64000$ (left to right). Under the perturbation, Eqs. (5.42) and (5.44) with $h = 0.01$, the water-bag initial QSS with $e = 0.65$ relaxes to an intermediate inhomogeneous QSS with $\langle m_x \rangle \approx 0.125$ (lower horizontal dash-dotted line) and then to the equilibrium state with $\langle m_x \rangle \approx 0.42$ (upper horizontal dashed line). The blue thick lines refer to running averages performed to smooth out local fluctuations.

homogeneous in the coordinate. In this case, we derived a closed form expression for the response function. We applied this formalism to the Hamiltonian mean-field model, and compared the theoretical predictions for three representative QSSs (the water-bag QSS, the Fermi-Dirac QSS and the Gaussian QSS) with N -particle simulations for large N . We also showed the long-time relaxation of the water-bag QSS to the Boltzmann-Gibbs equilibrium state.

The explicit application of Eq. (5.24) is possible with techniques very similar to those used to derive the Landau damping in Section 4.4.1. The results presented here has been also derived by Ogawa et al. [126]; in this work even some cases of spatially non-homogeneous f_0 is discussed. The technique, relying on the use of action-angle variables, follows the one employed to prove the Landau damping for non-homogeneous states in [163, 164] when the single-particle dynamics is integrable. An interesting observation of this work is that for the non-homogeneous equilibrium state, the prediction of the linear theory for the divergence of the susceptibility at the phase transition is different to the one obtained from statistical mechanics. We believe that the reason for this behavior is that, even if the system starts from equilibrium, it is found in a QSS after the action of the perturbation. Only finite size effects makes it relax to the new equilibrium of the perturbed Hamiltonian. Also for homogeneous QSS this behavior of the susceptibility would be possible, in principle; however, we have

seen that in this case, the prediction of the linear theory is exactly the same as the one of statistical mechanics.

After our work, we realized that some of the theoretical results obtained here were already noted in plasma physics, see [186].

Another approach to deal with non-homogeneous states, starting from Eq. (5.24), has been developed by Patelli et al. in [127]; the interesting point in this reference is that they do not suppose the one-particle dynamics to be integrable and hence they do not use action-angle variables. For their calculation it is supposed that the system, under a perturbation saturating to some value in time, does converge to a stationary state in the $t \rightarrow \infty$ limit (without proving it); moreover, only a finite number of Casimirs is taken into account. Their approach, even if approximate, compares very well with numerics performed on the HMF model and we think it deserves some attention in the future.

6

Stochastic forcing on particle systems

In this and in the next Chapter we study stochastically forced long-range interacting systems. We concentrate here on particle systems such as plasma or self-gravitating systems, whereas in the next Chapter we describe our first progress in generalizing the techniques developed to two-dimensional and geophysical turbulence models: this is the principal motivation and the long-term perspective of our work.

On the one hand, long-range interacting systems are often acted upon by external stochastic forces that drive them out of equilibrium. Unlike systems with short-range interactions, stochastic forces in long-range interacting systems can act coherently on all particles, and not independently on each particle. Consider, e.g., globular clusters being influenced by the gravitational potential of their galaxy, which produces a force that fluctuates. In addition, galaxies themselves feel the random potential of other surrounding galaxies, and their halos are subjected to transient and periodic perturbations, which may be due to the passing of dwarfs or to orbital decaying [121]. Dynamics of plasmas are also strongly influenced by fluctuating electric and magnetic fields due to the ever-changing ambience [123] or imposed external fields. In situations of stochastic driving, the systems at long times often reach a nonequilibrium stationary state that violates detailed balance. In such a state, the power injected by the external random fields balances on average the dissipation, and there is a steady flux of conserved quantities through the system. This situation is also very classical in geophysical turbulence, as will be discussed in Chapter 7.

On the other hand, the study of nonequilibrium stationary states (NESS) is an active area of research of modern day statistical mechanics. One of the primary challenges in this field is to formulate a tractable framework to analyze nonequilibrium systems on a common footing, similar to the one due to Gibbs and Boltzmann that has been established for equilibrium systems [117–120].

Our work provides, to the best of our knowledge, the first study of NESS in long-range systems with statistical mechanical perspectives.

As we have seen in Chapter 4, one of the main theoretical approaches to study isolated

CHAPTER 6. STOCHASTIC FORCING ON PARTICLE SYSTEMS

systems with long-range interactions is the kinetic theory description of relaxation towards equilibrium. In plasma physics and astrophysics, this approach leads to the Lenard-Balescu equation (see Section 4.6) or to the approximate Landau equation.

The main theoretical results of this Chapter is a detailed development of a generalization of this kinetic theory approach to describe nonequilibrium stationary states in systems with long-range interactions driven by external stochastic forces, valid in the limit of small external stochastic fields. We will see that the techniques on Lyapunov equations developed in Section 4.5 are applicable to this case, as well as they were to the derivation of the Lenard-Balescu equation. Our kinetic theory is quite general, being applicable to any long-range interacting system composed by particles. In the limit of small external forcing, the system settles into a stationary state, in which we find the one-particle momentum distribution to be non-Gaussian. The predictions of our kinetic equation for spatially homogeneous stationary states compare very well with results of our extensive N -particle numerical simulations on the stochastically forced HMF model.

The HMF model, at equilibrium, presents a second order phase transition below which the state is not homogeneous. It is thus natural to ask how such phase transition will be altered when the dynamics breaks the detailed balance. Our numerical simulations exhibit a nonequilibrium phase transition between homogeneous and inhomogeneous states. Close to the phase transition point, we demonstrate the occurrence of bistability between these two types of states, with a mean residence time that diverges as an exponential in the inverse of the strength of the external stochastic forces, in the limit of low values of such forces. Similar bistable behavior has recently been observed in two-dimensional turbulence with stochastic forcing [187] and thus looks a quite general phenomena for stochastically forced long-range interacting systems.

The structure of this Chapter is as follows. In the following section, we define the dynamics we are going to consider of a long-range interacting system driven by external stochastic forces. We also discuss the paradigmatic example of the stochastically forced (HMF) model. In section 6.2, we discuss the methods we adopt to analyze the dynamics. In particular, we give a detailed derivation of the kinetic theory to study spatially homogeneous stationary states of the dynamics. We describe the numerical simulation scheme that we employ to study the dynamics, specifically, to check the predictions of our kinetic theory. This is followed by a discussion in section 6.3 of the results obtained from the kinetic theory, and their comparison with numerical simulation results for spatially homogeneous stationary states. In section 6.4, we discuss the results of numerical simulations of spatially inhomogeneous stationary states. We report on the interesting bistable behavior in which the system in the course of its temporal evolution switches back and forth between homogeneous and inho-

mogeneous states, with a mean residence time that we show to be diverging as an exponential in the inverse of the strength of the external stochastic forcing, in the limit of low values of such forcing. We close the Section with concluding remarks. Some of the technical details of our computation are collected in the four appendices D.1, D.2, D.3 and D.4.

This Chapter mainly contains the results reported in [128, 129].

6.1 Long-range interacting systems driven by stochastic fields

Consider a system of N particles interacting through a long-range pair potential, and described by the Hamiltonian in Eq. (4.3). For simplicity, we regard q_i 's as scalar periodic variables of period 2π ; generalization to $q_i \in \mathbb{R}^n$, with $n = 1, 2$ or 3 , is straightforward.

We perturb the system (4.3) by a statistically homogeneous Gaussian stochastic field $F(q, t)$ with zero mean, and variance given by

$$\langle F(q, t)F(q', t') \rangle = C(|q - q'|)\delta(t - t'). \quad (6.1)$$

The resulting equations of motion for the i -th particle are

$$\dot{q}_i = \frac{\partial H}{\partial p_i}, \quad \text{and} \quad \dot{p}_i = -\frac{\partial H}{\partial q_i} - \alpha p_i + \sqrt{\alpha} F(q_i, t). \quad (6.2)$$

The property that the Gaussian fields $F(q_i, t)$ are statistically homogeneous, i.e., the correlation function C depends solely on $|q - q'|$, is consistent with any perturbation that respects space homogeneity. Such a property is necessary for the discussions later on the kinetic theory approach to describe spatially homogeneous stationary states of the dynamics (6.2). Note that $C(q)$ is the correlation, so that it is a positive-definite function [188], and its Fourier components are positive:

$$c_k \equiv \frac{1}{2\pi} \int_0^{2\pi} dq C(q)e^{-ikq} > 0; \quad c_{-k} = c_k, \quad C(q) = c_0 + 2 \sum_{k=1}^{\infty} c_k \cos(kq). \quad (6.3)$$

We find it convenient to use the equivalent Fourier representation of the Gaussian field $F(q, t)$ as follows:

$$F(q, t) = \sqrt{c_0} X_0(t) + \sum_{k=1}^{\infty} \sqrt{2c_k} [\cos(kq) X_k(t) + \sin(kq) Y_k(t)], \quad (6.4)$$

where $X_0(t)$, $X_k(t)$ and $Y_k(t)$ are independent scalar Gaussian white noises satisfying

$$\langle X_k(t) X_{k'}(t') \rangle = \delta_{k,k'} \delta(t - t'), \quad (6.5)$$

$$\langle Y_k(t) Y_{k'}(t') \rangle = \delta_{k,k'} \delta(t - t'), \quad (6.6)$$

$$\langle X_k(t) Y_{k'}(t') \rangle = 0. \quad (6.7)$$

CHAPTER 6. STOCHASTIC FORCING ON PARTICLE SYSTEMS

Using the Itô formula [165] to compute the time derivative of the energy density $e = H/N$, and averaging over noise realizations give

$$\left\langle \frac{de}{dt} \right\rangle + \langle 2\alpha\kappa \rangle = \frac{\alpha}{2}C(0), \quad (6.8)$$

where $\kappa = \sum_{i=1}^N p_i^2/(2N)$ is the kinetic energy density. On integration, we get

$$\langle k(t) \rangle = \left(\langle k(0) \rangle - \frac{C(0)}{4} \right) e^{-2\alpha t} + \frac{C(0)}{4}. \quad (6.9)$$

The average kinetic energy density in the stationary state is thus $\langle \kappa \rangle_{ss} = C(0)/4$. We define the kinetic temperature of the system as

$$\langle \kappa \rangle_{ss} \equiv \frac{T}{2}; \quad (6.10)$$

as a result, we have

$$T = \frac{C(0)}{2}. \quad (6.11)$$

Let us note that in the dynamics (6.2), fluctuations of intensive observables due to stochastic forcing are of order $\sqrt{\alpha}$, while those due to finite-size effects are of order $1/\sqrt{N}$. Moreover, the typical timescale associated with the effect of stochastic forces is $1/\alpha$, as is evident from Eq. (6.9), while the one associated with relaxation to equilibrium due to finite-size effects is of order N , see [90] and Chapter 4.

Our theoretical analysis to study the dynamics (6.2) by means of kinetic theory is valid for any general two-particle interaction potential $v(q)$. However, in order to perform simple numerical simulations with which we may check the predictions of the kinetic theory, we specifically make the choice $v(q) = 1 - \cos q$, that defines the stochastically-forced Hamiltonian mean-field (HMF) model, as detailed below. We note for later purpose that the Fourier transform of the HMF interparticle potential is, for $k \neq 0$, $v_k = -[\delta_{k,1} + \delta_{k,-1}]/2$, where $\delta_{k,i}$ is the Kronecker delta.

6.2 Methods of analysis

6.2.1 Kinetic theory for homogeneous stationary states

Here, we develop a suitable kinetic theory description to study the dynamics (6.2) in the joint limit $N \rightarrow \infty$ and $\alpha \rightarrow 0$. While the first limit is physically motivated on grounds that most long-range systems indeed contain a large number of particles, the second one allows us to study stationary states for small external forcing. Moreover, for small α , we will be able to develop a complete kinetic theory for the dynamics. For simplicity, we discuss here the continuum limit $N\alpha \gg 1$, when stochastic effects are predominant with respect to finite-size effects. The generalization of the following discussion to the cases $N\alpha$ of order one and

$N\alpha \ll 1$ is straightforward, as pointed out at the end of this subsection. For the development of the kinetic theory, we assume the system to be spatially homogeneous; a possible generalization to the non-homogeneous case will be discussed in the conclusions.

The development of the kinetic theory here strongly resemble the derivation of the Lenard-Balescu equation as presented in Chapter 4. As a starting point to develop the theory, we consider the Fokker-Planck equation associated with the equations of motion (6.2). This equation describes the evolution of the N -particle distribution function

$$f_N(q_1, \dots, q_N, p_1, \dots, p_N, t), \quad (6.12)$$

which is the probability density (after averaging over noise realizations) to observe the system with coordinates and momenta around the values $\{q_i, p_i\}_{1 \leq i \leq N}$ at time t . This equation can be derived by standard methods [165]; we have

$$\begin{aligned} \frac{\partial f_N}{\partial t} = & \sum_{i=1}^N \left[-p_i \frac{\partial f_N}{\partial q_i} + \frac{\partial(\alpha p_i f_N)}{\partial p_i} \right] + \frac{1}{2N} \sum_{i,j=1}^N \frac{\partial v(q_i - q_j)}{\partial q_i} \left[\frac{\partial}{\partial p_i} - \frac{\partial}{\partial p_j} \right] f_N \\ & + \frac{\alpha}{2} \sum_{i,j=1}^N C(|q_i - q_j|) \frac{\partial^2 f_N}{\partial p_i \partial p_j}. \end{aligned} \quad (6.13)$$

In D.1, by applying the so-called potential conditions [189] for the above Fokker-Planck equation, we prove that a necessary and sufficient condition for the stochastic process (6.2) to verify detailed balance is that the Gaussian noise is white in space, that is, $c_k = c$ for all k . This condition is not satisfied for a generic correlation function $C(q)$, in which case, the steady states of the dynamics are true nonequilibrium ones, characterized by non-vanishing probability currents in phase space, and a balance between external forces and dissipation.

Similar to the Liouville equation for Hamiltonian systems, the N -particle Fokker-Planck equation (6.13) is a very detailed description of the system. Using kinetic theory, we want to describe the evolution of the one-particle distribution function

$$f(z_1, t) = \int \prod_{i=2}^N dz_i f_N(z_1, \dots, z_N, t), \quad (6.14)$$

where we have used the notation $z_i \equiv (q_i, p_i)$. We note that with this definition, the normalization is $\int dz f(z, t) = 1$. Substituting in the Fokker-Planck equation (6.13) the reduced distribution functions

$$f_s(z_1, \dots, z_s, t) = \frac{N!}{(N-s)!N^s} \int \prod_{i=s+1}^N dz_i f_N(z_1, \dots, z_N, t), \quad (6.15)$$

we get a hierarchy of equations, similar to those of the BBGKY hierarchy presented in Sec-

CHAPTER 6. STOCHASTIC FORCING ON PARTICLE SYSTEMS

tion 4.3, as follows:

$$\begin{aligned} \frac{\partial f_s}{\partial t} + \sum_{i=1}^s p_i \frac{\partial f_s}{\partial q_i} - \frac{1}{N} \sum_{i,j=1}^s \frac{\partial v(q_i - q_j)}{\partial q_i} \frac{\partial f_s}{\partial p_i} - \sum_{i=1}^s \frac{\partial}{\partial p_i} [\alpha p_i f_s] \\ - \frac{\alpha}{2} \sum_{i,j=1}^s C(|q_i - q_j|) \frac{\partial^2 f_s}{\partial p_i \partial p_j} = \sum_{i=1}^s \int dz_{s+1} \frac{\partial}{\partial q_i} v(q_i - q_{s+1}) \frac{\partial f_{s+1}}{\partial p_i} \end{aligned} \quad (6.16)$$

for $s = 1, \dots, N-1$. With a slight abuse of the standard vocabulary, we will refer in this Chapter to Eq. (6.16) as the BBGKY hierarchy equation.

Now, as is usual in kinetic theory, we split the reduced distribution functions into connected and non-connected parts, e.g.,

$$f_2(z_1, z_2, t) = f(z_1, t)f(z_2, t) + \tilde{g}(z_1, z_2, t), \quad (6.17)$$

and similarly, for other f_s 's with $s > 2$. In D.2, we show that the connected part $\tilde{g}(z_1, z_2, t)$ of the two-particle correlation is of order α , so that we may write

$$f_2(z_1, z_2, t) = f(z_1, t)f(z_2, t) + \alpha g(z_1, z_2, t), \quad (6.18)$$

where g is of order unity; moreover, the connected part of the k -particle correlation is of higher order, with respect to α , in the small parameters α and $1/N$. Then, to close the BBGKY hierarchy, we neglect the effect of the connected part of the three-particle correlation on the evolution of the two-particle correlation function. This scheme is justified at leading order in the small parameter α , and is the simplest self-consistent closure scheme for the hierarchy while taking into account the effects of the stochastic forcing. With our assumption that the system is homogeneous, i.e., f depends on p , and g depends on $|q_1 - q_2|$, p_1 and p_2 only, the first two equations of the hierarchy are then

$$\frac{\partial f}{\partial t} - \alpha \frac{\partial}{\partial p} [pf] - \frac{\alpha}{2} C(0) \frac{\partial^2 f}{\partial p^2} = \alpha \frac{\partial}{\partial p} \int dq_1 dp_1 v'(q_1) g(q_1, p, p_1, t), \quad (6.19)$$

and

$$\frac{\partial g}{\partial t} + L_f^{(1)} g + L_f^{(2)} g = C(|q_1 - q_2|) f'(p_1, t) f'(p_2, t), \quad (6.20)$$

where $L_f^{(1)}$ and $L_f^{(2)}$ are the Vlasov operators linearized about the one-particle distribution f , and acting, respectively, on the first pair (q_1, p_1) and on the second pair (q_2, p_2) of variables of the function $g = g(q_1, p_1, q_2, p_2, t)$. Recall that the explicit expressions for L_f is given in Eq. (4.46).

Exactly as in the derivation of the Lenard-Balescu equation, to obtain from Eqs. (6.19) and (6.20) a single kinetic equation for the distribution function f , we have to solve Eq. (6.20) for g as a function of f and plug the result into the right hand side of Eq. (6.19). Observe now

that the difference between Eq. (6.20) and (4.80), stands only in the right hand side. Also in this case, because the two equations are coupled, we cannot go further without making any simplifying assumption. Nevertheless, we readily see from these equations that the two-particle correlation g evolves over a timescale of order one, whereas the one-particle distribution function $f(p, t)$ evolves over a timescale of order $1/\alpha$. We may then use this timescale separation and compute the long-time limit of g from Eq. (6.20) by assuming f to be steady in time; this is the equivalent of the Bogoliubov's hypothesis in the kinetic theory for isolated systems with long-range interactions. Note that for this timescale separation to be valid, we must also suppose that the one-particle distribution function $f(p, t)$ is a stable solution of the Vlasov equation at all times. Indeed, if this is not the case, g diverges in the limit $t \rightarrow \infty$, as can be readily seen from Eq. (4.74). The physical content of this hypothesis is that the system slowly evolves from the initial condition through a sequence of Quasi-Stationary States to the final stationary state.

Because we assume the system to be homogeneous in space, it is useful to Fourier transform Eqs. (6.19) and (6.20) with respect to the spatial variable; we get

$$\frac{\partial f}{\partial t} - \alpha \frac{\partial}{\partial p} [pf] - \frac{\alpha}{2} C(0) \frac{\partial^2 f}{\partial p^2} = -2\pi i \alpha \sum_{k=-\infty}^{\infty} k v_k \frac{\partial}{\partial p} \int dp' g_k(p, p', t), \quad (6.21)$$

and

$$\left(\frac{\partial g_k}{\partial t} + L_{f,k}^{(1)} g_k + L_{f,-k}^{(2)} g_k \right) (p_1, p_2, t) = c_k f'(p_1) f'(p_2), \quad (6.22)$$

where $g_k(p_1, p_2, t)$ is the Fourier transform of $g(q, p_1, p_2, t)$ with respect to the spatial variable, and v_k is the k -th Fourier coefficient of the pair potential $v(q)$. Remember that the explicit expression for the k -th Fourier component of the linear Vlasov operator $L_{f,k}$ is given by Eq. (4.85) and that $L_{f,k}^* = L_{f,-k}$.

The equation for g , i.e. Eq. (6.20) or equivalently Eq. (6.22), is a Lyapunov equation. Moreover, as in the derivation of the Lenard-Balescu equation, we see from Eq. (6.21), we see that to obtain a single kinetic equation, we need only the Fourier transform $g_k(p, p', t)$, more specifically, its integral with respect to the second momentum variable p' . We can thus compute

$$\int dp' g_k^\infty(p, p') = \lim_{t \rightarrow \infty} \int dp' g_k(p, p', t). \quad (6.23)$$

using Theorem 4.5.1. The fulfillment of the hypothesis is ensured, as in the derivation of the Lenard-Balescu equation, supposing f to be a stationary and stable solution of the Vlasov equation. By direct application of Theorem 4.5.1, we obtain

$$\int dp_1 g_k^\infty[f](p, p_1) = -\frac{1}{2\pi} \frac{c_k}{k v_k} f'(p) \int_{\Gamma} \frac{d\omega}{2\pi} \frac{1}{\omega - kp} \frac{1 - \epsilon(-k, -\omega)}{\epsilon(k, \omega) \epsilon(-k, -\omega)} \quad (6.24)$$

where Γ passes above all the poles of the integrand. To obtain such result, we have used that

$$\left(R_{f,k}(\omega) f' \right) (p) = \frac{1}{-i\omega + ikp} \frac{f'(p)}{\epsilon(k, \omega)} \quad (6.25)$$

CHAPTER 6. STOCHASTIC FORCING ON PARTICLE SYSTEMS

and that

$$\int dp \left(R_{f,-k}(\omega) f' \right)(p) = \frac{1}{2\pi i k v_k} \frac{\epsilon(-k, \omega) - 1}{\epsilon(-k, \omega)}. \quad (6.26)$$

Observe that Eq. (6.26) is valid for all $\omega \in \mathbb{C}$ once that ϵ is interpreted as the analytic continuation of Eq. (4.54).

To get from here the final form of the kinetic equation, we still have to observe that we are interested only in the real part of Eq. (6.21). It can be written, observing that the term $k = 0$ gives no contribution, as:

$$\text{Re} \left\{ i\alpha \sum_{k \neq 0} c_k \frac{\partial}{\partial p} f'(p) \int_{\Gamma} \frac{d\omega}{2\pi} \frac{1}{\omega - kp} \frac{1 - \epsilon(-k, -\omega)}{\epsilon(k, \omega) \epsilon(-k, -\omega)} \right\}, \quad (6.27)$$

where we have used Eq. (6.24). Using now the Plemelj formula to evaluate the integral containing the real part of the dielectric function (the choice of the sign is given by the position of Γ with respect to the pole $\omega = kp$), we get:

$$\alpha \sum_{k \neq 0} c_k \frac{\partial}{\partial p} f'(p) \left\{ \frac{1 - \text{Re}[\epsilon(k, kp)]}{2|\epsilon(k, kp)|^2} + i \text{Im} \left[\int^* \frac{d\omega}{2\pi} \frac{1}{\omega - kp} \frac{1 - \epsilon^*(k, \omega)}{|\epsilon(k, \omega)|^2} \right] \right\}, \quad (6.28)$$

where we have used that $\epsilon^*(k, \omega) = \epsilon(-k, -\omega)$ for $\text{Im}(\omega) = 0$ and the fact that in the Cauchy integral the variable ω is Real so that $\epsilon^*(k, kp) = \epsilon(-k, -kp)$.

Using now the expression for the dielectric function (4.58) for $\omega \in \mathbb{R}$ and observing that the terms in the sum labeled by k or by $-k$ give the same contribution, we get:

$$2\pi\alpha \sum_{k=1}^{\infty} v_k c_k \frac{\partial}{\partial p} f'(p) \left\{ \frac{1}{|\epsilon(k, kp)|^2} \int^* dp_1 \frac{f'(p_1)}{p_1 - p} + \int^* dp_1 \frac{f'(p_1)}{p_1 - p} \frac{1}{|\epsilon(k, kp_1)|^2} \right\}. \quad (6.29)$$

Finally, inserting such expression in the r.h.s. of Eq. (6.21) we get the final form of the kinetic equation (6.30):

$$\frac{\partial f}{\partial t} - \alpha \frac{\partial(p f)}{\partial p} - \alpha \frac{\partial}{\partial p} \left[D[f] \frac{\partial f}{\partial p} \right] = 0, \quad (6.30)$$

where

$$D[f](p) = \frac{1}{2} C(0) + 2\pi \sum_{k=1}^{\infty} v_k c_k \int^* dp_1 \left[\frac{1}{|\epsilon(k, kp)|^2} + \frac{1}{|\epsilon(k, kp_1)|^2} \right] \frac{1}{p_1 - p} f'(p_1, t). \quad (6.31)$$

We recall that v_k is the k -th Fourier coefficient of the pair potential $v(q)$, the quantity c_k is defined in Eq. (6.3), ϵ is the dielectric function defined (for real argument) in Eq. (4.58), and \int^* indicates the Cauchy integral or Principal Value.

The kinetic equation (6.30) is the central result of the kinetic theory developed in this Chapter. It has the form of a non-linear Fokker-Planck equation [189] because the diffusion

coefficient $D[f](p)$ is itself a functional of the one-particle distribution function f . The linear part of the diffusion coefficient $(1/2)C(0)$ is the mean-field effect of the stochastic forces, whereas the effect of two-particle correlation is encoded in the non-linear part. In the next section, we describe how we use this kinetic equation to get information about the nonequilibrium stationary states of the dynamics.

In the foregoing, we discussed the kinetic theory in the limit $N\alpha \gg 1$. The extension to the general case is straightforward: Because of the linearity of the equations of the hierarchy (6.19) and (6.20), the finite- N and stochastic effects give independent contributions. The kinetic equation at leading order of both stochastic and finite-size effects is

$$\frac{\partial f}{\partial t} = Q_\alpha[f] + Q_N[f], \quad (6.32)$$

where Q_α is the operator described in Eq. (6.30), and Q_N (of order $1/N$) is the Lenard-Balescu operator discussed in Section 4.6. For instance, in the case $N\alpha \ll 1$ and in dimensions greater than one, the operator Q_N is responsible for the relaxation to Boltzmann equilibrium after a timescale of order N , whereas the smaller effect of Q_α selects the actual temperature after a longer timescale of order $1/\alpha$.

6.2.2 Numerical simulations

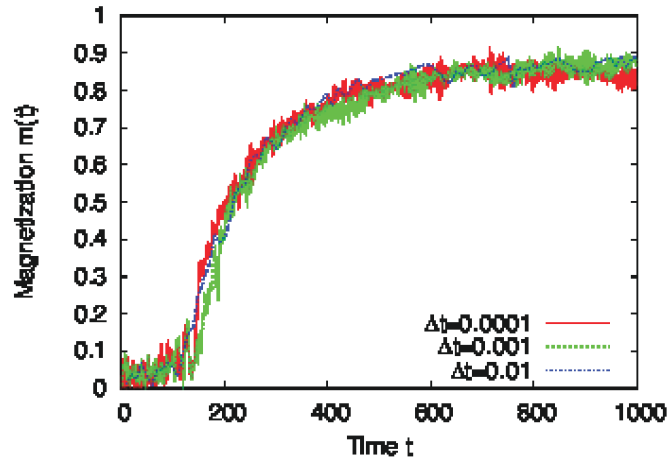


Figure 6.1 – Magnetization as a function of time, obtained from numerical simulation of the stochastically-forced HMF model with $N = 1000, \alpha = 0.01$ at kinetic temperature $T = 0.25$, and with $c_1 = c_2 = c_3 = \dots = c_{10} = C(0)/20, c_{k \geq 11} = 0$, where $C(0) = 2T$. The values of the integration step size Δt used are marked in the figure. The data are obtained by using the integration algorithm described in section 6.2.2. That the magnetization plots collapse onto one curve shows the stability of our algorithm with respect to variation in Δt .

Here we describe how we may simulate the dynamics (6.2) by means of a numerical integration scheme. The first possible choice is to use an Euler-like first-order scheme. However,

it turns out that this algorithm is unstable with respect to not-too-small Δt , in the sense that one obtains different magnetization profiles as a function of time $t = t_n \Delta t$. The situation gets worse for small α , when one needs to use very small Δt to obtain consistent results.

Implementing an higher order algorithm is not a trivial matter because in the Eq. (6.2) the noise is multiplicative. Therefore, for faster and efficient simulation, we adopted a “mixed” scheme which we describe now.

To simulate the dynamics over a given time interval $[0 : T]$, choose a time step size Δt , and set $t_n = n\Delta t$ as the n -th time step of the dynamics. Here, $n = 0, 1, 2, \dots, N_t$, where $N_t = T/\Delta t$. In our numerical scheme, at every time step, we first discard the effect of the noise and employ a fourth-order symplectic algorithm to integrate the deterministic Hamiltonian part of the dynamics [190]. Subsequently, we add the effect of noise and implement an Euler-like first-order algorithm to update the dynamical variables. Specifically, one step of the scheme from t_n to $t_{n+1} = t_n + \Delta t$ involves the following updates of the dynamical variables for $i = 1, 2, \dots, N$: For the symplectic part, we have, for $m = 1, \dots, 4$,

$$\begin{aligned}
 p_i\left(t_n + \frac{m\Delta t}{4}\right) &= p_i\left(t_n + \frac{(m-1)\Delta t}{4}\right) + b(m)\Delta t \left[-\frac{\partial H}{\partial q_i}(\{q_i\left(t_n + \frac{(m-1)\Delta t}{4}\right)\})\right], \\
 q_i\left(t_n + \frac{m\Delta t}{4}\right) &= q_i\left(t_n + \frac{(m-1)\Delta t}{4}\right) + a(m)\Delta t p_i\left(t_n + \frac{m\Delta t}{4}\right),
 \end{aligned}
 \tag{6.33}$$

where the constants $a(m)$'s and $b(m)$'s are given in Ref. [190]. At the end of the update (6.33), we have the set $\{q_i(t_{n+1}), p_i(t_{n+1})\}$. Next, one includes the effect of the stochastic noise by leaving $q_i(t_{n+1})$'s unchanged, but by updating $p_i(t_{n+1})$'s as

$$\begin{aligned}
 p_i(t_{n+1}) &\rightarrow p_i(t_{n+1}) \left[1 - \alpha\Delta t\right] + \sqrt{\alpha} \left[\sqrt{c_0} \Delta X^{(0)}(t_{n+1}) \right. \\
 &\left. + \sum_{k=1}^{N_R} \sqrt{2c_k} \left\{ \Delta X^{(k)}(t_{n+1}) \cos\left(kq_i(t_{n+1})\right) + \Delta Y^{(k)}(t_{n+1}) \sin\left(kq_i(t_{n+1})\right) \right\} \right].
 \end{aligned}
 \tag{6.34}$$

The outcome of implementing this mixed scheme for the stochastically-forced HMF model is shown in Fig. 6.1, where one may observe consistent results with respect to change of Δt over a wide range of values. In numerical simulations reported later, we exclusively used this mixed scheme to simulate the dynamics (6.2).

6.3 Predictions of the kinetic theory and comparison with simulations

We now focus on how to obtain from the kinetic equation (6.30) predictions for the nonequilibrium stationary states of the system. According to Eq. (6.30), $1/\alpha$ is only a timescale; thus, at leading order in α and except for a time rescaling, the parameter α does not affect the time evolution of the system. This statement holds also beyond the leading order for what

6.3. PREDICTIONS OF THE KINETIC THEORY AND COMPARISON WITH SIMULATIONS

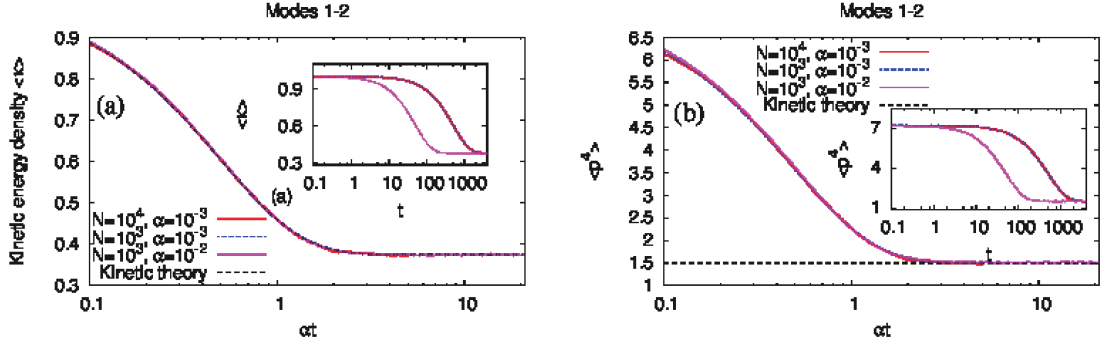


Figure 6.2 – (a) Kinetic energy density $\langle \kappa \rangle$, and (b) $\langle p^4 \rangle$ as a function of αt , at kinetic temperature $T = 0.75$, with modes 1 – 2 excited with amplitudes satisfying $c_1 = c_2 = C(0)/4$, where $C(0) = 2T$. The data for different N and α values are obtained from numerical simulations of the stochastically-forced HMF model with $\Delta t = 0.01$, and involve averaging over 50 histories for $N = 10^4$ and 10^3 histories for $N = 10^3$. The data collapse implies that α is the timescale of relaxation to the stationary state. The inset shows the data without time rescaling by α .

concerns the evolution of the kinetic energy; its evolution may be obtained directly from the equations of motion (6.2), as discussed in section 6.1, and can also be obtained from the kinetic equation (6.30), as detailed in D.3. For the evolution of other observables, there will be corrections at higher orders in α .

As previously discussed, the dynamics of the system does not respect detailed balance if the forcing is not white in space. At the level of the kinetic equation, by inspecting the definition of the diffusion coefficient, Eq. (6.31), we see that the effect of correlations induced by the stochastic forces is modulated by the Fourier component v_k of the interparticle potential. Then, taking the forcing spectral amplitudes c_k different from zero if and only if $v_k = 0$, the non-linear part of the diffusion coefficient vanishes. On the other hand, taking $c_k \neq 0$ for the modes for which $v_k \neq 0$ leads to a diffusion constant which has a non-vanishing non-linear part. To be concrete, let us discuss these two scenarios in the context of the stochastically-forced HMF model.

Since the Fourier transform of the HMF interparticle potential contains only the modes $k = \pm 1$, it follows that only the stochastic force mode with wave number $k = 1$ contributes to the non-linear part of the diffusion coefficient; all the other stochastic force modes result in only a mean-field contribution through the term $C(0)$. Thus, for the case $c_1 \neq 0$, the two relevant parameters that dictate the evolution of the stochastically-forced HMF model by the kinetic equation (6.30) with a non-linear diffusion coefficient are $C(0)$ and c_1 . From Eq. (6.11), since $C(0)$ is related to the kinetic temperature T , we take T and c_1 to be the two relevant parameters. From Eq. (6.10), we know that $2T$ equals the kinetic energy in the final stationary state. Also, Eq. (6.3) implies that $c_1 \leq C(0)/2$.

If however $c_1 = 0$, then, at leading order in α , the dynamics of the system is described by

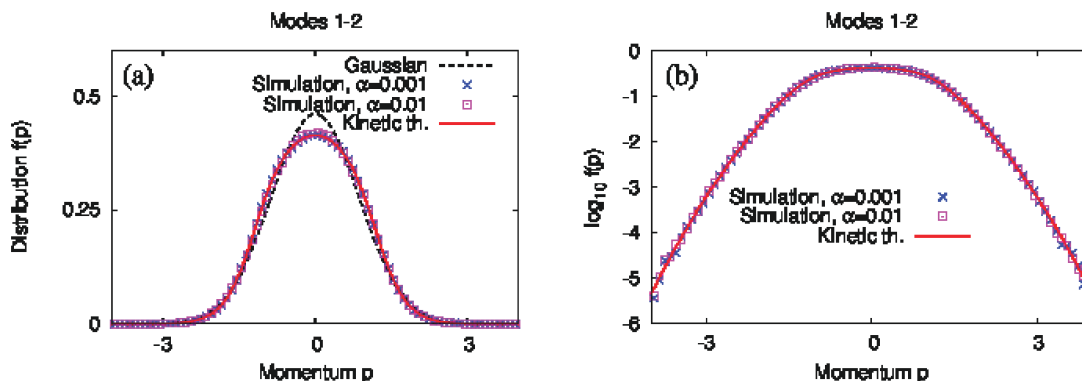


Figure 6.3 – Stationary momentum distribution $f(p)$, on (a) linear, and (b) semi-log scales, for $\alpha = 0.001$, and 0.01 at kinetic temperature $T = 0.75$. The plots correspond to modes 1 and 2 excited with amplitudes satisfying $c_1 = c_2 = C(0)/4$, where $C(0) = 2T$. The data denoted by crosses and squares are results of N -body simulations of the stochastically-forced HMF model with $N = 10000$, $\Delta t = 0.01$ and 1000 independent realizations of the dynamics, while the red continuous lines refer to the theoretical prediction from the kinetic theory. For comparison, the black broken line shows the Gaussian distribution with the same kinetic energy (stationary state of the stochastically-forced HMF model at $T = 0.75$, $c_0 = c_1 = 0$, $c_2 = 0.75$, $c_{k \geq 3} = 0$).

a linear Fokker-Planck equation; this equation is the same as the one which describes the HMF system when coupled to a Langevin thermostat, studied in [191–195]. This means that for this particular choice of the parameters, the detailed balance is broken for the dynamics, but this feature cannot be seen in the kinetic theory, being an effect at a higher order in α . In this case, the homogeneous stationary states of the kinetic equation have Gaussian momentum distribution $f(p)$. As has been studied thoroughly in the context of canonical equilibrium of the HMF model, these states are stable for kinetic energies greater than $1/4$, i.e., for $C(0) > 1$.

Except for the special case of $c_1 = 0$, the stationary velocity distribution of the kinetic equation (6.30) is in general not Gaussian. This can be seen semi-analytically by observing that the Gaussian distribution function

$$f_G(p) = A \exp(-\beta p^2), \quad A = \sqrt{\frac{\beta}{\pi}}, \quad \beta = \frac{1}{2T}, \quad (6.35)$$

with β chosen such that the value of the kinetic energy is the one selected by T , solves the linear Fokker-Planck equation with the diffusion coefficient given by

$$D_{mf} = T. \quad (6.36)$$

To prove that the Gaussian distribution function is not a stationary solution of Eq. (6.30), we have to prove that the contribution to $\partial f / \partial t$ from the non-linear part of $D[f](p)$ in Eq. (6.31) does not vanish. This result can be proven with an asymptotic expansion [136]

6.3. PREDICTIONS OF THE KINETIC THEORY AND COMPARISON WITH SIMULATIONS

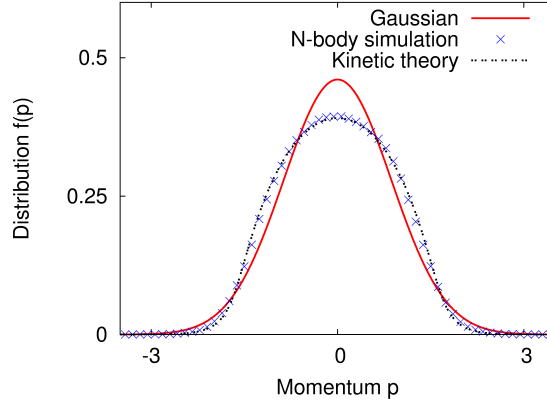


Figure 6.4 – The same as in Fig. 6.3 and 6.4 but only in linear scale, for $\alpha = 0.01$ and kinetic temperature $T = 0.75$. In this plot is excited only the mode 1 with amplitudes satisfying $c_1 = C(0)/2$, where $C(0) = 2T$. The difference with respect to the Gaussian is thus stronger. The value of N is 10000, $\Delta t = 0.01$ and 1000 independent realizations of the dynamics were been used to obtain the average.

for large momenta of the integrals which appear in the diffusion coefficient. We report the straightforward computation in D.4. From the same analysis, one can deduce that, even though the distribution function is not Gaussian, its tails are Gaussian.

On the basis of the above discussions, we expect that for values of T and c_1 such that $T > 0.5$ and $c_1 \ll 2T$, the stationary states will be close to homogeneous states with Gaussian momentum. In order to locate the actual stationary states of the kinetic equation, we have devised a simple numerical scheme, based on the observation that a linear Fokker-Planck equation whose diffusion coefficient $D(p)$ is strictly positive admits a unique stationary state

$$f_{ss}(p) = A \exp \left[- \int_0^p dp' \frac{p'}{D(p')} \right]. \quad (6.37)$$

For a given distribution $f_n(p)$, we compute the diffusion coefficient $D_n(p)$ through Eq. (6.31), and then f_{n+1} using D_n and Eq. (6.37). This procedure defines an iterative scheme. Whenever convergent, this scheme leads to a stationary state of Eq. (6.30). Each iteration involves integrations, so that we expect the method to be robust enough when starting not too far from an actual stationary state. However, we have no detailed mathematical analysis yet. Implementing this iterative scheme, we observed that the distribution f_∞ to which the scheme converges is independent of the initial distribution f_0 . Moreover, the convergence time is exponential in the number of steps n whenever T is not too close to loss of stability of f_∞ with respect to the linear Vlasov dynamics; in practice, we are able to get reliable results for $T \gtrsim 0.65$.

In order to check the theoretical predictions discussed above, we performed numerical simulations of the stochastically forced HMF model. Figure 6.2 shows the evolution of the kinetic energy and $\langle p^4 \rangle = (1/N) \sum_{i=1}^N p_i^4$, where they have been compared with our theoreti-

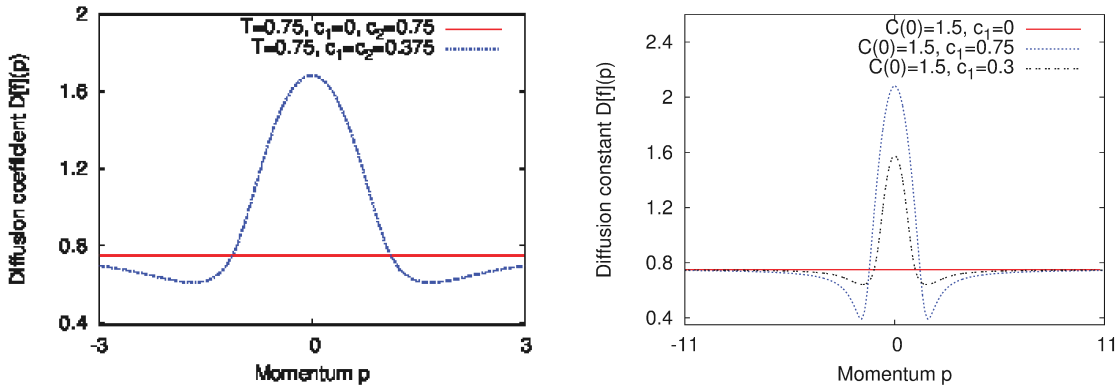


Figure 6.5 – Diffusion coefficient $D[f](p)$ for the stationary momentum distribution $f(p)$ at (a) kinetic temperature $T = 0.75$, with $c_0 = c_{k \geq 3} = 0$, and either (i) $c_1 = c_2 = 0.375$, or, (ii) $c_1 = 0, c_2 = 0.75$ and (b) kinetic temperature $T = 0.75$, with (i) $c_1 = 0$, (ii) $c_1 = 0.3$ or (iii) $c_1 = 0.75$.

cal predictions. In the case of $\langle p^4 \rangle$, we have compared the long-time asymptotic value with the kinetic theory prediction for the stationary state, computed numerically by using the iterative solution for the stationary distribution. The figure illustrates a very good agreement between the theory and simulations. For a more accurate check of the agreement, we have obtained the stationary momentum distribution from both N -body simulations and the numerical iterative scheme discussed above. A comparison between the two, shown in Fig. 6.3 and 6.4, both on linear and semi-log scales, shows a very good agreement between theory and simulations. In this figure, we also show the Gaussian distribution with the same kinetic energy, to illustrate the point that the stationary momentum distribution of the system is far from being Gaussian.

In passing, let us remark that, with an iterative scheme analogous to the one described above, one could have also obtained the full time evolution $f(p, t)$ that obeys the kinetic equation (6.30). However, we will not address this point here.

We also note that while a linear Fokker-Planck equation with non-degenerate diffusion coefficient can be proven to converge to a unique stationary distribution [189], this is not true in general for non-linear Fokker-Planck equations like Eq. (6.30). We expect that if the dynamics is not too far from detailed balance, the kinetic equation will have a unique stationary state. Although some methods to study this type of equation exist [196], we have only the numerical iterative scheme described above to provide some preliminary answers. A more rigorous mathematical analysis is left for future studies.

6.4 Nonequilibrium phase transition and collapse

Until now, we have considered homogeneous stationary states of the dynamics (6.2), and have discussed a kinetic theory to analyze them. Although our theory can in principle be ex-

6.4. NONEQUILIBRIUM PHASE TRANSITION AND COLLAPSE

tended to include inhomogeneous stationary states, its actual implementation to get, e.g., the single-particle distribution, would require more involved computations than the one we encountered for homogeneous states. In order to get preliminary answers, we have performed extensive numerical simulations of the dynamics in the context of the stochastically-forced HMF model. Our specific interest is to know about how the magnetization behaves as the kinetic temperature is reduced from high values.

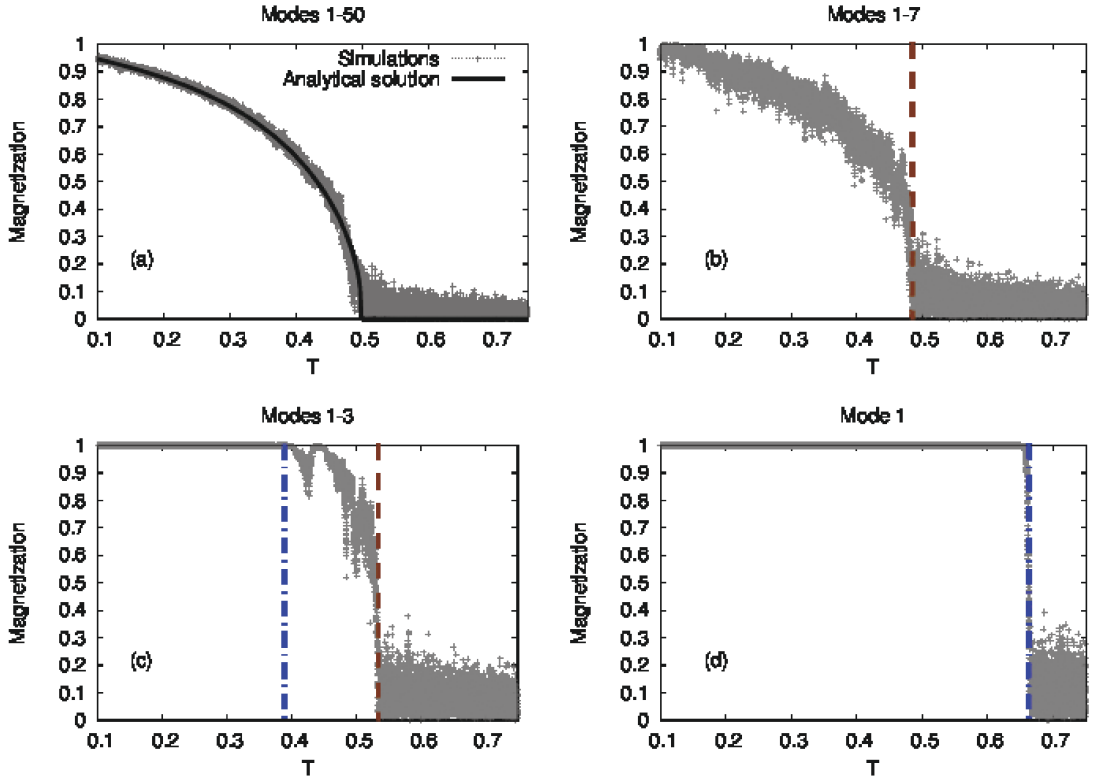


Figure 6.6 – Numerical simulation results for magnetization in the stochastically-forced HMF model as a function of adiabatically-tuned kinetic temperature T ; the different plots correspond to different number of modes excited in the spectrum with amplitudes satisfying $C(0) = c_0 + 2 \sum_{k=1}^{N_R} c_k$, where $C(0) = 2T$, the index $k = 1, 2, \dots, N_R$ denotes the mode number, while N_R is the total number of excited modes with $k \neq 0$. In all cases, the modes excited were chosen to have equal amplitudes, with $c_0 = 0, N = 5000, \alpha = 0.01, \Delta t = 0.01$, while the tuning rate for T is 10^{-5} . It may be noted that forcing equally a large number of modes (~ 50) reproduces the equilibrium magnetization profile as illustrated by the match with the analytical equilibrium solution in the panel (a). In panel (b), the first-order nonequilibrium phase transition is marked by the vertical dashed line. In panel (c), besides the first-order transition, we also show the dynamical transition to the collapsed state by the vertical dashed dotted line. In panel (d), the nonequilibrium phase transition and the dynamical transition almost coincide, and we just show the latter one by the vertical dashed dotted line.

In the case when the stochastic forcing respects detailed balance (i.e., when the noise spectrum is flat and all modes are excited), the stochastically-forced HMF model reduces to the Brownian mean-field (BMF) model studied previously [191]. Here, we know that the

system settles into an equilibrium state in which it exhibits a second-order phase transition at the kinetic temperature $T = T_c = 1/2$: on increasing T from low values, the magnetization decreases continuously to zero at T_c and remains zero at higher temperatures. In the following, we excite only a limited number of modes N_R , but the amplitudes of all excited modes are equal (c_k equals c for all $k \leq N_R$, and is zero otherwise, where the constant c is related to the temperature). Figure 6.6(a) shows that with $N_R = 50$, one reproduces very well the equilibrium profile of the magnetization as a function of temperature. On reducing the value of N_R , the system is driven more and more out of equilibrium. Indeed, Fig. 6.6(b) shows that with $N_R = 7$, the magnetization profile changes; in particular, it develops a discontinuity around a temperature $T_{trans} \approx 0.49$, reminiscent of a first-order phase transition. The transition temperature is denoted by the vertical dashed line. With $N_R = 3$, Fig. 6.6(c) shows that the discontinuity gets more pronounced, and T_{trans} is now shifted to a higher value (denoted again by the vertical dashed line). A new feature appears in this plot, namely, at a temperature $T_{dyn} \approx 0.4$, the magnetization attains the maximal value of unity, which it retains for all lower temperatures. This value of unity corresponds to a state in which the particles are very close to one another on the circle, thus defining a “collapsed” state. We found that this state, as well as the transition to it, persist on changing the system size N .

Now, it is known that trajectories of ensembles of dissipative dynamical systems forced by the same realization of a stochastic noise converge to a single one [197–200]. These attracting trajectories are referred to as the ones due to the so-called stochastic attractor. Although we did not perform a detailed characterization of the collapse in our model, we believe that the phenomenon is related to stochastic attractors.

Coming back to Fig. 6.6(c), we see that for temperatures $T_{dyn} < T < T_{trans}$, the magnetization shows strong fluctuations. Reducing the number of excited modes to a single one, namely, to the one that coincides with the Fourier mode of the HMF potential, it seems from Fig. 6.6(d) that only the dynamical transition to the collapsed state at a temperature $T_{dyn} \approx 0.66$ persists.

The hint that the nature of the phase transition at T_{trans} is of first-order comes from the hysteresis plots of Fig. 6.7. To obtain these plots, one monitors the magnetization while tuning adiabatically the kinetic temperature across T_{trans} from higher to lower values and back to complete a full cycle. As is evident from Fig. 6.7, the observed hysteresis is between the collapsed state and the zero-magnetization state. In principle, it should be possible to observe a hysteretical behavior between the magnetized and the zero-magnetization state. To achieve this in simulations involving adiabatic tuning of temperature, one should not allow the system to make the transition to the collapsed state, which requires conditions close to those that ensure detailed balance. However, a possible drawback of this method is that closeness to detailed balance might lead to narrow hysteresis loops. Moreover, the adiabatic tuning of temperature should not be very slow, as otherwise one observes bistability instead

6.4. NONEQUILIBRIUM PHASE TRANSITION AND COLLAPSE

of the hysteresis. All these factors make the observation of hysteresis between the magnetized and the zero-magnetization state difficult to observe numerically; further explorations of this will be the subject of future investigations.

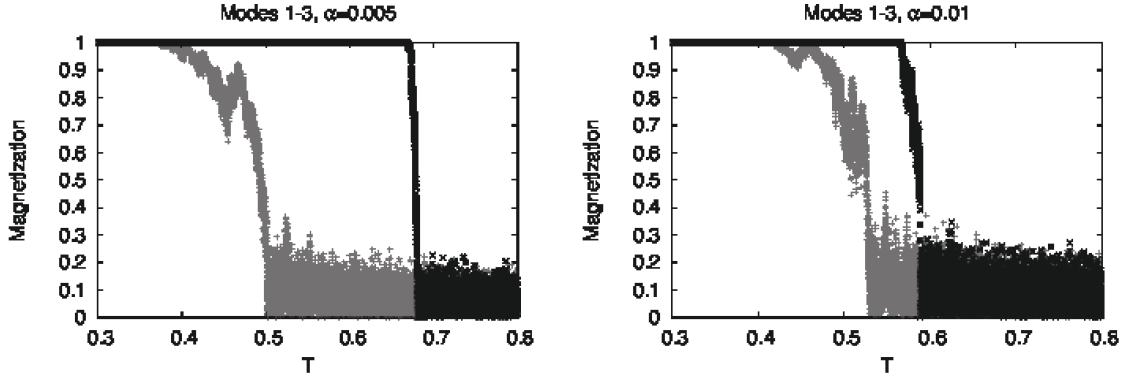


Figure 6.7 – Numerical simulation results for magnetization in the stochastically-forced HMF model as a function of adiabatically-tuned kinetic temperature T for two different values of α . In each case, the modes 1 – 3 are excited with amplitudes satisfying $c_1 = c_2 = c_3 = C(0)/6$, where $C(0) = 2T$. In all cases, $N = 5000$, $\Delta t = 0.01$, while the tuning rate for T is 10^{-5} . The grey points correspond to the case when the temperature is decreased from high values, while the black points correspond to the case when the temperature is increased from low values.

In order to explore further the region in Fig. 6.6(c) close to T_{trans} , and to ascertain the nature of the phase transition at T_{trans} , we fix the value of the temperature to be $T = 0.53$, and monitor the magnetization as a function of time. The time series of the magnetization is shown in Fig. 6.8(a), in which one observes clear signatures of bistability, whereby the system switches back and forth between homogeneous ($m \approx 0$) and inhomogeneous ($m > 0$) states. In addition, we show in Fig. 6.8(b) the distribution of the magnetization around the phase transition temperature: the distribution is bimodal with a peak around a zero value and another one around a positive value. When decreasing the temperature across the phase transition region, we clearly see that the peak heights of the distributions of the magnetization at the zero and non-zero values interchange. These two features, together with the hysteresis plots of Fig. 6.7, support the first-order nature of the transition around T_{trans} which can be estimated from Fig. 6.8(b) to be $T_{trans} \approx 0.532$. From Fig. 6.8, it is clear that the system has two well separated attractors, corresponding to the homogeneous and inhomogeneous states. A question of immediate interest is: How long does the system stay in one state before switching to the other? Let us define the residence time as the time the system stays in one state before it switches to the other. In the limit of low noise level α , there is a clear separation between the natural dynamical time and the typical residence time, as is evident from Fig. 6.8(a). As a result, one may conjecture that two successive switching events are statistically independent of one another. In case such a conjecture

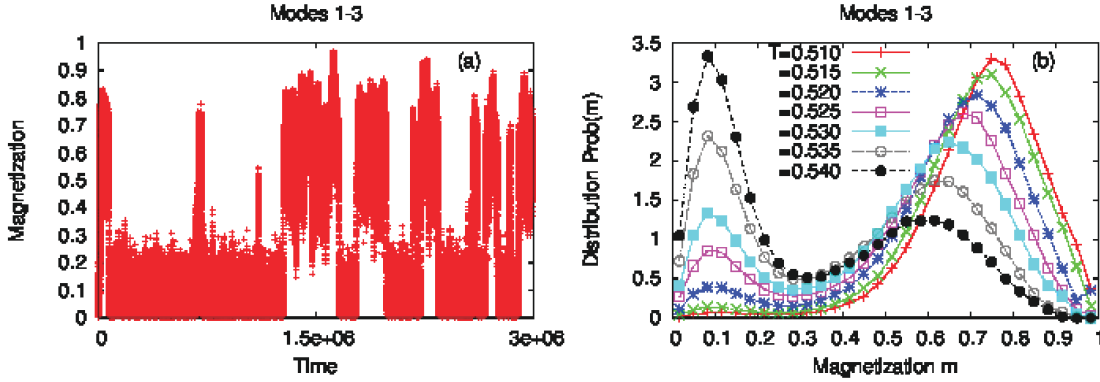


Figure 6.8 – (a) Numerical simulation results for magnetization in the stochastically-forced HMF model as a function of time at kinetic temperature $T = 0.53$, with $N = 5000$, $\alpha = 0.005$, $\Delta t = 0.01$, and with modes 1 – 3 excited, whose amplitudes satisfy $c_1 = c_2 = c_3 = C(0)/6$, where $C(0) = 2T$. The figure shows clear signatures of bistability in which the system during the course of evolution switches back and forth between spatially homogeneous ($m \sim O(0)$) and inhomogeneous ($m \sim O(1)$) states. (b) Distribution $Prob(m)$ of the magnetization m as a function of T at a fixed value of $\alpha = 0.01$. The data are obtained from numerical simulation results similar to those shown in Fig. 6.8(a) for magnetization in the stochastically-forced HMF model, with $N = 5000$, $\Delta t = 0.01$, and with modes 1 – 3 excited, whose amplitudes satisfy $c_1 = c_2 = c_3 = C(0)/6$, where $C(0) = 2T$.

holds for our model, the residence time statistics will be a Poisson process, characterized solely by the probability per unit time, λ_+ , of switching from the inhomogeneous state to the homogeneous state, and the probability per unit time, λ_- , for the reverse switch. The distribution of residence time τ in each phase is then exponential:

$$P_{\pm}(\tau) = \frac{1}{\lambda_{\pm}} \exp(-\lambda_{\pm}\tau), \quad (6.38)$$

so that the average residence times in the two states are $\tau_{\pm}^{res} = \frac{1}{\lambda_{\pm}}$. Such an exponential form of the residence time distribution is verified from our simulation data displayed in Fig. 6.9. Note that generating such a plot requires running simulations of the dynamics for long enough times so that the magnetization switches back and forth between the two states a sufficient number of times, and one has good statistics for the residence times. For low values of α , such as those used in Fig. 6.9, this was often not feasible due to very long simulation times. This results in bad statistics, and hence, the form of the plot displayed in Fig. 6.9, which, though good, may be improved upon by running longer simulations. We conclude that our conjecture of two successive jumps being independent holds for our model, and that the average residence time fully characterizes the switching process for small enough α .

We now discuss how the residence times depend on the system parameters, in particular, on α . For an equilibrium system, the type of switching process described above is an activation process with a residence time described by the Arrhenius law. A simple model of

6.4. NONEQUILIBRIUM PHASE TRANSITION AND COLLAPSE

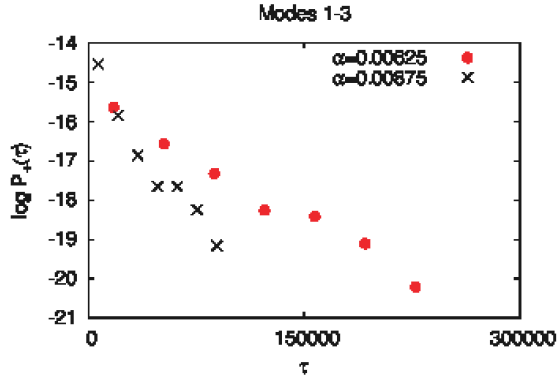


Figure 6.9 – Distribution of the residence time τ in the inhomogeneous state, for two values of α . The data are obtained from simulations with modes 1 – 3 excited, whose amplitudes satisfy $c_1 = c_2 = c_3 = C(0)/6$, where $C(0) = 2T$. Here, the kinetic temperature $T = 0.53$, while $\Delta t = 10^{-2}$, $N = 5000$.

such an activation process is the Langevin dynamics of a Hamiltonian system in a potential \mathcal{V} . The noise level is then related to the temperature, and the Arrhenius law takes the form [165, 201–203]

$$\tau_+^{res} \propto \exp(\Delta\mathcal{V}_{+-}/\alpha), \quad (6.39)$$

$$\tau_-^{res} \propto \exp(\Delta\mathcal{V}_{-+}/\alpha). \quad (6.40)$$

Here, $\Delta\mathcal{V}_{+-}$ and $\Delta\mathcal{V}_{-+}$ are respectively the potential energy barrier as observed from the inhomogeneous and the homogeneous state. In a non-equilibrium context such as ours, there is no obvious equivalent of a potential, but the law given by Eqs. (6.39) and (6.40) is expected to hold on a fairly general basis, in the limit of small noise. This may be established from the instanton theory, or, from the Freidlin-Wentzell theory, which allows to compute \mathcal{V} explicitly for a given model [109, 204]. Our system does not fulfill the hypothesis of Freidlin-Wentzell theory, nevertheless, it is interesting to check if the law given by Eqs. (6.39) and (6.40) holds. Our simulation data shown in Fig. 6.10 show that the dependence of τ_{\pm}^{res} on α , as in Eqs. (6.39) and (6.40), holds also for our model, thereby suggesting that in the limit of low noise, the system behaves as one with transitions activated by a weak noise.

We conclude this section by describing briefly the algorithm to find $P_{\pm}(\tau^{\pm})$ to produce Fig. 6.9, and τ_{\pm}^{res} to produce Fig. 6.10. To this end, one has to identify from the time series data of the magnetization (see Fig. 6.8(a) for an example) the switching time instants between the two states. In the limit of very small α , the distinction between two states should be obvious. However, we could not reach such a limit in our numerical simulations because the simulation time grows exponentially with $1/\alpha$ (see Fig. 6.10). For intermediate values of α , it is then a challenge to define precisely the two states. Indeed, as may be seen in Fig. 6.8(a), the data show strong fluctuations and hence, one needs to filter out “spurious” switching events and retain only the genuine ones. This may be done efficiently as we now discuss.

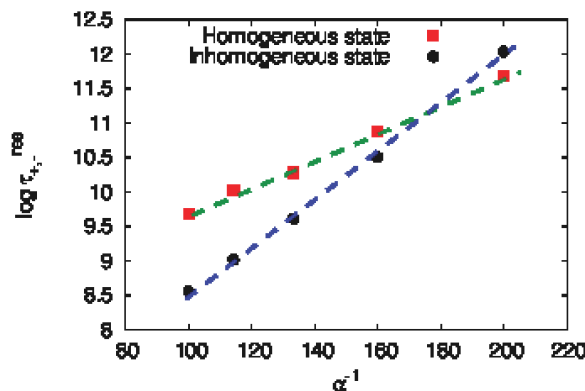


Figure 6.10 – The plot shows as a function of $1/\alpha$ the log of the mean residence time $\tau_{+,-}^{res}$ in the two bistable states, namely, the inhomogeneous ($m > 0$) state and the homogeneous state ($m \approx 0$). The plot is based on data obtained from simulations with modes 1–3 excited, whose amplitudes satisfy $c_1 = c_2 = c_3 = C(0)/6$, where $C(0) = 2T$. Here, the kinetic temperature $T = 0.53$, while $\Delta t = 10^{-2}$, $N = 5000$. The straight line fits imply that $\tau_{+,-}^{res} \sim \exp(1/\alpha)$, in accordance with Eqs. (6.39) and (6.40). That the slopes of the two straight lines in the plot are different could be due to the fact that the height of the barrier is different when observed from the inhomogeneous and the homogeneous state.

We first obtain from the data a rough estimate of the mean of the magnetization when the system is in the two states, the homogeneous and the inhomogeneous one. Let us denote by $m_>$ and $m_<$ these estimates when the system is in the inhomogeneous and the homogeneous state, respectively. Let us define a “threshold” value of the magnetization m_{th} as the average of $m_>$ and $m_<$; magnetization crossing this threshold to switch from one state to another however is not a precise enough criterion to define a switching event, as is obvious from Fig. 6.8. We thus resort to our algorithm which we now illustrate for the case when the system is in the homogeneous state; when the system is in the inhomogeneous state, the algorithm may be defined in a manner similar to the one below. In our algorithm, we identify a switching event as the one for which the following two conditions are satisfied, namely, (i) that the magnetization crosses the threshold to switch from the homogeneous to the inhomogeneous state, (ii) the magnetization after the switching reaches the value $m_>$ before reaching the value $m_<$. When a switching event occurs, the switching time is defined as the time at which the magnetization crossed the threshold. This algorithm allows us to precisely define the switching times, from which we compute the switching time statistics $P_{\pm}(\tau_{\pm})$, and hence, the mean residence time τ_{\pm}^{res} .

6.5 Conclusions and perspectives

In this Chapter, we have considered long-range interacting particle systems driven by external stochastic fields, thereby leading to generic nonequilibrium stationary states.

6.5. CONCLUSIONS AND PERSPECTIVES

To study spatially homogeneous stationary states, we developed a kinetic theory approach by generalizing the known results for isolated long-range systems. Our theoretical approach is quite general, being applicable to any long-range inter-particle potential, space dimensions and boundary conditions. Our extensive numerical simulations on a paradigmatic model of long-range interacting systems demonstrated a very good agreement with the theory. We observe that this is a non trivial result: On the one hand, the kinetic theory approach (mainly because of the truncation of the hierarchy) cannot be made rigorous. On the other hand, because of the difficulties introduced by strong non-linearities, even the Lenard-Balescu equation has not been tested extensively against numerical simulations [167, 171, 172]; the approximate Landau equation is more often used in plasma community and the analogous methods of Chandrasekar is used in astrophysics.

Besides kinetic theory, our simulations for the representative case of the stochastically forced HMF model, illustrated interesting bistable behavior between homogeneous and inhomogeneous states, with a mean residence time that diverges as an exponential in the inverse of the strength of the external stochastic forces in the limit of low values of such forces. Analogous bistable behaviors have been observed for the stochastically forced Euler equation in [187]. This kind of behavior is analogous to the one observed in real geophysical systems such as the reversal of Earth magnetic field [205], the multiple equilibrium of atmospheric flows [206] or the paths of the Kuroshio current [207]. We believe that such phase transitions are essential phenomena for geophysical flows and climate, for which the two-dimensional Euler equations are a simplified paradigmatic model. There exists a very strong analogy between the two-dimensional Euler equations and the Vlasov equation relevant for leading order dynamics of the model we discuss in this Chapter. One of the motivations of the present work is to be able to study analogous phenomena in a setup for which the theory can be more easily worked out.

Let us note that another route to deriving the kinetic theory studied in this paper is to adopt an approach similar to the one due to Klimontovich for isolated systems, by writing down the time evolution equation for the noise-averaged empirical measure $\rho(p, q, t) = (1/N) \sum_{i=1}^N \langle \delta(q_i(t) - q) \delta(p_i(t) - p) \rangle$. In the resulting equation, the noise appears as a multiplicative term, which can be treated perturbatively, leading to the kinetic equation (6.30). We note that Ref. [208] presents a computation of this kind, which do not quite agree with the ones obtained in our work; the reason for this disagreement is unknown, but the very good agreement between our theoretical predictions and numerical simulations (which have not been performed in [208]) give us confidence in the kinetic equation (6.30) derived here¹.

¹We also observe that, differently to our kinetic equation, the one derived in [208] does not respect the energy balance, Eq. (6.9).

CHAPTER 6. STOCHASTIC FORCING ON PARTICLE SYSTEMS

This work leaves open some interesting issues, e.g., for technical simplicity, we only studied the stationary states of the kinetic equation and not its dynamics. This could probably be done using a numerical method analogous to the one developed here to find stationary states.

Another open point is about the relevance of the kinetic theory to describe a single trajectory. Indeed, the kinetic theory as developed here describes the average over noise realizations of the dynamics of the system. However, it is not clear for the moment how close a single trajectory of the stochastic system is to the average. Preliminary analytical results in this direction show that the variance of the trajectories is smaller when forcing a large number of modes. Anyway, preliminary results from numerical simulations show that the description given by the kinetic theory is good for every forcing we have used.

Moreover, we assumed an homogeneous stationary state for the development of the kinetic theory. We think it is possible to generalize the theory to non-homogeneous states at least when the single particle dynamics is integrable so that action-angle variables can be used. In this regard, the method due to Heyvaerts reported recently [169], and the analysis of the Landau damping for some non-homogeneous states presented in [163, 164] are the technique we have in mind to handle the problem.

However, we expect that the resulting kinetic equation, similarly to the Lenard-Balescu equation for non-homogeneous states obtained in [169], will be so complex that it will not be simple to extract some information on the behavior of the system from it. For this reason, instead of aiming to write down analytically a kinetic equation, it could be more useful to solve numerically the second equation of the BBGKY hierarchy with techniques similar to those which will be presented in the next Chapter. Anyway, the fact that for non-homogeneous states different spatial modes do not decouple in the linear Vlasov equation (see Section 4.4.1) makes us wonder on the feasibility of such approach. In this respect, the techniques developed by Patelli et al. [127] to work out the linear response for non-homogeneous states without the using action-angle variable could come in help.

The most interesting perspective of this work is to develop kinetic theories similar to the one analyzed here for models relevant for geophysical applications. Models of two-dimensional and quasi-two dimensional turbulence such as the Euler equation, the beta-plane barotropic equations, the quasi-geostrophic equations and the shallow-water equations do share important properties with the Vlasov equation, relevant for leading order dynamics of the model we discuss in this Chapter. In the next one, we will start the develop of kinetic theory for the stochastically forced Euler equation, which is the simpler one among turbulence models.

7

Stochastic forcing on fluid models

Stochastically forced long-range interacting systems naturally arise in the context of geophysical flows. For example, in planetary atmospheres and in oceans, large scale structures with very long life-times are very common [108, 209–211]: jet streams, cyclones and anti-cyclones, currents such as the Gulf Stream, ocean rings, ... These structures emerge from a balance between the energy injected by the environment (due to, e.g. solar heating, wind on the surface of the oceans, action of different layers in the atmosphere, ...) resulting in turbulent fluctuations at small spatial scales, and dissipation due to boundary effects. Large scale structures can be interpreted as non-equilibrium stationary states.

How to model such phenomena depends both on the degree of accuracy and on the physical insight that one wants to obtain. On one side, there is the very detailed global circulation model, including not only fluid modeling but also thermodynamic terms for various energy sources, usually employed for weather forecasting and for climate modeling. However, as it usually happens for realistic models, the only method of analysis are numerical simulations and it is hard to get physical insight from the outcomes, because of the many parameters involved. For this reason, simplified models play an important role; in this respect, we can identify a hierarchy of models going from the primitive equations, through the shallow-water and quasi-geostrophic equations, to the barotropic beta-plane and two-dimensional Euler equations which are simpler and simpler but relevant for the physics of large scale structures.

Similar approaches to the kinetic theory have already been considered in the literature for the description of the formation, of the evolution and of the qualitative properties of large scale structures: we highlight in this respect the second order closure expansion [134, 212–214] and the stochastic structural stability theory [132, 215, 216]. However, most of these works are of phenomenological in nature, presenting and discussing results of direct numerical integration of equations similar to the first two equations of the BBGKY hierarchy presented in previous Chapters. In particular, it is usually not recognized that the kinetic theory is a perturbative approach in the limit of small forcing and dissipation parameter is not realized. Moreover, no analysis on the validity and the accuracy of the ap-

proximations is proposed; the presence of a time-scale separation between the time-scale of evolution of the mean flow and of the fluctuations.

We believe that it is important to develop a theoretical framework, both for clarifying when a kinetic theory approach is expected to give reliable results and to find the simplest possible way to obtain explicit predictions about the large scale structures attained and on their evolution.

In this Chapter we present preliminary results on the generalization of the kinetic theory developed in Chapter 6 to the case of fluid models. To begin with this study, we consider here the simplest possible case, the stochastically forced two-dimensional Euler equation under the hypothesis that the average flow is a jet stream. We show how the kinetic theory can be developed and we describe how one might predict the non-equilibrium stationary states and the slow evolution of the system. We do not discuss here explicit results, there being currently in development; we are working on this topic in collaboration with F. Bouchet and T. Tangarife [217].

The Chapter is organized as follows. In Section 7.1, we introduce the stochastic Euler equation and we describe the general structure of kinetic theory for fluid models. In Section 7.2, we discuss the Orr mechanism, an analogous phenomena to the Landau damping, which will be useful to prove the consistency of the kinetic theory approach. In Section 7.3 we consider the Lyapunov equation, analogous to the second equation of the BBGKY hierarchy in Chapter 6; we show that the quasi-linear approximation is well posed and that, also in this case, there is a time-scale separation in the evolution of the mean flow and of the fluctuations. Then, in Section 7.4, we discuss one possible way to find the stationary solution for two-point correlations. The difficulty with respect to Chapter 6 is that this solution cannot be found analytically but numerically techniques have to be employed. We conclude in Section 7.5 discussing how we think to pursue this work.

7.1 Quasi-linear approximation

We start from the stochastic two-dimensional Navier-Stokes equation

$$\partial_t \omega + \mathbf{v} \cdot \nabla \omega = \nu \Delta \omega - \alpha \omega + \sqrt{2\sigma} F(\mathbf{r}, t), \quad (7.1)$$

where $(x, y) = \mathbf{r} \in \mathcal{D}$, $\mathbf{v}(\mathbf{r}, t)$ is the two-dimensional non divergent velocity field ($\nabla \cdot \mathbf{v} = 0$), and $\omega = (\nabla \wedge \mathbf{v})$ the vorticity. We will consider periodic boundary conditions over $\mathcal{D} = [0, L_x] \times [0, L_y]$, even if the discussion can be easily generalized to more general settings. ν is the viscosity, α is the Rayleigh friction parameter: indeed, the term $-\alpha \omega$ modeling large scale friction due for example to boundary effects; σ is the energy injection rate (see below). The stream function $\psi(\mathbf{r}, t)$ is defined by $\mathbf{v} = (-\partial_y \psi, \partial_x \psi)$, and is related to the vorticity

7.1. QUASI-LINEAR APPROXIMATION

through $\omega = \Delta\psi$. The velocity can be reconstructed from the vorticity using a Green function formalism; we will use the notation

$$\mathbf{v}(\mathbf{r}, t) = \mathbf{G}[\omega](\mathbf{r}, t) \quad (7.2)$$

where \mathbf{G} is the linear operator transforming the vorticity in the velocity; we do not need its explicit expression, for which we refer the reader to [104, 218].

The forcing F is a Gaussian process with zero average and variance

$$\langle F(\mathbf{r}, t)F(\mathbf{r}', t') \rangle = C(\mathbf{r} - \mathbf{r}')\delta(t - t'), \quad (7.3)$$

where we have assumed F invariant with respect to space translations. Even if more general Gaussian processes could be considered, this hypothesis will be essential for the following discussion, as we will consider mainly translational invariant averaged vorticity distributions. We denote by $f_{\mathbf{k}}$ the \mathbf{k} -th Fourier component of the correlation function:

$$f_{\mathbf{k}} = \frac{1}{L_x L_y} \int_{\mathcal{D}} d\mathbf{r} C(\mathbf{r}) e^{-i\mathbf{k}\mathbf{r}}, \quad (7.4)$$

where $\mathbf{k} = (2\pi n_x/L_x, 2\pi n_y/L_y)$ with n_x and n_y integers. We have the equality $f_{\mathbf{k}} = f_{\mathbf{k}}^* = f_{-\mathbf{k}}$ because F is real; moreover, as the correlation C is a positive function, we have $f_{\mathbf{k}} \geq 0$ for all \mathbf{k} . We set

$$\frac{1}{2} \sum_{\mathbf{k}} \frac{f_{\mathbf{k}}}{|\mathbf{k}|^2} = 1 \quad (7.5)$$

so that σ is the energy injection rate.

In the stochastic Navier-Stokes equation, it is natural to fix the the average energy to be of order one, by using the typical turnover time as a new time unit. Putting $t' = t\sqrt{\sigma/(2\alpha)}$, $\omega' = \omega\sqrt{2\alpha/\sigma}$, $\alpha' = (2\alpha)^{3/2}/(2\sqrt{\sigma})$ and $\nu' = \nu\sqrt{2\alpha/\sigma}$ and dropping the primes, the dimensionless Navier-Stokes equation becomes

$$\partial_t \omega + \mathbf{v} \cdot \nabla \omega = \nu \Delta \omega - \alpha \omega + \sqrt{2\alpha} F(\mathbf{r}, t). \quad (7.6)$$

The unforced equation ($\alpha = \nu = 0$) is the Euler equation and conserves energy

$$\mathcal{E}[\omega] = \frac{1}{2} \int_{\mathcal{D}} \mathbf{v}^2(\mathbf{r}, t) d\mathbf{r} = -\frac{1}{2} \int_{\mathcal{D}} \omega(\mathbf{r}, t) \psi(\mathbf{r}, t) d\mathbf{r} \quad (7.7)$$

and all Casimirs, defined as

$$\mathcal{C}[\omega] = \int_{\mathcal{D}} s(\omega(\mathbf{r}, t)) d\mathbf{r} \quad (7.8)$$

for every function s ; the quadratic invariant $Z = \int_{\mathcal{D}} d\mathbf{r} \omega^2(\mathbf{r}, t)$ is called enstrophy. Euler equation shares many analogies with the Vlasov equation, both of them being advection equations of a scalar quantity [219, 220].

CHAPTER 7. STOCHASTIC FORCING ON FLUID MODELS

We can write the evolution of the energy for the dynamics (7.6). Taking the time derivative of the Energy functional in Eq. (7.7), using the Ito's formula and averaging over noise realizations, we get

$$\left\langle \frac{d\mathcal{E}}{dt} \right\rangle = -\nu \langle Z \rangle - 2\alpha \langle \mathcal{E} \rangle + \alpha. \quad (7.9)$$

The energy has, for small α and ν , a slow evolution on a time-scale determined by $1/\alpha$ and $1/\nu$.

For flows with large scale structures, Rayleigh friction dominates dissipation: $2\alpha \langle \mathcal{E} \rangle \gg \nu \langle Z \rangle$. Moreover, for most geophysical flows and experiments, the case of weak forcing and dissipation (inertial limit) is the relevant one. It is then natural to study the stochastic Navier-Stokes equation in the joint limits $\alpha \ll 1$ and $\nu \ll 1$, such that $\alpha/\nu \gg 1$. We then get the so-called stochastic Euler equation

$$\partial_t \omega + \mathbf{v} \cdot \nabla \omega = -\alpha \omega + \sqrt{2\alpha} F(\mathbf{r}, t), \quad (7.10)$$

for which we describe the kinetic approach in the following. From the energy balance for the stochastic Euler equation, Eq. (7.9) with $\nu = 0$, it is then natural to suppose that the evolution will be described at leading order by the Euler equation. Weak stochastic forces, of order α , lead to weak correlations that induce a long-time evolution on a time scale of order $1/\alpha$.

Let us now describe the kinetic approach¹: we use here the quasi-linear approximation [221]. Let us consider the projection operator \mathcal{P} on slow modes; in general, \mathcal{P} is the Fourier transform on the mode on which the system has a large scale structure. For simplicity, we will restrict here to the case of large scale structures invariant with respect to translations in the x direction, so that we set

$$h_0(y) \equiv \mathcal{P}[h](y) = \frac{1}{L_x} \int_0^{L_x} dx h(\mathbf{r}) \quad (7.11)$$

for any function h . We also suppose in the following $\mathcal{P}[F] = 0$, meaning that there is no forcing at large scales.

We call base flow the flow specified by $\omega_0 = \mathcal{P}[\omega]$, $\mathbf{v}_0 = \mathcal{P}[\mathbf{v}]$ and $\psi_0 = \mathcal{P}[\psi]$; we readily see that $\mathbf{v}_0(y) = (U(y), 0)$ for some function $U(y)$; this is called a shear flow. The fluctuations from the base flow will be denoted by

$$\sqrt{\alpha} \delta \omega = \omega - \mathcal{P}[\omega] = \omega - \omega_0 \quad (7.12)$$

and analogously for $\delta \mathbf{v}$ and $\delta \psi$. With this notation, we mean that $\delta \omega$ is of order one, and this is the analogous rescaling as we had in Chapter 6 for the connected part of two particle

¹A more formal treatment, which is the analogous to the BBGKY hierarchy presented in Chapters 4 and 6 for particle systems, could be also used and goes under the name of cumulant expansion, see for example [212].

7.1. QUASI-LINEAR APPROXIMATION

correlations. This can be expected because fluctuations are induced by a Gaussian process with variance proportional to $\sqrt{\alpha}$; however, a formal justification of this rescaling goes exactly as in Chapter 6 through the cumulant expansion, a hierarchy analogous to the BBGKY hierarchy. One starts introducing the cumulants

$$\mathcal{P}[\delta\omega(\mathbf{r}_1, t)\delta\omega(\mathbf{r}_2, t)] \quad (7.13)$$

$$\mathcal{P}[\delta\omega(\mathbf{r}_1, t)\delta\omega(\mathbf{r}_2, t)\delta\omega(\mathbf{r}_3, t)] \quad (7.14)$$

$$\dots \quad (7.15)$$

Then, with the same reasoning as in Appendix D.2, one can show that it is self-consistent to suppose

$$\alpha\mathcal{P}[\delta\omega(\mathbf{r}_1, t)\delta\omega(\mathbf{r}_2, t)] \sim \alpha \quad (7.16)$$

$$\alpha^{3/2}\mathcal{P}[\delta\omega(\mathbf{r}_1, t)\delta\omega(\mathbf{r}_2, t)\delta\omega(\mathbf{r}_3, t)] \sim \alpha^{3/2} \quad (7.17)$$

$$\dots \quad (7.18)$$

and thus we have $\alpha\delta\omega \sim \sqrt{\alpha}$. We do not enter in such a derivation², being very similar to the case of Chapter 6.

Taking the projection of the stochastic Euler equation (7.10), we get

$$\partial_t \omega_0 + \alpha\mathcal{P}[\delta\mathbf{v} \cdot \nabla \delta\omega] = -\alpha\omega_0, \quad (7.19)$$

where we have used that, by definition, we have $\mathcal{P}[\delta\omega] = 0$ and that any shear flow is a stationary solution of the Euler equation ($\mathbf{v}_0 \cdot \nabla \omega_0 = 0$).

The evolution of the base flow, in Eq. (7.19), is coupled to the equation which determines the evolution of $\delta\omega$. The equation for $\delta\omega$ can be obtained subtracting Eq. (7.19) from the stochastic Euler equation (7.10)

$$\partial_t \delta\omega + L_{\omega_0} \delta\omega + \sqrt{\alpha}[\delta\mathbf{v} \cdot \nabla \delta\omega - \mathcal{P}[\delta\mathbf{v} \cdot \nabla \delta\omega]] = -\alpha\delta\omega + \sqrt{2}F, \quad (7.20)$$

where $L_{\omega_0} \delta\omega$ is the linearized Euler operator around the base flow ω_0 and acting on $\delta\omega$. Explicitly, it reads

$$L_{\omega_0} \delta\omega = \mathbf{v}_0 \cdot \nabla \delta\omega + \delta\mathbf{v} \cdot \nabla \omega_0. \quad (7.21)$$

The term in square brackets of Eq. (7.20) describes fluctuations of a two-point function. The quasi-linear approximation consists in neglecting this term to obtain, instead of Eq. (7.20), the following

$$\partial_t \delta\omega + L_{\omega_0} \delta\omega = -\alpha\delta\omega + \sqrt{2}F. \quad (7.22)$$

²We only stress that, for such an argument to be valid, the hypothesis that $\mathcal{P}[F] = 0$ is necessary.

CHAPTER 7. STOCHASTIC FORCING ON FLUID MODELS

The quasi-linear approximation is analogous to discard three-particles and higher order correlations in the BBGKY hierarchy for particle systems, as it can be seen by writing the cumulant expansion³. As in that case, it is not rigorously justified, but it is self-consistent, because the quantity

$$\sqrt{\alpha}[\delta\mathbf{v}\cdot\nabla\delta\omega - \mathcal{P}[\delta\mathbf{v}\cdot\nabla\delta\omega]] \quad (7.23)$$

is negligible in the limit $\alpha \ll 1$. Moreover, the quasi-linear approximation does not alter the energy balance, Eq. (7.9) with $\nu = 0$. This can be proven using the fact that \mathcal{P} is a projection operator ($\mathcal{P}^2 = 1$) and the same argument holds for the enstrophy.

We are mainly interested in the average of physical quantities over a time scale which is long with respect to the time-scale of the microscopic dynamics but short with respect to the time-scale of the evolution of the large scale structures. If the system has only one attractor, we can replace such average with an average over noise realizations, which will be denoted by $\langle \cdot \rangle$; we thus get from Eq. (7.19)

$$\partial_t \langle \omega_0 \rangle + \alpha \langle \mathcal{P}[\delta\mathbf{v}\cdot\nabla\delta\omega] \rangle = -\alpha \langle \omega_0 \rangle. \quad (7.24)$$

Moreover, replacing Eq. (7.19) by Eq. (7.24), we do not address the question of how close a single trajectory obtained from Eq. (7.19) is to the average. Of course this is a very important point both at theoretical level and for what concern applications. This question could be answered studying the variance of the term $\mathcal{P}[\delta\mathbf{v}\cdot\nabla\delta\omega]$. Even if the calculation is probably feasible, it goes beyond the scope we have here and we leave it for future investigations.

Equations (7.24) and (7.22) are still complicated because they are coupled: the simplest approximation is the Markovianization hypothesis, and it is based on the presence of a time-scale separation. From Eq. (7.24), we readily see that the base flow evolves on a time-scale of order $1/\alpha$. On the other hand, in Eq. (7.22), we see the presence of two separated time-scales in the evolution of $\delta\omega$: a time-scale of order one due to the term L_{ω_0} and a much longer time scale of order $1/\alpha$, given by the term $-\alpha\delta\omega$. It is then natural to approximate the dynamics replacing $\langle \mathcal{P}[\delta\mathbf{v}\cdot\nabla\delta\omega] \rangle$ in Eq. (7.24) by its steady state

$$\lim_{t \rightarrow \infty} \langle \mathcal{P}[\delta\mathbf{v}(\mathbf{r}, t) \cdot \nabla \delta\omega(\mathbf{r}, t)] \rangle = g^\infty[\omega_0](y), \quad (7.25)$$

where $g^\infty[\omega_0]$ is calculated from Eq. (7.22) supposing ω_0 fixed in time. Section 7.3 is devoted to prove that this procedure is well posed in the sense that $\langle \mathcal{P}[\delta\mathbf{v}\cdot\nabla\delta\omega] \rangle$ actually converges to a well defined function. This is due to the so-called algebraic Orr mechanism, which is the analogous to the exponential Landau damping for Euler equation present for homogeneous systems with long-range interactions, see the following.

Let us observe that, in Eq. (7.20), the term $-\alpha\delta\omega$ is of higher order in α , so that one could think to neglect it. However, as we will see in Section 7.3, such term just makes the

³Writing the cumulant expansions, one easily sees that the quasi-linear approximation exactly corresponds to discard three-points and higher order projections: $\mathcal{P}[\delta\omega(\mathbf{r}_1, t)\delta\omega(\mathbf{r}_2, t)\delta\omega(\mathbf{r}_3, t)], \dots$

7.2. THE LINEARIZED TWO-DIMENSIONAL EULER EQUATION

value of $\langle \mathcal{P}[\delta \mathbf{v} \cdot \nabla \delta \omega] \rangle$ in the regime $1 \ll t \ll 1/\alpha$ very similar to the asymptotic value. This is consistent with the physical interpretation of the $t \rightarrow \infty$ limit in Eq. (7.25). Indeed, on a time-scale of order $1/\alpha$, the base flow ω_0 changes so that the Markovianization hypothesis surely breaks down.

As in the case of the stochastically forced systems with long range interactions, a necessary condition for the time-scale separation to be valid is that the base flow is a stable solution of the Euler equation for all times t . Indeed if the initial condition is not stable, the average of the base flow $\langle \omega_0 \rangle$ will have a fast evolution on a time scale of order one, breaking down the time-scale separation. Next Section is devoted to a brief review of some notions of stability of a stationary flow of the Euler equation.

To summarize we obtained the kinetic equation

$$\partial_t \langle \omega_0 \rangle + \alpha g^\infty[\omega_0] = -\alpha \langle \omega_0 \rangle \quad (7.26)$$

where $g^\infty[\omega_0]$ is defined by Eq. (7.25) and $\delta \omega$ satisfies Eq. (7.22) with ω_0 fixed in time. We will not write explicitly a single kinetic equation for the evolution of $\langle \omega_0 \rangle$, because we are not able to compute analytically $g^\infty[\omega_0]$; however, we believe that the computation of $g^\infty[\omega_0]$ can be afforded numerically, as it is described in Section 7.4.

7.2 The linearized two-dimensional Euler equation

Before proving that the limiting procedure in Eq. (7.25) is actually well defined, we need to briefly review the notions of linear stability for the two-dimensional Euler equation. We concentrate here on the notions of spectral and asymptotic stability, the latter mechanism being the analogous for the Euler equation to the Landau damping for the Vlasov equation. The presentation we gave in this Section is very partial: only the results useful for the following have been discussed. We address the reader to [218, 222] and references therein for more complete expositions on the Orr mechanism and to [223] general discussion of stability concepts in fluid dynamics.

7.2.1 Spectral stability

Let us consider the two-dimensional Euler equation linearized around the base flow ω_0

$$\partial_t \tilde{\omega} + L_{\omega_0}[\tilde{\omega}] = 0. \quad (7.27)$$

As we have supposed the system to be translational invariant along x , it is useful to consider the Fourier transform in the x direction: we use the notation $\tilde{\omega}_m(y, t)$ for the Fourier

CHAPTER 7. STOCHASTIC FORCING ON FLUID MODELS

transform with respect to the first variable of $\tilde{\omega}(x, y, t)$ and analogous expressions for other quantities. In Fourier transform, Eq. (7.27) is

$$\partial_t \tilde{\omega}_m + L_{\omega_0, m} [\tilde{\omega}_m] = 0. \quad (7.28)$$

Observe that, as ω_0 is a shear flow, each mode of the Fourier transform in the x direction is decoupled from the others.

The spectral stability is defined looking for solutions of the form $\tilde{\omega}_m(y)e^{-imst}$ which thus verify

$$L_{\omega_0, m} [\tilde{\omega}_m] = im s \tilde{\omega}_m, \quad (7.29)$$

and are called proper modes. The explicit expression for the m -th component of the Fourier transform of the Euler operator linearized around ω_0 and acting on $\tilde{\omega}_m$ is given by

$$(L_{\omega_0, m} \tilde{\omega}_m)(y, t) = im U(y) \tilde{\omega}_m(y, t) - U''(y) \tilde{\mathbf{v}}_m^{(y)}(y, t), \quad (7.30)$$

where we have used that $\mathbf{v}_0 = (U(y), 0)$ and we denote by $\tilde{\mathbf{v}}^{(x)}$ and $\tilde{\mathbf{v}}^{(y)}$ the first and second component of $\tilde{\mathbf{v}}$. Observe that $L_{\omega_0, -m} = L_{\omega_0, m}^*$.

If a base of regular solutions $\{\tilde{\omega}_m^s\}$ of this equation can be found, one can write every solution of Eq. (7.28) as a superposition of them. One may thus study the asymptotic stability of a given initial condition, as a function of the sign of $\text{Im}(s)$. This is the so called spectral stability. However, in many cases⁴, Eq. (7.29) does not admit any solution except, of course, for $m = 0$. This is due to the fact that the operator $L_{\omega_0, m}$ acts on a infinite dimensional space.

If $\{\tilde{\omega}_m, s\}$ is a solution of Eq. (7.29), then also $\{\tilde{\omega}_m^*, s^*\}$ is a solution: stable proper modes exist ($\text{Im}(s) < 0$) if and only if unstable proper modes exist ($\text{Im}(s) > 0$). Very classical results [223, 224] on the stability of stationary flows are focused on the absence of unstable proper modes. For example, Rayleigh proved [223] that a necessary condition for spectral instability is the presence of points y_I such that $U''(y_I) = 0$.

7.2.2 Asymptotic stability: the Orr mechanism

Let us consider the case in which no modes (neither unstable nor neutral) are present. In this case, the Euler equation show a mechanism analogous to the Landau damping that we have seen in Chapter 4 for the Vlasov equation. This phenomena, called Orr mechanism [225], was first studied in the case of a linear profile $U(y) = \sigma y$ in [222]. We briefly review here the results contained in [218], in which the problem is addressed for a shear flow, even in the case in which the profile $U(y)$ admit stationary points y_c such that $U'(y_c) = 0$. The authors of [218] have shown that the asymptotic behavior of the vorticity is given by

$$\tilde{\omega}_m(y, t) \sim_{t \rightarrow \infty} \tilde{\omega}_m^\infty(y) e^{-imU(y)t}. \quad (7.31)$$

⁴A simple example of a flow without modes is given by the linear shear flow $U(y) = \sigma y$, as it can be easily checked.

For the m -th velocity components one has:

$$\tilde{\mathbf{v}}_m^{(x)}(y, t) \sim_{t \rightarrow \infty} \frac{\tilde{\omega}_m^\infty(y)}{imU'(y)} \frac{e^{-imU(y)t}}{t} \quad (7.32)$$

for the x component, and

$$\tilde{\mathbf{v}}_m^{(y)}(y, t) \sim_{t \rightarrow \infty} \frac{\tilde{\omega}_m^\infty(y)}{im(U'(y))^2} \frac{e^{-imU(y)t}}{t^2} \quad (7.33)$$

for the y component. Analogously, for the stream function, it is proven that

$$\tilde{\psi}_m(y, t) \sim_{t \rightarrow \infty} \frac{\tilde{\omega}_m^\infty(y)}{(imU'(y))^2} \frac{e^{-imU(y)t}}{t^2}. \quad (7.34)$$

In all the above formula, higher order corrections are present and decay with higher powers in $1/t$. One should also observe that the initial condition enters only in $\tilde{\omega}_m^\infty(y)$, which can be numerically computed from the initial condition $\tilde{\omega}(y, 0)$ without integrating the Euler equation.

These results are valid for every shear flow $U(y)$ also in the case of presence of stationary points y_c in the profile $U(y)$, but for points $y \neq y_c$. For $y = y_c$, the damping is still algebraic but no theoretical prediction is available⁵.

One thus find an algebraic damping of the velocity which is the analogous to the exponential damping of the potential given by the Landau damping for homogeneous states. The emergence of an algebraic behavior is due to the singularities of the Green functions necessary to invert the relations between the velocity and the vorticity.

7.3 Stochastic Orr mechanism

In Section 7.1, using the quasi-linear approximation, we have obtained the two equations (7.26) and (7.22) describing, respectively, the averaged evolution of the base flow and of the fluctuations. Thanks to the presence of a time-scale separation, we have decoupled these two equations, reducing the problem to the computation of $g^\infty[\omega_0]$, defined in Eq. (7.25). However, we have not checked that the limiting procedure in Eq. (7.25) is well-posed, that is the quantity $\langle \mathcal{P}[\delta \mathbf{v} \cdot \nabla \delta \omega] \rangle$ actually converges: this is the topic of the present Section. As we will see, an exponential convergence is ensured by the term $-\alpha \delta \omega$ in Eq. (7.22); however also neglecting such term, which in principle is of higher order in α , the Orr mechanism ensures an algebraic convergence.

Taking the Fourier transform of Eq. (7.22), we have that every component of the vorticity ($m \neq 0$) obeys a Ornstein-Uhlenbeck process

$$\partial_t \delta \omega_m + L_{\omega_0, m} \delta \omega_m + \alpha \delta \omega_m = \sqrt{2} \eta_m(y, t), \quad (7.35)$$

⁵See [218] for precise numerical results in the case $y = y_c$.

CHAPTER 7. STOCHASTIC FORCING ON FLUID MODELS

where $\eta_m(y, t)$ are independent complex Gaussian processes with correlation

$$\langle \eta_m(y, t) \eta_{m'}^*(y', t) \rangle = \delta_{m,m'} \sum_l f_{\mathbf{k}} e_l(y) e_l^*(y'), \quad (7.36)$$

where $\mathbf{k} = (m, l)$, components $f_{\mathbf{k}}$ being defined in Eq. (7.4) and $e_l(y) = e^{-ily}$.

The Lyapunov equation associated to Eq. (7.35) is

$$\partial_t \phi_m + L_{\omega_0, m}^{(1)} \phi_m + L_{\omega_0, -m}^{(2)} \phi_m + 2\alpha \phi_m = \sum_l f_{(m,l)} e_l(y) e_l^*(y'), \quad (7.37)$$

where

$$\phi_m(y, y', t) = \langle \delta \omega_m(y, t) \delta \omega_{-m}(y', t) \rangle. \quad (7.38)$$

Because of the linearity of the Lyapunov equation, we will consider in the following just the case in which the right hand side is given by $c_m(y)c_{-m}(y')$, where c_m are generic function such that $c_m^* = c_{-m}$; the general case can be recovered using Eq. (4.66).

We are interested in computing $\langle \mathcal{P} [\nabla \delta \omega \cdot \delta \mathbf{v}] \rangle$. Using the Fourier transform, it can be written as

$$\begin{aligned} \langle \mathcal{P} [\nabla \delta \omega(\mathbf{r}, t) \cdot \delta \mathbf{v}(\mathbf{r}, t)] \rangle = & \quad (7.39) \\ = \sum_m i m \langle \delta \omega_m(y, t) \delta \mathbf{v}_{-m}^{(x)}(y, t) \rangle + \langle (\partial_y \delta \omega_m(y, t)) \delta \mathbf{v}_{-m}^{(y)}(y, t) \rangle, \end{aligned}$$

and each component of the sum can be obtained as a linear transform of $\phi_m(y, y', t)$. We denote by $\mathbf{G}_m^{(x)}$ and $\mathbf{G}_m^{(y)}$ the first and second components of the linear operator \mathbf{G}_m which transforms the m -th component of the vorticity in the m -th component of the velocity. We then have

$$\mathbf{G}_{-m}^{(x)(2)}[\phi_m](y, y, t) = \langle \delta \omega_m(y, t) \delta \mathbf{v}_{-m}^{(x)}(y, t) \rangle, \quad (7.40)$$

where $\mathbf{G}_{-m}^{(x)(2)}$ acts on the second variable of ϕ , and analogously for the second quantity in the sum in Eq. (7.39).

We can then use Eq. (4.74) to compute $\langle \mathcal{P} [\delta \mathbf{v} \cdot \nabla \delta \omega] \rangle$. We have, for the two terms in Eq. (7.39)

$$\langle \delta \omega_m(y, t) \delta \mathbf{v}_{-m}^{(x)}(y, t) \rangle = 2 \int_0^t du \tilde{\omega}_m(y, u) \tilde{\mathbf{v}}_{-m}^{(x)}(y, u) e^{-2\alpha u} \quad (7.41)$$

and

$$\langle (\partial_y \delta \omega_m(y, t)) \delta \mathbf{v}_{-m}^{(y)}(y, t) \rangle = 2 \int_0^t du (\partial_y \tilde{\omega}_m(y, u)) \tilde{\mathbf{v}}_{-m}^{(y)}(y, u) e^{-2\alpha u} \quad (7.42)$$

where $\tilde{\omega}_m$ obeys to the linearized Euler equation (7.28) with the initial condition

$$\tilde{\omega}_m(y, t=0) = c_m(y) \quad (7.43)$$

and $\tilde{\mathbf{v}}_m$ is the associated velocity field.

From the previous expressions and the results presented in Section 7.2, one easily realizes that Eq. (7.39) converges for $t \rightarrow \infty$ to a well defined function whenever ω_0 has no unstable, nor neutral, modes. Clearly, the exponential term in Eq. (7.41) and (7.42), due to the effect of the Rayleigh friction on the evolution of the fluctuations, gives an exponential damping on a time-scale of order $1/(2\alpha)$. However, such a damping is not necessary to prove that the limiting procedure (7.39) is well defined.

At first sight, one could expect a logarithmic divergence of Eq. (7.39) if the exponential damping is neglected: indeed, both terms in the sum have this behavior. However, the detailed computation⁶ shows that the leading order behavior given by Eq. (7.41) and (7.42) exactly cancels out. Equation (7.39) does converge because the higher order corrections to the long-time behavior of the vorticity and the velocity are in powers of $1/t$. We thus conclude⁷ that, even neglecting the exponential damping given by the dissipation, the function $g^\infty[\omega_0]$ is well defined by the limiting procedure of Eq. (7.25).

Let us also comment on the effect of the friction term in Eq. (7.22): as anticipated before, it only gives an exponential damping to the integrands in Eq. (7.41) and (7.42). This is in agreement with the physical interpretation of the Markovianization: indeed, for every small α , we should remember that $1/\alpha$ is the typical time-scale on which ω_0 changes. Taking into account the Rayleigh friction on the evolution of the fluctuations, the value attained by $\langle \mathcal{P}[\delta\mathbf{v} \cdot \nabla \delta\omega] \rangle$ in the regime $1 \ll t \ll 1/2\alpha$ does not differ much with respect to the one attained in the $t \rightarrow \infty$ limit.

We conclude that the kinetic approach to the stochastic Euler equation as obtained here through the quasi-linear approximation is well posed. In next Section, we propose a method to numerically compute $\langle \mathcal{P}[\delta\mathbf{v} \cdot \nabla \delta\omega] \rangle$ and to evaluate the stationary state and the evolution of the kinetic equation (7.26).

7.4 How to obtain explicit results?

Differently to the case of stochastically forced particle systems, the analytic evaluation of Eq. (7.25), which would permit to explicitly write the kinetic equation (7.26), is probably not feasible. However, we expect that this does not restrict the applicability of the kinetic approach because we can numerically compute Eq. (7.25). We describe in this Section one of the methods that can be employed for this scope; other possibilities are currently under investigation.

⁶This has been already observed in [218, 226] for the self-consistency of the quasi-linear approximation for the two-dimensional Euler equation without the stochastic forcing and dissipation.

⁷This results can be extended even to the case of $y = y_c$ on the base of the numerical results reported in [218].

CHAPTER 7. STOCHASTIC FORCING ON FLUID MODELS

The filamentation phenomena given by the Orr mechanism (but this is a general phenomena in fluid dynamics, at least on a qualitative level) indicates the presence of structures which becomes finer and finer as the time goes on. From a numerical point of view, this fact leads to numerical instabilities in the solution of, for example, the linearized Euler equation; in general, a viscosity (or hyperviscosity) term regularizes these instabilities. However, for geophysical flows, the viscosity is often negligible on the time-scale of formation and evolution of large scale structures and it looks unphysical to add such a term just for numerical reasons. We thus looked for an integral equation to compute directly Eq. (7.25), which we expect to be simpler to be solved.

It is useful to rewrite Eq. (7.39) in the following way

$$\langle \mathcal{P} [\nabla \delta \omega(\mathbf{r}, t) \delta \mathbf{v}(\mathbf{r}, t)] \rangle = -\frac{d}{dy} \sum_m i m h_m(y, y, t), \quad (7.44)$$

where

$$h_m(y, y', t) = \langle \delta \omega_m(y, t) \delta \psi_{-m}(y', t) \rangle, \quad (7.45)$$

is called the Reynolds tensor. We recall that

$$\delta \omega_m(y, t) = \left(\frac{d^2}{dy^2} - m^2 \right) \delta \psi_m(y, t) \quad \Longleftrightarrow \quad \delta \psi_m(y, t) = \int dy' H_m(y, y') \delta \omega_m(y', t),$$

where H_m is the Green function of the Fourier transform of the Laplacian [218]. With this definition of h_m , the kinetic equation (7.26) is

$$\partial_t \langle \omega_0 \rangle(y, t) - \alpha \frac{d}{dy} \sum_m i m h_m^\infty(y, y) + \alpha \langle \omega_0 \rangle(y, t) = 0, \quad (7.46)$$

with⁸

$$h_m^\infty(y, y') = \lim_{t \rightarrow \infty} h_m(y, y', t) \quad (7.47)$$

and where we have used that

$$g^\infty[\omega_0](y) = -\frac{d}{dy} \sum_m i m h_m^\infty(y, y). \quad (7.48)$$

We want to write an integral equation for $h_m^\infty(y, y')$. For this scope, we first consider $\phi_m(y, y', t)$ defined in Eq. (7.38), that we recall obeys to

$$\partial_t \phi_m + L_{\omega_0, m}^{(1)} \phi_m + L_{\omega_0, -m}^{(2)} \phi_m - 2\alpha \phi_m = c_m(y) c_m^*(y'). \quad (7.49)$$

⁸With a similar reasoning to the one of the previous Section, we can prove that the $t \rightarrow \infty$ limit of h_m is well defined.

7.4. HOW TO OBTAIN EXPLICIT RESULTS?

Explicitly, this equation reads

$$\begin{aligned} \partial_t \phi_m(y, y', t) + [im(U(y) - U(y')) + 2\alpha] \phi_m(y, y', t) = \\ = imU''(y)h_m^*(y', y, t) - imU''(y')h_m(y, y', t) + c_m(y)c_m^*(y'). \end{aligned} \quad (7.50)$$

We can formally integrate such an equation, by regarding the terms on the r.h.s. as a source terms

$$\begin{aligned} \phi_m(y, y', t) = c_m(y)c_m^*(y') \int_0^t ds e^{-[im(U(y) - U(y')) + 2\alpha](s-t)} + \\ + im \int_0^t ds [U''(y)h_m^*(y', y, s) - U''(y')h_m(y, y', s)] e^{[im(U(y) - U(y')) + 2\alpha](s-t)} \end{aligned} \quad (7.51)$$

Using the relation between h_m and ϕ_m , the change of variables $s' = s - t$ and performing the $t \rightarrow \infty$ limit, we get the integral equation for $h_m^\infty(y, y')$

$$\begin{aligned} h_m^\infty(y, y') = -\frac{i}{m} \int dy_1 \frac{H_m(y', y_1) c_m(y) c_m^*(y_1)}{U(y) - U(y_1) - \frac{2i\alpha}{m}} + \\ + \int dy_1 \frac{H_m(y', y_1)}{U(y) - U(y_1) - \frac{2i\alpha}{m}} [U''(y)h_m^{\infty*}(y_1, y) - U''(y_1)h_m^\infty(y, y_1)]. \end{aligned} \quad (7.52)$$

The integral equation (7.52) is the main result of this Section. It is a closed integral equation for h_m of the form

$$r = S + T[r], \quad (7.53)$$

where S is a source term, not depending on the unknown h_m^∞ while T is the linear operator entering in Eq. (7.52). We can thus try to solve such an equation iteratively with a scheme of the form

$$r^{(k+1)} = S + T[r^{(k)}]. \quad (7.54)$$

On the one hand, we want to stress that we have no mathematical proof that such a scheme does converge to a self-consistent solution, neither in the case $\alpha = 0$ nor in the case $\alpha \neq 0$. On the other hand, we expect this equation to be simpler to solve with respect to the associated differential problem. Indeed, the quantities entering in Eq. (7.52) are only averaged quantities, in which the effect of filamentation is smoothed out. Some encouraging preliminary results on the solution of Eq. (7.52) has been obtained, in collaboration with F. Bouchet and T. Tangarife, numerically implementing the iterative algorithm [217]. We are not going to present them, being incomplete for the moment.

Once that one is able to obtain $h_m^\infty(y, y')$ for a generic base flow ω_0 , one can apply a first order Euler algorithm to integrate the kinetic equation (7.26). Otherwise, in the case

in which one is interested only in the stationary flow predicted by the kinetic equation, one can apply a second iterative scheme to the equation

$$g^\infty[\omega_0] = -\langle \omega_0 \rangle. \quad (7.55)$$

The stability of these methods in the actual case, as well as their practical implementation, is currently under investigation.

7.5 Conclusions and perspectives

We have presented in this Chapter some preliminary results on the generalization of the kinetic theory to the stochastically forced two-dimensional Euler equation, concentrating on the case of shear flows. We have seen how to develop the theory which we have shown to be well-posed.

Differently to the case of particle systems treated in Chapter 6, it is probably not possible to write explicitly a kinetic equation. Anyway, we do not expect that this does limit the predictions that is possible to obtain with the kinetic theory. We have proposed a numerical scheme that can be employed to evaluate the Reynold stresses; other ways are probably possible, even if not explored for the moment: indeed, the problem is reduced to solve the linear Euler equation. Semi-analytical (see for example [227]) or purely numerical methods may be employed for this scope.

We have not presented the explicit results we have on the iterative solution of the integral equation (7.52), being incomplete for the moment. We are currently working in collaboration with F. Bouchet and T. Tangarife [217] on these topics.

We expect that the techniques presented here can be used both to obtain the non equilibrium stationary states attained by the system at long times and the time-evolution of the mean flow using a simple Euler scheme to integrate Eq. (7.26). Our program is to compare these results with direct numerical simulations of the stochastically forced Euler equation.

As in the case of particle systems, we have only considered the evolution of the averaged base flow with respect to noise realizations. As in that case, an important question is to understand how far it is a single trajectory from the mean flow. We think that it is possible to answer to this question but our results are not conclusive for the moment.

The kinetic theory, as well as the numerical method presented in Section 7.4, has been sketched here for the two-dimensional Euler equation. The generalization to the barotropic beta-plane equation⁹, defined by

$$\partial_t q + \mathbf{v} \cdot \nabla q = -\alpha q + \sqrt{2\alpha} F, \quad q = \omega + \beta y, \quad (7.56)$$

⁹The term βy (beta effect) takes into account in the most simple way the effect of the Coriolis force.

7.5. CONCLUSIONS AND PERSPECTIVES

should present no additional difficulties. This simple model is already relevant for geophysical applications [108], for example for what concern the formation of jet streams in planetary atmospheres, and has already been studied using the quasi-linear approximation [134] with encouraging results.

On the other hand, more work is necessary to generalize the kinetic theory to quasi-geostrophic and shallow-water equations, as well to the primitive equations, or to cases where the mean flow is given by a vortex or by a dipole. An important point we understood in this respect is that it is probably not necessary to study the analogous to the Orr mechanism, which poses strong difficulties in many cases. Indeed, as we have seen in Section 7.3, the Rayleigh friction on the evolution of the fluctuations gives an exponential damping to the stochastic Orr mechanism which is not present in the deterministic case. Some weaker result on the asymptotic stability of the base flow, without an explicit computation of the decay rates of the velocity for large times as in Section 7.2, may thus be sufficient for the kinetic theory to be well-posed.

Conclusions and perspectives

We have discussed the results we obtained on long-range interacting systems forced by some external fields, considering both the cases of a deterministic and stochastic external driving.

In the case of deterministic perturbations (see Chapter 5), we asked the following question: how does a long-range interacting system prepared in a QSS react to an external forcing? We have performed a linear study obtaining the analogous to the Kubo formula which is valid for any Vlasov stationary state. However, the explicit application of such a formula is possible essentially with the techniques by which the Landau damping is derived. We thus obtained explicit theoretical predictions in the case of homogeneous stationary states. The results agree quite well with N -body simulations.

Later on, Ogawa et al. [126] obtained predictions also for non-homogeneous states in the cases in which the single-particle dynamics is integrable, so that action-angle variables can be used. Their work relies on the results obtained in [163, 164] on the Landau damping for these kind of states. Patelli et al. [127] have also obtained results for non-homogeneous states but without invoking action-angles variables: they assume that, under a perturbation saturating in time to some value, the system will converge to a stationary state; in the case it does, they obtain (with further approximations involving the conservation of the Casimirs) the time asymptotic behavior. However, the hypothesis and approximations they use have still to be investigated. We are working with Patelli to understand on the basis of his work if the techniques they developed could be useful to define the stability of a generic stationary state of the Vlasov equation, even in the cases in which the single-particle dynamics is not integrable.

Most of the work in this part of the thesis is devoted to the study of stochastically driven long-range interacting systems, in which the dynamics breaks the detailed balance and stationary states are maintained by currents of conserved quantities. Unlike systems with short-range interactions, stochastic forces in long-range interacting systems can act coherently on all the degrees of freedom, and not independently on each particle (e.g., gravitational or electric fields). Beside the fact that we are dealing with long-range interacting systems, the study of nonequilibrium stationary states (NESS) is an active area of research of modern day statistical mechanics. Our work provides, to the best of our knowledge, the first study of NESS in long-range systems with statistical mechanical perspectives.

Non equilibrium stationary states of this kind are very common in geophysics, where the energy injection on large scale structures is provided by turbulent fluctuations and the dissipation is given by friction at the boundaries of these structures. Unfortunately, the direct theoretical analysis of models which are relevant for geophysical applications is complicated at technical level. Because they are amenable for analytical results, we mainly concentrated

on particle systems.

In this case, we generalized the kinetic theory leading to the Lenard-Balescu equation for isolated long-range interacting systems, to describe the evolution of homogeneous stochastically driven systems in the limit of small forcing. To do it, we carefully reviewed the derivation of the Lenard-Balescu equation in Chapter 4, putting it on a general basis. We then used this general formulation to develop the kinetic theory for stochastically forced long-range interacting particle systems. Our theoretical approach is quite general, being applicable to any long-range inter-particle potential, space dimensions and boundary conditions.

Extensive numerical simulations on the stochastically forced HMF model demonstrated a very good agreement with the theory, predicting with a very high accuracy the velocity profile of homogeneous stationary states. We observe that this is a non trivial result: indeed, the kinetic theory approach (mainly because of the truncation of the hierarchy) cannot be made rigorous and it was not clear a priori how good are the predictions. In this respect we observe that, because of the difficulties introduced by strong non-linearities, even the Lenard-Balescu equation has not been tested extensively against numerical simulations; the only results we know in this direction are those in [167, 171, 172]. The approximate Landau equation is more often used in plasma community and the analogous method of Chandrasekhar is used in astrophysics.

A simple step forward, with respect to our work, is to work out explicitly the full time evolution as predicted by the kinetic equation (6.30) and to compare it with numerical simulations. In this respect, we also note that the kinetic theory as developed here does describe the average of the evolution over noise realizations. But how far is typically a single trajectory from this average? For the moment we have no final answer for this question, but we have some preliminary results saying that more the dynamics of the system is close to the detailed balance, smaller is the variance of the trajectories.

Other open questions concerning these works are: the possible generalization of the kinetic theory to describe the evolution of non-homogeneous states using the techniques developed in [163, 164, 169] when the single particle dynamics is integrable or those in [127] which, albeit approximate, do not rely on the hypothesis of integrability.

Beside kinetic theory, we numerically observed a very interesting bistable behavior between homogeneous and non-homogeneous states that we observed numerically when the parameters of the forcing are set in such a way that the system is close to a phase transition. We believe that such behaviors, already observed in stochastically forced Euler equations [187], are quite general phenomena in long-range interacting systems whose dynamics breaks the detailed balance and we believe that they are essential phenomena for geophysical flows. Similar phenomena indeed happen to the Earth magnetic field, to the Kuroshio current and in other systems. The theoretical understanding of such phenomena may be affordable with large deviations techniques; J. Laurie, F. Bouchet and O. Zaboronski have

preliminary results on this topic [228] for the two-dimensional Euler equation and the applicability of such methods to particle systems is actually under investigation.

One of the most interesting perspective of our work is, in our opinion, the generalization of the kinetic theory approach to fluids and, in particular, to models relevant for geophysical applications. In this respect, we have described our first efforts to generalize the kinetic theory to the stochastically forced Euler equation. There are already some approaches in literature, called second order closure expansion or stochastic structural stability theory, which are very close to kinetic theory, see for example [130–134]. However, these studies are of phenomenological nature and mainly based on direct numerical solution of the quasi-linear system. No theory is developed: they did not realized that the quasi-linear approximation is valid for small external forcing; they did not try to verify if the quasi-linear approximation is a well-posed procedure and, moreover, they do not use the time scale separation between the time-scale governing evolution of the mean flow and the one governing the relaxation of correlations.

It is necessary to develop a theoretical framework at least for two reasons: to clarify when the kinetic theory gives reliable predictions and to find the simplest possible way to obtain explicit results on the stationary state attained and on the evolution of the mean flow. In Chapter 7 we have described our first results in this direction working on the stochastically forced 2d Euler equation in the case of shear flows. We have however not shown the explicit predictions we have because the results are not satisfactory for the moment.

It is simple to generalize what we have presented in Chapter 7 to the barotropic dynamics on a beta plane, the model considered for example in [134], which is already relevant for geophysical applications in the explanation of strong jets in the planetary atmospheres. More effort is however necessary to deal with mean flows represented by vortices or to deal with more complicated models such as the Shallow water or the Quasi-geostrophic equations.

A

Appendix to Chapter 2

A.1 Density of states of the effective model

To solve the model in the microcanonical ensemble we need to calculate the density of states (2.41), i.e.,

$$\begin{aligned} \omega_N(E) &= \sum_{N_g=0}^N \frac{N!}{N_g!(N-N_g)!} \int_{-\infty}^{\infty} dp_1 \cdots dp_N \int_{-\pi}^{\pi} d\vartheta_1 \cdots d\vartheta_{N_g} \int_{-\infty}^{\infty} d\vartheta_{N_g+1} \cdots d\vartheta_N \\ &\times \delta \left[\frac{1}{2} \sum_{i=1}^N p_i^2 + \frac{\mu}{2} \sum_{i,j=N_g+1}^N (\vartheta_i - \vartheta_j)^2 - V_0 - E \right]. \end{aligned} \quad (\text{A.1})$$

To compute the above integral we follow a procedure similar to that used in [55, 69]. First, we expand the square in the last sum, obtaining

$$\begin{aligned} \omega_N(E) &= \frac{1}{\mu} \sum_{N_g=0}^N \frac{N!}{N_g!(N-N_g)!} \int_{-\infty}^{\infty} dp_1 \cdots dp_N \int_{-\pi}^{\pi} d\vartheta_1 \cdots d\vartheta_{N_g} \int_{-\infty}^{\infty} d\vartheta_{N_g+1} \cdots d\vartheta_N \\ &\times \delta \left[\frac{1}{2\mu} \sum_{i=1}^N p_i^2 + (N-N_g) \sum_{i=N_g+1}^N \vartheta_i^2 - \left(\sum_{i=N_g+1}^N \vartheta_i \right)^2 - \frac{V_0 + E}{\mu} \right], \end{aligned} \quad (\text{A.2})$$

and then we search for a coordinate transformation diagonalizing the coupling between the ϑ 's. As to this point, we note that

$$(N-N_g) \sum_{i=N_g+1}^N \vartheta_i^2 - \left(\sum_{i=N_g+1}^N \vartheta_i \right)^2 = (\vartheta_{N_g+1}, \dots, \vartheta_N) \mathbb{A} (\vartheta_{N_g+1}, \dots, \vartheta_N)^T, \quad (\text{A.3})$$

where the symmetric $(N-N_g) \times (N-N_g)$ matrix \mathbb{A} reads as

$$\mathbb{A} = - \begin{pmatrix} 1 & \cdots & 1 \\ \vdots & \ddots & \vdots \\ 1 & \cdots & 1 \end{pmatrix} + (N-N_g) \mathbb{I}_{N-N_g} \quad (\text{A.4})$$

APPENDIX A. APPENDIX TO CHAPTER 2

and \mathbb{I}_d is the $d \times d$ identity matrix. The matrix \mathbb{A} has eigenvalues $\lambda_1 = 0$ and $\lambda_2 = \dots = \lambda_{N-N_g} = N - N_g$, and can be diagonalized by an orthogonal transformation that does not change the integration measure. Hence we can write

$$\begin{aligned} \omega_N(E) &= \frac{1}{\mu} \sum_{N_g=0}^N \frac{N!}{N_g! (N - N_g)!} (2\pi)^{N_g} \int_{-\infty}^{\infty} dp_1 \cdots dp_N \int_{-\infty}^{\infty} d\vartheta_{N_g+1} \cdots d\vartheta_N \\ &\times \delta \left[\frac{1}{2\mu} \sum_{i=1}^N p_i^2 + (N - N_g) \sum_{i=N_g+1}^{N-1} \vartheta_i^2 - \frac{V_0 + E}{\mu} \right], \end{aligned} \quad (\text{A.5})$$

where we have also performed the N_g integrals over the circle. With the change of variables $\psi_i = \vartheta_i \sqrt{N - N_g}$, $i = N_g + 1, \dots, N - 1$ we get

$$\begin{aligned} \omega_N(E) &= \frac{1}{\mu} \sum_{N_g=0}^N (2\pi)^{N_g} \frac{N! (N - N_g)^{-(N - N_g - 1)/2}}{N_g! (N - N_g)!} \int_{-\infty}^{\infty} dp_1 \cdots dp_N \int_{-\infty}^{\infty} d\psi_{N_g+1} \cdots d\psi_{N-1} \\ &\times \delta \left[\frac{1}{2\mu} \sum_{i=1}^N p_i^2 + (N - N_g) \sum_{i=N_g+1}^{N-1} \psi_i^2 - \frac{V_0 + E}{\mu} \right] \int_{-\infty}^{\infty} d\vartheta_N. \end{aligned} \quad (\text{A.6})$$

The last integral in Eq.(A.6) stems from the zero mode due to the $O(2)$ invariance of the Hamiltonian; it is divergent but does not affect the thermodynamic quantities so that from now on we will ignore it.

When $\frac{1}{2\mu} \left[2(V_0 + E) - \sum_{i=1}^N p_i^2 \right] \geq 0$, the integrals over the ψ 's give the volume of the $(N - N_g - 2)$ -dimensional sphere $\mathbb{S}_R^{N - N_g - 2}$ of radius $R = \frac{1}{2\mu} \left[2(V_0 + E) - \sum_{i=1}^N p_i^2 \right]$; on the other hand, when $\frac{1}{2\mu} \left[2(V_0 + E) - \sum_{i=1}^N p_i^2 \right] < 0$ the same integrals vanish. As to the integrations over the momenta, we note that the integrand depends only on

$$p = \sqrt{\sum_{i=1}^N p_i^2}, \quad (\text{A.7})$$

so that we can write

$$\begin{aligned} \omega_N(E) &= \frac{1}{\mu} \sum_{N_g=0}^N (2\pi)^{N_g} \frac{N! (N - N_g)^{-(N - N_g - 1)/2}}{N_g! (N - N_g)!} \frac{2\pi^{(N - N_g - 1)/2}}{\Gamma\left(\frac{N - N_g - 1}{2}\right)} \frac{2\pi^{N/2}}{\Gamma\left(\frac{N}{2}\right)} \\ &\times 2^{N/2} \int_0^{\infty} dp p^{N-1} \left[\frac{2E' - p^2}{2\mu} \right]^{(N - N_g - 2)/2} \Theta \left[\frac{2E' - p^2}{2\mu} \right], \end{aligned} \quad (\text{A.8})$$

where $\Gamma(x)$ is the Euler gamma function, $\Theta(x)$ is the Heaviside step function and $E' = V_0 + E$.

We want to compute

$$s(\varepsilon) = \lim_{N \rightarrow \infty} \frac{1}{N} \log \omega_N(N\varepsilon), \quad (\text{A.9})$$

where we have introduced the energy density $\varepsilon = \frac{E}{N}$. Clearly,

$$\omega_N(N\varepsilon) \equiv 0 \text{ if } \varepsilon < \varepsilon_{\min}, \quad (\text{A.10})$$

A.1. DENSITY OF STATES OF THE EFFECTIVE MODEL

where ε_{\min} is the absolute minimum of the potential energy per degree of freedom,

$$\varepsilon_{\min} = -\frac{1}{2\sqrt{2\alpha}}, \quad (\text{A.11})$$

so that the domain of the entropy density (A.9) is $\varepsilon > \varepsilon_{\min}$. For large N , computing the integral in Eq.(A.8) with the Laplace (or saddle-point) method we get

$$\begin{aligned} \omega_N(N\varepsilon) &= \frac{2^{N/2}}{\mu} \sum_{N_g=0}^{N_g^{\max}(\varepsilon)} (2\pi)^{N_g} \frac{N! (N - N_g)^{-(N - N_g - 1)/2}}{N_g! (N - N_g)!} \frac{2\pi^{(N - N_g - 1)/2}}{\Gamma\left(\frac{N - N_g - 1}{2}\right)} \frac{2\pi^{N/2}}{\Gamma\left(\frac{N}{2}\right)} \\ &\times \left[N^2 2(2\alpha)^{3/2} \right]^{(N - N_g - 2)/2} \exp \left\{ N \left[\frac{1}{2} \log \left(\frac{N}{2 - n_g} \right) \right. \right. \\ &\left. \left. + \frac{2 - n_g}{2} \log a(n_g, \alpha, \varepsilon) + \frac{1 - n_g}{2} \log \left(\frac{1 - n_g}{2 - n_g} \right) \right] \right\} + o(e^N), \end{aligned} \quad (\text{A.12})$$

where

$$a(n_g, \alpha, \varepsilon) = \frac{\gamma}{2\sqrt{2}} n_g (2 - n_g) + \frac{(1 - n_g)^2}{2\sqrt{2\alpha}} + \varepsilon, \quad (\text{A.13})$$

and we have introduced the fraction of gas particles $n_g = \frac{N_g}{N}$; $N_g^{\max}(\varepsilon)$ is the maximum number of gas particles allowed at a given energy density ε , so that the quantity $a(n_g, \alpha, \varepsilon)$ given by Eq.(A.13) is positive in the domain $\varepsilon > \varepsilon_{\min}$ with $0 \leq N_g \leq N_g^{\max}$.

Neglecting the sub-exponential terms and using the Stirling approximation, Eq.(A.12) can be written as

$$\omega_N(N\varepsilon) = \int_0^{n_g^{\max}(\varepsilon)} dn_g \exp [Ns(\varepsilon, n_g)], \quad (\text{A.14})$$

where¹

$$n_g^{\max}(\varepsilon) = \frac{N_g^{\max}(\varepsilon)}{N} = 1 - \sqrt{1 - \frac{1 + 2\varepsilon\sqrt{2\alpha}}{\sqrt{2} - \gamma\sqrt{\alpha}}} \quad (\text{A.15})$$

and

$$\begin{aligned} s(\varepsilon, n_g) &= \frac{1 - n_g}{2} \log \left[\frac{4\pi(2\alpha)^{3/2}}{(1 - n_g)(2 - n_g)} \right] + \frac{1}{2} \log \left(\frac{2\pi\sqrt{2}}{2 - n_g} \right) \\ &+ \frac{2 - n_g}{2} [1 + \log a(n_g, \alpha, \varepsilon)] + n_g \log(2\pi) \\ &- n_g \log n_g - (1 - n_g) \log(1 - n_g); \end{aligned} \quad (\text{A.16})$$

hence, we can write the entropy (A.9) as

$$s(\varepsilon) = \sup_{n_g \in [0, n_g^{\max}]} s(\varepsilon, n_g). \quad (\text{A.17})$$

¹Eq. (A.15) holds for sufficiently small α , i.e., such that $\sqrt{2} - \gamma\sqrt{\alpha} > 0$.

B

Appendix to Chapter 3

B.1 Specific heat critical exponent from Eq. (3.14)

In Chapter 3, we have discussed the implications of Eqs. (3.14) and (3.15) in case they would exactly hold. Here we give the details about the predictions on the specific heat critical exponent α obtained by assuming that the density of states has the form given by Eqs. (3.14) or (3.15), respectively. Let us recall that, in the microcanonical ensemble, the specific heat is defined as

$$C(\varepsilon) = -\frac{[s'(\varepsilon)]^2}{s''(\varepsilon)}, \quad (\text{B.1})$$

where $s(\varepsilon)$ is the entropy density and the temperature is defined as $T(\varepsilon) = 1/s'(\varepsilon)$. With $s'(\varepsilon)$ and $s''(\varepsilon)$ we denote the first and second derivative of the function $s(\varepsilon)$.

Let us consider a short-range $O(n)$ model and assume the relation (3.14) holds as an equality. We assume in the following that the phase transition occurs for a value of the energy density in the interior of the domain of the entropy density¹. Without loss of generality, let us shift the energy density ε such that $\varepsilon_c = 0$. The entropy density of the continuous model can then be written as:

$$s(\varepsilon) = s_I(\varepsilon) + \log f(\varepsilon), \quad (\text{B.2})$$

where here and in the following we use the notation $s_I(\varepsilon)$ instead of $s^{(1)}(\varepsilon)$ for the entropy density of the Ising model, to avoid possible misunderstanding with derivatives. We also omit the symbol (n) indicating which $O(n)$ model we are considering because our arguments do not depend on it. Finally, we denoted $g^{(n)}(\varepsilon)^{1/N}$ by $f(\varepsilon)$.

Let us now consider, for the moment, only energy densities larger than the critical one, i.e., $\varepsilon > 0$. Three facts are relevant for the following:

1. we consider $0 < \alpha_I < 1$, i.e., the case $d > 2$. Moreover, because the critical temperature of the Ising models is finite, $s_I''(\varepsilon) \propto \varepsilon^{\alpha_I}$ for $\varepsilon \rightarrow 0^+$.

¹As a consequence, what follows does not apply to the mean-field and 1-d Xy models.

APPENDIX B. APPENDIX TO CHAPTER 3

2. $s'(\varepsilon)$ is finite around $\varepsilon = 0$ because the critical temperature of the continuous model does not vanish at the transition.
3. we assume $f(\varepsilon)$ is analytical. We can then expand $f(\varepsilon)$ in a Taylor series around $\varepsilon = 0$.

Inserting Eq.(B.2) into Eq.(B.1), we get

$$C(\varepsilon) = - \frac{\left[s'_I(\varepsilon) + \frac{g'(\varepsilon)}{f(\varepsilon)} \right]^2}{s''_I(\varepsilon) + \frac{g''(\varepsilon)}{f(\varepsilon)} - \left[\frac{g'(\varepsilon)}{f(\varepsilon)} \right]^2}. \quad (\text{B.3})$$

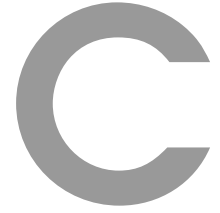
Using the expansions described above around $\varepsilon = 0$, neglecting the higher order terms and expanding the fraction, we obtain

$$C(\varepsilon) \simeq a_+ + b_+ \varepsilon^{\alpha_I} \quad (\varepsilon \rightarrow 0^+), \quad (\text{B.4})$$

where a_+ and b_+ are constants whose exact value is irrelevant to our purposes. We can repeat the same calculations for $\varepsilon < 0$, obtaining the same result as in Eq.(B.4) but for that $\varepsilon \rightarrow -\varepsilon$ and that the constants may be different. Hence the specific heat close to $\varepsilon = 0$ is

$$C(\varepsilon) \simeq a_{\pm} + b_{\pm} |\varepsilon|^{\alpha_I}. \quad (\text{B.5})$$

We then obtain the result stated in Sec. 3.3: the specific heat of the continuous model does not diverge at the transition and the critical exponent α of the continuous model is related to the one of the Ising model via $\alpha = -\alpha_I$.



Appendix to Chapter 5

C.1 Normalization, energy density, and stability criterion for the Fermi-Dirac distribution

Normalization: Consider the distribution Eq. (5.64). The normalization A satisfies

$$A \int_{-\infty}^{\infty} \frac{dp}{1 + e^{\beta(p^2 - \mu)}} = 1. \quad (\text{C.1})$$

Changing variables and doing an integration by parts, we get

$$2\beta A \int_0^{\infty} dx \frac{\sqrt{x} e^{\beta(x - \mu)}}{[1 + e^{\beta(x - \mu)}]^2} = 1. \quad (\text{C.2})$$

The left hand side may be written in terms of the derivative $\partial f_{\text{FD}}(x)/\partial x$ of the Fermi-Dirac-like function $f_{\text{FD}}(x) = 1/[1 + e^{\beta(x - \mu)}]$. We get

$$2A \int_0^{\infty} dx \sqrt{x} \left(\frac{-\partial f_{\text{FD}}(x)}{\partial x} \right) = 1. \quad (\text{C.3})$$

In the limit of large β , the derivative $\partial f_{\text{FD}}(x)/\partial x$ approaches the Delta function: $\lim_{\beta \rightarrow \infty} \partial f_{\text{FD}}(x)/\partial x = -\delta(x - \mu)$. In this limit, we may expand \sqrt{x} in a Taylor series about μ ,

$$\sqrt{x} = \sqrt{\mu} + \frac{x - \mu}{2\sqrt{\mu}} - \frac{(x - \mu)^2}{8\mu^{3/2}} + \dots, \quad (\text{C.4})$$

which on substituting in Eq. (C.3) gives

$$A \left(2\sqrt{\mu} I_0 + \frac{1}{\beta\sqrt{\mu}} \mathcal{I}_1 - \frac{1}{4\beta^2\mu^{3/2}} \mathcal{I}_2 + \dots \right) = 1. \quad (\text{C.5})$$

Here,

$$\mathcal{I}_0 = \int_0^{\infty} dx \left(\frac{-\partial f_{\text{FD}}(x)}{\partial x} \right) = \int_{-\beta\mu}^{\infty} dy \frac{e^y}{(1 + e^y)^2} \xrightarrow{\beta \rightarrow \infty} \int_{-\infty}^{\infty} dy \frac{e^y}{(1 + e^y)^2} = 1, \quad (\text{C.6})$$

APPENDIX C. APPENDIX TO CHAPTER 5

$$\mathcal{I}_1 = \beta \int_0^\infty dx (x - \mu) \left(\frac{-\partial f_{\text{FD}}(x)}{\partial x} \right) = \int_{-\beta\mu}^\infty dy \frac{y e^y}{(1 + e^y)^2} \xrightarrow{\beta \rightarrow \infty} \int_{-\infty}^\infty dy \frac{y e^y}{(1 + e^y)^2} = 0, \quad (\text{C.7})$$

$$\mathcal{I}_2 = \beta^2 \int_0^\infty dx (x - \mu)^2 \left(\frac{-\partial f_{\text{FD}}(x)}{\partial x} \right) = \int_{-\beta\mu}^\infty dy \frac{y^2 e^y}{(1 + e^y)^2} \xrightarrow{\beta \rightarrow \infty} \int_{-\infty}^\infty dy \frac{y^2 e^y}{(1 + e^y)^2} = \frac{\pi^2}{3}. \quad (\text{C.8})$$

Thus, to order $1/\beta^2$, we find from Eq. (C.5) that

$$A \left(2\sqrt{\mu} - \frac{\pi^2}{12\beta^2 \mu^{3/2}} \right) = 1, \quad (\text{C.9})$$

which gives

$$A = \frac{1}{2\sqrt{\mu}} \left(1 + \frac{\pi^2}{24\beta^2 \mu^2} \right). \quad (\text{C.10})$$

Average energy: The average energy density is obtained from Eq. (5.38) as

$$e = A \int_{-\infty}^\infty dp \frac{p^2/2}{1 + e^{\beta(p^2 - \mu)}} + \frac{1}{2}. \quad (\text{C.11})$$

Changing variables and doing an integration by parts, we get

$$e = \frac{A}{3} \int_0^\infty dx x^{3/2} \left(\frac{-\partial f_{\text{FD}}(x)}{\partial x} \right) + \frac{1}{2}. \quad (\text{C.12})$$

Expanding $x^{3/2}$ in a Taylor series about μ and substituting in Eq. (C.12) give

$$\begin{aligned} e &= \frac{A}{3} \left(\mu^{3/2} \mathcal{I}_0 + \frac{3}{2\beta} \sqrt{\mu} \mathcal{I}_1 + \frac{3}{8\beta^2 \sqrt{\mu}} \mathcal{I}_2 + \dots \right) + \frac{1}{2} \\ &= \frac{A\mu^{3/2}}{3} \left(1 + \frac{\pi^2}{8\beta^2 \mu^2} \right) + \frac{1}{2}. \end{aligned} \quad (\text{C.13})$$

Using Eq. (C.10), we find that to $O(1/\beta^2)$, the energy density is

$$e = \frac{\mu}{6} \left(1 + \frac{\pi^2}{6\beta^2 \mu^2} \right) + \frac{1}{2}. \quad (\text{C.14})$$

Dielectric function: Using Eqs. (5.64), we get

$$\epsilon(1, 0) = 1 - A \int_0^\infty dx \frac{1}{\sqrt{x}} \left(\frac{-\partial f_{\text{FD}}(x)}{\partial x} \right). \quad (\text{C.15})$$

Expanding $1/\sqrt{x}$ in a Taylor series about μ , and substituting in Eq. (C.15) give

$$\epsilon(1, 0) = 1 - A \left(\frac{\mathcal{I}_0}{\sqrt{\mu}} - \frac{\mathcal{I}_1}{2\beta\mu^{3/2}} + \frac{3\mathcal{I}_2}{8\beta^2\mu^{5/2}} + \dots \right), \quad (\text{C.16})$$

so that to $O(1/\beta^2)$, we get

$$\epsilon(1, 0) = 1 - \frac{1}{2\mu} \left(1 + \frac{\pi^2}{6\beta^2 \mu^2} \right), \quad (\text{C.17})$$

where we have used Eq. (C.10).

D

Appendices to Chapter 6

We report in these appendices some computations relative to Chapter (6) which have not found space in the text.

D.1 Condition of detailed balance for the dynamics (6.2)

We prove here that the dynamics defined by the equations of motion (6.2) satisfies detailed balance if and only if $c_k = c$ for all k , that is, if the stochastic forcing has a white spectrum in space.

We start from the N -particle Fokker-Planck equation (6.13) associated with the equations of motion (6.2). It will be useful to rewrite it in the following way:

$$\frac{\partial f_N(\mathbf{x})}{\partial t} = - \sum_{i=1}^{2N} \frac{\partial}{\partial x_i} [A_i(\mathbf{x}) f_N(\mathbf{x})] + \frac{1}{2} \sum_{i,j=1}^{2N} \frac{\partial^2}{\partial x_i \partial x_j} [B_{i,j}(\mathbf{x}) f_N(\mathbf{x})], \quad (\text{D.1})$$

where $x_i = q_i$ for $i = 1, \dots, N$, $x_i = p_{i-N}$ for $i = (N+1), \dots, 2N$, and we use the notation $\mathbf{x} = \{x_i\}$. The drift vector $A_i(\mathbf{x})$ is a function of the x_i 's, and is given by

$$A_i(\mathbf{x}) = p_i \quad \text{for} \quad i = 1, \dots, N, \quad (\text{D.2})$$

$$A_i(\mathbf{x}) = -\alpha p_{i-N} - \frac{1}{N} \sum_{j=1}^N \frac{\partial v(q_{i-N} - q_j)}{\partial q_{i-N}} \quad \text{for} \quad i = (N+1), \dots, 2N. \quad (\text{D.3})$$

Similarly, the expression for the (symmetric) diffusion matrix $B_{i,j}$ is:

$$B_{i,j}(\mathbf{x}) = \alpha C(|q_{i-N} - q_{j-N}|) \quad \text{for} \quad i > N \wedge j > N, \quad (\text{D.4})$$

and $B_{i,j}(\mathbf{x}) = 0$ otherwise. We moreover introduce the constants $\epsilon_i = \pm 1$, which denote the parity with respect to time inversion of the variables x_i , and the notation $\epsilon \mathbf{x} = \{\epsilon_i x_i\}$.

It can be shown (see [165], Sect. 5.3.5, or [189], Sect. 6.4) that the dynamics described by a Fokker-Planck equation of the form (D.1) satisfies detailed balance if and only if the following two conditions are satisfied ($i = 1, \dots, 2N$):

$$\epsilon_i \epsilon_j B_{i,j}(\epsilon \mathbf{x}) = B_{i,j}(\mathbf{x}), \quad (\text{D.5})$$

and

$$\epsilon_i A_i(\epsilon \mathbf{x}) f_N^s(\mathbf{x}) = -A_i(\mathbf{x}) f_N^s(\mathbf{x}) + \sum_{j=1}^{2N} \frac{\partial}{\partial x_j} B_{i,j}(\mathbf{x}) f_N^s(\mathbf{x}), \quad (\text{D.6})$$

where $f_N^s(\mathbf{x})$ is the stationary solution of (D.1).

In our case, in which the drift and the diffusion terms are given by Eqs. (D.2) and (D.4), respectively, the condition (D.5) is trivially satisfied. Our proof goes as follows: we solve formally Eq. (D.6), and show that $f_N^s(\mathbf{x})$ is a stationary solution of Eq. (D.1) if and only if the non-vanishing part of $B_{i,j}$ is proportional to the identity matrix. Then, it is simple to show that this implies that the spectrum of the forcing has to be white in space.

Equation (D.6) for $i = 1, \dots, N$ is also trivially satisfied. On the other hand, for what concerns $i = (N + 1), \dots, 2N$, we have

$$2p_k f_N^s(\mathbf{x}) = - \sum_{j=1}^N C(|q_k - q_j|) \frac{\partial f_N^s(\mathbf{x})}{\partial p_j}, \quad (\text{D.7})$$

where $k = i - N$. We introduce the $N \times N$ matrix \mathcal{C} whose components are given by $\mathcal{C}_{k,j}(\mathbf{x}) = C(|q_k - q_j|)$, and observe that, for generic values of the q_i 's, \mathcal{C} admits an inverse \mathcal{C}^{-1} . Integrating Eq. (D.7), we thus have

$$f_N^s(\mathbf{x}) = d(q_1, \dots, q_N) \exp \left[- \sum_{k,j=1}^N p_k (\mathcal{C}^{-1})_{k,j} p_j \right], \quad (\text{D.8})$$

where $d(q_1, \dots, q_N)$ is an undetermined function. Inserting Eq. (D.8) into the Fokker-Planck equation (D.1), imposing that it is a stationary solution, and with some calculations, we get

$$\sum_{i=1}^N \left[- \frac{\partial f_N^s}{\partial q_i} \frac{\partial H}{\partial p_i} + \frac{\partial H}{\partial q_i} \frac{\partial f_N^s}{\partial p_i} \right] = 0. \quad (\text{D.9})$$

Then, f_N^s is a function of the Hamiltonian H , that is $f_N^s(\mathbf{x}) = \psi(H(\mathbf{x}))$ for some function ψ . On the other hand, because f_N^s is given by the formula in Eq. (D.8), we can also deduce that ψ is an exponential, and thus, that f_N^s is Gaussian in the velocities. We conclude that \mathcal{C}^{-1} (and hence, \mathcal{C}) has to be independent of the q_i 's and proportional to the identity. Finally, from the form of $C(|q_i - q_j|)$ in Eq. (6.3), we see that this condition on \mathcal{C} is satisfied if and only if the spectrum of the forcing is white in space.

D.2 Closure of the BBGKY hierarchy

We analyze here in detail the closure of the BBGKY hierarchy discussed in the text, in particular, the reasons for which the connected part of the two-particle correlation is of order α , while higher correlations are negligible at leading order in α , so that this closure is self-consistent.

D.2. CLOSURE OF THE BBGKY HIERARCHY

In the following, we expand the functions f_2 and f_3 as

$$f_2(z_1, z_2, t) = f(z_1, t)f(z_2, t) + \tilde{g}(z_1, z_2, t), \quad (\text{D.10})$$

and

$$\begin{aligned} f_3(z_1, z_2, z_3, t) &= f(z_1, t)f(z_2, t)f(z_3, t) + f(z_1, t)\tilde{g}(z_2, z_3, t) \\ &\quad + f(z_2, t)\tilde{g}(z_1, z_3, t) + f(z_3, t)\tilde{g}(z_1, z_2, t) + h(z_1, z_2, z_3, t), \end{aligned} \quad (\text{D.11})$$

and similarly, for other f_s 's for $s \geq 4$.

Now, let us write explicitly the first two equations of the BBGKY hierarchy (6.16). The first one, obtained from Eqs. (6.16) and (D.10), is

$$\frac{\partial f}{\partial t} + p \frac{\partial f}{\partial q} - \frac{\partial f}{\partial p} \frac{\partial \Phi[f]}{\partial q} - \alpha \frac{\partial}{\partial p} [pf] - \frac{\alpha}{2} C(0) \frac{\partial^2 f}{\partial p^2} = \frac{\partial}{\partial p} \int dq_1 dp_1 v'(q - q_1) \tilde{g}(z, z_1, t), \quad (\text{D.12})$$

where

$$\Phi[f](q) = \int dq_1 dp_1 v(q - q_1) f(q_1, p_1, t) \quad (\text{D.13})$$

is the mean-field potential. For the second equation of the hierarchy, we use Eqs. (D.11) and (D.12) to get

$$\begin{aligned} \frac{\partial \tilde{g}(z_1, z_2, t)}{\partial t} &= \left[-p_1 \frac{\partial \tilde{g}}{\partial q_1} + \frac{\partial \tilde{g}}{\partial p_1} \frac{\partial \Phi[f]}{\partial q_1} + \frac{f(z_2)}{N} \frac{\partial v(q_1 - q_2)}{\partial q_1} \frac{\partial f}{\partial p_1} + \frac{1}{N} \frac{\partial v(q_1 - q_2)}{\partial q_1} \frac{\partial \tilde{g}}{\partial p_1} \right. \\ &\quad \left. + \frac{\partial f}{\partial p_1} \int dz_3 \frac{\partial v(q_1 - q_3)}{\partial q_1} \tilde{g}(z_2, z_3) + \frac{\partial}{\partial p_1} [\alpha p_1 \tilde{g}] + \frac{\alpha}{2} C(|q_1 - q_2|) \frac{\partial f}{\partial p_1} \frac{\partial f}{\partial p_2} \right. \\ &\quad \left. + \frac{\alpha}{2} C(0) \frac{\partial^2 \tilde{g}}{\partial p_1^2} + \frac{\alpha}{2} C(|q_1 - q_2|) \frac{\partial^2 \tilde{g}}{\partial p_1 \partial p_2} + \int dz_3 \frac{\partial v(q_1 - q_3)}{\partial q_1} \frac{\partial h}{\partial p_1} \right] \\ &\quad + \{1 \leftrightarrow 2\}, \end{aligned} \quad (\text{D.14})$$

where the symbol $\{1 \leftrightarrow 2\}$ stands for an expression obtained from the bracketed one on the right hand side by exchanging the subscripts 1 and 2.

Let us analyze the order of magnitude of various terms in Eq. (D.14). First of all, we have $f \sim 1$, as it is normalized to unity. However, we do not know a priori the order of magnitude of \tilde{g} and h . Thus, the order of magnitude of all but the terms $\frac{f(z_2)}{N} \frac{\partial v(q_1 - q_2)}{\partial q_1} \frac{\partial f}{\partial p_1}$ and $\frac{\alpha}{2} C(|q_1 - q_2|) \frac{\partial f}{\partial p_1} \frac{\partial f}{\partial p_2}$ is unknown. In the continuum limit $N\alpha \gg 1$, we have

$$\frac{f(z_2)}{N} \frac{\partial v(q_1 - q_2)}{\partial q_1} \frac{\partial f}{\partial p_1} \sim \frac{1}{N} \ll \alpha \sim \frac{\alpha}{2} C(|q_1 - q_2|) \frac{\partial f}{\partial p_1} \frac{\partial f}{\partial p_2}, \quad (\text{D.15})$$

so that it is natural to guess that $\tilde{g} \sim \alpha$. Let us also observe that in the limit $N\alpha \ll 1$, we have

$$\frac{f(z_2)}{N} \frac{\partial v(q_1 - q_2)}{\partial q_1} \frac{\partial f}{\partial p_1} \sim \frac{1}{N} \gg \alpha \sim \frac{\alpha}{2} C(|q_1 - q_2|) \frac{\partial f}{\partial p_1} \frac{\partial f}{\partial p_2}, \quad (\text{D.16})$$

APPENDIX D. APPENDICES TO CHAPTER 6

so that we obtain $\tilde{g} \sim 1/N$. In the limit $N\alpha \ll 1$, the kinetic theory leads to the Lenard-Balescu equation.

Once we have established that $\tilde{g} \sim \alpha$, one can write down the equation of the hierarchy for h and, with similar reasoning as above, one then finds that h is at least of order $\alpha/N \ll \alpha$ (or, α^2 depending on whether $\alpha/N \ll \alpha^2$, or, the converse), so that the term $\int dz_3 \frac{\partial v(q_1 - q_3)}{\partial q_1} \frac{\partial h}{\partial p_1}$ is negligible in Eq. (D.14), as may be straightforwardly checked. The iterative procedure can be repeated at all orders of the hierarchy. Discarding three-particle and higher-order correlations is thus a self-consistent procedure. Moreover, note that in Eq. (D.14), some of the terms are of higher orders (α^2 , α/N ,...) with respect to α , and thus, can be discarded. The final form of the second equation of the BBGKY hierarchy is thus

$$\begin{aligned} \frac{\partial \tilde{g}(z_1, z_2)}{\partial t} = & \left[-p_1 \frac{\partial \tilde{g}}{\partial q_1} + \frac{\partial \tilde{g}}{\partial p_1} \frac{\partial \Phi[f]}{\partial q_1} + \frac{\partial f}{\partial p_1} \int dz_3 v'(q_1 - q_3) \tilde{g}(z_2, z_3) \right. \\ & \left. + \frac{\alpha}{2} C(|q_1 - q_2|) \frac{\partial f}{\partial p_1} \frac{\partial f}{\partial p_2} \right] + \{1 \leftrightarrow 2\}. \end{aligned} \quad (\text{D.17})$$

Note that $\tilde{g} \sim \alpha$ implies, see Eq. (D.12), that the mean-field effect of the stochastic forces gives a contribution at the same order to the two-particle correlation induced by them.

D.3 Evolution of the kinetic energy for the dynamics

We derive here the evolution of the kinetic energy as obtained from the kinetic equation (6.30). Let us recall that the average kinetic energy density at time t in the continuous limit can be written as

$$\langle k(t) \rangle = \frac{1}{2} \int dp p^2 f(p, t). \quad (\text{D.18})$$

The starting point to obtain its time evolution is to multiply the kinetic equation (6.30) by $\frac{1}{2}p^2$, and then, to integrate over p . Neglecting for the moment the non-linear part of the diffusion coefficient, and integrating by parts, we get

$$\left\langle \frac{\partial k(t)}{\partial t} \right\rangle + 2\alpha \langle k(t) \rangle - \frac{\alpha}{2} C(0) = 0, \quad (\text{D.19})$$

which gives

$$\langle k(t) \rangle = \left(\langle k(0) \rangle - \frac{C(0)}{4} \right) e^{-2\alpha t} + \frac{C(0)}{4}. \quad (\text{D.20})$$

The kinetic energy density in the stationary state is thus $\langle k \rangle_{ss} = C(0)/4$.

We now have to prove that the non-linear part of the diffusion coefficient (6.31) does not contribute to the time evolution of the kinetic energy. Such a result is expected and is usually valid for collisional terms (i.e., those terms in the kinetic equations which are given by two-particle correlation), for example, in the Boltzmann equation or in the Lenard-Balescu

D.4. PROOF THAT THE KINETIC EQUATION ADMITS NON-GAUSSIAN STATIONARY DISTRIBUTION WITH GAUSSIAN TAILS

equation [111]. The contribution to $k(t)$ from the non-linear part of the diffusion coefficient is a sum of terms proportional to

$$T = \frac{1}{2} \int dp p^2 \times \frac{\partial}{\partial p} \left\{ f'(p, t) \left[\frac{1}{|\epsilon(k, kp)|^2} \int^* dp_1 \frac{f'(p_1, t)}{p_1 - p} + \int^* dp_1 \frac{f'(p_1, t)}{p_1 - p} \frac{1}{|\epsilon(k, kp_1)|^2} \right] \right\}; \quad (\text{D.21})$$

we will show that each of such terms vanishes independently. Indeed, integrating the last expression over p_1 by parts, we get that

$$T = - \int dp \int^* dp_1 p f'(p, t) \left[\frac{f'(p_1, t)}{p_1 - p} \frac{1}{|\epsilon(k, kp)|^2} + \frac{f'(p_1, t)}{p_1 - p} \frac{1}{|\epsilon(k, kp_1)|^2} \right]. \quad (\text{D.22})$$

Exchanging now the variables p_1 and p and the order of integration, we get that the above equation may be rewritten as

$$T = \int dp \int^* dp_1 p_1 f'(p_1, t) \left[\frac{f'(p, t)}{p_1 - p} \frac{1}{|\epsilon(k, kp_1)|^2} + \frac{f'(p, t)}{p_1 - p} \frac{1}{|\epsilon(k, kp)|^2} \right]. \quad (\text{D.23})$$

Summing up the last two equations, we therefore have

$$T = \frac{1}{2} \int dp \int^* dp_1 f'(p_1, t) f'(p, t) \left[\frac{1}{|\epsilon(k, kp_1)|^2} + \frac{1}{|\epsilon(k, kp)|^2} \right], \quad (\text{D.24})$$

which vanishes on integrating by parts both with respect to p_1 and p .

D.4 Proof that the kinetic equation admits non-Gaussian stationary distribution with Gaussian tails

We prove here that for a general forcing spectra, the Gaussian distribution function in Eq. (6.35) is not a stationary solution of the kinetic equation (6.30), and that the tails of any stationary state are Gaussian. For the first point, we have to prove that the contribution to $\partial f / \partial t$ from the non-linear part of $D[f](p)$ in Eq. (6.31) is not vanishing. This result can be proven with an asymptotic expansion [136] for large momenta of the integrals which appear in the diffusion coefficient. Given any function $g(p)$, we approximate integrals of the form

$$\int^* dp_1 \frac{g(p_1)}{p_1 - p} \quad (\text{D.25})$$

by expanding $\frac{1}{p_1 - p}$ in Taylor series. We get, for example,

$$\int^* dp_1 \frac{f'_G(p_1)}{p_1 - p} \simeq \frac{2}{\sqrt{\pi}} \beta^{3/2} \int_{-\infty}^{\infty} e^{-\beta p_1^2} \left[\frac{p_1}{p} + \left(\frac{p_1}{p} \right)^2 + \left(\frac{p_1}{p} \right)^3 + \dots \right] \simeq \frac{1}{p^2}, \quad (\text{D.26})$$

APPENDIX D. APPENDICES TO CHAPTER 6

where, in the last equality, we have taken into account the fact that the Gaussian distribution being even, the terms containing $\left(\frac{p_1}{p}\right)^k$ with k odd do not contribute. In a similar way, we have

$$|\epsilon(k, kp)|^2 \simeq 1 - \frac{4\pi\nu(k)}{p^2}, \quad (\text{D.27})$$

and

$$\int^* dp_1 \left[\frac{f'_G(p_1)}{p_1 - p} \frac{1}{|\epsilon(k, kp_1)|^2} \right] \simeq \frac{2\beta^{3/2}}{\sqrt{\pi} p^2} \int dp_1 \frac{p_1^2 e^{-\beta p_1^2}}{|\epsilon(k, kp_1)|^2}, \quad (\text{D.28})$$

where we have used the fact that $|\epsilon(k, kp)|^2$ is an even function of p . With these results, we can evaluate the non-linear part of the kinetic equation: for large p_1 , the non-linear contribution to $\partial f / \partial t$ is

$$2\pi\alpha \sum_{k=1}^{\infty} \nu_k c_k \left[1 + \frac{2\beta^{3/2}}{\sqrt{\pi}} \int dp \frac{p^2 e^{-p^2}}{|\epsilon(k, kp)|^2} \right] \left[\frac{4\beta^{5/2}}{\sqrt{\pi}} e^{-\beta p_1^2} \right]. \quad (\text{D.29})$$

It can be shown that such a term is a non-vanishing function of p_1 . This completes the proof: for a generic forcing spectra, the stationary state, when exists, is not Gaussian.

Using the same asymptotic expansion as before, it can be checked that the diffusion coefficient $D[f](p)$ converges to $C(0)/2$ for any distribution f . From this observation and Eq. (6.37), it follows that any stationary solution of the kinetic equation (6.30) has Gaussian tails.

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