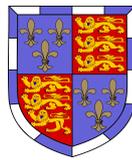




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Quantitative studies and Hydrodynamical limits for interacting particle systems

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Summary

The main results of my work contribute to the mathematical study of microscopic non-equilibrium systems that were first introduced in order to derive macroscopic physical laws such as Fourier's law. In particular the main objective is to determine the scaling of the spectral gap, i.e. the relaxation rate, in terms of the number of the particles for a paradigmatic model describing heat transport, the chain of oscillators. The mathematical study of this model started at the end of 90s and it is challenging due to the degeneracy of the dynamics as the noise is not assumed to act to all the degrees of freedom, leading to lack of ellipticity and coercivity. We give bounds on the spectral gap for weak nonlinearities of the chain, i.e. perturbations around linear homogeneous chains and also a complete answer for the linear, homogeneous and disordered, chain of oscillators as well as d -dimensional grids of oscillators. The methods range from hypocoercivity inspired techniques, in the sense of Villani, to spectral analysis of discrete Schrödinger operators. Moreover we study heat conduction in gases addressing, with both analytic and probabilistic techniques, the question of the existence, and properties, of a non-equilibrium steady state for the nonlinear BGK model, introduced by Bhatnagar, Gross and Krook, with diffusive boundary conditions. The case that we address concerns large boundary temperatures away from the equilibrium case. Furthermore, besides non-equilibrium phenomena in many particle systems, this thesis deals with the question of deriving nonlinear diffusion equations from microscopic stochastic processes. We present a new, quantitative, unified method to show that the particle densities of one-dimensional processes on a periodic lattice, including the zero-range and simple exclusion jump processes as well as diffusion processes of Ginzburg-Landau type, converge to the solution of a nonlinear diffusion equation with an explicit, uniform in time, convergence rate. We discuss how we can extend the result to all the dimensions. Finally a study of the scaling of the spectral gap for all the mean field $\mathcal{O}(n)$ models of Ginzburg-Landau type using semiclassical tools, is included in this thesis. This concerns the spectral gap as a function of the number of particles, spins, for the dynamics below and at the critical temperature, with and without an external magnetic field.

Declaration

This dissertation is the result of my own work and includes nothing which is the outcome of work done in collaboration except as declared in the Preface and specified in the text. It is not substantially the same as any that I have submitted for a degree or diploma or other qualification at any other university.

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ΑΝΑΤΟΛΗ ΗΛΙΟΥ

Είταν η ώρα που επρόκειτο να ανάψουν οι φανοστάτες. Δεν είχε καμιά αμφιβολία, το 'ξερε πως όπου νά ναι θα ανάβανε, όπως και κάθε βράδυ άλλωστε. Πήγε και στάθηκε στη διασταύρωση, για την ακρίβεια στη νησίδα ασφαλείας, για να δει τούς φανοστάτες να ανάβουν ταυτόχρονα, τόσο στον κάθετο, όσο και στον οριζόντιο δρόμο.

Με το κεφάλι ασάλευτο, έστριψε το δεξί του μάτι δεξιά, το αριστερό του αριστερά. Περίμενε, μα οι φανοστάτες δεν ανάβανε. Τα μάτια του κουράστηκαν, άρχισαν να πονάνε, σ'εκείνη την άβολη στάση. Σε λίγο δεν άντεξε και έφυγε. Ωστόσο, το επόμενο σούρουπο, πιστός στο καθήκον, πήγε και ξαναστάθηκε στη νησίδα του. Οι φανοστάτες και πάλι δεν ανάψανε, ούτε εκείνο το βράδι, ούτε τις άλλες νύχτες, μα τα μάτια του συνήθιζαν λίγο λίγο, δεν κουράζονταν πια, δεν πονούσαν.

Και κάποτε, εκεί που στεκόταν και περίμενε, χάραζε εντελώς ξαφνικά. Εντελώς ξαφνικά, είδε τον ήλιο να ανατέλει, ταυτόχρονα, απ'τον κάθετο δρόμο και απ' τον άλλον, τον οριζόντιο. . .

Αρης Αλεξάνδρου,
Παρίσι, 1971

Declaration on collaboration and publication of results

Chapter 1 is my own review of the background and the current literature together with a summary of the results contained in the following Chapters from 2 to 6.

Chapter 2 is published in [Men20] and contains my own results.

Chapter 3 contains a work in collaboration with Simon Becker from the University of Cambridge and it follows the article [BM22].

Chapter 4 contains results obtained in collaboration with Josephine Evans from the University of Warwick, which are published in [EM21].

Chapter 5 is the result of a collaboration with Daniel Marahrens who is a quantitative researcher and Clément Mouhot from the University of Cambridge and has not been published yet.

Chapter 6 is a work in collaboration with Simon Becker from the University of Cambridge and it follows the article [BM20].

Contents

1	Introduction	17
1.1	Evolution of Microscopic Interacting Particle Systems	19
1.1.1	Hamiltonian dynamics	19
1.1.2	Stochastic dynamics	20
1.1.3	Examples	22
1.2	Long Time behaviour	25
1.2.1	Elliptic case	25
1.2.1.1	Relaxation of the semigroup via Poincaré Inequality	27
1.2.1.2	Relaxation of the semigroup via Log-Sobolev Inequality	27
1.2.1.3	Curvature-Dimension Inequalities	29
1.2.2	Hypoellipticity and Hypocoercivity	29
1.2.2.1	Hypoellipticity	29
1.2.2.2	Convergence rates towards stationary measure in the hypoelliptic case	32
1.3	Hydrodynamical behaviour for stochastic interacting particle systems	35
1.3.1	Introduction of our basic examples	38
1.3.2	In the literature	43
1.4	List of the works and perspectives	44
2	Quantitative Rates of Convergence to Non-Equilibrium Steady State for a Weakly Anharmonic Chain of Oscillators	59
2.1	Introduction	59
2.1.1	Description of the model	60
2.1.1.1	State of the art	61
2.1.2	Notation	62
2.1.3	Set up and main results	63
2.1.4	Plan of the Chapter	68
2.2	Carré du Champ operators and curvature condition	69
2.2.1	Introduction to Carré du Champ operators	69
2.2.2	Description of the method	70

2.3	Functional inequalities in the modified setting	72
2.4	Convergence to equilibrium in Kantorovich-Wasserstein distance	82
2.5	Entropic Convergence to equilibrium	83
2.6	Estimates on the spectral norm of b_N	85
2.6.1	Matrix equations on Lyapunov equation	87
2.6.2	Calculations for $m = 0, 1, 2$	88
2.6.3	Preliminaries: compute the blocks z_N, y_N, x_N of b_N	93
3	The optimal spectral gap for regular and disordered harmonic networks of oscillators	111
3.1	Introduction	112
3.1.1	Description of the model	112
3.1.2	State of the art and motivation	114
3.1.3	Main results	116
3.2	Mathematical preliminaries	120
3.3	Proofs of the main results	124
3.3.1	Reduction method from scattering theory	124
3.3.2	One-dimensional homogeneous chain	125
3.3.3	Higher-dimensional homogeneous networks	130
3.3.4	Single impurities in the chain	138
3.3.5	Disordered chains	143
	Appendices	149
3.A	Proposition 2.1 on the chain of oscillators (2.5)	149
3.B	Matrix-valued Rouché's theorem	150
4	Existence of a Non-Equilibrium Steady State for the non-linear BGK equation on an interval	153
4.1	Introduction	154
4.1.1	Description of the model	154
4.1.2	State of the Art	155
4.2	Mathematical Preliminaries	157
4.2.1	Notation	157
4.2.2	Plan of the paper	157
4.3	Main Results	158
4.4	Proofs	159
4.4.1	Strategy of Proof	159
4.4.2	Definition of the map $\mathcal{F}(T)$	160
4.4.3	L^∞ Bounds on $\mathcal{F}(T)$	167

4.4.4	Hölder continuity of $\mathcal{F}(T)(x)$.	177
4.4.5	Continuity of the map \mathcal{F}	180
4.4.6	Fixed Point Argument	184
4.5	Discussion of the results and future work	185
5	A quantitative perturbative approach to hydrodynamic limits	187
5.1	Introduction	188
5.1.1	Zero-Range process	193
5.1.2	Simple Exclusion model	196
5.1.3	Ginzburg-Landau type models	197
5.1.4	State of the art	200
5.2	Quantitative Local Law of Large Numbers	202
5.3	Proof of the main abstract Theorem	205
5.4	Proof of (H1)-(H2)-(H3) for the Zero-Range Process	206
5.4.1	Consistency estimate	209
5.4.2	Microscopic Stability estimate	216
5.5	Proof of (H1)-(H2)-(H3) for the Simple Exclusion process	219
5.5.1	Consistency estimate	220
5.5.2	Microscopic stability estimate	225
5.6	Proof of (H1)-(H2)-(H3) for the Ginzburg-Landau process	227
5.6.1	Consistency estimate	229
5.6.2	Microscopic stability estimate	232
5.7	Perspectives-Work in progress	234
5.7.1	The case of $d \geq 2$ dimensions	234
5.7.2	Convergence of the microscopic entropy to the macroscopic entropy	234
	Appendices	237
5.A	Regularity properties of the quasilinear diffusion equation	237
6	Spectral gap in mean-field $\mathcal{O}(n)$-model	243
6.1	Introduction and main results	244
6.1.1	$\mathcal{O}(n)$ -model	244
6.1.2	State of the art and motivation	244
6.1.3	Organization of the chapter	247
6.2	The mean-field $\mathcal{O}(n)$ -model	248
6.3	Renormalized measure and mathematical preliminaries	249
6.4	The mean-field Ising model	254
6.4.1	Lower bound on spectral gap in weak field $h < h_c(\beta)$ regime	254
6.4.2	Upper bound on spectral gap in weak field $h < h_c(\beta)$ regime.	257

6.4.3	Spectral gap in strong magnetic field regime $h > h_c(\beta)$	259
6.4.4	Critical magnetic fields in $n = 1$	260
6.5	Multi-component $\mathcal{O}(n)$ -models	264
6.5.1	$n \geq 2$: Zero magnetic field, $h = 0$	264
6.5.2	Zero magnetic field- A lower bound on the spectral gap	265
6.5.3	Nonzero magnetic fields for $n \geq 2$	270
6.6	The critical regime, Proof of Theo. 1.3	273
6.6.1	Critical Ising model	273
6.6.2	Critical multi-component systems	279

Appendices **285**

6.A	Numerical results	285
6.B	Asymptotic properties of the Ising model	286
6.C	SUSY Quantum Mechanics	288
6.D	Asymptotic properties	288

Bibliography **291**

Chapter 1

Introduction

The aim of this thesis is to study problems in mathematical physics motivated by kinetic theory and non-equilibrium statistical mechanics. The main motivation is to understand the scaling of certain quantities in many-particle systems in terms of the number of the particles or other physical parameters of interest. In particular, in many cases we are interested in making precise how the spectral gap of the associated dynamics (the speed of the convergence to the steady state) scales. This contributes towards an answer to one of the most important open problems in statistical physics which is the rigorous derivation of Fourier's law in an appropriate regime or a mathematical proof of its breakdown. Fourier's law was proposed by Fourier in 1808 and it is a physical macroscopic law that relates the local thermal flux $J(t, x)$ to small variations of temperature $\nabla T(t, x)$ through a proportionality constant $\kappa(T)$ known as *thermal conductivity*:

$$J(t, x) = -\kappa(T)\nabla T(t, x). \quad (0.1)$$

Given that Fourier's law (0.1) holds, one can deduce the following diffusion equation for the temperature

$$c(T)\partial_t T(t, x) = \nabla \cdot [\kappa(T)\nabla T(t, x)] \quad (0.2)$$

where $c(T)$ is the specific heat of the system per unit volume. Apart from Fourier's law discussed here, there are other similar laws in physics discovered during the nineteenth century, including Ohm's law for electric currents or Fick's law.

At the microscopic scale, matter is made out of particles assumed to evolve according to the classical laws of mechanics, and one of the goals of statistical physics is to model heat conductivity through a system of interacting atoms and to achieve a rigorous derivation of constitutive laws such as Fourier's law [BLRB00, FB19, Lep16, Dha08]. Understanding macroscopic laws of matter when starting from a microscopic system of interacting atoms

is a challenge addressed to mathematicians by Hilbert in his 6th problem [Hil02]:

“6. Mathematical Treatment of the Axioms of Physics. The investigations on the foundations of geometry suggest the problem: To treat in the same manner, by means of axioms, those physical sciences in which already today mathematics plays an important part; in the first rank are the theory of probabilities and mechanics.”

In a further explanation Hilbert proposed two specific problems: first, an axiomatic treatment of probability with limit theorems for the foundation of statistical physics and second, the rigorous theory of limiting processes *“which lead from the atomistic view to the laws of motion of continua.”*

A paradigmatic set up where Fourier’s law is observed to hold with high precision is when one considers a fluid in a cylindrical slab of height h and uniform cross sectional area A , coupled at the two boundaries, the top and the bottom of the cylinder, to two heat reservoirs at different temperatures. This is known as the Benard experiment [BLRB00]. The two heat reservoirs keep the system out of equilibrium and produce a stationary heat flow. If there is a non-equilibrium steady state (NESS) that is described by a phase-space measure, one would like to prove that the following limit exists:

$$0 < \kappa(N) := \lim_{N \rightarrow \infty} \frac{\langle J^N(t, x) \rangle}{A(\Delta T/N)} < \infty \quad (0.3)$$

where N is the microscopic length of the cylinder,

$$\frac{\Delta T}{N} = \frac{T_2 - T_1}{N}$$

is the effective temperature gradient, $\langle J^N(t, x) \rangle$ is the expectation of the heat flux with respect to the non equilibrium steady state and where we write $J^N(t, x)$ to stress the dependence of J on N . The above limit allows us to define the thermal conductivity and the very existence of the limit is a formulation of Fourier’s law.

Our main objective is to investigate how certain quantities, such as the relaxation rates to the NESS of such systems (the spectral gap of the associated dynamics), scale with the system size, since these are crucial to making sure that the thermal conductivity has a thermodynamic limit.

A subclass of models describing thermal transport are one dimensional chain of atoms [LLP03, Dha08]. These models have been the subject of many studies from a mathematical and a numerical point of view, mainly after the end of 90s. Deriving Fourier’s law from this model however turned out to be particularly challenging since the thermal conductivity of one-dimensional chains does not have a well-defined thermodynamical limit as the number of the particles goes to infinity. Nevertheless, interestingly, these caricatural systems are

in fact physically relevant when one looks at promising new (one-dimensional or two-dimensional) materials like carbon nanotubes or graphene sheets. It was experimentally observed that the thermal conductivity diverges in actual sufficiently clean experimental samples of such materials [ZOC⁺20], as predicted by numerical simulations. This is also discussed in the introduction of [IOS21].

The introduction that follows provides the mathematical tools and framework for the articles contained in the following chapters. In Section 1.1, I briefly recall some classical features of the microscopic description of Hamiltonian systems. I introduce general Markov processes and semigroups, describe their evolution laws, I briefly recall their properties and finish with some examples from both equilibrium and non-equilibrium mechanics of elliptic and hypoelliptic type. In Section 1.2, I review the main results about the long-time behaviour of dynamics described by both elliptic and hypoelliptic operators, focusing mainly on the examples that I introduced just before in section 1.1. I introduce the notion of an invariant measure, I state the conditions for its existence and uniqueness and introduce the notion of non-equilibrium stationary states. I present some existing methodologies to study quantitatively the long time behavior of the systems. Next, in Section 1.3 I discuss about some hydrodynamic limits, i.e. limits as the number of the particles goes to infinity, connecting stochastic interacting particle systems to macroscopic partial differential equations and I review known results on the topic. In the last section of this introduction there is a summary of the results presented in each of the following Chapters.

1.1 Evolution of Microscopic Interacting Particle Systems

1.1.1 Hamiltonian dynamics

The state of a microscopic system that consists of N point-like particles in d -dimensions, $d \geq 1$, is determined by the values of the coordinates $(q_1, \dots, q_{Nd}) \in X_N$, where the dimension of X_N is dN , and the momenta $(p_1, \dots, p_{Nd}) \in \mathbb{R}^{dN}$. The phase space is then $\Omega_N = X_N \times \mathbb{R}^{dN}$.

The total internal energy of the system is the sum of its total kinetic energy and its potential energy. The energy is described by a Hamilton function $H : \Omega_N \rightarrow \mathbb{R}$,

$$H(p, q) = \frac{1}{2} p^T \text{diag}(m_1^{-1} \text{Id}_d, \dots, m_N^{-1} \text{Id}_d) p + U(q), \quad q \in X_N, \quad p \in \mathbb{R}^{dN} \quad (1.4)$$

where $m_i > 0$, $i = 1, \dots, N$ are the masses.

The microscopic dynamics is governed by the following classical Hamiltonian equations:

$$\begin{aligned}
dq(t) &= \nabla_p H(p, q) dt = \text{diag}(m_1^{-1} \text{Id}_d, \dots, m_N^{-1} \text{Id}_d) p(t) dt = M^{-1} p(t) dt \\
dp(t) &= (-\nabla_q H(p, q)) dt = -\nabla_q U(q) dt \\
(p(0), q(0)) &= (p_0, q_0), \quad q \in X_N, \quad p \in \mathbb{R}^{dN}.
\end{aligned} \tag{1.5}$$

We consider the Hamiltonian flow of the dynamics ϕ_t , which is a semigroup, *i.e.* $\phi_{t+s} = \phi_t \circ \phi_s$ for all $t, s \in \mathbb{R}$, and is so that

$$\phi_t(p_0, q_0) = (p_t, q_t). \tag{1.6}$$

Let $f \in C^1(X_N \times \mathbb{R}^{dN})$ and compute the time-derivative of $t \mapsto f(\phi_t(p_0, q_0))$:

$$\begin{aligned}
\frac{d}{dt} f(p_t, q_t) &= \frac{d}{dt} f(\phi_t(p_0, q_0)) = p^T \text{diag}(m_1^{-1} \text{Id}_d, \dots, m_N^{-1} \text{Id}_d) \nabla_q f - \nabla_q U(q)^T \nabla_p f \\
&=: \mathcal{L}f.
\end{aligned} \tag{1.7}$$

We then say that the differential operator \mathcal{L} is the infinitesimal generator of the Hamiltonian dynamics so that when $f \in C^1(\Omega_N)$ as before,

$$f(p_t, q_t) = (e^{t\mathcal{L}} f)(p_0, q_0) = (f \circ \phi_t)(p_0, q_0).$$

1.1.2 Stochastic dynamics

In this subsection we consider first the SDE of the following form

$$dz_t = b(z_t) dt + \sigma(z_t) dW_t, \quad z_t \in \Omega \tag{1.8}$$

where W_t are d -dimensional Wiener processes, $b : \Omega \rightarrow \mathbb{R}^n$ is the drift vector and $\sigma : \Omega \rightarrow \mathbb{R}^{n \times d}$ is the diffusion matrix. The solution to (1.8) forms a Markov process and so we define the transition probabilities for all $z \in \Omega$,

$$P_t^*(z, dy) = \mathbb{P}(z_t \in dy | z_0 = z) \quad \text{with} \quad \int_{\Omega} P_t^*(z, dy) = 1$$

where z is the initial condition and P_t^* satisfies the Chapman-Kolmogorov relation

$$P_{t+s}^*(z, dy) = \int_{w \in \Omega} P_t^*(z, dw) P_s^*(w, dy) \tag{1.9}$$

which is the semigroup property. Thus we consider a semigroup $\{P_t^*, t \geq 0\}$ ¹ on the space of Borel probability measures on the space Ω such that

$$(P_t^* \mu)(B) = \int_{\Omega} P_t^*(x, B) d\mu(x), \quad B \in \mathcal{B}(\Omega).$$

Now, one can similarly consider the *dual* semigroup $\{P_t, t \geq 0\}$ acting on observables.² For any measurable function $f : \Omega \rightarrow \mathbb{R}$ we define

$$P_t f(z) = \int_{\Omega} f(y) P_t(z, dy) = \mathbb{E}_z(f(z_t))$$

where $z_t = (p_t, q_t)$ solves (1.1) and $\mathbb{E}_z(f(z_t))$ is the expectation taking over all the realizations of the Brownian motion starting from $z \in \Omega$.

It is clear now that P_t is indeed a semigroup because of the relation (1.9). The Markov semigroup P_t preserves mass, positivity and it is bounded (hence it is a contractive semigroup), i.e.

$$P_t(1) = 1, \quad P_t(f) \geq 0, \quad \text{for } 0 \leq f \in L^1 \quad \text{and} \quad \|P_t f\|_{L^\infty(\Omega)} = \left| \int_{\Omega} f(y) P_t(x, dy) \right| \leq \|f\|_{L^\infty(\Omega)}.$$

These properties allow to make sense of the following definition of the *generator* of the semigroup $\{P_t\}_{t \geq 0}$ (which is due to the so-called Hille-Yosida Theorem, see for instance [Paz83] or [BGL14, Section 1.4] and references therein):

$$\mathcal{L}f := \lim_{t \rightarrow 0^+} \frac{P_t f - f}{t} \tag{1.10}$$

for every $f \in C_c^\infty(\Omega)$. An application of Ito's formula then gives that the generator \mathcal{L} on $f(z_t)$ when z_t is solution to the process (1.8), is

$$\mathcal{L} = b \cdot \nabla + \frac{1}{2} \sigma \sigma^T : \nabla^2 \tag{1.11}$$

where the symbol $:$ denotes the Frobenius inner product, i.e.

$$\mathcal{L}f = b \cdot \nabla f + \frac{1}{2} \sum_{i,j,l} \sigma_{i,l} \sigma_{j,l} \partial_{x_i x_j} f.$$

Regarding the existence and uniqueness of solutions to the SDE (1.8) it is well-known [Ok03, RB06a] that if the fields b, σ are locally Lipschitz and either

- (i) $|b(x)| + |\sigma(x)| \lesssim c(1 + |x|)$ for all $x \in \Omega$, i.e. existence of a linear bound

¹The semigroup interprets how a probability measure μ propagates in time, i.e. $P_t^* \mu$ is the distribution at time t if the initial probability distribution is μ .

²An observable is a bounded and continuous function of the microscopic state $f(q, p)$.

or

- (ii) there exists a Lyapunov function W with $W \geq 1$ and $\lim_{|x| \rightarrow \infty} W(x) = \infty$ with $\mathcal{L}W(x) \leq cW(x)$, for $c > 0$,

we have a unique global in time solution.

1.1.3 Examples

Here we expose the main examples of our interest and on which we will work on later chapters.

- **(i) Equilibrium mechanics: Langevin dynamics.** A paradigmatic example of equilibrium dynamics in the form of the SDE (1.8) is the *Langevin dynamics*, namely

$$\begin{aligned} dq_t &= M^{-1}p_t dt \\ dp_t &= (-\nabla U(q_t) - \gamma M^{-1}p_t) dt + \sqrt{\frac{2\gamma}{\beta}} dW_t, \quad q_t \in X_N, p_t \in \mathbb{R}^{dN} \end{aligned} \quad (1.12)$$

where $M = \text{diag}(m_1^{-1}\text{Id}_d, \dots, m_N^{-1}\text{Id}_d)$, so that the state space is $\Omega = X_N \times \mathbb{R}^{dN}$ of dimension $2dN$, $\gamma > 0$ is a positive friction constant, W_t a dN -dimensional Wiener process and β the inverse temperature of the system.

As discussed in [LRS10, Section 2.2.4] one can consider the limit $\gamma \rightarrow \infty$ under the time rescaling $t \mapsto \gamma t$, to recover the so-called *overdamped Langevin dynamics*:

$$dq_t = -\nabla U(q_t) dt + \sqrt{\frac{2\gamma}{\beta}} dW_t. \quad (1.13)$$

This limiting process (1.13) can be also obtained when $M = m\text{Id}$, as the limit $m \rightarrow 0$.

The explicit expression of the generator of the Langevin dynamics is then given by

$$\mathcal{L} = M^{-1}p \cdot \nabla_q - \nabla_q U(q) \cdot \nabla_p + \gamma (\beta^{-1} \Delta_p - M^{-1}p \cdot \nabla_p) \quad (1.14)$$

for *inhomogeneous dynamics* and

$$\mathcal{L} = -\nabla_q U(q) \cdot \nabla_q + \beta^{-1} \Delta_p \quad (1.15)$$

for *overdamped Langevin dynamics*.

The Langevin dynamics (and generalized Langevin dynamics³) have been studied extensively in [IOS19, Iac17, PSV21] and references therein, where questions of existence

³In general generalized Langevin dynamics (GLE) is a non-Markovian stochastic integro-differential equation more complicated to study than the Langevin and overdamped Langevin equations. This is why in many mathematical works quasi-Markovian approximation are studied instead, see [PSV21] and references therein.

and uniqueness of invariant measures and rates of convergence towards the stationary measure are tackled, as well as analytical and numerical results on how several parameters of physical interest, such as friction coefficients for example, affect the convergence rates.

Before we present the second example, let us make a brief introduction. Apart from the example regarding Langevin dynamics from equilibrium dynamics, in this thesis we are mainly interested in *non-equilibrium perturbations of equilibrium dynamics*. We study the effects of some external forcings on the system, so that they perturb the equilibrium dynamics and keep the system in a non-equilibrium state. From a physical viewpoint, the irreversibility of the evolution is characterised by the existence of non-zero currents, which represent the response of the system to the perturbation. Typically, the external action can be either an external force, like a potential force, or it can be caused by letting different parts of the system interact with heat baths at different temperatures, which is a localized forcing.

Here we will focus on a family of heat-conducting systems. We consider a classical system of N particles, each of which in d dimensions. As before, we denote by q_i the position and by p_i the momentum of each particle $i \in \{1, \dots, N\}$. The phase space is denoted by Ω . The two usual cases, depending on the domain of q_i , that have been considered in the literature are (for more details we refer to the thesis [Cun16] and references therein):

- Oscillators: $\Omega = \mathbb{R}^{dN} \times \mathbb{R}^{dN}$. That is, $q_i, p_i \in \mathbb{R}^d$.
- Rotors: $\Omega = \mathbb{T}^{dN} \times \mathbb{R}^{dN}$. We then have that the q_i 's are on the torus and $p_i \in \mathbb{R}^{dN}$. In this case one sees each particle as a rotor, i.e. rotating disk.

We consider a rod (typically an electrical insulator) in contact at two ends with heat reservoirs at different temperatures $T_L > T_R$. The motivation of considering this model is the derivation of Fourier's law, according to which we expect to see a heat flux along the rod moving from left to right, which is proportional to the temperature difference $T_L - T_R$ (which has been experimentally tested when the temperature difference is small), and inversely proportional to the length of the rod. A model of a heat-conducting medium is typically a network of interacting sites, which can be thought of as atoms, coupled to some reservoirs (heat baths). We will focus on the case of oscillators such that at the bulk of the system they undergo Hamiltonian dynamics. Regarding the reservoirs (heat baths), there are several ways to model the thermostats, see the review [BLRB00, section 4]. Here we will model the coupling through Langevin thermostats, which is the simplest coupling for our purposes, as we will see below. Lastly, we will consider nearest neighbor interaction among the oscillators and the geometry of our network will be either a line (one-dimensional) or d -dimensional grids.

• (ii) **Non-Equilibrium mechanics: Hamiltonian systems in contact with Langevin thermostats.**

We consider a chain (or network) of oscillators, the energy of which is described by a Hamilton function $H : T^*\mathbb{R}^{dN} \rightarrow \mathbb{R}$, where $T^*\mathbb{R}^{dN}$ is the cotangent bundle phase space and can, of course, be identified with \mathbb{R}^{2dN} ,

$$H(q, p) = \frac{\langle p, m_N^{-1} p \rangle}{2} + V(q) \quad \text{where } V(q) = \sum_{i=1}^N V_1(q_i) + \sum_{i \sim j} V_2(q_i - q_j) \quad (1.16)$$

where \sim indicates nearest neighbors on the $\{1, \dots, N\} \subset \mathbb{Z}$ lattice. The above form of the potential describes particles that are fixed by a *pinning* potential $V_1(q)$ and interact through an *interaction* potential $V_2(q_i - q_j)$ for i, j such that $\|i - j\|_\infty = 1$, i.e. the neighboring particles. For simplicity we assume that the masses m_i are all equal and normalized to 1.

The dynamics of this model is such that the particles at the boundary are coupled to heat baths at (possibly) different temperatures $\beta_i^{-1}, i \in \mathcal{F}$ are subject to friction. $\mathcal{F} \subset \{1, \dots, N\}$ here is the subset of the particles on which we impose friction and noise and we also denote by $\gamma_i > 0$ the friction strength at the i -th particle. The time evolution is then for particles $i \in \{1, \dots, N\}$ described by a coupled system of SDEs:

$$\begin{aligned} dq_i(t) &= (\nabla_{p_i} H) dt \quad \text{and} \\ dp_i(t) &= \left(-\nabla_{q_i} H - \gamma_i p_i \delta_{i \in \mathcal{F}} \right) dt + \delta_{i \in \mathcal{F}} \sqrt{\frac{2\gamma_i}{\beta_i}} dW_i \end{aligned} \quad (1.17)$$

where β_i is the inverse temperature at the boundary of the chain of oscillators, W_i with $i \in \mathcal{F}$ are independent identically distributed Wiener processes, $\gamma_i > 0$ a friction parameter, and $\mathcal{F} \subset \{1, \dots, N\}$ the set of the particles subject to friction. Let us consider for this example here the case $\mathcal{F} = \{1, N\}$, i.e. where the noise and the friction are imposed only on the particles on the boundary of the chain (the first and the last particle).

The generator of the dynamics in this case is given by

$$\mathcal{L} = \sum_{j=1}^N p_j \cdot \nabla_{q_j} - [\nabla_{q_j} V(q)] \cdot \nabla_{p_j} + \gamma_1 p_1 \cdot \nabla_{p_1} - \gamma_N p_N \cdot \nabla_{p_N} + \gamma_1 T_L \Delta_{p_1} + \gamma_N T_R \Delta_{p_N} \quad (1.18)$$

where T_L, T_R are the (possibly) different temperatures at the left and right boundary of the network of oscillators. One remark about our choice of Langevin thermostats, comparatively with works-stations on this problem, as [EPRB99a, EPRB99b, RBT02] is the following: The authors there considered ‘infinite’ Hamiltonian heat baths. That is each heat bath was an infinite dimensional linear Hamiltonian system, where it was chosen

as the classical field theory associated with linear wave equations. The initial assumption was that the initial states of the reservoirs are distributed according to Gibbs distribution with given (possibly) different temperatures. Integrating the variables of the heat baths then, would lead to a system of random integro-differential equations, the generalized Langevin equations (GLE). Even though this way of modeling the thermostats would not give immediately Markov solutions, it is shown that the resulting process can become Markovian under a specific interaction between the chain and the fields. In particular one can introduce a finite number of auxiliary variables in such a way that the evolution of the chain, together with these variables, is described by a system of Markovian stochastic differential equations.

Nevertheless, even in this more complicated scenario, the equation (1.17) can be recovered by taking some appropriate limit as discussed in [RBT02] (see comments above the equation (10)) and [FKM65].

1.2 Long Time behaviour

1.2.1 Elliptic case

Here we briefly review the long time analysis of the dynamics for the elliptic case, an example of which is the overdamped Langevin dynamics, introduced in the example (i) in subsection 1.1.3. We start by giving the definitions of certain functional inequalities that are useful for establishing convergence to the invariant measure (i.e. equilibrium measure).

Definition 2.1 (Entropy, Log-Sobolev Inequalities and Poincaré Inequalities). *Given a probability measure μ on some Borel space Ω the entropy $\text{Ent}_\mu(F)$ of a positive measurable function $F : \Omega \rightarrow \mathbb{R}_{\geq 0}$ is defined as*

$$\text{Ent}_\mu(F) := \int_\Omega F(x) \log \left(F(x) / \int_\Omega F(y) d\mu(y) \right) d\mu(x) \in [0, \infty]. \quad (2.19)$$

We say that μ satisfies a logarithmic Sobolev inequality with constant k , denoted LSI(k), iff

$$\text{Ent}_\mu(f^2) \leq \frac{2}{k} \|\nabla f\|_{L^2(d\mu)}^2 \quad (2.20)$$

for all smooth functions f . The LSI(k) implies [Led99, Prop. 2.1] that μ satisfies a spectral gap inequality with constant k , denoted SGI(k), also called Poincaré Inequality, iff

$$\text{Var}_\mu(f) \leq \frac{1}{k} \|\nabla f\|_{L^2(d\mu)}^2. \quad (2.21)$$

Logarithmic Sobolev (and other functional) inequalities are very effective tools to study the concentration of measure phenomenon and to quantify the relaxation rates, i.e. the

mixing properties, of the dynamics of many-particle systems [Gro93, BE85, Led99, Led01, GZ03, ABC⁺00]. This is since the spectral gap (the speed of relaxation) is known to be determined by the constant in the Log-Sobolev inequalities. We define the spectral gap to be the size of the gap between 0 and the rest of the spectrum of the associated generator L . The gap then can be also characterized by

$$\lambda_S := \inf_{f \in L^2(\mu) \setminus \{0\}} \frac{-\langle Lf, f \rangle_{L^2(d\mu)}}{\text{Var}_\mu(f)}$$

where Var_μ is the variance relative to the equilibrium measure μ . The generator L and the reference measure μ are specified for the dynamics of our interest, in the following chapters. In what follows, we briefly discuss the fulfillment of some functional inequalities and convergence to equilibrium for the overdamped Langevin dynamics. This is an example where the generator is an elliptic operator, since the matrix $\beta^{-1}\text{Id}$ corresponding to the second order derivatives, is positive definite.

Overdamped Langevin dynamics: In the case of the overdamped Langevin dynamics, equation (1.15), the invariant measure

$$\rho(dq) = Z^{-1} e^{-\beta U(q)} dq, \quad q \in X_N \tag{2.22}$$

is the solution to the stationary Fokker Planck equation $\mathcal{L}^\dagger \psi = 0$, where \mathcal{L}^\dagger is the L^2 -adjoint and \mathcal{L} is given by (1.15). Note that this generator in the weighted space $L^2(d\rho)$ is self-adjoint, see [BGL14, Section 3.3] and writing \mathcal{L}^* for the $L^2(d\rho)$ -adjoint we have

$$\mathcal{L}^* = -\beta^{-1} \nabla_q^* \nabla_q, \quad \text{where } \nabla_q^* = -\nabla_q + \beta \nabla_q U(q) \tag{2.23}$$

i.e. ∇_q^* is the adjoint of ∇_q in the weighted space $L^2(d\rho)$. Also note that $\text{Ker}(\mathcal{L}) = \text{span}(\mathbf{1})$. Regarding the long time behavior of this dynamics, i.e. the convergence to the invariant measure, we consider the density $f(t, q)$ with respect to the invariant measure $\rho(dq)$, i.e. $f(t, q) = \psi(t, q) dq / \rho(dq)$. Then we see that $f(t, q)$ satisfies the Kolmogorov equation

$$\partial_t f(t, q) = \mathcal{L}^* f(t, q), \quad f(0, q) = f_0(q)$$

with initial data $f_0 \in L^1(d\rho)$, $\int_X f_0(q) \rho(dq) = 1$, and so $f_t(q) = e^{t\mathcal{L}^*} f_0(q)$. The convergence to equilibrium then reads

$$e^{t\mathcal{L}^*} (f_0 - \mathbf{1}) \rightarrow 0, \quad \text{as } t \rightarrow \infty. \tag{2.24}$$

In order to state quantitative convergence results involving exponential rates, we exploit functional inequalities such as the Poincaré and logarithmic Sobolev inequalities.

1.2.1.1 Relaxation of the semigroup via Poincaré Inequality

For the overdamped generator (1.15) we have that

$$\langle -\mathcal{L}\phi, \phi \rangle_{L^2(d\rho)} = \beta^{-1} \|\nabla_q \phi\|_{L^2(d\rho)}^2 \quad (2.25)$$

so that if we have a Poincaré Inequality (2.21) and restrict to the functional space $L_0^2(d\rho) := \{\phi \in L^2(d\rho) : \int_X \phi(q) d\rho(q) = 0\}$, we have

$$\langle -\mathcal{L}\phi, \phi \rangle_{L^2(d\rho)} = \beta^{-1} \|\nabla_q \phi\|_{L^2(d\rho)}^2 \geq \beta^{-1} k \|\phi\|_{L^2(d\rho)}^2 \quad \text{for all } \phi \in L_0^2(d\rho). \quad (2.26)$$

In other words, Poincaré Inequality implies the coercivity of the operator with respect to the $L^2(d\rho)$ -inner product. The Grönwall's inequality then implies exponential relaxation of the associated semigroup:

$$\|e^{t\mathcal{L}} \phi\|_{L^2(d\rho)} \leq e^{-\frac{k\beta^{-1}t}{2}} \|\phi\|_{L^2(d\rho)}.$$

We can summarize this in the following statement.

Proposition 2.2. *The semigroup $e^{t\mathcal{L}}$ satisfies*

$$\|e^{t\mathcal{L}}\| \leq e^{-\frac{k\beta^{-1}t}{2}}, \quad \text{for all } t \geq 0$$

if and only if the reference measure ρ satisfies a Poincaré Inequality with constant $k > 0$, SGI(k). This implies that \mathcal{L} is invertible with $\mathcal{L}^{-1} = -\int_0^\infty e^{t\mathcal{L}} dt$ and

$$\|\mathcal{L}^{-1}\| \leq \beta k^{-1}.$$

One more important property of Spectral Gap Inequalities, is the tensorization. It will prove to be particularly useful when we study the spectral gap for the $\mathcal{O}(n)$ model by employing the renormalization group procedure. The following proposition holds.

Proposition 2.3 ([BGL14]). *Given m probability measure ρ_1, \dots, ρ_m which all satisfy the Poincaré Inequality with constants $k_i, i = 1, \dots, m$, the product measure $\rho_1 \otimes \rho_2 \otimes \dots \otimes \rho_m$ satisfies the Poincaré Inequality with constant $k = \min\{k_1, \dots, k_m\}$.*

1.2.1.2 Relaxation of the semigroup via Log-Sobolev Inequality

This inequality was introduced by L. Gross in [Gro75] to prove the hypercontractivity result of Nelson (see [Nel73]) for the Ornstein-Uhlenbeck semigroup. Even though we will restrict ourselves here to the case of diffusions, this inequality is valid in more general settings and in infinite dimensional situations.

Consider two probability measures μ, ν , so that $\nu \ll \mu$ and define

$$f^2 = \frac{d\nu}{d\mu},$$

then the entropy defined in 2.1 is

$$\text{Ent}_\mu(f^2) = \int \log f^2 d\nu$$

which is the relative entropy of ν with respect to μ and it is denoted $H(\mu|\nu) = H_\nu(\mu)$.

Recalling now the definition of the Log-Sobolev Inequality in 2.1:

$$\text{Ent}_\mu(f^2) \leq \frac{2}{k} \|\nabla f\|_{L^2(d\mu)}^2,$$

we first observe that it is homogeneous so that without loss of generality we assume that $\int f^2 d\mu = 1$ and then we can write $d\nu = f^2 d\mu := g d\mu$, so that the inequality takes the form

$$H(\nu|\mu) \leq \frac{1}{2k} \int \frac{|\nabla g|^2}{g} d\mu.$$

The quantity in the right-hand side $I_\mu(\nu) := \int \frac{|\nabla g|^2}{g} d\mu$ is called the relative *Fisher Information* of ν with respect to μ .

Note that the Log-Sobolev Inequality is stronger than the Poincaré inequality, so that if a measure μ satisfies a LSI(k) then it satisfies a SGI with the constant $k/2 > 0$. As a matter of fact Poincaré is a linearization of the LSI. To see this, it suffices to apply the LSI to $(1 + \epsilon f)$ and then let ϵ go to 0. For that and more details, see the book [BGL14, Section 5]. Let us also mention [OV00] which draws connections with other functional inequalities, such as the Talagrand Inequality.

We can now state the convergence result: If $\psi_t(q)$ solves the Kolmogorov equation (or the Fokker-Planck equation) $\partial_t \psi_t(q) = \mathcal{L}^\dagger \psi_t(q)$, i.e. $\psi_t(q) = e^{t\mathcal{L}^\dagger} \psi_0(q)$, then we have the following equivalence:

$$\begin{aligned} H(\psi_t|\rho) &\leq e^{-2kt\beta^{-1}} H(\psi_0|\rho) \quad \text{for all } t \geq 0, \quad \text{if and only if} \\ \rho &\text{ satisfies a } LSI(k) \end{aligned} \tag{2.27}$$

for any initial state ψ_0 such that $\int_X \psi_0(q) dq = 1$ and $H(\psi_0|\mu) < \infty$. Once we have established a convergence in relative entropy as above, by exploiting the Pinsker-Csiszár-Kullback Inequality which in general reads: $\|\mu - \nu\|_{TV}^2 \leq 2H(\mu|\nu)$, we have

$$\|\psi_t - \rho\|_{TV}^2 \leq 2H(\psi_t|\rho) \leq e^{-2kt\beta^{-1}} H(\psi_0|\rho) \quad \text{for all } t \geq 0, \tag{2.28}$$

or equivalently if ψ_t has density f_t with respect to the reference measure ρ , we write

$$\|f_t - 1\|_{L^1(\rho)}^2 \leq 2 \text{Ent}_\rho(f_0) e^{-2kt\beta^{-1}} \quad \text{for all } t \geq 0. \quad (2.29)$$

There are several ways to obtain Log-Sobolev Inequalities for measures of the form of the canonical measure ρ , as in (2.22) for example. In the particular case of a measure which is a product of m measures and each one satisfies a LSI, then the whole measure satisfies a LSI with constant $k = \min_i k_i$. Just like Poincaré Inequalities, the LSI has the tensorization property as well (see [Gro75]).

1.2.1.3 Curvature-Dimension Inequalities

As in the works by Bakry-Emery [BE85], see also [ABC⁺00, Bak06, BGL14], one way to get to the functional inequalities described above, and as a consequence to obtain quantitative rates of convergence to the stationary state, is to study the local structure of the generator and prove a so-called Curvature-Dimension Inequalities. Let \mathcal{A} be an algebra, included in the domain of the generator L of the semigroup, $D(L)$. We introduce the bilinear map $\Gamma : \mathcal{A} \times \mathcal{A} \rightarrow \mathcal{A}$, called the *Carré Du Champ Operator*:

$$\Gamma(f, g) = \frac{1}{2} (L(fg) - fLg - gLf) \quad \text{for all } f, g \in \mathcal{A}. \quad (2.30)$$

We iterate this and in the same way that we defined Γ having as action the standard inner product, now we define Γ_2 on $\mathcal{A} \times \mathcal{A}$ having as action the action of Γ :

$$\Gamma_2(f, g) = \frac{1}{2} (L\Gamma(f, g) - \Gamma(f, Lg) - \Gamma(g, Lf)). \quad (2.31)$$

We say that the operator L satisfies the *curvature-dimension condition* $CD(\lambda, n)$ with curvature $\lambda \in \mathbb{R}$ and dimension $n \in [1, \infty]$, if and only if for any function $f \in \mathcal{A}$, we have

$$\Gamma_2(f, f) \geq \lambda \Gamma(f, f) + \frac{1}{n} (Lf)^2. \quad (2.32)$$

It is well-known then that if $CD(\lambda, \infty)$ holds true with $\lambda \in \mathbb{R}$, then this is equivalent to having a Poincaré and a Log-Sobolev Inequality with constant proportional to λ , so that the spectral gap is proportional to λ . We refer to [BGL14, ABC⁺00], [Bak06, Proposition 3.3].

1.2.2 Hypoellipticity and Hypocoercivity

1.2.2.1 Hypoellipticity

We are also interested in degenerate dynamics such as the inhomogeneous Langevin dynamics introduced in Example (i) in subsection 1.1.3, as well as dynamics describing non-equilibrium transport phenomena as in the Example (ii) in subsection 1.1.3. In contrast to the overdamped Langevin dynamics, the generators in such cases is not elliptic.

When \mathcal{L} is elliptic, the regularization properties of the Laplacian imply that if $\mathcal{L}f = g$ with $g \in H^m(W)$ and W a bounded open subset of the state space, the solution f is in $H^{m+2}(W)$. Now when the generator is not elliptic, as for the (inhomogenous) Langevin dynamics where the second order derivatives are not acting on all the degrees of freedom, we still can have regularizing properties, under certain conditions on the operator, thanks to the theory of *hypoellipticity*. We start by presenting Hörmander's condition, [Hö67]. We denote by $[A, B] = AB - BA$ the commutator between two operators. We recall that a differential operator A is called hypoelliptic if

$$\text{sing supp } u = \text{sing supp } \mathcal{L}u \quad \text{for all } u \in \mathcal{D}'(X) \quad (2.33)$$

where X is the state space, $\mathcal{D}'(X)$ is the space of distributions on the infinitely differential functions with compact support and for $u \in \mathcal{D}'(X)$, $\text{sing supp } u$ (i.e. the singular support of u) is the set of points $x \in X$ so that there is no open neighborhood of x where u restricted in that region is C^∞ .

Let the operator \mathcal{L} be of the form

$$\mathcal{L} = \sum_{j=1}^M X_j^2 + X_0,$$

where the X_i 's, $i \in \{1, \dots, M\}$ are C^∞ vector fields.

Definition 2.4 (Hörmander's condition). *The family of vector fields $\{X_i\}_i$ satisfies Hörmander's condition if the Lie algebra spanned by $\{X_i\}$, $i \in \{1, \dots, M\}$ has rank $\dim X$ at every point.*

The celebrated Hörmander's Theorem [Hö7b, Theorem 22.2.1] that states that if an operator \mathcal{L} satisfies Definition 2.4, then \mathcal{L} is hypoelliptic. In particular it can be shown, [RB06c], that in this case the solution f to $\mathcal{L}f = g$ with $g \in H^m(W)$ and W is a compact subset of the state space X , is in $H^{m+\epsilon}(W)$ for some $\epsilon > 0$. In particular of course when $g \in C^\infty(X)$ then $f \in C^\infty(X)$. Note that if \mathcal{L} satisfies Hörmander's condition, then one may easily check that any of the following operators also satisfy it and are therefore hypoelliptic: $\mathcal{L}, \mathcal{L}^\dagger, \partial_t - \mathcal{L}, \partial_t - \mathcal{L}^\dagger$.

As immediate consequence we have that the transition probabilities of the associated Markov process have a smooth density with respect to the Lebesgue measure. The latter implies that if we assume that an invariant measure exists, then it should have a smooth density.

As an example of how the generator of the Langevin dynamics satisfy the Hörmander's condition, we take X_0 to be the first order part of the generator, i.e.

$$X_0 = M^{-1}p \cdot \nabla_q - \nabla_q U(q) \cdot \nabla_p + \gamma M^{-1}p \cdot \nabla_p$$

and

$$X_i = \sqrt{\gamma\beta^{-1}}\partial_{p_i} \quad \text{for } i = 1 \dots, Nd.$$

Then the first commutator between X_0 and X_i gives

$$[X_i, X_0] = M^{-1}\sqrt{\gamma\beta^{-1}}(\partial_{q_i} - \partial_{p_i})$$

so that we can recover the vector field ∂_{q_i} by linear combination of X_i and $[X_0, X_i]$. Hence, by considering successive commutators, the family of vector fields $\{[X_i, [X_j, X_0]]_{i,j}$ has maximum rank $2Nd$. Similar discussion for the oscillator chains model in particular can be found in Chapter 2.

Invariant measure. From the definition of the generator (1.10) and integrating both sides with respect to the measure μ on the state space X , we get the following characterization of the invariant measure μ : For all $f \in C_c^\infty(X)$,

$$\int_X \mathcal{L}f d\mu = 0 \tag{2.34}$$

where \mathcal{L} is the generator of the dynamics. By duality the invariant measure can be also obtained as a solution to the Fokker-Planck equation

$$\mathcal{L}^\dagger \psi = 0$$

where \mathcal{L}^\dagger is the L^2 -dual operator of \mathcal{L} . In the weighted $L^2(\mu)$ space, the adjoint is denoted by \mathcal{L}^* and it satisfies

$$\int_X \phi_1(\mathcal{L}\phi_2) d\mu = \int_X (\mathcal{L}^*\phi_1)\phi_2 d\mu.$$

Combining this with (2.34) for $\phi_1 = \mathbf{1}$, then μ is invariant measure iff $\mathcal{L}^*\mathbf{1} = 0$.

Concerning the Langevin dynamics (1.12), it is easy to see that an invariant measure is the Gibbs measure $e^{-\beta H(p,q)} dpdq$.

The existence and uniqueness of invariant measures for a stochastic Markov processes is guaranteed by [RB06c, HM11]:

Proposition 2.5. *Let $(x_t)_t$ be a Markov stochastic process on the phase space X with transition kernel $P_t(x, dy)$ and with generator \mathcal{L} . Then if*

(a) *X is a compact phase space with $(x_t)_t$ being irreducible, i.e. there exists $t_* > 0$ so that $P_{t_*}(x, A) > 0$ for all $x \in X$ and all open sets $A \subset X$, and $P_t(x, dy)$ admits a smooth density.*

(b) *$X = \mathbb{R}^{2dN}$ and (i) $(x_t)_t$ is irreducible, (ii) $P_t(x, dy)$ admits a smooth density and (iii) we have a Lyapunov condition: There exists a Lyapunov function $W : X \rightarrow [1, \infty)$ so that $(\mathcal{L}W)(x) \leq -aW(x) + b$, for all $x \in X$ and some constants $a > 0, b \geq 0$,*

there exists a unique invariant measure μ for $(x_t)_t$.

Note that the first assumption (in both cases, compact and non-compact) about the irreducibility ensures the ergodicity of the invariant measure, while the second assumption implies hypoellipticity and therefore ensures us about the regularity of the invariant measure. In order to have existence and uniqueness in the second (non-compact) case which is the one we are interested in for our example of Langevin dynamics, we need the Lyapunov condition to ensure stability. With this assumption we ensure that the process $(x_t)_t$ stays most of the time in a compact subset of X , where the Lyapunov function takes small values.

Equilibrium and non-equilibrium invariant measures. Regarding non-equilibrium invariant measures, the steady state is induced by external forcing. Examples of such forcings are interactions with thermal reservoirs coupled to some particles of our system as in the Example (ii) in subsection 1.1.2, or interactions with some externally generated field. The steady state is then reached due to the dissipation mechanism which prevents the external forcing to cause an uncontrolled growth of the energy of the system.

For the purpose of describing non-equilibrium steady states we do not make a distinction here between non-equilibrium dynamics and non-reversible dynamics since the dynamics perturbed by some external forcing are irreversible in the sense that the law of forward trajectories is different from the law of backward trajectories. This is discussed in [LS16]. In contrast with equilibrium systems which can be characterized by the self-adjointness of the generator \mathcal{L} on the weighted Hilbert space $L^2(\mu)$, where μ is the invariant measure, which interprets the reversibility for such dynamics, in non-equilibrium systems such property does not hold.

1.2.2.2 Convergence rates towards stationary measure in the hypoelliptic case

As explained above in the cases where our operator fails to be elliptic, i.e. the noise is degenerate and it acts only on a subset of our degrees of freedom (in the overdamped

Langevin case, it acts only on momentum variables), Hörmander's theorem implies regularizing properties by taking advantage of the commutators and transferring the smoothing to all the variables, i.e. hypoellipticity.

The main observation here is that similar phenomena arise when one wants to study the convergence to the equilibrium as well for degenerate systems. In particular, in contrast with the overdamped Langevin (elliptic) case, the operator corresponding to degenerate dynamics is not coercive, and the lack of second-order derivatives, i.e. diffusion, in the position variables leads to the non-coercivity of the operator.

In order to overcome this problem, we exploit the theory of *hypo-coercivity*, which is inspired by hypoellipticity and gives a way through commutators to retrieve some dissipation in the position-variables. The idea is to introduce a modified scalar product with additional correctors by mixed derivatives-terms in the momentum and position variables, see the equation below, (2.35). This new inner product induces a norm different but equivalent to the original norm. Through this norm, one is able to prove and estimate coercivity of the operator which leads (as discussed above) to an exponentially fast convergence to the invariant measure. The price to pay is that we have this convergence in the modified norm, so that when we go back to the original norm (thanks to their equivalence) we end up with a prefactor greater than 1 in front of the exponential.

The first idea of hypo-coercivity goes back to Talay [Tal02] and it was generalized a bit later by Villani [Vil09a]. Related methods were also employed by Hérau and Nier in [HN04] earlier than Villani. Originally, Villani worked in the $H^1(\mu)$ setting, where μ is an invariant measure, and the modified scalar product he introduced was of the following form

$$\langle\langle f, g \rangle\rangle := \langle f, g \rangle + a \langle \nabla_p f, \nabla_p g \rangle + b (\langle \nabla_p f, \nabla_q g \rangle + \langle \nabla_q f, \nabla_p g \rangle) + c \langle \nabla_q f, \nabla_q g \rangle \quad (2.35)$$

where $\langle \cdot, \cdot \rangle$ is the original $L^2(\mu)$ -inner product and $a, b, c \in \mathbb{R}$ with $a, c > 0$, $ac - b^2 > 0$.

The scalar product $\langle\langle \cdot, \cdot \rangle\rangle$ is equivalent to the original $H^1(\mu)$ scalar product. It allows us to prove coercivity in the space $H^1(\mu) \cap L_0^2(\mu)$, where $L_0^2(\mu)$ is the weighted L^2 space with functions that have zero average. Provided that $\mu(dq)$ satisfies a Poincaré inequality, it yields a convergence of the form

$$\|f_t\|_{H^1(\mu)}^2 \leq C e^{-\lambda t} \|f_0\|_{H^1(\mu)}^2 \quad (2.36)$$

with explicit constants C and λ . This is the concept of the so-called H^1 -hypo-coercivity.

Once we have a quantitative convergence result in $H^1(\mu)$, we can combine it with an independent regularity study (hypoelliptic regularization) applied on the initial data to get also a convergence in $L^2(\mu)$, see [H07a, HP08]. This is also discussed in [LS16, Vil09a].

Regarding hypo-coercivity in L^2 , there is a more direct approach first proposed in

[H06] and then extended in a series of papers [DMS15, BDM⁺20, CDH⁺] and references therein. This approach is based on the introduction of a modified L^2 -scalar product via a well-chosen regularization operator. Then the idea is to see hypocoercivity as a combination of two effects: the microscopic coercivity and the macroscopic coercivity.

Alongside with the H^1 -hypocoercivity in Villani's monograph, hypocoercivity in relative entropy was also developed, where instead of the H^1 -norm, we have a combination of two functionals: the relative entropy and the relative Fisher information. In order to have entropic hypocoercivity we assume that the reference measure μ satisfies the stronger Log-Sobolev Inequality instead of Poincaré Inequality.

Other ways to show hypocoercivity include Lyapunov techniques, probabilistic techniques based on coupling methods or on Harris' theorem or on Malliavin calculus. See for instance the recent PhD thesis [Eva19], for more explanations and for an interesting implementation of hypocoercivity through Malliavin calculus. Techniques from Γ calculus can also be used to get quantitative rates of convergence [Bau17, Mon19]. In the following we explain a bit more the hypocoercivity through Γ calculus, as this is applied in the Chapter 2 to study the evolution of the microscopic system, the chain of oscillators, which is a specific case of the Example (ii) in subsection 1.1.3.

Hypocoercivity through generalized Bakry-Emery criteria. Even though the Bakry-Emery theory [BGL14] through Γ -calculus works very well in the elliptic setting, since one can easily confirm that we have a curvature-dimension inequality $\text{CD}(\rho, \infty)$ and then immediately get a $\text{SGI}(\rho)$ and a $\text{LSI}(\rho)$.

However in the hypoelliptic case the Γ and Γ_2 bilinear forms, we see that it seems impossible to bound from below Γ_2 by Γ , and to get the desired inequality of the form (2.31). For example, in the Langevin case (normalizing to 1 for now the constants: mass, friction temperature), we get that

$$\begin{aligned}\Gamma(f, f) &= \|\nabla_p f\|^2 \quad \text{and} \\ \Gamma_2(f, f) &= \Gamma(f, f) + \|\nabla_p^2 f\|^2 + \nabla_q f \cdot \nabla_p f.\end{aligned}\tag{2.37}$$

It is clear then that we can not bound the term $\nabla_q f \cdot \nabla_p f$ from below, and thus in this case we don't have immediately the curvature-dimension inequality.

Nevertheless, this method has been extended to hypoelliptic cases in a number of works recently [Bau17, BG17, BB12, Mon19]. Instead of modifying the norm, we modify the Γ -functional. We introduce a new bilinear form \mathcal{T} that is different but equivalent to the original gradient, so that the twisted form does not depend directly anymore on \mathcal{L} . In general it takes the form

$$\mathcal{T}(f, g) := \sum_{i,j=1}^n \sigma_{ij}(x) \frac{\partial f}{\partial x_i} \frac{\partial g}{\partial x_j}\tag{2.38}$$

where $\sigma_{ij} : \mathbb{R}^n \rightarrow \mathbb{R}$ are smooth functions so that for every $x \in \mathbb{R}^n$, $(\sigma_{ij}(x))_{1 \leq i, j \leq n}$ is symmetric positive definite matrix. Then we analogously define

$$\mathcal{T}_2(f, f) := \frac{1}{2}(\mathcal{L}\mathcal{T}(f, f) - 2\mathcal{T}(\mathcal{L}f, f)). \quad (2.39)$$

Now once we have a ‘twisted’ curvature dimension inequality of the form $\mathcal{T}_2(f, f) \geq \lambda\mathcal{T}(f, f)$, for $\lambda > 0$, we can prove an exponential convergence in Wasserstein distances. Mimicking also the basic ideas of Bakry-Emery, we can prove a Poincaré, SGI(λ) and a Log-Sobolev Inequality, LSI(λ), which allows us to conclude convergence in relative entropy as well.

1.3 Hydrodynamical behaviour for stochastic interacting particle systems

Apart from looking at the long-time behavior of microscopic interacting particle systems, a part of this thesis concerns the ‘hydrodynamic limit’ from stochastic interacting particle systems to macroscopic PDEs, i.e. looking at the limit as the number of the particles N goes to infinity.

The derivation of limit PDE from interacting particle systems has a long history that can be traced back to the founders of the kinetic theory, J. C. Maxwell and L. Boltzmann. We recall here that a rigorous derivation of the Boltzmann equation from molecular dynamics on short time intervals was obtained by O.E. Lanford in [Lan75]. Also ‘formal’ derivations of the Euler system for compressible fluids from molecular dynamics were discussed by C.B. Morrey in [Mor55] and later on, J. Fritz, S.R.S. Varadhan and their collaborators considered stochastic variants of molecular gas dynamics and obtained rigorous derivations of macroscopic PDE models from these variants: see for instance [Var95] and the references therein.

In this thesis we present a quantitative version of such limits for the following stochastic processes: the (jump) processes zero-range and simple exclusion processes and the (diffusion) Ginzburg-Landau process.

We consider these processes on the discrete torus $\mathbb{T}_N^d = \{1, \dots, N\}^d$ with state space X_N which will be either $\mathbb{N}^{\mathbb{T}_N^d}$ for jump processes and $\mathbb{R}^{\mathbb{T}_N^d}$ for diffusion processes. Let $\eta \in X_N$ be a particle configuration with $\eta(x)$ denoting the number of particles at each site $x \in \mathbb{T}_N^d$ (or the value of the charge). Regarding the zero-range and simple exclusion processes, the particles randomly jump to neighboring sites, with the restriction in the simple-exclusion process that at most one particle per site is allowed.

The distribution of particle configurations for time $t > 0$ is a probability measure on

X_N , $\mu_t^N \in P(X_N)$. The evolution of the state $\mu_t^N \in P(X_N)$ solves

$$\frac{d}{dt} \langle \mu_t^N, f \rangle = \langle \mu_t^N, \mathcal{L}_N f \rangle \quad \text{for all } f \in C_b(X_N) \quad (3.40)$$

where the generator $\mathcal{L}_N : C_b(X_N) \rightarrow C_b(X_N)$ is given by

$$\mathcal{L}_N f(\eta) = \sum_{x \sim y \in \mathbb{T}_N^d} c(x, y, \eta) (f(\eta^{xy}) - f(\eta)), \quad \text{for all } f \in C_b(X_N) \quad (3.41)$$

for jump processes, while for the Ginzburg-Landau process the operator is

$$\mathcal{L}_N := \sum_{x \sim y \in \mathbb{T}_N} \left(\frac{\partial}{\partial \eta(x)} - \frac{\partial}{\partial \eta(y)} \right)^2 - \sum_{x \sim y \in \mathbb{T}_N} \left(\frac{\partial V}{\partial \eta(x)} - \frac{\partial V}{\partial \eta(y)} \right) \left(\frac{\partial}{\partial \eta(x)} - \frac{\partial}{\partial \eta(y)} \right). \quad (3.42)$$

Here $\sum_{x \sim y \in \mathbb{T}_N}$ denotes the sum over all the neighboring sites to x , i.e. $y \in \mathbb{T}_N^d$ so that $|x - y| = 1$ and $c(x, y, \cdot)$ is the jump rate, and $\eta^{x,y}$ is the configuration of the particle system after one jump from x to y :

$$\eta^{x,y}(z) = \begin{cases} \eta(x) - 1 & \text{if } z = x, \\ \eta(y) + 1 & \text{if } z = y, \\ \eta(z) & \text{otherwise.} \end{cases}$$

In the diffusion case, $V : \mathbb{R} \rightarrow \mathbb{R}$ is a $C^2(\mathbb{R})$ potential.

We assume that the jump rate is not degenerate: $g(n+1) > g(n)$ for $n > 0$. This monotonicity condition implies in the limit the ellipticity of the diffusion equation, in the diffusive scaling. That means that the limit equation in the diffusive rescaling, has regularizing properties.

We call a measure $\nu^N \in P(X_N)$ invariant under the evolution of the process if

$$\langle \nu^N, \mathcal{L}_N f \rangle = 0 \quad \text{for all } f \in C_b(X_N).$$

For the three processes above, which we will present in more detail below, there exists a family of invariant measures ν_α^N indexed by some positive constant $\alpha > 0$ ($\alpha \in [0, 1]$ for the simple-exclusion process) that satisfy

$$\int \mathcal{L}_N f d\nu_\alpha^N = 0, \quad \int \eta(0) d\nu_\alpha^N = \alpha, \quad \int \tau_x f(\eta) d\nu_\alpha^N(\eta) = \int f(\eta) d\nu_\alpha^N \quad (3.43)$$

where τ_x is the translation operator defined by $\tau_x f(\eta) = f(\tau_x \eta)$ and $\tau_x \eta(y) = \eta(x + y)$. Note that under the law ν_α^N the $\eta(x)$'s are independent.

Here we also introduce an example of a *local equilibrium*, we define a measure with a slowly varying parameter instead of a constant parameter just as above.

Definition 3.1 (measure with slowly varying parameter). *For every f_0 smooth function, we consider $\nu_{f_0(\cdot)}^N$ to be the product measure on X_N so that*

$$\nu_{f_0(\cdot)}^N(\{\eta : \eta(x) = k\}) = \nu_{f_0(x/N)}^N(\{\eta : \eta(0) = k\}) \quad (3.44)$$

and under $\nu_{f_0(\cdot)}^N$ the variables $\{\eta(x) : x \in \mathbb{T}_N^d\}$ are independent.

A specific formula for this measure in each process will be given in Chapter 5.

In order to get a continuum description via a PDE, we also need to embed the discrete torus \mathbb{T}_N^d into the continuous (macroscopic) torus $\mathbb{T}^d = \mathbb{R}^d/\mathbb{Z}^d$ by mapping $x \mapsto x/N \in \mathbb{T}^d$ assuming the microscopic scale to be of order $\mathcal{O}(N^{-1})$.

We assume that the total number of particles $N^{-d} \sum_{x \in \mathbb{T}_N^d} \eta(x)$ is conserved and this is our only conserved quantity, so the only information we expect to get in the limit as $N \rightarrow \infty$ is the macroscopic particle density. The quantity we use in order to measure the particle density is the empirical measure (associated with a configuration η)

$$\alpha_\eta^N(du) = N^{-d} \sum_{x \in \mathbb{T}_N^d} \eta(x) \delta_{\frac{x}{N}}(du). \quad (3.45)$$

With the empirical measure at hand we can mathematically formulate the convergence of the microscopic particle densities as follows. Let $\phi \in C(\mathbb{T}^d)$ be a test function, then we say that the empirical measure α_η^N converge in probability to a deterministic object f_t if for all $\delta > 0$

$$\lim_{N \rightarrow \infty} \mathbb{P}_{\mu_t^N} (|\langle \alpha_\eta^N, \phi \rangle - \langle f_t, \phi \rangle| > \delta) \rightarrow 0 \quad (3.46)$$

where $\mathbb{P}_{\mu_t^N}(A)$ is the probability that the event A will occur under the law μ_t^N and where f_t solves a PDE of the form $\partial_t f_t = L f_t$ for some differential operator L which is determined from the scaling we do in time (it is either hyperbolic or parabolic/diffusive).

In particular, when our stochastic process is asymmetric, i.e. if $p(\cdot)$ are the transition probabilities and we have that $\sum_z z p(z) \neq 0$, then we rescale time by N (the same as the scaling we do in x , so we apply the *hyperbolic scaling*) and in the limit we get the solution of the following conservation law

$$\partial_t f_t = \gamma \cdot \nabla \sigma(f_t), \quad \text{where } \gamma = \sum_z z p(z).$$

When the stochastic process has mean zero, i.e. $\gamma = 0$, in order to see a limit we need to rescale the time by N^2 (and so we shall apply the *diffusive scaling*). In this case we have

that the particle densities converge to the solution of

$$\partial_t f_t = \Delta_c \sigma(f_t)$$

where Δ_c is the weighted Laplacian $\Delta_c = \sum_{1 \leq i, j \leq d} c_{ij} \partial_{u_i} \partial_{u_j}$ and c_{ij} are the covariances $c_{ij} = \sum_{i, j} p(x) x_i x_j$.

The nonlinearity σ appearing in both cases, will be determined from the jump rates of the stochastic processes.

1.3.1 Introduction of our basic examples

- *Simple-Exclusion Process.*

The simple exclusion process allows at most one particle per site. The jump is therefore suppressed if it leads to an already occupied site. The state space therefore in this case is $X_N = \{0, 1\}^{\mathbb{T}_N^d}$ and the generator of the process is given by

$$\mathcal{L}_N f(\eta) = \sum_{x, y \sim x} p(y-x) (\eta(x)(1-\eta(y)) [f(\eta^{x,y}) - f(\eta)]) \quad (3.47)$$

for each $f^N \in C_b(X_N)$, where $\eta^{x,y}$ is the configuration of the particle system after one particle has jumped from site x to a neighboring site y :

$$\eta^{x,y}(z) = \begin{cases} \eta(y) & \text{if } z = x, \\ \eta(x) & \text{if } z = y, \\ \eta(z) & \text{otherwise.} \end{cases}$$

Given a density $\alpha \in (0, 1)$, the invariant measure is the Bernoulli product measures with parameter α :

$$\nu_\alpha^N(\eta) = \prod_{x \in \mathbb{T}_N^d} \alpha^{\eta(x)} (1-\alpha)^{1-\eta(x)}.$$

Diffusive scaling. We assume that the mean $\gamma = \sum_z z p(z) = 0$ and we accelerate the process $(\eta_t)_t$ by a factor N^2 , i.e. the microscopic x -variable scales with N , while the time scales with N^2 . The generator then is for all $f \in C_b(X_N)$,

$$\mathcal{L}_N f(\eta) = N^2 \sum_{x, y \sim x} p(y-x) \eta(x)(1-\eta(y)) [f(\eta^{x,y}) - f(\eta)].$$

Under diffusive scaling and with initial decorrelation, the empirical measure of the simple exclusion process converges to the solution f_t to the *diffusion equation*

$$\partial_t f_t = \Delta_c f_t, \quad \text{where } \Delta_c = \sum_{1 \leq i, j \leq d} c_{i,j} \partial_{u_i} \partial_{u_j} \quad (3.48)$$

and the diffusion matrix is given by

$$c_{i,j} := \sum_{x \in \mathbb{Z}^d} p(x) x_i x_j.$$

Hydrodynamic limit under hyperbolic scaling. We accelerate the process $(\eta_t)_t$ by a factor N , i.e. both the microscopic spatial variables and the time scale with N , and we assume that the mean $\gamma = \sum_z z p(z) \neq 0$. The generator in this case is for all $f \in C_b(X_N)$,

$$\mathcal{L}_N f(\eta) = N \sum_{x,y \sim x} p(y-x) \eta(x) (1 - \eta(y)) [f(\eta^{x,y}) - f(\eta)].$$

Under the hyperbolic scaling, the empirical measure of the process converges to the solution f_t to the *conservation law*

$$\partial_t f_t = \gamma \cdot \nabla \sigma(f_t) \tag{3.49}$$

where $\sigma(f_t) = f_t(1 - f_t)$. Due to the nonlinearity, the solution of (3.49) may develop shocks and it is thus understood in the sense of distributions, after a finite time T , even for smooth data [Daf16, Chapter 4]. Up to the time T of the appearance of the first shock, the solution is smooth. Therefore, most techniques for the hydrodynamic limit under Euler scaling, hold up to this time T since usually some regularity of the limit PDE is required. The only proof of such limit for all times, by exploiting the notion of *entropy* and *measure-valued entropy solutions*, was done by Rezakhanlou in [Rez91].

- *Zero-Range process.* Here there is no restriction on the number of the particles per site, so that $X_N = \mathbb{N}^{\mathbb{T}^d}$. The generator is given by, for all $f \in C_b(X_N)$,

$$\mathcal{L}_N f(\eta) = \sum_{x,y \sim x} p(y-x) g(\eta(x)) [f(\eta^{x,y}) - f(\eta)] \tag{3.50}$$

where g is the *jump rate* and $\eta^{x,y}$ is the configuration of the particle system after one particle has jumped from site x to a neighboring site y :

$$\eta^{x,y}(z) = \begin{cases} \eta(x) - 1 & \text{if } z = x, \\ \eta(y) + 1 & \text{if } z = y, \\ \eta(z) & \text{otherwise.} \end{cases}$$

We assume that $g(k) = 0$ if and only if $k = 0$, meaning that the rate at which particles leave a site is zero if and only if the site is empty. The process is called zero-range as the hopping rate only depends on the particles at the same site. The *jump rate* $g : \mathbb{N} \rightarrow [0, \infty)$ can be thought of as describing the interactions of particles occupying the same site. In

order for our process to be well-defined we also assume that g satisfies for some $g^* > 0$:

$$\text{for all } n \geq 0, \quad 0 \leq |g(n+1) - g(n)| \leq g^* < +\infty.$$

A special case is the case of linear g , $g(n) = n$, where the particles perform independent random walks on the lattice.

An important family of invariant measures is given by the *grand-canonical* or *Gibbs* measures, given $\rho \geq 0$:

$$\nu_\rho^N(\eta) = \prod_{x \in \mathbb{T}_N^d} \frac{\sigma(\rho)^{\eta(x)}}{g(\eta(x))! Z(\sigma(\rho))}, \quad (3.51)$$

where Z is the *partition function* of the zero range process given by,

$$Z(\phi) = \sum_{n=0}^{\infty} \frac{\phi^n}{g(n)!} \quad (3.52)$$

with $g(n)! := g(1) \cdot g(2) \cdots g(n)$ and $g(0)! := 1$. The function $\sigma(\rho)$ is then chosen uniquely such that

$$\langle \nu_\rho^N, \eta(0) \rangle = \rho.$$

We shall elaborate on the construction of σ in Chapter 5. Since the number of particles is conserved and the process has no other conserved quantities, another important set of invariant measure is given by the *canonical measures*: given $K \in \mathbb{N}$,

$$\nu^{N,K}(\eta) = \nu_\rho^N(\eta \mid \sum_x \eta(x) = K), \quad (3.53)$$

which are the grand-canonical measures conditioned on hyperplanes of constant number of particles.

In order to get a hydrodynamic limit we add two more assumptions on g : attractivity and spectral gap. We assume that g is monotonously increasing,

$$\text{for all } n \in \mathbb{N} \quad g(n+1) \geq g(n)$$

and that there exists $n_0 > 0$ and $\delta > 0$ such that

$$\text{for all } j \in \mathbb{N}, \quad n \geq j + n_0 \quad g(n) - g(j) \geq \delta.$$

The fact that $g(\cdot)$ is increasing is a sufficient and necessary condition for zero-range processes to be attractive⁴, [KL99, Theorem 5.2]. The attractivity assumption helps in defining a coupling between two copies of this process: this is a property used in the

⁴An interacting particle system is said to be attractive if its semigroup preserves the partial order, i.e. if $\mu_{0,1}^N \leq \mu_{0,2}^N$ then $\mu_{t,1}^N \leq \mu_{t,2}^N$.

proof in subsection 5.4.2 of Chapter 5. The spectral gap condition ensures that the limit equation is elliptic.

Diffusive scaling. We accelerate the zero-range process $(\eta_t)_t$ by a factor N^2 , *i.e.* the microscopic spatial variables scale with N and time with N^2 , and we assume that the mean $\gamma = 0$. The generator in this case is

$$\mathcal{L}_N f(\eta) = N^2 \sum_{x,y \sim x} p(y-x)g(\eta(x)) [f(\eta^{x,y}) - f(\eta)].$$

Under diffusive scaling, the empirical measure of the zero range process converges to the solution f_t to the nonlinear *diffusion equation*

$$\partial_t f_t = \sum_{1 \leq i,j \leq d} c_{i,j} \partial_{u_i} \partial_{u_j} \sigma(f_t) \quad (3.54)$$

where the diffusion matrix is given by

$$c_{i,j} := \sum_{x \in \mathbb{Z}^d} p(x) x_i x_j$$

and the nonlinearity $\sigma : [0, \infty) \rightarrow [0, \infty)$ appears in (3.51) and more specifically it satisfies $\langle \nu_\rho^N, g(\eta(x)) \rangle = \sigma(\rho)$ (see details in the Chapter 5).

Hydrodynamic limit under hyperbolic scaling. We accelerate the zero-range process $(\eta_t)_t$ by a factor N , *i.e.* both the microscopic spatial variables and the time scale like N , and we assume that the mean $\gamma = \sum_z z p(z) \neq 0$. The generator in this case is, for all $f \in C_b(X_N)$,

$$\mathcal{L}_N f(\eta) = N \sum_{x,y \sim x} p(y-x)g(\eta(x)) [f(\eta^{x,y}) - f(\eta)].$$

Under the hyperbolic scaling, the empirical measure of the zero-range process converges to the solution f_t to the *conservation law*

$$\partial_t f_t = \gamma \cdot \nabla \sigma(f_t) \quad (3.55)$$

where σ is given by $\langle \nu_\rho^N, g(\eta(x)) \rangle = \sigma(\rho)$.

- *Process of Ginzburg-Landau type.* Let $\mathbb{T}_N = \mathbb{Z}/(N\mathbb{Z})$ the one-dimensional periodic integer lattice. To each lattice site $x \in \mathbb{T}_N$ we associate the continuous variable $\eta(x) \in \mathbb{R}$ which represents a charge at this site and $\eta = (\eta(x))_{x \in \mathbb{T}_N} \in \mathbb{R}^{\mathbb{T}_N}$ is then a field configuration. After time $t > 0$ the configuration is $\eta_t = (\eta_t(x))_{x \in \mathbb{T}_N}$. The charges are relocated among adjacent sites randomly according to a diffusion law. In this model we apply only the diffusive scaling, *i.e.* speed up the time by N^2 and shrink the space between charges by N so that we obtain a system of spins (charges) located at points x/N with $x = 1, \dots, N$ of

the circle $\mathbb{S} = \mathbb{R}/\mathbb{Z}$.

The Ginzburg-Landau dynamics for η is described by the set of stochastic differential equations, for all $x \in \mathbb{T}_N$,

$$d\eta_t(x) = \frac{N^2}{2} \left[V'(\eta(x+1)) - 2V'(\eta(x)) + V'(\eta(x-1)) \right] dt + N [dW_t(x) - dW_t(x+1)],$$

$$x \in \mathbb{T}_N$$
(3.56)

where $W_t(i)$, $i = 1, \dots, N$ are independent Brownian motions and $V : \mathbb{R} \rightarrow \mathbb{R}$ is a $C^2(\mathbb{R})$ function for which we assume the following.

Assumption 1. (A1) $\int_{\mathbb{R}} e^{-V(u)} du = 1$,

(A2) There is $C_1, C_2, R > 0$ so that $\forall u \in \mathbb{R}$, $|u| > R$, $V''(u) > C_2$ and $V''(u) \leq C_1$,

(A3) for all $\lambda \in \mathbb{R}$, $M(\lambda) := \int_{\mathbb{R}} e^{\lambda u - V(u)} du < \infty$.

The attractivity here corresponds to V being a convex potential, at least away from the origin. The infinitesimal generator of the diffusion process $\eta(x)$ is

$$\mathcal{L}_N := \frac{N^2}{2} \sum_{x \sim y \in \mathbb{T}_N} \left(\frac{\partial}{\partial \eta(x)} - \frac{\partial}{\partial \eta(y)} \right)^2 - \frac{N^2}{2} \sum_{x \sim y \in \mathbb{T}_N} \left(\frac{\partial V}{\partial \eta(x)} - \frac{\partial V}{\partial \eta(y)} \right) \left(\frac{\partial}{\partial \eta(x)} - \frac{\partial}{\partial \eta(y)} \right).$$
(3.57)

The generator \mathcal{L}_N is symmetric with respect to the invariant (Gibbs) product measure

$$d\nu^N(\eta) := \prod_{i \in \mathbb{T}_N} e^{-V(\eta(x_i))} d\eta(x_i) \quad \text{on } \mathbb{R}^N.$$

Consider a function f_0^N and a law $\psi_0^N(\eta) := f_0^N d\nu^N(\eta)$. At later time $t > 0$, the law ψ_t^N system will have a density f_t^N relative to $d\nu^N$ satisfying the equation

$$\partial_t f_t^N = \mathcal{L}_N^* f_t^N.$$

Associated with the charge configuration η we define as before the empirical measure

$$\alpha_\eta^N = \frac{1}{N} \sum_x \eta(x) \delta_{\frac{x}{N}} \quad \text{on } \mathbb{S}.$$

In order to describe the hydrodynamical equation in this case, let us introduce some notation. Let $M(\lambda)$ the function defined in assumption (A3) above and consider

$$p(\lambda) = \log M(\lambda), \quad h(y) := \sup_{\lambda \in \mathbb{R}} (\lambda y - p(\lambda)).$$

Then h and p are a pair of conjugate convex functions and

$$h'(y) = \lambda \quad \text{iff} \quad y = p'(\lambda)$$

where

$$p'(\lambda) = \frac{M'(\lambda)}{M(\lambda)} = \frac{\int_{\mathbb{R}} u e^{\lambda u - V(u)} du}{M(\lambda)}$$

i.e. h' and p' are inverse of each other. Moreover h' and p' are smooth and strictly increasing functions. The empirical density of the Ginzburg-Landau dynamics has a macroscopic profile f_t that solves the diffusion equation

$$\partial_t f_t(u) = \partial_{uu} h'(f_t(u)), \quad (t, u) \in (0, \infty) \times \mathbb{S}. \quad (3.58)$$

1.3.2 In the literature

Regarding the state of the art of this problem, the qualitative behavior of these hydrodynamic limits is well-known and was first proven by Fritz in [Fri89]. This was done for the Ginzburg-Landau model for which another method was invented later by Guo-Papanicolaou-Varadhan in [GPV88], called *the entropy method*, as it involved estimates on the entropy and Fischer information. The entropy method has been generalized to prove the hydrodynamic limit for several other models, including jump processes such as zero-range and exclusion processes, in [KL99]. Apart from this method, further results include the *relative entropy method* due to H.-T. Yau [Yau91] which shows convergence of the relative entropy with respect to local equilibrium states. Both of these methods are not quantitative, so there is no explicit rate of the convergence to the limit PDE and from their techniques there is no reason to expect the convergence in N to be uniform in time. The method in [GPV88] is based on compactness while the method in [Yau91] is closer to being quantitative, apart from one step. Also, as the key estimate in relative entropy method is a Grönwall estimate, the error in terms of the time is growing exponentially in time. However both the many-particle systems and the limit systems are *dissipative*, therefore ergodicity and relaxation should win over stochastic fluctuations at the level of the laws: As $t \rightarrow \infty$, the system relaxes to an invariant measure, for which the hydrodynamic limit holds, as shown in the figure below, so that we expect the limit in N to be uniform in time t .

$$\begin{array}{ccc} f_t^N \in \mathcal{P}(X_N) & \xrightarrow{N \rightarrow \infty} & f_t \in L^\infty(\mathbb{T}^d) \\ \downarrow t \rightarrow \infty & & \downarrow t \rightarrow \infty \\ \nu_{\sigma(\rho)}^N \in \mathcal{P}(X_N) & \xrightarrow{N \rightarrow \infty} & f_\infty \end{array}$$

In terms of quantitative results, the first result was obtained for the Ginzburg-Landau model by Grunewald, Otto, Villani, and Westdickenberg, in [GOVW09]. The method is based on a coarse-graining of the state-space. The results there however are not fully quantitative. For this specific model, recently a fully quantitative result was obtained in [DMOWa], by a modification of the method that was applied in [GOVW09]. This result holds for Ginzburg Landau models with Kawasaki dynamics, including potentials that are non-convex, like the double well potential. On the negative side, their result does not hold uniform in time and it is not clear how to extend the method to get the result for jump processes as well.

Our contribution to the theory is a new approach to quantify the rate of convergence for several processes, both jump and diffusion, and make it uniform in time, in the diffusive case where it is expected to be.

1.4 List of the works and perspectives

In this section I am presenting the main results of each chapter while explaining the main tools and ideas.

- **Quantitative Rates of Convergence to Non-Equilibrium Steady State for a Weakly Anharmonic Chain of Oscillators.**

This work is the article [Men20] and has been published in *Journal of Statistical Physics*. It is presented in Chapter 2.

The main objective is to find estimates on the speed of the convergence to a stationary state for a heat conducting system. The model consists of a one-dimensional chain of N interacting oscillators on the phase space \mathbb{R}^{2N} , where the variables are q_i, p_i for $i = 1, \dots, N$: the displacements of the particles from their equilibrium positions and their momenta, respectively. Each particle has its own *pinning potential* and it interacts with its nearest neighbors through an *interaction potential*. We call H the Hamiltonian energy. The two ends of the chain $\{1, N\}$, are in contact with heat baths, modeled by *Langevin* (Ornstein–Uhlenbeck) processes at two (possibly) different inverse temperatures $\beta_1^{-1}, \beta_N^{-1}$. The dynamics therefore is described by a coupled system of SDEs (1.17): for $i \in \{1, \dots, N\}$,

$$\begin{aligned} dq_i(t) &= (\nabla_{p_i} H) dt \text{ and} \\ dp_i(t) &= \left(-\nabla_{q_i} H - \gamma_i p_i \delta_{i \in \{1, N\}} \right) dt + \delta_{i \in \{1, N\}} \sqrt{\frac{2\gamma_i}{\beta_i}} dW_i \end{aligned} \tag{4.59}$$

where $\gamma_i, i \in \{1, N\}$ are the friction coefficients.

The non-equilibrium steady state for the purely harmonic chain, i.e. when both potentials are quadratic (harmonic), was made precise in [RLL67]. Anharmonic chains

were studied in various works [JP98, EPRB99a, EPRB99b, Car07, RBT02, CEHRB18], where existence, uniqueness of a non-equilibrium steady state and exponential convergence towards it were proven in certain cases. More specifically the existence, uniqueness of a steady state and exponential convergence, hold under the assumptions that both the interaction and pinning potentials behave as polynomials near infinity and that the interaction is stronger than the pinning potential. The last assumption is important as there are some works which exhibit cases where the relaxation rate is not exponential, i.e. where there is lack of spectral gap [Hai09, HM09]. The existing results are however not quantitative, i.e. they do not give information on the scaling of these rates in terms of N , since compactness arguments are employed. Quantitative results for the spectral gap are therefore missing and even in the simplest case of the linear (harmonic) chain, the dependence on the dimension of the spectral gap was not known. Attempts have been made through hypocoercive techniques to get N -dependent estimates under certain conditions on the potentials: see the discussion in [Vil09a, Section 9.2] where this question was first raised. The techniques discussed in Villani's monograph however only yield non-optimal estimates.

The Chapter 2 gives a partial answer to this question by Villani: we prove explicit rates of convergence to the non-equilibrium steady state (with optimal lower bound) in a weakly anharmonic scenario, i.e. when both potentials are N -dependent perturbations of the harmonic ones. The proof relies on (i) an application of a generalized version of the Γ_2 -calculus of Bakry-Emery [BE85] for elliptic operators recently generalized by Baudoin for hypoelliptic operators [Bau17], as explained in the Section 1.2.2.2, and (2) a careful analysis of a high-dimensional matrix equation.

We first prove the following contraction property in Wasserstein-2 distance. First we recall the definition of the Kantorovich-Rubinstein-Wasserstein L^2 -distance $W_2(\mu, \nu)$ between two probability measures μ, ν :

$$W_2(\mu, \nu)^2 = \inf \int_{\mathbb{R}^N \times \mathbb{R}^N} |x - y|^2 d\pi(x, y)$$

where the infimum is taken over the set of all the couplings, i.e. the joint measures π on $\mathbb{R}^N \times \mathbb{R}^N$ with left and right marginals μ and ν respectively.

Theorem 4.1 (Theorem 1.4 in Chapter 2). *We consider a 1-dimensional chain of coupled oscillators with rigidly fixed edges so that the dynamics are described by the system (4.59) with*

$$H(p, q) = \sum_{i=1}^N \left(\frac{p_i^2}{2} + a \frac{q_i^2}{2} + U_{pin}^N(q_i) \right) + \sum_{i=1}^{N-1} \left(c \frac{(q_{i+1} - q_i)^2}{2} + U_{int}^N(q_{i+1} - q_i) \right) + c \frac{q_1^2}{2} + c \frac{q_N^2}{2} \quad (4.60)$$

for $a \geq 0, c > 0$ and under the assumption that

$$\sup_{q_i} \|\nabla^2 U_{pin}^N(q_i)\|_2, \quad \sup_{r_i} \|\nabla^2 U_{int}^N(r_i)\|_2 \leq C^N \quad (4.61)$$

where $r_i = q_{i+1} - q_i$ and $C^N \lesssim N^{-9/2}$.⁵ For a fixed number of particles N , there is a unique stationary state, in particular, for initial data f_0^1, f_0^2 we have:

$$W_2(P_t^* f_0^1, P_t^* f_0^2) \leq C_{a,c} N^{\frac{3}{2}} e^{-\frac{\lambda_0}{N^3} t} W_2(f_0^1, f_0^2) \quad (4.62)$$

for $C_{a,c}, \lambda_0$ dimensionless constants.

After having proved a Log-Sobolev inequality for the invariant measure, we also give a convergence to the stationary measure in relative entropy as in [Vil09a, Section 6]. We first recall the definitions of the following functionals:

For two probability measures μ and ν on \mathbb{R}^{2N} with $\nu \ll \mu$, we define the Boltzmann H functional

$$H_\mu(\nu) = \int_{\mathbb{R}^{2N}} h \log h \, d\nu, \quad \nu = h\mu \quad (4.63)$$

and the relative Fisher information

$$I_\mu(\nu) = \int_{\mathbb{R}^{2N}} \frac{|\nabla h|^2}{h} d\nu, \quad \nu = h\mu. \quad (4.64)$$

Theorem 4.2 (Theorem 1.6 in Chapter 2). *We consider a weakly anharmonic 1-dimensional chain of coupled oscillators with rigidly fixed edges whose dynamics are described by the system (4.59) under the same assumptions as in the Theorem 4.1 above. For a fixed number of particles N , assuming that (i) μ is the invariant measure for P_t and (ii) that it satisfies a Log-Sobolev inequality with constant $C_N > 0$, for all $0 < f \in L^1(\mu)$ with*

$$\mathcal{E}(f) < \infty, \quad \text{and} \quad \int f d\mu = 1,$$

we have a convergence to the non-equilibrium steady state in the following sense:

$$H_\mu(P_t f \mu) + I_\mu(P_t f \mu) \leq \lambda_{a,c} N^3 e^{-\lambda_0 N^{-3} t} \left(H_\mu(f \mu) + I_\mu(f \mu) \right) \quad (4.65)$$

for dimensionless constants $\lambda_{a,c}, \lambda_0$.

Theorem 4.1 implies exponential relaxation with rate bigger than N^{-3} for the weakly anharmonic chain (4.59) with energy (4.60) and (4.61). In the purely harmonic case, we have that the convergence rate is between $C_1 N^{-3}$ and $C_2 N^{-1}$ for some constants C_1, C_2 that are independent of N .

⁵This is what we call a weakly anharmonic chain of oscillators.

- **The optimal spectral gap for regular and disordered harmonic networks of oscillators.**

This work has been done in collaboration with Simon Becker and it is submitted for publication, see [BM22] in the bibliography. It is presented in Chapter 3 and it is a continuation of the work in Chapter 2. We explore the behavior of the spectral gap for purely harmonic chains in higher dimensions and different settings.

We study the spectral gap for purely harmonic chains and d -dimensional grids of oscillators, and proved the optimal lower and upper bounds. We also treat non-homogeneous scenarios where the coefficients of the pinning potentials are not identical. In particular we look at chains of oscillators with an impurity (so that the particle in the middle of the chain has pinning potential significantly weaker than the pinning potential of all the other particles) as well as at disordered chains of oscillators. As regards the d -dimensional grids, the spectral gap depends on which particles are exposed to friction. These are explained in the statement below. Our setting is the following, we look at the system (1.17) with $\mathcal{F} \subset \{1, \dots, N\}^d$ and

$$H(q, p) = \frac{\langle p, m_{[N]^d}^{-1} p \rangle}{2} + V_{a,c}(q) \text{ where } V_{a,c}(q) = \sum_{i \in [N]^d} a_i |q_i|^2 + \sum_{i \sim j} c_{ij} |q_i - q_j|^2. \quad (4.66)$$

Our method of proof relies on a new approach for studying non-symmetric spectral problems that reduces the problem to spectral analysis of discrete Schrödinger operators. Using a *Wigner matrix* representation we reduce the study of this high dimensional spectral analysis to the study of resolvents involving only the heat bath sites.

In general, if the friction parameters do not grow faster than the number of boundary particles, i.e. $\sup_{i \in \mathcal{F} \subset \partial[N]^d} \gamma_i \leq \mathcal{O}(N^{d-1})$, where $\partial[N]^d$ denoted the boundary of the grid, the spectral gap of the chain of oscillators always decays as a function of N and the rate is at least of order $\mathcal{O}(1/N)$.

Our main results give sharper and usually optimal bounds in each specific case. They are summarized in the following statement:

Theorem 4.3 (Theorem 1.1 in Chapter 3). *Let the positive masses m_i and interaction strengths c_i of all oscillators coincide, N^d be the number of oscillators, placed in a square grid with N oscillators on each side, and d the dimension of the network.*

- **(Homogeneous chain):** *Let the pinning strength a_i be the same for all oscillators, then*
 1. *if two particles located at the corners $(1, \dots, 1), (N, \dots, N)$, see Fig. 3.6, are exposed to the same non-zero friction and non-zero diffusion, the spectral gap*

of the generator decays at the optimal rate N^{-3d} :

$$\lambda_S = \mathcal{O}(N^{-3d}).$$

In particular for the one-dimensional chain of oscillators $\lambda_S = \mathcal{O}(N^{-3})$.

2. if the same non-zero friction and non-zero diffusion for particles located at the center of two opposite edges of the network

$$(1, \lceil N/2 \rceil, \dots, \lceil N/2 \rceil), (N, \lceil N/2 \rceil, \dots, \lceil N/2 \rceil),$$

see Fig. 3.7, the spectral gap of the generator decays at the optimal rate $N^{-3-(d-1)}$: $\lambda_S = \mathcal{O}(N^{-3-(d-1)})$.

3. if $d = 2$ and the particles exposed to the same non-zero friction are located at opposite edges of the network, the spectral gap satisfies $\lambda_S \leq \mathcal{O}(N^{-5/2})$.

- **(Chain with impurity):** Let N be even. We assume that all masses and interaction parameters are positive and coincide and the friction parameters γ_i of the boundary particles

$$\partial[N]^d := \{i \in [N]^d; \exists i_n : i_n \in \{1, N\}\} \quad \text{of} \quad [N]^d := \{1, \dots, N\}^d$$

satisfy $\sup_{i \in \partial[N]^d} \gamma_i \in (0, c)$ where c is independent of N and the friction is non-zero on at least one boundary edge. Then, if the pinning strength $a_{c_d(N)}$ at the center point $c_d(N) = (N/2, \dots, N/2)$ of the network is sufficiently small compared to the pinning strength of all other oscillators, the spectral gap λ_S of the generator decays at least exponentially fast in N , for all $d \geq 1$.

In dimension 1 this rate is the optimal one.

- **(Disordered chain):** We assume that all masses and interaction parameters are positive and coincide and the friction parameters γ_i of the particles at the boundary

$$\partial[\pm N]^d := \{i \in [\pm N]^d; \|i\|_\infty = N\} \quad \text{of the network} \quad [\pm N]^d := \{-N, \dots, N\}^d$$

satisfy $\sup_{i \in \partial[\pm N]^d} \gamma_i \in (0, c)$ where c is independent of N and the friction is non-zero on at least one boundary edge. Then, if the pinning strengths are iid random variables distributed according to some compactly supported density $\rho \in C_c(0, \infty)$, the spectral gap λ_S of the generator decays exponentially fast in N , for all $d \geq 1$ for all but finitely many N .

Existence of a Non-Equilibrium Steady State for the non-linear BGK equation

on an interval.

This work has been done in collaboration with Josephine Evans and it is published in *Pure and Applied Analysis*, see [EM21] in the bibliography. It is exposed in Chapter 4.

In this article we study a non-equilibrium system that describes heat conduction in gases, through the so-called BGK equation. Historically the first examples of microscopic description of heat conduction goes back to Clausius, Maxwell and Boltzmann [Max67, Bol03] who obtained formally (0.1), through a ‘kinetic theory’ analysis, see [BLRB00, Section 2] for more details.

For the stationary Boltzmann equation, the rigorous proof of (0.1), was given in [ELM94, ELM95] in the slab geometry, and when the temperature difference of the two reservoirs is small. In [EGKM13], solutions to the 3-dim steady problem were constructed, with sufficiently small difference of the temperatures as well (in the kinetic regime). In these works, the coupling with the reservoirs is ensured by the “*diffusive boundary conditions*”, i.e. when a particle hits one of the boundary walls it gets reflected with a new velocity drawn from the Maxwellian

$$\mathcal{M}_i(v) := \frac{1}{(2\pi T_i)^{d/2}} \exp\left(-\frac{|v|^2}{2T_i}\right), \quad i = 1, 2,$$

where d is the dimension.

Motivated by the series of papers [CLM15, CEL⁺18, CEL⁺19] as well as [EGKM13], we study the *non-linear* BGK equation on an interval with diffusive boundary conditions. The BGK model was introduced by Bhatnagar, Gross and Krook in [BGK54] as a toy model for Boltzmann flows (as a simplified Boltzmann equation). In particular we consider a gas of particles in $(0, 1)$ with the distribution function $f(x, v)$ in position x and velocity $v \in \mathbb{R}$. The Knudsen number $\text{Kn} > 0$ is defined as the ratio between the mean free path (this is the average distance a particle travels between collisions in a gas) and the typical observation length.

The collisions then are described by the right-hand side of the following equation

$$\partial_t f + v \partial_x f = \frac{1}{\text{Kn}} (\rho_f \mathcal{M}_{T_f} - f). \quad (4.67)$$

We are interested in the stationary boundary value problem:

$$v \partial_x f = \frac{1}{\text{Kn}} (\rho_f \mathcal{M}_{T_f} - f), \quad (4.68)$$

$$f(0, v) = \mathcal{M}_1(v) \int_{v' < 0} |v'| f(0, v') dv', \quad v > 0, \quad (4.69)$$

$$f(1, v) = \mathcal{M}_2(v) \int_{v' > 0} |v'| f(1, v') dv', \quad v < 0, \quad (4.70)$$

where $\rho_f(x), T_f(x)$ are the *spatial density* and the *local temperature* corresponding to f :

$$\rho_f(x) = \int_{-\infty}^{\infty} f(x, v) dv, \quad \rho_f(x)T_f(x) = \int_{-\infty}^{\infty} v^2 f(x, v) dv. \quad (4.71)$$

We denote by $\mathcal{M}_{T_f}(v)$ the Maxwellian with temperature T_f ,

$$\mathcal{M}_{T_f}(v) = \frac{1}{(2\pi T_f)^{1/2}} \exp\left(-\frac{1}{2T_f}v^2\right)$$

which is the non-linear term of the system, and by $\mathcal{M}_1, \mathcal{M}_2$ the Maxwellians at the boundary temperatures T_1, T_2 respectively. We show existence of a non-equilibrium steady state when the boundary temperatures are large and their difference is not small, in the kinetic regime, when the Knudsen number is kept fixed.

Our proof differs from the previous perturbative techniques as we do not assume the temperature difference to be small. It relies on a fixed point argument that relates the non-linear BGK model to the linear BGK model, which is

$$v\partial_x f = \frac{1}{\text{Kn}}(\rho(x)\mathcal{M}_{T(x)} - f) \quad (4.72)$$

with the same boundary conditions (4.69)-(4.70) and for temperature profile $T(x) \in [T_1, T_2]$. In particular, (i) we show existence and uniqueness of a solution f to (4.72)-(4.69)-(4.70) by purely probabilistic techniques. Then the existence of a solution to (4.68)-(4.69)-(4.70) is implied by a fixed point of the mapping $\mathcal{F}(T) = \tau$, where $\tau(x)$ is the temperature profile of the non-equilibrium steady state of (4.72).

The main result with all the details is:

Theorem 4.4 (Theorem 3.1 in Chapter 4). *For every two fixed temperatures T_1, T_2 satisfying*

$$(C1) \quad (\text{Kn})^2 T_1 > \gamma_2 \text{ and}$$

$$(C2) \quad \sqrt{T_2} - \sqrt{T_1} \geq \gamma_1 (\text{Kn})^{1/2} T_2^{1/4}$$

for γ_1, γ_2 positive constants, there exists a steady state which satisfies equation (4.68) with boundary conditions (1.2) and (1.3). Furthermore, this steady state has the following properties:

- It has zero momentum uniformly in $x \in (0, 1)$.
- It has constant density $\rho_f(x)$ and the pressure $P_f(x)$ is equal to $\sqrt{T_1 T_2}$ asymptotically

with T_1 . More specifically, for all $x \in (0, 1)$,

$$1 - \gamma_0 \frac{1}{(\text{Kn})^{1/2}} \frac{1}{T_1^{1/4}} \leq \rho_f(x) \leq 1 + \gamma_1 \frac{1}{(\text{Kn})^{1/2}} \frac{1}{T_1^{1/4}}$$

$$\sqrt{T_1 T_2} \lesssim P_f(x) \lesssim \sqrt{T_1 T_2}.$$

- Its temperature profile is $1/2$ -Hölder continuous and also it is asymptotically equal to $\sqrt{T_1 T_2}$ with the deviation from $\sqrt{T_1 T_2}$ decreasing as T_1 increases: for all $x \in (0, 1)$,

$$\sqrt{T_1 T_2} \left(1 - \gamma_1 \frac{1}{(\text{Kn})^{1/2}} \frac{1}{T_1^{1/4}} \right) \lesssim T_f(x) \lesssim \sqrt{T_1 T_2} \left(1 + \gamma_0 \frac{1}{(\text{Kn})^{1/2}} \frac{1}{T_1^{1/4}} \right),$$

for some constants γ_0, γ_1 and (Kn) the constant in front of the collisional operator in (4.68).

Quantitative Scaling limits for interacting particle systems.

This work in progress is a joint work with Daniel Marahrens and Clément Mouhot. We intend to submit it for publication in the near future with additional results. The exposition of the results we have so far is in Chapter 5.

The objective of this work is the rigorous derivation of macroscopic PDEs when one starts from microscopic interacting particle systems and we present an abstract quantitative method to prove the hydrodynamic limit, with a rate uniform in time (in the diffusive scaling) and unified in the sense that it can be applied to several models, introduced in Section 1.3. The method is also simpler compared with the existing literature.

It is inspired by the approach of F. Rezakhanlou in [Rez91] who proved the hydrodynamic limit under hyperbolic scaling for the simple exclusion/zero-range process, and by the approach of H.-T. Yau in [Yau91], who proved convergence in relative entropy with respect to the local Gibbs measure for the Ginzburg-Landau process.

In particular, instead of working with the relative entropy as Yau did, we work with the Wasserstein-1 distance with cost being the microscopic ℓ^1 distance among two processes: Let $\mu_{t,1}^N, \mu_{t,2}^N$ be two measures describing the state of the particle process at time t , we define

$$W_1(\mu_{t,1}^N, \mu_{t,2}^N) := N^{-d} \sum_{x \in \mathbb{T}_N^d} \inf \iint_{X_N^2} |\eta(x) - \zeta(x)| d\tilde{\mu}_t^N(\eta, \zeta) \quad (4.73)$$

where the infimum is taken over all the set of coupling measures on X_N^2 .

Due to the attractivity assumption we can properly define a coupling between two copies of the same process, let us say with generator $\tilde{\mathcal{L}}$. To fix ideas on the coupling, let us consider just the zero-range process. For two copies of a zero-range process then, we

define [Lig85], see also [Rez91, KL99], a coupling with generator $\tilde{\mathcal{L}} : C_b(X_N^2) \rightarrow C_b(X_N^2)$ given by

$$\begin{aligned} \tilde{\mathcal{L}}_N f(\eta, \zeta) &:= N^2 \sum_{x,y} p(y-x) g(\eta(x)) \wedge g(\zeta(x)) (f(\eta^{xy}, \zeta^{xy}) - f(\eta, \zeta)) \\ &+ N^2 \sum_{x,y} p(y-x) \left(g(\eta(x)) - g(\eta(x)) \wedge g(\zeta(x)) \right) (f(\eta^{xy}, \zeta) - f(\eta, \zeta)) \\ &+ N^2 \sum_{x,y} p(y-x) \left(g(\zeta(x)) - g(\eta(x)) \wedge g(\zeta(x)) \right) (f(\eta, \zeta^{xy}) - f(\eta, \zeta)). \end{aligned} \quad (4.74)$$

The intuition behind this coupling is that the η -particles and the ζ -particles try to jump together as much as possible (this is called the basic coupling or Wasserstein coupling).

The idea is to compare the law of our original process (simple-exclusion, zero-range or Ginzburg-Landau process) with an ‘artefact’, which is chosen to be the *local Gibbs state*. This comparison will take place through an appropriate coupling that will allow us to employ the W_1 -distance as defined in (4.73). Let f_t be a solution to our limit PDE:

$$\partial_t f_t = L f_t \quad (4.75)$$

for a differential operator L .

We call

$$\psi_t^N = \frac{d\nu_{f_t(\cdot)}^N}{d\nu_\alpha^N}$$

the density of the local Gibbs measure as was defined in Definition 3.1 (i.e. the Gibbs measure with slowly varying parameter associated to f_t) relative to a reference measure with parameter $\alpha > 0$.

The density ψ_t^N can be shown to satisfy $\partial_t \psi_t^N(\zeta) - \mathcal{L}_N^* \psi_t^N(\zeta) = E^N(t, \zeta) \rightarrow 0$ as N diverges. In other words, the local Gibbs state does not satisfy of course the Kolmogorov equation, but it is a good approximation of the solution.

Then we consider the coupled density $G^N(\eta, \zeta)$ on X_N^2 between the law of the stochastic process $f_t^N := d\mu_t^N / d\nu_\alpha^N$ and the artificial process. This solves the equation

$$\partial_t G_t^N(\eta, \zeta) - \tilde{\mathcal{L}}_N^* G_t^N(\eta, \zeta) = S^N(t, \eta, \zeta) := \frac{d\nu_\alpha^N}{d\nu_\alpha^N}(\eta) \otimes E^N(t, \zeta) \quad (4.76)$$

with initial data $G_0^N(\eta, \zeta)$ to be the *optimal coupling* between $f_0^N := d\mu_0^N / d\nu_\alpha^N$ and the local Gibbs density ψ_0^N .

Having this set up, here are the key steps:

First step: Consistency Estimate. First we prove an estimate of the following form, which we call a *consistency estimate* and it should be satisfied by the ‘artificial’ density

ψ_t^N : There exists a rate $\mathcal{E}^N \rightarrow 0$ as N goes to infinity so that for all $\alpha \geq 0$,

$$\iint_{X_N^2} \frac{1}{N^d} \sum_x |\eta(x) - \zeta(x)| (\partial_t - \mathcal{L}^*) \psi_t^N(\zeta) d\nu_\alpha^N(\eta) d\nu_\alpha^N(\zeta) \lesssim \mathcal{E}^N \max_{k \in \{1, \dots, 4\}} \|D^k(f_t - f_\infty)\|_H \quad (4.77)$$

where $(H, \|\cdot\|_H)$ is the space of our solutions to the limit PDE, like $H = L^\infty(\mathbb{T}^d)$ and $f_\infty = \lim_{t \rightarrow \infty} f_t$.

Second step: Microscopic Stability Estimate. We adapt parts of the proof of [Rez91, Theorem 3.1] to prove the pointwise estimate

$$\tilde{\mathcal{L}} \left(N^{-d} \sum_x |\eta(x) - \zeta(x)| \right) \leq 0 \quad (4.78)$$

where $\tilde{\mathcal{L}}$ is the generator of the coupled process. We call the density of our coupled process G^N acting on X_N^2 .

Third step: Macroscopic Stability Estimate. In the last step we prove stability estimates on the limit PDE, which we call *macroscopic stability*. This concerns estimates on the derivatives in an appropriate space of solutions for the limit PDE. More specifically we would like to have that there exists $K > 0$, $T \in (0, \infty]$, so that

$$\|D^k f_t\|_H \leq K, \text{ for all } t \in [0, T] \quad (4.79)$$

and multi-indices k so that $|k| \leq 4$. When $T = \infty$, there is $R(t) \xrightarrow{t \rightarrow \infty} 0$ so that

$$\|D^k(f_t - f_\infty)\|_H \lesssim_{\|f_0\|_H} R(t), \text{ and } R(t) \in L^1((0, \infty))$$

for $f_\infty \in H$.

The abstract theorem reads:

Theorem 4.5 (Theorem 1.1 in Chapter 5). *Let $d = 1$, $F \in Lip(\mathbb{R})$ and $\phi \in C_c^\infty(\mathbb{T}^d)$. Let f_0 be the initial data to the hydrodynamical equation (4.75) and μ_0^N be the initial distribution of the stochastic process. We also consider the density of the local Gibbs measure that we call $\psi_t^N := d\nu_{f_t(\cdot)}^N / d\nu_\lambda^N$ for some $\lambda \geq 0$ and then the coupling G_t^N between ψ_t^N and $f_t^N := d\mu_t^N / d\nu_\lambda^N$. We assume that for $C_0 < \infty$ independent of N there exists a rate $\mathcal{R}^N \rightarrow 0$ as $N \rightarrow \infty$ so that*

$$\begin{aligned} \int_{X_N} \left| N^{-d} \sum_x \eta(x) \phi\left(\frac{x}{N}\right) - \int f_0(u) \phi(u) du \right| d\mu_0^N(\eta) &\leq C_0 \mathcal{R}^N, \\ \int_{X_N^2} \sum_x |\eta(x) - \zeta(x)| G_0^N(d\eta, d\zeta) &\leq C_0 \mathcal{R}^N. \end{aligned} \quad (4.80)$$

Then, assuming (4.77)-(4.78)-(4.79), for $t > 0$, there exists constant $0 < C_1, C_2 < \infty$

independent of N, t and $r(t)$ which is in $L^1((0, \infty))$ if $T = \infty$ and $r(t) = tK$ if $T < \infty$, such that

$$\left| \int_{X_N} F \left(N^{-d} \sum_{x \in \mathbb{T}_N^d} \eta(x) \phi \left(\frac{x}{N} \right) \right) - F \left(\int_{\mathbb{T}^d} f_t(u) \phi(u) du \right) d\mu_t^N(\eta) \right| \leq C_1 r(t) \mathcal{E}^N + \mathcal{R}^N + C_2 N^{-d/(d+2)}$$

where $f_t(\cdot)$ solves the hydrodynamical equation

$$\partial_t f(t, u) = Lf(t, u), \quad f(0, \cdot) = f_0(u). \quad (4.81)$$

We then prove (4.77)-(4.78)-(4.79) for the zero-range, simple exclusion and Ginzburg-Landau type processes, so that we can apply the abstract Theorem to obtain a rate.

Spectral gap for the mean field $\mathcal{O}(n)$ models.

This paper is a joint work with Simon Becker and it has been published in *Communications in Mathematical Physics*, see [BM20] in the bibliography. It is presented in Chapter 6.

We study the spectral gap for the overdamped Langevin operator on a sphere or the Ginzburg-Landau model. Here we write n for the spatial dimension and N for the number of spins. We consider N spins interacting with each other on an n -dimensional sphere \mathbb{S}^{n-1} , through the *mean-field Laplacian*

$$(\Delta_{MF}\sigma)(x) := \frac{1}{N} \sum_{y \in \{1, \dots, N\}} [\sigma(y) - \sigma(x)] \quad (4.82)$$

where $\sigma : \{1, \dots, N\} \rightarrow \mathbb{S}^{n-1}$ is the spin configurations. The energy function is given by the *Curie-Weiss Hamiltonian*⁶

$$H(\sigma) = \frac{1}{2} \sum_{x \in \{1, \dots, N\}} \sigma(x) (-\Delta_{MF}\sigma)(x) - \beta^{-1} \sum_{x \in \{1, \dots, N\}} \langle h, \sigma(x) \rangle \quad (4.83)$$

where the constant vector $h \in \mathbb{R}^n$ represents an external magnetic field, while β is the inverse temperature. The $\mathcal{O}(n)$ model is the Ising model when $n = 1$, and it is also called the rotator model when $n = 2$ and the classical Heisenberg model for $n = 3$, [BBS19]. The critical temperature for the $\mathcal{O}(n)$ -models is when $\beta = n$.

We estimate the dependence in N of the spectral gap of the *Langevin dynamics*, i.e.

$$\partial_t f = \sum_{x \in [N]} \left\langle \nabla_{\mathbb{S}^{n-1}}^{(x)}, \beta^{-1} \nabla_{\mathbb{S}^{n-1}}^{(x)} f + f \nabla_{\mathbb{S}^{n-1}}^{(x)} H \right\rangle_{\mathbb{R}^n} \quad (4.84)$$

⁶We refer to the book [BBS19, Section 1.4] and the references therein.

for all the mean-field $\mathcal{O}(n)$ models with $n \geq 1$ and $\beta \geq n$, i.e. both in the critical and in the supercritical regimes (i.e. low temperature regime) and we include the case of an external magnetic field h . We extend the results in [BB19] where Bauerschmidt and Bodineau prove uniform in N spectral gap for sufficiently high temperatures.

The invariant distribution is the Gibbs measure

$$d\rho(\sigma) := Z^{-1} e^{-\beta H(\sigma)} dS_{\mathbb{S}^{n-1}}^{\otimes N}(\sigma)$$

with Z the normalizing constant and $dS_{\mathbb{S}^{n-1}}$ is the normalized surface measure on the n -sphere.

Note that the operators $\langle f, -\Delta_{\mathbb{S}^{n-1}}^{(x)} f \rangle := \langle \nabla_{\mathbb{S}^{n-1}}^{(x)} f, \nabla_{\mathbb{S}^{n-1}}^{(x)} f \rangle$ and $\nabla_{\mathbb{S}^{n-1}}^{(x)}$ are the standard Laplace-Beltrami and gradient operator on \mathbb{S}^{n-1} acting on spin x , while for a function $F : \mathbb{S}^0 \rightarrow \mathbb{R}$ the gradient is given by

$$(\nabla_{\mathbb{S}^0} F)(\sigma) = F(\sigma) - F(-\sigma).$$

For the proof, we apply one step of renormalization [BBS19, Section 1.4] decomposing the stationary measure $d\rho$ on $(\mathbb{S}^{n-1})^N$ into two measures, which we call the *renormalized measure* and the *fluctuation measure*. The fluctuation measure $d\mu_\varphi(\sigma)$ is a measure on $(\mathbb{S}^{n-1})^N$ but on simpler form than the original $\mathcal{O}(n)$ measure and the renormalized measure $d\nu_N(\varphi)$ is a measure on \mathbb{R}^n such that

$$\mathbb{E}_\rho(F) = \mathbb{E}_{\nu_N}(\mathbb{E}_{\mu_\varphi}(F)).$$

We skip in this part their specific form and we refer either to Chapter 6 or to [BBS19, Lemma 1.4.3]. The fluctuation measure satisfies a Log-Sobolev inequality with a uniform in N constant, [ABC⁺00, Led01, SC97, ZQM11], it suffices therefore to study the renormalized measure.

Before I present the exact Theorems, let me explain with words our findings. Our results for $\beta > n$ can be summarized as follows. For $n = 1$ (Ising model), *for a weak magnetic field*: a direct analysis shows an exponentially fast decaying of the spectral gap in N , which is the optimal order. In contrast to that, *for a magnetic field with strength over its critical value*, an asymptotic analysis of the eigenvalues of a Schrödinger operator [Sim83] associated to the renormalized measure, yields uniformly bounded spectral gap in N whereas *for a magnetic field with strength exactly at its critical value* the decay of the spectral gap is no faster than a polynomially in N .

For $n \geq 2$, similar analysis as in [Sim83] shows that: when $h = 0$ the gap decays as N^{-1} which is the optimal rate, while when $h \neq 0$ it is bounded uniformly in N .

Finally for the critical case $\beta = n$, we see a different behavior of the spectral gap:

namely *zero magnetic fields* it decays at a polynomial rate $N^{-1/2}$, which is optimal, while for all $h \neq 0$ it remains uniformly bounded.

The specific statements with all the details and the exact parameters are as follows:

The first statement is about the Ising model case ($n = 1$).

Theorem 4.6 (Theorem 1.1 in Chapter 6, Supercritical Mean-field Ising models, $\beta > 1$).

Let N be the number of spins and n the number of components.

For the supercritical mean-field Ising model ($n = 1, \beta > 1$), the spectral gap λ_N of the generator

- for the case of small magnetic fields $|h| < h_c$, decays as $N \rightarrow \infty$ exponentially fast, $\lambda_N = e^{-N\Delta_{\text{small}}(V)(1+o(1))}$, which is the optimal rate. In particular, for magnetic fields $h \in [0, h_c)$

$$\Delta_{\text{small}}(V) := \int_{\gamma_1(\beta)}^{\gamma_2(\beta)} \beta (\varphi - \tanh(\beta\varphi + h)) d\varphi$$

where $\gamma_1(\beta) \leq \gamma_2(\beta) \in \mathbb{R}$ are the two smallest numbers satisfying the condition

$$\gamma(\beta) = \tanh(\gamma(\beta) \beta + h).$$

- For critical magnetic fields $|h| = h_c$, the spectral gap does not decay faster than $\mathcal{O}(N^{-1/3})$: $\lambda_N \gtrsim N^{-1/3}$.
- Finally, for strong magnetic fields $|h| > h_c$, it is bounded away from zero uniformly in N .

Where h_c is defined as $h_c = \sqrt{\beta(\beta - 1)} - \text{arccosh}(\sqrt{\beta})$.⁷

Theorem 4.7 (Theorem 1.2 in Chapter 6, Supercritical Mean-field $\mathcal{O}(n)$ -models, $\beta > n \geq 2$).

Let N be the number of spins and n the number of components.

For the supercritical mean-field $\mathcal{O}(n)$ -models ($n \geq 2, \beta > n$), the spectral gap λ_N of the generator

- decays at the optimal rate N^{-1} : $\lambda_N = \mathcal{O}(N^{-1})$, if there is no external magnetic field $h = 0$.
- is bounded away from zero uniformly in N for all $h \in \mathbb{R}^n \setminus \{0\}$.

Theorem 4.8 (Theorem 1.3 in Chapter 6, Critical Mean-field $\mathcal{O}(n)$ models, $\beta = n$). For all critical, $\beta = n$, $h = 0$ mean-field $\mathcal{O}(n)$ -models the spectral gap decays at the optimal rate

⁷We define the critical magnetic field strength h_c in the Ising model $h_c(\beta) := \sqrt{\beta(\beta - 1)} - \text{arccosh}(\sqrt{\beta})$ for temperatures $\beta \geq 1$ as the supremum of all $h > 0$ such that $x = \tanh(\beta x + h)$ has three distinct solutions for $x \in [-1, 1]$.

$N^{-1/2}$: $\lambda_N = \mathcal{O}(N^{-1/2})$. In particular, the rate $N^{-1/2}$ is attained for the magnetization

$$M(\sigma) = N^{-1/2} \sum_{x \in [N]} \sigma(x).$$

We emphasize that at the critical points ($\beta = n$, $h = 0$), the gap does no longer decay once a non-zero magnetic field is present and in this case it stays uniformly bounded from below:

Theorem 4.9 (Theorem 1.4 in Chapter 6, Mean-field $\mathcal{O}(n)$ models, $\beta = n$, $h \neq 0$). *For all, $\beta = n$ and $h \neq 0$, the spectral gap of all mean-field $\mathcal{O}(n)$ -models uniformly bounded.*

Chapter 2

Quantitative Rates of Convergence to Non-Equilibrium Steady State for a Weakly Anharmonic Chain of Oscillators

This chapter is published in the Journal of Statistical Physics [Men20].

We study a 1-dimensional chain of N weakly anharmonic classical oscillators coupled at its ends to heat baths at different temperatures. Each oscillator is subject to pinning potential and it also interacts with its nearest neighbors. In our set up both potentials are homogeneous and bounded (with N dependent bounds) perturbations of the harmonic ones. We show how a generalised version of Bakry-Emery theory can be adapted to this case of a hypoelliptic generator which is inspired by F. Baudoin (2017). By that we prove exponential convergence to non-equilibrium steady state in Wasserstein-Kantorovich distance and in relative entropy with quantitative rates. We estimate the constants in the rate by solving a Lyapunov-type matrix equation and we obtain that the exponential rate, for the homogeneous chain, has order bigger than N^{-3} . For the purely harmonic chain the order of the rate is in $[N^{-3}, N^{-1}]$. This shows that, in this set up, the spectral gap decays at most polynomially with N .

2.1 Introduction

2.1.1 Description of the model

We consider a model for heat conduction consisting of a one-dimensional chain of N coupled oscillators. The evolution is a Hamiltonian dynamics with Hamiltonian

$$H(p, q) = \sum_{1 \leq i \leq N} \left(\frac{p_i^2}{2} + U_{\text{pin}}(q_i) \right) + \sum_{i=0}^N U_{\text{int}}(q_{i+1} - q_i),$$

where (p, q) belong in the phase space \mathbb{R}^{2N} and q_0, q_{N+1} describe the boundaries which here are considered to be fixed: $q_0 = q_{N+1} = 0$. We denote by $q = (q_1, \dots, q_N) \in \mathbb{R}^N$ the displacements of the atoms from their equilibrium positions and by $p = (p_1, \dots, p_N) \in \mathbb{R}^N$ the momenta. Each particle has its own pinning potential U_{pin} and it also interacts with its nearest neighbors through an interaction potential U_{int} . Notice that here all the masses are equal and we take them $m_i = 1$. So we consider a homogeneous chain, where both the masses and the potentials that act on each oscillator, are the same. The classical Hamiltonian dynamics is perturbed by noise and friction in the following way: the two ends of the chain are in contact with heat *Langevin* baths at two different temperatures $T_L, T_R > 0$. So our dynamics is described by the following system of SDEs:

$$\begin{aligned} dq_i(t) &= p_i(t)dt \quad \text{for } i = 1, \dots, N, \\ dp_i(t) &= (-\partial_{q_i} H)dt \quad \text{for } i = 2, \dots, N-1, \\ dp_1(t) &= (-\partial_{q_1} H - \gamma_1 p_1)dt + \sqrt{2\gamma_1 T_L} dW_1(t), \\ dp_N(t) &= (-\partial_{q_N} H - \gamma_N p_N)dt + \sqrt{2\gamma_N T_R} dW_N(t) \end{aligned} \tag{1.1}$$

where γ_i are the friction constants, T_i are the two temperatures and W_1, W_N are two independent normalised Wiener processes.

The dynamics (1.1) is equivalently described by the following Liouville equation on the law of the process

$$\partial_t f = \mathcal{L}^* f \quad \text{with } f(0, p, q) = f_0(p, q) \tag{1.2}$$

where \mathcal{L} is the second order differential operator

$$\mathcal{L} = \sum_{i=1}^N (p_i \partial_{q_i} - \partial_{q_i} H \partial_{p_i}) - \gamma_1 p_1 \partial_{p_1} - \gamma_N p_N \partial_{p_N} + \gamma_1 T_L \partial_{p_1}^2 + \gamma_N T_R \partial_{p_N}^2 \tag{1.3}$$

which is the generator of the semigroup P_t acting on the space $C_b^2(\mathbb{R}^{2N})$ of bounded real-valued, C^2 functions on the phase space. We denote by \mathcal{L}^* the generator of the dual semigroup that acts on probability measures.

2.1.1.1 State of the art

The model described by the SDEs (1.1), was first used to describe heat diffusion and derive rigorously Fourier's law (for an overview see [BLRB00], [Lep16, Dha08] and [FB19]). Since then, it has been the subject of many studies, both from a numerical and from a theoretical perspective. First, the purely harmonic case with several idealised reservoirs at different temperatures has been solved explicitly in [RLL67]. In this paper the authors found exactly how the non-equilibrium stationary state looks like: it is Gaussian in the positions and momenta of the system. For the anharmonic chain there are no explicit results in general. However it has been studied numerically for many different potentials and many kinds of heat baths, including the Langevin heat baths that we consider here. See for instance [ALS06] [GLPV00, LLP03] and references therein.

There are two facts in this model that make its rigorous study very challenging: first of all, we do not know explicitly the form of the invariant measure of (1.1) and also our generator is highly degenerate, having the dissipation and noise acting only on two variables of momenta at the end of the chain. It is not difficult to see, though, that in the equilibrium case, *i.e.* when the two temperatures are equal $T_L = T_R = T = \beta^{-1}$, the stationary measure is the Gibbs-Boltzmann measure $d\mu(p, q) = \exp(-\beta H(p, q)) dp dq$: after explicit calculations we have $\mathcal{L}^* e^{-\beta H(p, q)} = 0$.

Since we are interested in the theoretical aspects of the model, we refer to [EPRB99a, EPRB99b], which is the first rigorous study of the anharmonic case. The existence of a steady state has only been obtained in some cases where the potentials act like polynomials near infinity. In particular under the following assumptions on the potentials:

$$\lim_{\lambda \rightarrow \infty} \lambda^{-k} U(\lambda q) = a_k |q|^k \text{ and } \lim_{\lambda \rightarrow \infty} \lambda^{1-k} U'(\lambda q) = k a_k |q|^{k-1} \text{sign}(q)$$

for constants $a_k > 0$, where for the interaction: $k \geq 2$ and for the pinning $k \geq 1$ (the exponent k for the pinning was improved in [Car07]) and assuming that *the interaction potential is at least as strong as the pinning*, the existence and uniqueness of an invariant measure was first proved in [EPRB99a] using functional analytic methods. In particular it was proved that the resolvent of the generator of (1.1) is compact in a suitable weighted L^2 space. Later it was proved in [RBT02] that the rate of convergence to the steady state is exponential using probabilistic tools. Note that in the above-mentioned papers, the coupling of the chain with the heat baths is slightly different and a bit more complicated than considering Langevin thermostats, with physical interpretation: the model of the reservoirs is the classical field theory given by linear wave equations with initial conditions distributed with respect to appropriate Gibbs measures at different temperatures, see also

[RB06b, Section 2]. Later, an adaptation of a very similar probabilistic proof was provided in [Car07] for the Langevin thermostats. The difference with the Langevin heat baths is that the dissipation and the noise act on the momenta only indirectly through some auxiliary variables. Finally let us mention that the relaxation rates have been studied for short chains of rotors with Langevin thermostats in [CP17, CEP15].

Regarding the existence, uniqueness of a non-equilibrium stationary state and exponential convergence towards it in more complicated networks of oscillators (multi-dimensional cases) see [CEHRB18]. The proofs there are inspired by the above-mentioned works in the 1-dimensional chains.

There are also cases where there is no convergence to equilibrium, when for instance $l > k$, *i.e.* when the pinning is stronger than the coupling potential, see for example [Hai09, HM09]. In [HM09] the resolvent of the generator fails to be compact or/and there is lack of spectral gap, under some scenarios included in $l > k$. In particular, when the interaction is harmonic, 0 belongs in the essential spectrum of the generator as soon as the pinning potential is of the form $|q|^k$ for $k > 3$. The conjecture is that this is true as soon as $k > \frac{2n}{2n-1}$ if n is the center of the chain.

2.1.2 Notation

$\{e_i\}_{i=1}^n$ denote the elements of the canonical basis in \mathbb{R}^n and $|\cdot|$ to denote the Euclidean norm on \mathbb{R}^n , from the usual inner product $\langle \cdot, \cdot \rangle$. For a square matrix $A = (a_{ij})_{1 \leq i, j \leq n} \in \mathbb{R}^{n \times n}$, we write $\|A\|_2$ for the operator (spectral) norm, induced by the Euclidean norm for vectors :

$$\|A\|_2 = \max_{x \in \mathbb{R}^n} \frac{|Ax|_2}{|x|_2} = (\text{maximum eigenvalue of } A^T A)^{1/2}.$$

We also write $A^{1/2}$ for the square root of a (positive definite) matrix A , *i.e.* the matrix such that $A^{1/2}A^{1/2} = A$, for $A^{1/2}$ a positive definite matrix as well. Moreover, by $C_b^\infty(\mathbb{R}^n)$ we denote the space of the smooth and bounded functions, by ∇_z we denote the gradient on z -variables in a metric space X with respect to the Euclidean metric. We write $\mathcal{P}_2(\mathbb{R}^n)$ for the space of the probability measures on \mathbb{R}^n that have second moment finite, *i.e.*

$$\mathcal{P}_2(\mathbb{R}^n) = \left\{ \rho \in \mathcal{P}(\mathbb{R}^n) : \int_{\mathbb{R}^n} |x|^2 d\rho(x) < \infty \right\}.$$

$[N]$ denotes the set $\{1, 2, \dots, N\}$ and we use the notation $g(x) \lesssim \mathcal{O}(f(x))$ to indicate that there is a dimensionless constant $C > 0$ so that $|g(x)| \leq C|f(x)|$.

2.1.3 Set up and main results

Let us state two assumptions: one on the boundary conditions of the chain and one on the potentials.

- **(H1)** Regarding the boundary conditions, we consider the oscillators chain with *rigidly fixed edges*: the left boundary of the chain is an oscillator labelled 0 and the right is an oscillator labelled $N + 1$ under the hypothesis that $q_0 = q_{N+1} = 0$. The first and the last particle are pinned with additional harmonic forces, corresponding to their attachment to a wall.

Note that these boundary conditions and heat baths modelled by two Ornstein-Uhlenbeck processes at both ends as explained above, is the same model as in [RLL67] and is known as the *Casher-Lebowitz model*, since it is also one of the models considered in [CL71]¹.

- **(H2)** The chain is *weakly anharmonic*: both pinning and interaction potentials differ from the quadratic ones by perturbing potentials $U_{\text{pin}}^N, U_{\text{int}}^N \in \mathcal{C}^2(\mathbb{R})$ with bounded Hessians in the following sense:

$$\sup_{\substack{q_i \in \mathbb{R}, \\ i=1, \dots, N}} \|\text{Hess } U_{\text{pin}}^N(q_i)\|_2 \leq C_{\text{pin}}^N \quad \text{and} \quad \sup_{\substack{r_i \in \mathbb{R}, \\ i=1, \dots, N}} \|\text{Hess } U_{\text{int}}^N(r_i)\|_2 \leq C_{\text{int}}^N \quad (1.4)$$

where $r_i := q_{i+1} - q_i$, $i = 1, \dots, N$. The positive constants $C_{\text{pin}}^N, C_{\text{int}}^N$ scale with the dimension like

$$C_{\text{pin}}^N + C_{\text{int}}^N \leq C_0 N^{-9/2} \quad (1.5)$$

and C_0 is a dimensionless constant.

Under Assumptions **(H1)** and **(H2)** for $a \geq 0, c > 0$, the Hamiltonian takes the form

$$H(p, q) = \sum_{i=1}^N \left(\frac{p_i^2}{2} + a \frac{q_i^2}{2} + U_{\text{pin}}^N(q_i) \right) + \sum_{i=1}^{N-1} \left(c \frac{(q_{i+1} - q_i)^2}{2} + U_{\text{int}}^N(q_{i+1} - q_i) \right) + \frac{cq_1^2}{2} + \frac{cq_N^2}{2} \quad (1.6)$$

and denoting by \mathcal{L} the infinitesimal generator, we look at the Liouville equation

¹The other one considered for studying the N -dependence of the energy flux was first introduced by Rubin-Greer, [RG71], where the heat baths are semi-infinite chains distributed according to Gibbs equilibrium measures of temperatures T_L, T_R (free boundaries). In both [CL71] and [RG71] the purpose was to study the heat flux behaviour in disordered harmonic chains

$\partial_t f = \mathcal{L}^* f$, where the generator of the dynamics now is

$$\begin{aligned} \mathcal{L} = & p \cdot \nabla_q - q \cdot B \nabla_p - \sum_{i=1}^N (U_{\text{pin}}^N)'(q_i) \partial_{p_i} - \gamma p_1 \partial_{p_1} - \gamma p_N \partial_{p_N} + \gamma T_L \partial_{p_1}^2 + \gamma T_R \partial_{p_N}^2 - \\ & - \sum_{i=1}^N \left((U_{\text{int}}^N)'(q_{i+1} - q_i) \partial_{p_i} - (U_{\text{int}}^N)'(q_i - q_{i-1}) \partial_{p_i} \right) \end{aligned}$$

where we take all the friction constants equal $\gamma_1 = \gamma_N = \gamma$, for the two temperatures T_L, T_R we assume that they satisfy $T_L = T + \Delta T$, $T_R = T - \Delta T$, for some temperature difference $\Delta T > 0$. Also, B is the symmetric tridiagonal (Jacobi) matrix

$$B := \begin{bmatrix} (a+2c) & -c & 0 & 0 & \dots & 0 & 0 & 0 \\ -c & (a+2c) & -c & 0 & \dots & 0 & 0 & 0 \\ 0 & -c & (a+2c) & -c & \dots & 0 & 0 & 0 \\ \vdots & \vdots & & & & & & \\ \vdots & \vdots & & & \ddots & \ddots & \ddots & \\ 0 & 0 & 0 & 0 & & -c & (a+2c) & -c \\ 0 & 0 & 0 & 0 & \dots & 0 & -c & (a+2c) \end{bmatrix}. \quad (1.7)$$

It is convenient to see the above form of the generator in the following block-matrix form:

$$\mathcal{L} = -z^T M \nabla_z - \nabla_q \Phi(q) \cdot \nabla_p + \nabla_p \cdot \mathfrak{F} \Theta \nabla_p \quad (1.8)$$

where $z = (p, q)^T \in \mathbb{R}^{2N}$, $\Phi(q)$ corresponds to the perturbing potentials so that

$$\Phi(q) = \sum_{i=1}^N U_{\text{pin}}^N(q_i) + \sum_{i=1}^N U_{\text{int}}^N(q_{i+1} - q_i) + U_{\text{int}}^N(q_1) + U_{\text{int}}^N(-q_N),$$

the matrix \mathfrak{F} is the friction matrix

$$\mathfrak{F} = \text{diag}(\gamma, 0, \dots, 0, \gamma)$$

the matrix Θ is the temperature matrix

$$\Theta = \text{diag}(T_L, 0, \dots, 0, T_R)$$

and M in blocks is the following

$$M = \begin{bmatrix} \mathfrak{F} & -I \\ B & 0 \end{bmatrix} \quad (1.9)$$

where I is the identity matrix, so that it corresponds to the transport part of the operator, while B and \mathfrak{F} correspond to the harmonic part of the potentials and the drift from both ends, respectively.

Motivation. This study is motivated by a discussion opened in C. Villani's memoir on hypocoercivity, see Section 9.2 in [Vil09a], concerning open questions on the heat conduction model as defined above, and how to approach them by hypocoercive techniques. This chain of coupled oscillators corresponds to a hypocoercive situation, where the diffusion only at the ends of the chain leads to a convergence to the stationary distribution exponentially fast, under the following assumptions on the potentials: strict convexity on the interaction potential (being stronger than the pinning one) and bounded Hessians for both potentials. In particular, he points out that it might be possible to recover the previous results of exponential convergence in the weighted $H^1(\mu)$ -norm for this different class of potentials (than the potentials assumed in [EPRB99b] for instance) by applying a generalised version of Theorem 24 in [Vil09a]. For that, one needs to know some properties of the, non-explicit, non-equilibrium steady state μ : for instance, if it satisfies a Poincaré inequality or if the Hessian of the logarithm of its density is bounded.

Finally we note that entropic hypocoercivity has been applied in [LO17] in order to develop estimates and to get quantitative convergence results to the limit equation, for anharmonic chains but with thermostats in contact with all the particles along the chain.

Main results. Here, considering a perturbation of the harmonic chain (homogeneous case), instead we follow an approach that combines hypocoercivity techniques and the Bakry-Émery theory of Γ calculus and curvature conditions as in [BE85]. We prove the validity of the Bakry-Émery criterion in a modified setting. This is explained in more details and is implemented in Section 3. The whole idea was inspired by F. Baudoin in [Bau17]: using this combination, Baudoin proved exponential convergence to equilibrium for the Kinetic Fokker-Planck equation in H^1 -norm and in Kantorovich-Wasserstein distance.

Thus we show, for the dynamics (1.1) as well, exponential convergence to the stationary state in Kantorovich-Wasserstein distance and in relative entropy and we get quantitative rates of convergence in these distances, *i.e.* we obtain information on the N -dependence of the rate. In particular our estimates show that the convergence rate in the harmonic chain approach 0 as N tends to infinity at a *polynomial* rate with order between C_1/N^3 and C_2/N and that the scaling of the rate is bigger than C_3N^{-3} in the weakly anharmonic chain.

In order to quantify the above rates, we estimate $\|b_N\|_2$, where b_N is a block matrix defined in Section 3 as a solution of a matrix equation, (1.10). Since $\|b_N\|_2$ appears in the rates in the Theorems 1.4, 1.6 and the Proposition 1.2, we start by stating this result:

Proposition 1.1. *Let $\Pi_N = \text{diag}(2T_L, 1, \dots, 1, 2T_R, 1, 1, \dots, 1, 1) \in \mathbb{R}^{2N \times 2N}$ and $M \in \mathbb{R}^{2N \times 2N}$ given by (1.9), with pinning and interaction coefficients $a \geq 0, c > 0$. For all $N \in \mathbb{N}$, there exists a unique symmetric positive definite block matrix $b_N \in \mathbb{R}^{2N \times 2N}$ such that*

$$b_N M + M^T b_N = \Pi_N. \quad (1.10)$$

Moreover there exists $C_{a,c} > 0$, that depends only on the coefficients a, c , such that for all $N \in \mathbb{N}$, $\|b_N\|_2 \leq C_{a,c} N^3$ and $\|b_N^{-1}\| \leq C_{a,c}$.

Second, we state the following Proposition, that is restricted to the harmonic chain, and provides us with a lower bound on the spectral gap (given the estimates on $\|b_N\|_2$ by Proposition 1.1):

Proposition 1.2 (Lower bound on the spectral gap of the harmonic chain). *For the spectral gap ρ of the chain described by the generator (1.8) without the perturbing potentials (the harmonic chain), which is given by the relation*

$$\min\{\rho > 0 : (z - \mathcal{L})^{-1} \text{ is invertible with bounded inverse, for } -\rho \leq \text{Re}(z) < 0\},$$

we have the following property: there exists $\kappa > 0$ such that for all $N \in \mathbb{N}$,

$$\rho \geq \kappa N^{-3}.$$

This lower bound is in fact the optimal rate in the case of the harmonic homogeneous chain. In the work [BM22, Proposition 9.1] an upper bound is provided as well and thus the scaling of ρ is exactly N^{-3} . This is done by exploiting the form of the matrix M , (1.9), and more specifically using information on the spectrum of the discrete Laplacian. In [BM22] we study also the case of disordered chains by considering different pinning coefficients for each oscillator. Compared to the homogeneous case, as in this paper, where the decay is *polynomial*, in a disordered chain the spectral gap decays at an *exponential rate* in terms of N . Regarding the adaptation of the generalised Bakry-Emery theory presented in this paper to a non-homogeneous scenario, we can prove existence of a spectral gap for the weakly anharmonic chain as soon as the matrix M has a spectral gap (and this is the case as soon as all the interaction coefficients $c_i \neq 0$). The difficulty in a non-homogeneous scenario will be the second part (as described in the Section 2): to solve the high-dimensional matrix equation (1.10) in order to estimate the spectral norm.

Remark 1.3. *We expect the bound on the $\|b_N\|_2$, from Proposition 1.1, to be optimal, since from the proof of Proposition 1.2 combined with [BM22, Proposition 9.1]: there exist*

$c_1 > 0$, such that

$$c_1 N^{-3} \geq \rho \geq \frac{1}{\|b_N\|_2}.$$

In the following, we consider b_N as given by Proposition 1.1. Before we state the first main Theorem, we recall the definition of the Kantorovich-Rubinstein-Wasserstein L^2 -distance $W_2(\mu, \nu)$ between two probability measures μ, ν :

$$W_2(\mu, \nu)^2 = \inf \int_{\mathbb{R}^N \times \mathbb{R}^N} |x - y|^2 d\pi(x, y)$$

where the infimum is taken over the set of all the couplings, *i.e.* the joint measures π on $\mathbb{R}^N \times \mathbb{R}^N$ with left and right marginals μ and ν respectively.

It is easy to see that W_2 is indeed a metric. We restrict ourselves on the subspace $\mathcal{P}_2(\mathbb{R}^{2N})$, where μ and ν have second moments finite, so that their distance $W_2(\mu, \nu)$ will be finite. For more information on this distance we refer the reader for instance to [Vil09b] and references therein.

Theorem 1.4. *We consider a chain of coupled oscillators whose dynamics are described by the system (1.1) under Assumptions (H1) and (H2). For a fixed number of particles N , there is a unique stationary state f_∞ , in particular, for initial data f_0^1, f_0^2 of the evolution equation, we have the following contraction property:*

$$W_2(P_t^* f_0^1, P_t^* f_0^2) \leq C_{a,c} N^{\frac{3}{2}} e^{-\frac{\lambda_0}{N^3} t} W_2(f_0^1, f_0^2) \quad (1.11)$$

for $C_{a,c}, \lambda_0$ dimensionless constants.

Moreover, in the set up of Theorem 1.4, we get some qualitative information about the non-equilibrium steady distribution, like the validity of a Poincaré inequality and even better, a Log-Sobolev inequality:

Proposition 1.5 (Log-Sobolev inequality). *Let \mathcal{T} be the quadratic form*

$$\mathcal{T}(f, g) = \nabla_z f^T b_N \nabla_z g + \nabla_z g^T b_N \nabla_z f.$$

Under Assumption (H2), the unique invariant measure $\mu = f_\infty$ from the Theorem 1.4 satisfies a Log-Sobolev inequality (LSI(C_N)) :

$$\int_{\mathbb{R}^{2N}} f \log f \, d\mu - \int_{\mathbb{R}^{2N}} f \, d\mu \log \left(\int_{\mathbb{R}^{2N}} f \, d\mu \right) \leq C_N \int_{\mathbb{R}^{2N}} \frac{\mathcal{T}(f, f)}{f} d\mu. \quad (1.12)$$

where

$$C_N := \frac{\gamma T_L \|b_N^{-1}\|_2}{2 \left(\min(1, 2T_R) \|b_N\|_2^{-1} - (C_{pin}^N + C_{int}^N) \|b_N\|_2^{1/2} \|b_N^{-1}\|_2^{1/2} \right)} \leq \gamma T_L C_{a,c} \lambda_0^{-1} N^3$$

where $\gamma, T_L, C_{a,c}, \lambda_0 := \lambda_0(C_0)$ are all dimensionless constants with the prefactor in (1.5), C_0 , to satisfy $C_0 < \min(1, 2T_R)C_{a,c}^{-2}$.

Consequently we have convergence to the non-equilibrium steady state in Entropy. Let us first define the following information-theoretical functionals. For two probability measures μ and ν on \mathbb{R}^{2N} with $\nu \ll \mu$, we define the Boltzmann H functional

$$H_\mu(\nu) = \int_{\mathbb{R}^{2N}} h \log h \, d\mu, \quad \nu = h\mu \quad (1.13)$$

and the relative Fisher information

$$I_\mu(\nu) = \int_{\mathbb{R}^{2N}} \frac{|\nabla h|^2}{h} d\mu, \quad \nu = h\mu. \quad (1.14)$$

We have entropic convergence in the following sense, as in [Vil09a, Section 6]:

Theorem 1.6. *We consider a chain of coupled oscillators whose dynamics are described by the system (1.1) under Assumptions **(H1)** and **(H2)**. For a fixed number of particles N , assuming that (i) μ is the invariant measure for P_t and (ii) that it satisfies a Log-Sobolev inequality with constant $C_N > 0$, for all $f > 0$ with*

$$\mathcal{E}(f) < \infty, \quad \text{and} \quad \int f d\mu = 1,$$

we have a convergence to the non-equilibrium steady state in the following sense:

$$H_\mu(P_t f \mu) + I_\mu(P_t f \mu) \leq \lambda_{a,c} N^3 e^{-\lambda_0 N^{-3} t} \left(H_\mu(f \mu) + I_\mu(f \mu) \right) \quad (1.15)$$

for dimensionless constants $\lambda_{a,c}, \lambda_0$.

From Theorem 1.4 we get an exponential rate of order bigger than N^{-3} for the weakly anharmonic chain. In the purely harmonic case, we have that the convergence rate is between $C_1 N^{-3}$ and $C_2 N^{-1}$ for some constants C_1, C_2 that are independent of N .

Remark 1.7. *Note that a generalised version of Γ calculus has been applied for a toy model of the dynamics (1.1) by P. Monmarché, [Mon19]: working with the unpinned, non-kinetic version, with convex interaction and given that the center of the mass is fixed, he proves the same kind of convergences and ends up with explicit and optimal N -dependent rates, of order $\mathcal{O}(N^{-2})$, for the overdamped dynamics.*

2.1.4 Plan of the Chapter

Sections 2 to 5 concern the proofs of the convergence to the steady state by hypocoercive arguments (applying the generalized Bakry-Emery criterion) while Section 6 is devoted to

estimating the spectral norm of b_N , which is crucial in the final estimate for the scaling of the spectral gap. In particular, Section 2 contains an introduction to Bakry-Emery theory and an explanation of the method that is used. In Section 3 we obtain the estimates that lead to the proof of Proposition 1.5. In Section 5 and Section 4 we give the proof of Theorem 1.6 and Theorem 1.4 respectively. Finally in Section 6 we prove Propositions 1.1 and 1.2.

2.2 Carré du Champ operators and curvature condition

2.2.1 Introduction to Carré du Champ operators

Consider a Markov semigroup P_t with at least one invariant measure μ and infinitesimal generator $L : D(L) \subset L^2(\mu) \rightarrow L^2(\mu)$. Here we restrict ourselves to the case of the diffusion operators and we associate with the operator L , a bilinear quadratic differential form Γ , the so-called *Carré du Champ* operator, which is defined as follows: for every pair of functions (f, g) in $C^\infty \times C^\infty$

$$\Gamma(f, g) := \frac{1}{2} \left(L(fg) - fLg - gLf \right). \quad (2.16)$$

In other words Γ measures the *default of the distributivity* of L . Then we define its iteration Γ_2 , where instead of the multiplication we use the action of Γ :

$$\Gamma_2(f, g) := \frac{1}{2} \left(L(\Gamma(f, g)) - \Gamma(f, Lg) - \Gamma(g, Lf) \right). \quad (2.17)$$

From the theory of Γ -calculus we have that a curvature condition of the form

$$\Gamma_2(f, f) \geq \lambda \Gamma(f, f) \quad (2.18)$$

for all f in a suitable algebra \mathcal{A} dense in the $L^2(\mu)$ -domain of L and $\lambda > 0$ is equivalent to the following gradient estimate

$$\Gamma(P_t f, P_t f) \leq e^{-2\lambda t} P_t(\Gamma(f, f)), \quad t \geq 0$$

where P_t is the semigroup generated by \mathcal{L} . The uniqueness of the invariant measure then follows from the contraction property in W_2 distance (which is equivalent to the gradient estimate above thanks to Kuwada's duality, see [Kuw10] or Theorem 4.1 later on). This also implies a Log-Sobolev inequality (and thus a Poincaré inequality), see [BE85] or [Bak06, Section 3].

Attempt to apply the classical Γ theory to the generator \mathcal{L} given by (1.8): For the generator of the dynamics (1.1), given by (1.8), we can not bound Γ_2 by Γ from below. Explicit calculations give

$$\Gamma(f, f) = 2\gamma_1 T_L (\partial_{p_1} f)^2 + 2\gamma_N T_R (\partial_{p_N} f)^2$$

while

$$\begin{aligned} \Gamma_2(f, f) = & 2(\gamma_1 T_L)^2 (\partial_{p_1}^2 f)^2 + 2(\gamma_N T_R)^2 (\partial_{p_N}^2 f)^2 + 2T_L \gamma_1^2 (\partial_{p_1} f)(\partial_{q_1} f) + \\ & + 2T_R \gamma_N^2 (\partial_{p_N} f)(\partial_{q_N} f) + \Gamma(f, f). \end{aligned}$$

Since we can not control the terms $\partial_{p_i} f \partial_{q_i} f$, we can not bound Γ_2 from below by Γ . In cases like this, we say that the particle system has $-\infty$ Bakry-Emery curvature.

2.2.2 Description of the method

In order to overcome this problem, we are doing the following:

(1) First we modify the classical Γ theory: we define a new quadratic form, different, but equivalent, to the $|\nabla_z f|^2$ that will play the role of the Γ functional. This will spread the noise from p_1 and p_N to all the other degrees of freedom as well. The general idea comes from Baudoin [Bau17]. We make a suitable choice of a positive definite matrix, $b_N \in \mathbb{R}^{2N \times 2N}$, to define a new quadratic form that will replace the Γ functional, so that we obtain a 'twisted' curvature condition: an estimate of the form (2.18). This implies also a modified gradient estimate, and thus a Poincaré and Log-Sobolev inequality. We choose this matrix to be the unique solution of a *Lyapunov* equation with *positive definite r.h.s.*:

$$b_N M + M^T b_N = \Pi_N > 0.$$

In general in order to deal with a hypocoercive situation in H^1 - setting, one can perturb the norm to an equivalent norm, so that exponential convergence results can be deduced with this new norm. The idea is originally due to Talay in [Tal02] and it was later generalised by Villani in [Vil09a]. Then one can have convergence in the usual norm thanks to their equivalence. Here, instead of the norm, we modify the gradient and thus the Γ *Carré du Champ*, and work with a generalised Γ - theory.

The idea of working with the matrix that solves the above-mentioned Lyapunov equation came from the fact that (i) we need to control from below the quantity $b_N M + M^T b_N$ and

(ii) in the linear chain, the covariance matrix $b_0 \in \mathbb{R}^{2N \times 2N}$ solves

$$b_0 M + M^T b_0 = \text{diag}(2T_L, 0, \dots, 2T_R, 0, \dots, 0) \quad (2.19)$$

and determines the stationary solution of the corresponding Liouville equation. Therefore, tackling the hypoellipticity problem, i.e. spreading the dissipation to all the degrees of freedom, corresponds to working with a Lyapunov equation with *positive definite* r.h.s. A way to think of it is as a sequence of *Lyapunov* equations:

$$\begin{aligned} b_0 M + M^T b_0 &= \text{diag}(2T_L, 0, \dots, 2T_R, 0, \dots, 0) \\ b_1 M + M^T b_1 &= \text{diag}(2T_L, 0, \dots, 0, 2T_R, 1, 0, \dots, 0, 1) := \Pi_1 \\ b_2 M + M^T b_2 &= \text{diag}(2T_L, 1, 0, \dots, 0, 1, 2T_R, 1, 1, 0, \dots, 0, 1, 1) := \Pi_2 \\ &\vdots \\ b_N M + M^T b_N &= \text{diag}(2T_L, 1, \dots, 1, 2T_R, 1, 1, \dots, 1, 1) := \Pi_N \end{aligned}$$

so that in each step we add a positive entry in the diagonal of the r.h.s. from both sides. This corresponds to spreading the noise and dissipation to the next oscillator from both ends until the center of the chain, like the commutators would do in a classical hypoelliptic setting, see also Figure 2.1. So in the last step we have $\Pi_N > 0$ which corresponds to having spread the noise everywhere in the space. This allows us to prove the validity of the generalised Bakry-Emery criterion (3.23), which is the key estimate in order to have exponential convergence to the non-equilibrium steady state.

(2) In order to make our estimates quantitative, we estimate the spectral norm of the matrix b_N and its inverse. Regarding the bound on the norm of b_N , we estimate its entries using that it solves the Lyapunov equation, while for the norm of b_N^{-1} , we compare it to the norm of b_0^{-1} which is uniformly bounded in N . This corresponds to the proof of Proposition 1.1 which is the subject of Section 6.

For those familiar with Hörmander's method we describe briefly here the similarity with the spreading of dissipation-mechanism: in Hörmander's theory the *smoothing* mechanism is the one transferred through the interacting particles inductively by the use of commutators: the generator has the form

$$\mathcal{L} = X_0 + X_1^2 + X_N^2$$

where

$$X_0 = p \cdot \nabla_q - \nabla_q H \cdot \nabla_p - \gamma p_1 \partial_{p_1} - \gamma p_N \partial_{p_N} \quad \text{and} \quad X_i = \sqrt{T_i} \partial_{p_i}.$$

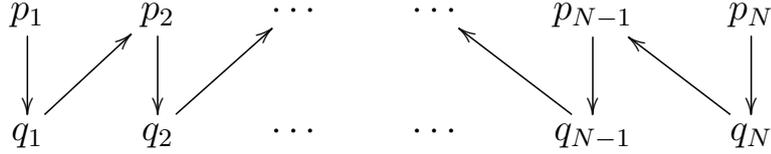


Figure 2.1: Spreading of dissipation by commutators as in Hörmander’s hypoellipticity theory.

Then $[\partial_{p_1}, X_0] = -\partial_{p_1} + \partial_{q_1}$. Now commuting ∂_{q_1} with the first order terms of the generator: $[\partial_{q_1}, X_0] = \partial_{q_1 q_1} H \partial_{p_1} - \partial_{q_1 q_2} H \partial_{p_2}$. Given that $\partial_{q_1 q_2} H$ is non-vanishing we have ‘spread the smoothing mechanism’ to p_2 . Continuing like that, commuting the ‘new’ variable with the first order terms of \mathcal{L} , inductively we cover all the particles of the chain.

2.3 Functional inequalities in the modified setting

In order to apply a ‘twisted’ Bakry-Emery machinery, introduced by Baudoin in Section 2.6 of [Bau17], we work with the positive definite matrix b_N chosen to be the solution of the *Lyapunov equation* (1.10). The following Proposition gives us existence of such a solution.

Proposition 3.1. *There exists a positive solution to (1.10) if and only if the r.h.s. of it, is positive definite and all the eigenvalues of M have positive real parts.*

Proof. It is a matrix reformulation of a well known and classical result of Lyapunov that can be found for instance in [Gan59, page 224] or [Lia47, Section 20]. \square

The eigenvalues of M have strictly positive real part ([JPS17, Lemma 5.1]) and the right hand side of (1.10) is positive definite. Therefore there exists a positive solution of (1.10). Also, we can easily see that the solution is given by the formula

$$b_N = \int_0^\infty e^{-tM^T} \Pi_N e^{-tM} dt.$$

We define the following quadratic quantity for $f, g \in C^\infty(\mathbb{R}^{2N})$,

$$\mathcal{T}(f, g) := \nabla_z f^T b_N \nabla_z g + \nabla_z g^T b_N \nabla_z f \tag{3.20}$$

so that

$$\mathcal{T}(f, f) = 2\nabla_z f^T b_N \nabla_z f.$$

Then we consider the functional

$$\mathcal{T}_2(f, f) = \frac{1}{2} \left(\mathcal{L}\mathcal{T}(f, f) - 2\mathcal{T}(f, \mathcal{L}f) \right).$$

Here $\mathcal{T}(f, f)$ is always positive since $b_N \geq 0$ (and in fact positive definite since $b_N > 0$: this is proven in the last part of the proof of Proposition 1.1). In contrast with the original operator Γ , our modified quadratic form \mathcal{T} is related to \mathcal{L} only indirectly through the different steps of commutators.

We have an equivalence of the following form between \mathcal{T} and $|\nabla_z|^2$:

$$\frac{1}{\|b_N^{-1}\|_2} |\nabla_z f|^2 \leq \mathcal{T}(f, f) \leq \|b_N\|_2 |\nabla_z f|^2. \quad (3.21)$$

Combining this with the conclusion of Proposition 1.1, we write

$$C_{a,c}^{-1} |\nabla f|^2 \leq \mathcal{T}(f, f) \leq C_{a,c} N^3 |\nabla f|^2.$$

Proposition 3.2. *With the above notation, under Assumption **(H2)**, for all $N \in \mathbb{N}$ there exists constant*

$$\lambda_N = \min(1, 2T_R) \|b_N\|_2^{-1} - (C_{pin}^N + C_{int}^N) \|b_N\|_2^{1/2} \|b_N^{-1}\|_2^{1/2} \quad (3.22)$$

such that for $f \in C^\infty(\mathbb{R}^{2N})$,

$$\mathcal{T}_2(f, f) \geq \lambda_N \mathcal{T}(f, f). \quad (3.23)$$

Proof. We use the form of the generator \mathcal{L} as in (1.8):

$$\mathcal{L} = -z^T M \nabla_z - \nabla_q \Phi(q) \cdot \nabla_p + \gamma T_L \partial_{p_1}^2 + \gamma T_R \partial_{p_N}^2$$

where Φ is the function that corresponds to the perturbing potentials. We write

$$2\mathcal{T}_2(f, f) = \mathcal{L}\mathcal{T}(f, f) - 2\mathcal{T}(f, \mathcal{L}f) = \mathcal{L}\mathcal{T}(f, f) - 2\nabla_z f^T b_N \nabla_z \mathcal{L}f - 2\nabla_z \mathcal{L}f^T b_N \nabla_z f.$$

About the $(-z^T M \nabla_z)$ -part of \mathcal{L} , the last equation of the above formula gives

$$2\nabla_z f^T b_N M \nabla_z f + 2\nabla_z f^T M^T b_N \nabla_z f.$$

Similarly, concerning the $(-\nabla_q \Phi(q) \cdot \nabla_p)$ -part of \mathcal{L} we get

$$\nabla_z f^T b_N \text{Hess}(\Phi)^T \nabla_z f + \nabla_z f^T \text{Hess}(\Phi) b_N \nabla_z f$$

and finally regarding the second order terms of the generator we end up with

$$\begin{aligned}
& 4\gamma T_L \nabla_z \partial_{p_1} f^T b_N \nabla_z \partial_{p_1} f + 2\gamma T_L \nabla_z \partial_{p_1}^2 f^T b_N \nabla_z f + 2\gamma T_L \nabla_z f^T b_N \nabla_z \partial_{p_1}^2 f \\
& \quad - 2\gamma T_L \nabla_z f^T b_N \nabla_z \partial_{p_1}^2 f - 2\gamma T_L \nabla_z \partial_{p_1}^2 f^T b_N \nabla_z f \\
& \quad + 4\gamma T_R \nabla_z \partial_{p_N} f^T b_N \nabla_z \partial_{p_N} f + 2\gamma T_R \nabla_z \partial_{p_N}^2 f^T b_N \nabla_z f + 2\gamma T_R \nabla_z f^T b_N \partial_{p_N}^2 \nabla_z f \\
& \quad - 2\gamma T_R \nabla_z f^T b_N \nabla_z \partial_{p_N}^2 f - 2\gamma T_R \nabla_z \partial_{p_N}^2 f^T b_N \nabla_z f.
\end{aligned}$$

We eventually write

$$\begin{aligned}
\mathcal{T}_2(f, f) &= \nabla_z f^T b_N M \nabla_z f + \nabla_z f^T M^T b_N \nabla_z f + \nabla_z f^T b_N \text{Hess}(\Phi)^T \nabla_z f \\
& \quad + \nabla_z f^T \text{Hess}(\Phi) b_N \nabla_z f + 2\gamma T_L \mathcal{T}(\partial_{p_1} f, \partial_{p_1} f) + 2\gamma T_R \mathcal{T}(\partial_{p_N} f, \partial_{p_N} f) \\
& \geq \nabla_z f^T (b_N M + M^T b_N) \nabla_z f + \nabla_z f^T b_N (\text{Hess}(U_{pin}^N) + \text{Hess}(U_{int}^N)) \nabla_z f \\
& \quad + \nabla_z f^T (\text{Hess}(U_{pin}^N) + \text{Hess}(U_{int}^N))^T b_N \nabla_z f \\
& = \nabla_z f^T (b_N M + M^T b_N) \nabla_z f + \nabla_z f^T (b_N \text{Hess}(U_{pin}^N) + \text{Hess}(U_{pin}^N)^T b_N) \nabla_z f \\
& \quad + \nabla_z f^T (b_N \text{Hess}(U_{int}^N) + \text{Hess}(U_{int}^N)^T b_N) \nabla_z f
\end{aligned}$$

where for the second inequality we used that the terms $\mathcal{T}(\partial_{p_i} f, \partial_{p_i} f)$ for $i = 1, N$, are positive. We write the second and third term of the last equation as

$$\begin{aligned}
\nabla_z f^T (b_N \text{Hess}(U_{pin}^N)) \nabla_z f &= \nabla_z f^T b_N^{1/2} b_N^{1/2} \text{Hess}(U_{pin}^N) b_N^{-1/2} b_N^{1/2} \nabla_z f \\
&= (b_N^{1/2} \nabla_z f)^T (b_N^{1/2} \text{Hess}(U_{pin}^N) b_N^{-1/2} (b_N^{1/2} \nabla_z f))
\end{aligned}$$

and then from the boundedness assumption on the operator norms of the Hessians for both perturbing potentials and the Lyapunov equation (1.10), we get the following

$$\begin{aligned}
\mathcal{T}_2(f, f) &\geq \nabla_z f \pi_N \nabla_z f^T - \|b_N^{1/2} \text{Hess}(U_{pin}^N) b_N^{-1/2}\|_2 \mathcal{T}(f, f) - \|b_N^{1/2} \text{Hess}(U_{int}^N) b_N^{-1/2}\|_2 \mathcal{T}(f, f) \\
&\geq \min(1, 2T_L, 2T_R) |\nabla_z f|^2 - \sup_z \|\text{Hess}(U_{pin}^N)(z)\|_2 \|b_N\|_2^{1/2} \|b_N^{-1}\|_2^{1/2} \mathcal{T}(f, f) - \\
&\quad - \sup_z \|\text{Hess}(U_{int}^N)(z)\|_2 \|b_N\|_2^{1/2} \|b_N^{-1}\|_2^{1/2} \mathcal{T}(f, f) \\
&\geq \min(1, 2T_R) \|b_N\|_2^{-1} \mathcal{T}(f, f) - (C_{pin}^N + C_{int}^N) \|b_N\|_2^{1/2} \|b_N^{-1}\|_2^{1/2} \mathcal{T}(f, f).
\end{aligned}$$

We conclude by gathering the terms. □

The assumption **(H2)** combined with the conclusion of the Proposition 1.1 ensures us that λ_N is positive, by choosing suitable pre-factors, as we do in the proofs of the main Theorems 1.4 and 1.6. We state now the following lemma that gives the 'twisted' gradient bound.

Lemma 3.3 (Gradient bound). *Under Assumption **(H2)**, for all $N \in \mathbb{N}$, $t \geq 0$, $(p, q) \in$*

\mathbb{R}^{2N} and $f \in C_c^\infty(\mathbb{R}^{2N})$, we have the following twisted gradient estimate

$$\mathcal{T}(P_t f, P_t f)(p, q) \leq e^{-2\lambda_N t} P_t(\mathcal{T}(f, f))(p, q) \quad (3.24)$$

for λ_N given by Proposition 3.2.

Proof. We shall first present a formal derivation of the estimate (3.24). If $\mathcal{T}(P_t f, P_t f)$ is compactly supported we consider the functional, for fixed $t > 0$, $(p, q) \in \mathbb{R}^{2N}$,

$$\Psi(s) = P_s(\mathcal{T}(P_{t-s} f, P_{t-s} f))(p, q), \quad s \in [0, t]$$

for $f \in C_c^\infty(\mathbb{R}^{2N})$. Since from the semigroup property we have

$$\frac{d}{ds} P_s = \mathcal{L} P_s = P_s \mathcal{L},$$

by differentiating and using the above inequality we get

$$\frac{d}{ds} \Psi(s) = 2P_s(\mathcal{T}_2(P_{t-s} f, P_{t-s} f)) \geq 2\lambda_N P_s(\mathcal{T}(P_{t-s} f, P_{t-s} f)) = 2\lambda_N \Psi(s)$$

and since $\Psi(0) = \mathcal{T}(P_t f, P_t f)$, $\Psi(t) = P_t(\mathcal{T}(f, f))$, by Grönwall's lemma we get the desired inequality for every smooth and bounded function f .

In general we need $\mathcal{T}(P_t f, P_t f)$ to belong in $L^\infty(\mathbb{R}^{2N})$ because then we know that $P_s(\mathcal{T}(P_{t-s} f, P_{t-s} f))$ is well defined. So we do the following:

First we take $W(p, q) = 1 + |p|^2 + |q|^2$ as a Lyapunov structure that satisfies the following conditions: $W > 1$, $\mathcal{L}W \leq CW$, the sets $\{W \leq m\}$ are compact for each m , and $\mathcal{T}(W) \leq CW^2$. This W satisfy the conditions thanks to the bounded-Hessians assumption, *i.e.* $|\nabla(U_{int}^N + U_{pin}^N)|$ will be Lipschitz. In particular, for the inequality $\mathcal{L}W \leq CW$ using Cauchy-Schwarz and Young's inequalities, we write

$$\begin{aligned} \mathcal{L}W &= 2p \cdot q - 2q \cdot Bp - 2p \cdot \nabla_q \Phi - 2\gamma_1 p_1^2 - 2\gamma_N p_N^2 + 2T_L \gamma_1 + 2T_R \gamma_N \\ &\leq 2|p||q| + 2|Bq||p| + 2|\nabla_q \Phi||p| + 2T_L \gamma_1 + 2T_R \gamma_N \\ &\leq |p|^2 + |q|^2 + C_{C_{ip}, \|B\|_2}(|p|^2 + |q|^2) + 2T_L \gamma_1 + 2T_R \gamma_N \\ &\leq \max\{\max(1, C_{C_{ip}, \|B\|_2}), 2T_L \gamma_1 + 2T_R \gamma_N\}(1 + |p|^2 + |q|^2) = C_1 W \end{aligned}$$

while the inequality $\mathcal{T}(W) \leq C_2 W^2$ obviously holds. So we end up with the same constant by choosing $C := \max\{C_1, C_2\}$.

Now using the function W combined with a localization argument as in the work

by F.Y. Wang [Wan, Lemma 2.1] or [Bau, Theorem 2.2] we prove the boundedness of $\mathcal{T}(P_t f, P_t f)$. For this we approximate the generator \mathcal{L}_n with truncated operators so that the approximating diffusion processes remain in compact sets. Consider $h \in C_c^\infty([0, \infty))$ decreasing such that $h|_{[0,1]} = 1$ and $h|_{[2,\infty)} = 0$ and define

$$h_n = h(W/n) \quad \text{and} \quad \mathcal{L}_n = h_n^2 \mathcal{L}.$$

Then \mathcal{L}_n has compact support in $K_n := \{W \leq 2n\}$, in the sense that it is 0 outside of it, due to the definition of h_n . Let P_t^n be the semigroup generated by \mathcal{L}_n , which is given as the unique bounded solution of

$$\mathcal{L}_n P_t^n f = \partial_t P_t^n f \quad \text{for } f \in L^\infty(\mathbb{R}^{2N}).$$

Then we also have that for every bounded $f \in L^\infty(\mathbb{R}^{2N})$, pointwise

$$P_t^n f \xrightarrow{n \rightarrow \infty} P_t f.$$

We do the 'interpolation semigroup argument' as before for \mathcal{L}_n and for $f \in C_c^\infty(\mathbb{R}^{2N})$ supported in $\{W \leq n\}$. Define

$$\Psi_n(s) = P_s^n(\mathcal{T}(P_{t-s}^n f, P_{t-s}^n f))(p, q), \quad s \in [0, t]$$

for fixed $t > 0$, $n \geq 1$ applied to a fixed point (p, q) in the support inside the set $\{W \leq n\}$. It is true, due to the properties of W , that $\mathcal{T}(P_t^n f, P_t^n f) \leq C_{f,t}$ with $C_{f,t}$ independent of n and so we have a bound on $\mathcal{T}(P_t^n f, P_t^n f)$ uniformly on the set $\{W \leq n\}$. Indeed

$$\begin{aligned} \Psi_n'(s) &= P_s^n(\mathcal{L}_n \mathcal{T}(P_{t-s}^n f, P_{t-s}^n f) - 2\mathcal{T}(\mathcal{L}_n P_{t-s}^n f, P_{t-s}^n f)) \\ &= P_s^n(2h_n^2 \mathcal{T}_2(P_{t-s}^n f, P_{t-s}^n f) - 4h_n \mathcal{L} P_{t-s}^n f \mathcal{T}(h_n, P_{t-s}^n f)) \\ &\geq P_s^n(2h_n^2 \lambda_N \mathcal{T}(P_{t-s}^n f, P_{t-s}^n f) - 4h_n \mathcal{L} P_{t-s}^n f \mathcal{T}(h_n, P_{t-s}^n f)) \\ &\geq P_s^n(2h_n^2 \lambda_N \mathcal{T}(P_{t-s}^n f, P_{t-s}^n f) - 4P_{t-s}^n \mathcal{L} f \mathcal{T}(\log h_n, P_{t-s}^n f)) \\ &\geq P_s^n(2h_n^2 \lambda_N \mathcal{T}(P_{t-s}^n f, P_{t-s}^n f) - 4\|\mathcal{L} f\|_\infty \sqrt{\mathcal{T}(\log h_n, \log h_n)} \sqrt{\mathcal{T}(P_{t-s}^n f, P_{t-s}^n f)}) \\ &\stackrel{\text{Young's ineq.}}{\geq} P_s^n(- (2|\lambda_N| + 2)\mathcal{T}(P_{t-s}^n f, P_{t-s}^n f) - C_1 \mathcal{T}(\log h_n, \log h_n)) \end{aligned}$$

with C_1 constant independent of n . About the last term:

$$\mathcal{T}(\log h_n, \log h_n) = -\frac{1}{n^2 h_n^2} h'(W/n)^2 \mathcal{T}(W) \leq \frac{C}{h_n^2}$$

with C independent of n . Now calculate

$$\mathcal{L}_n \left(\frac{1}{h_n^2} \right) = -\frac{2h'(W/n)\mathcal{L}W}{nh_n} - \frac{2h''(W/n)\Gamma(W)}{n^2h_n} + \frac{6h'(W/n)^2\Gamma(W)}{n^2h_n^2} \leq \frac{C_2}{h_n^2}$$

with $C_2 > 0$ some constant again independent of n (from the assumptions on the Lyapunov functional W). Therefore

$$P_s^n \left(\frac{1}{h_n^2} \right) \leq \frac{e^{sc_2}}{h_n^2}.$$

Combining this last estimate with the above bounds we end up with the differential inequality

$$\Psi_n'(s) \geq -(2|\lambda_N| + 2)\Psi_n(s) - C_3$$

and $C_3 = C_3(f, t)$ is again independent of n . We multiply both sides with $e^{(2|\lambda_N|+2)s}$ so that the above inequality implies

$$(e^{(2|\lambda_N|+2)s}\Psi_n(s))' \geq -C_3e^{(2|\lambda_N|+2)s}$$

or equivalently, after integrating both sides in time from 0 to t , that

$$\Psi_n(0) \leq e^{(2|\lambda_N|+2)t}\Psi_n(t) + \bar{C}_3(f, t) \leq e^{(2|\lambda_N|+2)t}\|\mathcal{T}(f, f)\|_\infty + \bar{C}_3(f, t)$$

which gives the boundedness of $\mathcal{T}(P_t^n f, P_t^n f) = \Psi_n(0)$ uniformly in n , on the set $\{W \leq n\}$. Now if d' is the intrinsic distance induced by \mathcal{T}

$$d'(x, y) = \sup_{\mathcal{T}(f, f) \leq 1} |f(x) - f(y)|,$$

from the above bound we have that

$$|P_t^n f(x) - P_t^n f(y)| \leq Cd'(x, y)$$

for n large enough with $x, y \in \{W \leq n\}$ and $f \in C_c^\infty(\mathbb{R}^{2N})$ with support in $\{W \leq n\}$. This comes from the formula

$$P_t^n f(y) - P_t^n f(x) = \int_0^1 \nabla P_t^n f(x + t(y-x)) \cdot (y-x) dt.$$

Now C does not depend on n (from before), so passing to the limit we have

$$|P_t f(x) - P_t f(y)| \leq Cd'(x, y)$$

and so $\mathcal{T}(P_t f, P_t f)$ is also bounded. Now we can repeat the standard Bakry-Emery calculations as in the beginning of the proof. \square

Remark 3.4. Note that using the equivalence of \mathcal{T} and $|\nabla_z|^2$:

$$\frac{1}{\|b_N^{-1}\|_2} |\nabla_z f|^2 \leq \mathcal{T}(f, f) \leq \|b_N\|_2 |\nabla_z f|^2,$$

we get the following L^2 - gradient estimate

$$|\nabla_z P_t f|^2 \leq \|b_N\|_2 \|b_N^{-1}\|_2 e^{-2\lambda_N t} P_t(|\nabla_z f|^2) \quad (3.25)$$

Once we have a curvature condition of the form (3.23) we are also able to show that the stationary measure satisfies a Poincaré inequality.

Proposition 3.5. Let \mathcal{L} be the generator of the dynamics described by the SDEs (1.1) and \mathcal{T} the perturbed quadratic form defined in (3.20). Under Assumption **(H2)**, for all $N \in \mathbb{N}$, if $f \in C^\infty(\mathbb{R}^{2N})$, invariant measure μ satisfies a Poincaré inequality

$$\text{Var}_\mu(f) \leq C_N \int_{\mathbb{R}^{2N}} \mathcal{T}(f, f) d\mu.$$

where $C_N = \frac{\gamma T_L \|b_N^{-1}\|_2}{\lambda_N}$, with λ_N defined in Proposition 3.2.

Proof. For $f \in C^\infty(\mathbb{R}^{2N})$, we consider the functional

$$\Psi(s) = P_s((P_{t-s}f)^2), \quad s \in [0, t].$$

We denote by Γ the *Carré du Champ* operator defined in (2.16). By differentiating we have

$$\Psi'(s) = \mathcal{L}P_s((P_{t-s}f)^2) - 2P_s(P_{t-s}f \mathcal{L}P_{t-s}f) = 2P_s(\Gamma(P_{t-s}f, P_{t-s}f)).$$

Now by integrating from 0 to t

$$\begin{aligned} P_t(f^2) - (P_t f)^2 &= 2 \int_0^t P_s(\Gamma(P_{t-s}f, P_{t-s}f)) ds \leq 2\gamma T_L \int_0^t P_s(|\nabla P_{t-s}f|^2) ds \\ &\leq 2\gamma T_L \|b_N^{-1}\|_2 \int_0^t P_s(\mathcal{T}(P_{t-s}f, P_{t-s}f)) ds \\ &\leq 2\gamma T_L \|b_N^{-1}\|_2 \int_0^t P_s(e^{-2\lambda_N(t-s)} P_{t-s} \mathcal{T}(f, f)) ds \\ &= 2\gamma T_L \|b_N^{-1}\|_2 e^{-2\lambda_N t} P_t \mathcal{T}(f, f) \int_0^t e^{2\lambda_N s} ds \\ &= 2\gamma T_L \|b_N^{-1}\|_2 e^{-2\lambda_N t} P_t \mathcal{T}(f, f) \left(\frac{e^{2\lambda_N t} - 1}{2\lambda_N} \right) \end{aligned}$$

where in the first inequality we used that

$$\Gamma(f, f) = \gamma T_L (\partial_{p_1} f)^2 + \gamma T_R (\partial_{p_N} f)^2 \leq \gamma T_L |\nabla f|^2,$$

for the second we used the gradient bound from Lemma 3.3 and just right after that, the semigroup property. The last line can be rewritten like

$$P_t(f^2) - (P_t f)^2 = \gamma T_L \|b_N^{-1}\|_2 \frac{1 - e^{-2\lambda_N t}}{\lambda_N} P_t \mathcal{T}(f, f).$$

Now letting t to go to ∞ , thanks to the ergodicity, we have the desired inequality. \square

In fact it is possible to show a stronger pointwise gradient bound, that we exploit for the proof of a Log-Sobolev inequality for the invariant measure of the dynamics.

Proposition 3.6 (Strong gradient bound). *For $f \in C_c^\infty(\mathbb{R}^{2N})$, $\forall t \geq 0$ and $(p, q) \in \mathbb{R}^{2N}$*

$$\mathcal{T}(P_t f, P_t f)(p, q) \leq \left(P_t(\sqrt{\mathcal{T}(f, f)}) \right)^2(p, q) e^{-2\lambda_N t}. \quad (3.26)$$

Remark 3.7. *This is a better estimate than (3.24) in Lemma 3.3 because of Cauchy-Schwarz inequality.*

Proof. The rigorous justification, *i.e.* boundedness of $\sqrt{\mathcal{T}(P_{t-s} f, P_{t-s} f)}$, of the following formal calculations is exactly like in the proof of Lemma 3.3.

Here for $f \in C_c^\infty(\mathbb{R}^{2N})$, and for fixed $t \geq 0$, $(p, q) \in \mathbb{R}^{2N}$, instead we define

$$\Phi(s) = P_s \left(\sqrt{\mathcal{T}(P_{t-s} f, P_{t-s} f)} \right)(p, q), \quad s \in [0, t].$$

We denote by $g = P_{t-s}f$, we differentiate and perform the standard calculations we have

$$\begin{aligned}
\Phi'(s) &= P_s \left(\mathcal{L}(\sqrt{\mathcal{T}(g, g)}) - \frac{\nabla \mathcal{L} g^T b_N \nabla g + \nabla g^T b_N \nabla \mathcal{L} g}{2\sqrt{\mathcal{T}(g, g)}} \right) \\
&= P_s \left(\mathcal{L}(\sqrt{\mathcal{T}(g, g)}) + \frac{2\mathcal{T}_2(g, g) - \mathcal{L}\mathcal{T}(g, g)}{2\sqrt{\mathcal{T}(g, g)}} \right) \\
&= P_s \left(\frac{1}{\sqrt{\mathcal{T}(g, g)}} \left(-\Gamma(\sqrt{\mathcal{T}(g, g)}, \sqrt{\mathcal{T}(g, g)}) + \mathcal{T}_2(g, g) \right) \right) \\
&= P_s \left(\frac{1}{\sqrt{\mathcal{T}(g, g)}} \left(\mathcal{T}_2(g, g) - \frac{2\gamma T_L(\mathcal{T}(\partial_{p_1}g, \partial_{p_1}g))^2 + 2\gamma T_R(\mathcal{T}(\partial_{p_N}g, \partial_{p_N}g))^2}{4\mathcal{T}(g, g)} \right) \right) \\
&\geq P_s \left(\frac{1}{4\mathcal{T}(g, g)^{3/2}} \left(4\lambda_N(\mathcal{T}(g, g))^2 + 4\gamma T_L(\mathcal{T}(\partial_{p_1}g))^2 \right. \right. \\
&\quad \left. \left. + 4\gamma T_R(\mathcal{T}(\partial_{p_N}g))^2 - 2\gamma T_L(\partial_{p_1}\mathcal{T}(g, g))^2 - 2\gamma T_R(\partial_{p_N}\mathcal{T}(g, g))^2 \right) \right) \\
&\geq P_s \left(\frac{4\lambda_N(\mathcal{T}(g, g))^2}{4\mathcal{T}(g, g)^{3/2}} \right) = \lambda_N \Phi(s)
\end{aligned}$$

where in the first equality we used that

$$\mathcal{L}(g) = \frac{\mathcal{L}(g^2)}{2g} - \frac{\Gamma(g, g)}{g}.$$

In the first inequality we used the formula

$$\mathcal{T}_2(f, f) \geq \lambda_N \mathcal{T}(f, f) + \gamma T_L \mathcal{T}(\partial_{p_1}f, \partial_{p_1}f) + \gamma T_R \mathcal{T}(\partial_{p_N}f, \partial_{p_N}f)$$

from the proof of Proposition 3.2, that

$$\Gamma(f, g) = \gamma T_L(\partial_{p_1}f)(\partial_{p_1}g) + \gamma T_R(\partial_{p_N}f)(\partial_{p_N}g)$$

where Γ is the *Carré du Champ* operator defined in (2.16), and that \mathcal{T} and ∂_{p_1} obviously commute. Now from Grönwall's lemma we get

$$\Phi(t) \geq e^{\lambda_N t} \Phi(0) \Rightarrow \mathcal{T}(P_t f, P_t f) \leq e^{-2\lambda_N t} \left(P_t(\sqrt{\mathcal{T}(f, f)}) \right)^2.$$

□

This pointwise, strong gradient bound implies a Log-Sobolev inequality.

Proof of Proposition 1.5. For $f \in C_c^\infty(\mathbb{R}^{2N})$, we introduce the functional

$$H(s) = P_s \left(P_{t-s}f \log P_{t-s}f \right)$$

for fixed $s \in [0, t]$ evaluated at a fixed point in the phase space. We denote by Γ the *Carré du Champ* operator defined in (2.16) and following again Bakry's recipes, we get

$$\begin{aligned}
H'(s) &= P_s \left(\mathcal{L}(P_{t-s}f \log P_{t-s}f) - \mathcal{L}P_{t-s}f \log P_{t-s}f - \mathcal{L}(P_{t-s}f) \right) \\
&= P_s \left(\Gamma(P_{t-s}f, \log P_{t-s}f) \right) \\
&= P_s \left(\frac{\gamma T_L (\partial_{p_1} P_{t-s}f)^2}{P_{t-s}f} + \frac{\gamma T_R (\partial_{p_N} P_{t-s}f)^2}{P_{t-s}f} \right) \\
&= P_s \left(\frac{\Gamma(P_{t-s}f, P_{t-s}f)}{P_{t-s}f} \right) \\
&\leq \gamma T_L \|b_N^{-1}\|_2 P_s \left(\frac{\mathcal{T}(P_{t-s}f, P_{t-s}f)}{P_{t-s}f} \right) \\
&\leq \gamma T_L \|b_N^{-1}\|_2 P_s \left(e^{-2\lambda_N(t-s)} \frac{(P_{t-s}(\sqrt{\mathcal{T}(f, f)}))^2}{P_{t-s}f} \right) \\
&\leq \gamma T_L \|b_N^{-1}\|_2 P_t \left(\frac{\mathcal{T}(f, f)}{f} \right) e^{-2\lambda_N(t-s)}
\end{aligned}$$

where for the second inequality we used the bound from Proposition 3.6, while for the last inequality we applied Jensen's and the fact that the function y^2/x is convex for x, y positive. Now integrating from 0 to t , we get

$$\begin{aligned}
H(t) - H(0) &\leq \frac{\gamma T_L \|b_N^{-1}\|_2}{2\lambda_N} (1 - e^{-2\lambda_N t}) P_t \left(\frac{\mathcal{T}(f, f)}{f} \right) \\
&\leq \frac{\gamma T_L \|b_N^{-1}\|_2 \|b_N\|_2}{2\lambda_N} (1 - e^{-2\lambda_N t}) P_t \left(\frac{|\nabla_z f|^2}{f} \right)
\end{aligned}$$

Letting $t \rightarrow \infty$ and thanks to the ergodicity of the semigroup, we get the LSI with constant $\frac{\gamma T_L \|b_N^{-1}\|_2 \|b_N\|_2}{2\lambda_N}$ corresponding to the constant with the non-perturbed Fischer information. Therefore, applying the estimates from Proposition 1.1 we have

$$\begin{aligned}
\frac{\gamma T_L \|b_N^{-1}\|_2}{2\lambda_N} &= \frac{\gamma T_L \|b_N^{-1}\|_2}{2 \left(\min(1, 2T_R) \|b_N\|_2^{-1} - (C_{pin}^N + C_{int}^N) \|b_N\|_2^{1/2} \|b_N^{-1}\|_2^{1/2} \right)} \\
&\leq \frac{\gamma T_L C_{a,c}}{N^{-3} (\min(1, 2T_R) C_{a,c}^{-1} - C_0 C_{a,c})} := \lambda_0^{-1} \gamma T_L C_{a,c} N^3
\end{aligned}$$

where C_0 is the constant in (1.5) which we choose small enough, *i.e.* to satisfy

$$C_0 < \min(1, 2T_R) C_{a,c}^{-2},$$

so that $\lambda_0 > 0$. □

2.4 Convergence to equilibrium in Kantorovich-Wasserstein distance

We use that the gradient estimate (3.25) is equivalent to an estimate in Wasserstein distance (Kuwada's duality, [Kuw10]). More specifically, we have the following Theorem, here stated only in the Euclidean space with the Lebesgue measure $(\mathbb{R}^{2N}, |\cdot|, \lambda)$ and only for the Wasserstein-2 distance:

Theorem 4.1 (Theorem 2.2 of [Kuw10]). *Let a Markov semigroup P on \mathbb{R}^{2N} , that has a continuous density with respect to the Lebesgue measure. For $c > 0$, the following are equivalent:*

(i) *For all probability measures μ, ν we have,*

$$W_2(P_t^* \mu, P_t^* \nu) \leq c W_2(\mu, \nu).$$

(ii) *For all bounded and Lipschitz functions f and $z \in \mathbb{R}^{2N}$,*

$$|\nabla P_t f|(z) \leq c P_t(|\nabla f|^2)(z)^{1/2}$$

where this estimate is associated with the Lipschitz norm defined just above.

Now we are ready to prove Theorem 1.4.

Proof of Theorem 1.4. The convergence follows if we apply Kuwada's duality from Theorem 4.1 since we have the estimate (3.25) with $c = \|b_N^{-1}\|_2^{1/2} \|b_N\|_2^{1/2}$. Therefore the contraction reads

$$W_2(P_t^* f_0^1, P_t^* f_0^2) \leq \|b_N\|_2^{1/2} \|b_N^{-1}\|_2^{1/2} e^{-\lambda_N t} W_2(f_0^1, f_0^2). \quad (4.27)$$

Since λ_N , as defined in (3.22), is:

$$\lambda_N = \min(1, 2T_R) \|b_N\|_2^{-1} - (C_{pin}^N + C_{int}^N) \|b_N\|_2^{1/2} \|b_N^{-1}\|_2^{1/2},$$

by exploiting the estimates on $\|b_N\|_2$ and $\|b_N^{-1}\|_2$ from the Proposition 1.1 we quantify the rate:

$$\lambda_N \geq \min(1, 2T_R) C_{a,c}^{-1} N^{-3} - C_0 N^{-9/2} C_{a,c} N^{3/2} = (\min(1, 2T_R) C_{a,c}^{-1} - C_0 C_{a,c}) N^{-3} := \lambda_0 N^{-3}$$

Choosing $C_0 < \min(1, 2T_R) C_{a,c}^{-2}$ gives us $\lambda_N > 0$ for all N . This gives us the statement of

the Theorem:

$$W_2(P_t^* f_0^1, P_t^* f_0^2) \leq C_{a,c} N^{\frac{3}{2}} e^{-\frac{\lambda_0}{N^3} t} W_2(f_0^1, f_0^2). \quad (4.28)$$

Finally, for the uniqueness of the stationary solution f_∞ , we see that all the solutions f_t will converge towards it if we make the choice $f_0^2 = f_\infty$. \square

2.5 Entropic Convergence to equilibrium

If μ is the invariant measure of the system, we prove here convergence to the stationary state in Entropy as stated in Theorem 1.6: first with respect to the functional

$$\mathcal{E}(f) := \int_{\mathbb{R}^{2N}} f \log f + f \mathcal{T}(\log f, \log f) d\mu$$

and then using the equivalence of $\mathcal{T}(f, f)$ with $|\nabla f|^2$.

Proof of Theorem 1.6. We consider the functional

$$\Lambda(s) = P_s \left(P_{t-s} f \log P_{t-s} f \right) + P_s \left(P_{t-s} f \mathcal{T}(\log P_{t-s} f, \log P_{t-s} f) \right)$$

and by differentiating and repeating similarly the steps from the Propositions 3.6 and 1.5 we end up with

$$\begin{aligned} \Lambda'(s) &= P_s \left(\Gamma(P_{t-s} f, \log P_{t-s} f) \right) + P_s \mathcal{L} \left(P_{t-s} f \mathcal{T}(\log P_{t-s} f, \log P_{t-s} f) \right) \\ &\quad - 2P_s \left(P_{t-s} f \mathcal{T} \left(\log P_{t-s} f, \frac{\mathcal{L} P_{t-s} f}{P_{t-s} f} \right) \right) - P_s \left(\mathcal{L} P_{t-s} f \mathcal{T}(\log P_{t-s} f, \log P_{t-s} f) \right) \\ &\geq P_s \left(P_{t-s} f \mathcal{L} \mathcal{T}(\log P_{t-s} f) \right) + 2P_s \left(\Gamma(P_{t-s} f, \mathcal{T}(\log P_{t-s} f, \log P_{t-s} f)) \right) \\ &\quad - 2P_s \left(P_{t-s} f \mathcal{T}(\log P_{t-s} f, \Gamma(\log P_{t-s} f, \log P_{t-s} f) + \mathcal{L}(\log P_{t-s} f)) \right) \\ &= 2P_s \left(P_{t-s} f \mathcal{T}_2(\log P_{t-s} f, \log P_{t-s} f) \right) \\ &\geq 2\lambda_N P_s \left(P_{t-s} f \mathcal{T}(\log P_{t-s} f, \log P_{t-s} f) \right) \end{aligned}$$

where we have used that for the second inequality

$$\begin{aligned} \Gamma(P_{t-s} f, \log P_{t-s} f) &\geq 0, \quad \mathcal{L}(\log P_{t-s} f) = \frac{\mathcal{L} P_{t-s} f}{P_{t-s} f} - \Gamma(\log P_{t-s} f, \log P_{t-s} f) \text{ and} \\ \mathcal{T}(\log P_{t-s} f, \Gamma(\log P_{t-s} f, \log P_{t-s} f)) &= \Gamma(\log P_{t-s} f, \mathcal{T}(\log P_{t-s} f, \log P_{t-s} f)) \end{aligned}$$

and in the last inequality we used the bound (3.23). We introduce a constant η on which we will optimize later, we integrate against the invariant measure μ and we apply the

Log-Sobolev inequality from Proposition 1.5:

$$\begin{aligned} \int_{\mathbb{R}^{2N}} \Lambda'(s) d\mu &\geq 2\eta \frac{\lambda_N}{C_N} \int_{\mathbb{R}^{2N}} P_s \left(P_{t-s} f \log P_{t-s} f \right) d\mu \\ &\quad + 2(1-\eta) \lambda_N \int_{\mathbb{R}^{2N}} P_s \left(\mathcal{T}(\log P_{t-s} f, \log P_{t-s} f) P_{t-s} f \right) d\mu \\ &\geq 2\lambda_N \min \left(\frac{\eta}{C_N}, 1-\eta \right) \int_{\mathbb{R}^{2N}} \Lambda(s) d\mu \end{aligned}$$

since $\int_{\mathbb{R}^{2N}} P_s \left(P_{t-s} f \log P_{t-s} f \right) d\mu = \int_{\mathbb{R}^{2N}} P_s \left(P_{t-s} f \log P_{t-s} f - P_{t-s} f + 1 \right) d\mu$ which is non-negative. For $\eta := \frac{C_N}{1+C_N}$ we have

$$\int_{\mathbb{R}^{2N}} \Lambda'(s) d\mu \geq 2\lambda_N \frac{C_N}{1+C_N} \int_{\mathbb{R}^{2N}} \Lambda(s) d\mu.$$

Finally, from Grönwall's inequality we have

$$\int \Lambda(0) d\mu \leq e^{-2\lambda_N \frac{C_N}{1+C_N} t} \int \Lambda(t) d\mu$$

or equivalently the desired convergence, thanks to the invariance of the measure. Since $\lim_{N \rightarrow \infty} \lambda_N \frac{C_N}{1+C_N} = \lim_{N \rightarrow \infty} \lambda_N$, we have that the exponential rate is indeed of order λ_N (as in the convergence in Theorem 1.4):

$$\mathcal{E}(P_t f) \leq e^{-\lambda_N t} \mathcal{E}(f) \quad (5.29)$$

Since \mathcal{T} and $|\nabla_z|^2$ are equivalent, see (3.21), we get the above convergence in the non-perturbed setting with equivalence-constant $\max(1, \|b_N^{-1}\|_2) \|b_N\|_2$.

In particular, both the Boltzmann entropy $H_\mu(P_t f \mu)$, given by (1.13), and the Fisher information $I_\mu(P_t f \mu)$, given by (1.14), decay:

$$H_\mu(P_t f \mu) + I_\mu(P_t f \mu) \leq \frac{\max(1, \|b_N\|_2)}{\min(1, \|b_N^{-1}\|_2^{-1})} e^{-\lambda_N t} \left(H_\mu(f \mu) + I_\mu(f \mu) \right) \quad (5.30)$$

Thus, combining with the conclusion of Proposition 1.1, the denominator is of order 1 with the dimension, and, as in the proof of Theorem 1.4, $\lambda_N \geq \lambda_0 N^{-3}$ and we conclude. \square

Remark 5.1. (i) *The rate of the convergence to the stationary state, λ_N , does not depend on the difference of the temperatures ΔT : under the assumption **(H2)** we get existence of spectral gap for all ΔT , since the twisted curvature condition from Proposition 3.2 sees only the first order terms of the generator. The scaling of λ_N relies on the result of the Proposition 1.1 and we can see through its proof that it is not affected by ΔT . Therefore, the same scaling holds in the equilibrium case $\Delta T = 0$ as well.*

- (ii) Regarding the boundary conditions: Assumption **(H1)** is not necessary in order to obtain existence of a spectral gap with a lower bound N^{-3} when the chain is pinned. In fact, we have spectral gap as soon as there is a solution to the matrix equation (1.10). This requires (see Proposition 3.1) M to be positively stable. Therefore, the proof of Proposition 1.1 still holds, with minor differences, when we consider the following b.c. as well (free in a sense): $q_0 = q_1$, $q_N = q_{N+1}$ with $a > 0$. See also in the next chapter the first item of Prop. 2.2.
- (iii) A comment on the choice of Π_N : We have the curvature condition from Proposition 3.2 by considering any positive definite r.h.s. of (1.10). We choose specifically π_N , since then we can compare b_N to b_0 that solves (2.19) (b_0 is the covariance matrix for the harmonic chain) and then we bound $\|b_N^{-1}\|_2$. See the end of proof of the Proposition 1.1.
- (iv) A convergence to equilibrium in total variation norm for a similar small perturbation of the harmonic oscillator chain, has been shown recently in [Raq19]. There, a version of Harris' ergodic Theorem was applied making it possible to treat more general cases of the oscillator chain with different kind of noises, as well. However, this is a non-quantitative version of Harris' Theorem, which provides no information on the dependency of the convergence rate in N .

2.6 Estimates on the spectral norm of b_N

First, let us state the following Proposition on the optimal exponential rate of convergence for the *purely harmonic chain*.

Proposition 6.1 (Proposition 7.1 and 7.2 (3) in [BM22]). *We write λ_N^H for the spectral gap of the dynamics which evolution is described by the generator (1.8), without the perturbing potentials, i.e. dynamics of the linear chain, and $\rho := \inf\{Re(\mu) : \mu \in \sigma(M)\}$. We have*

$$\lim_{N \rightarrow \infty} \frac{\lambda_N^H}{\rho} \in \mathbb{R}.$$

Moreover the spectral gap approaches 0 as N goes to infinity as follows:

$$\rho \leq \frac{C}{2N} \tag{6.31}$$

for some constant C independent of N .

Proof. We exploit the results by Arnold and Erb in [AE] or by Monmarché in [Mon19,

Proposition 13]: working with an operator of the form

$$Lf(x) = -(M^T x) \cdot \nabla_x f(x) + \operatorname{div}(\mathfrak{F}\Theta \nabla_x f)(x)$$

under the conditions that (i) no non-trivial subspace of $\operatorname{Ker}(\mathfrak{F}\Theta)$ is invariant under M and (ii) the matrix M is positively stable, *i.e.* all the eigenvalues have real part greater than 0, then the associated semigroup has a unique invariant measure and if $\rho > 0$, then for the exponential rate λ_N^H of the above Ornstein-Uhlenbeck process we have

$$\rho - \epsilon \leq \lambda_N^H \leq \rho$$

for every $\epsilon \in (0, \rho)$. Fix such an $\epsilon > 0$ and conclude the first statement of the Proposition. In particular, when m is the maximal dimension of the Jordan block of M corresponding to the eigenvalue λ such that $\operatorname{Re}(\lambda) = \rho$, the quantity $(1 + t^{2(m-1)})e^{-2\rho t}$ is the optimal one regarding the long time behaviour, [Mon19]. This implies that the spectral gap of the generator is $\rho - \epsilon$, whereas the constant in front of the exponential is

$$c(\epsilon, m) := \sup_t (1 + t^{2(m-1)})e^{-2\epsilon t}.$$

The harmonic chain satisfies the conditions (i) and (ii): the first condition is equivalent to the hypoellipticity of the operator L , [Hö7, Section 1], and our generator (1.8) is indeed hypoelliptic: it is proven, [EPRB99b, Section 3, page 667] and [Car07, Section 3], for more general classes of potentials than the quadratic ones, that the generator satisfies the rank condition of Hörmander's hypoellipticity Theorem, [Hö7b, Theorem 22.2.1]. Also the matrix M is stable for every N , *i.e.* $\operatorname{Re}(\lambda) > 0$ for all the eigenvalues λ , see [JPS17, Lemma 5.1].

For the second conclusion of the Proposition, we recall that the matrix M is given by (1.9) and we write,

$$2\gamma = \operatorname{Tr}(\mathfrak{F}) = \operatorname{Re}(\operatorname{Tr}(\mathfrak{F})) = \operatorname{Re}(\operatorname{Tr}(M)) = \sum_{\lambda \in \sigma(M)} \operatorname{Re}(\lambda).$$

In the r.h.s. we have a sum of $2N$ (counting multiplicity) positive terms, since $\inf\{\operatorname{Re}(\lambda)\}$ is strictly positive, [JPS17, Lemma 5.1(2)]. Now note that the $\operatorname{Tr}(\mathfrak{F})$ does not depend on the number of oscillators, so the r.h.s. of the above displayed equation should be uniformly bounded in N . Since

$$\sum_{\lambda \in \sigma(M)} \operatorname{Re}(\lambda) \geq 2N \inf\{\operatorname{Re}(\lambda) : \lambda \in \sigma(M)\}$$

we have that $2N \inf\{\operatorname{Re}(\lambda) : \lambda \in \sigma(M)\}$ is bounded asymptotically with N , which implies

the second part of the statement. \square

Remark 6.2. B can be seen as the Schrödinger operator : $B = -c \Delta^N + \sum_{i=1}^N a\delta_i$ where $c > 0$, Δ^N is the Dirichlet Laplacian on $l^2(\{1, \dots, N\})$ and δ_i the projection on the i -th coordinate. We give the following definition for the (discrete) Laplacian on $l^2(\{1, \dots, N\})$ with Dirichlet boundary conditions:

$$-\Delta^N := \sum_{i=1}^{N-1} L^{i,i+1}$$

where $L^{i,i+1}$ are uniquely determined by the quadratic form

$$\begin{aligned} \langle u, L^{i,i+1}u \rangle &= (u(i) - u(i+1))^2 \quad \text{with} \\ u(0) &= u(N+1) = 0 \quad \text{Dirichlet b.c.} \end{aligned}$$

We will use this information in the last part of the proof of Proposition 1.1, to bound the spectral norm of the inverse, $\|b_N^{-1}\|_2$.

The rest of this section is devoted to the study of the solution of the matrix equation (1.10). Note that [RLL67, RS19] are two other cases where a Lyapunov equation is explicitly solved in order to study the thermal transport in atom harmonic chains. The right hand side of the equation in the two above-mentioned cases is much simpler though, therefore it is easier to provide an analytical formula which represents the unique solution as in [RS19].

Here we split the $2N \times 2N$ dimensional problem into 4 equal-sized blocks of dimension $N \times N$. Then we exploit all the information we get about each block from the following Lemma (6.3). In order to ease the readability of the proof we split it into several lemmas until the end of the section.

2.6.1 Matrix equations on Lyapunov equation

Lemma 6.3. For $0 \leq m \leq N$, we have the following equations for the blocks x_m, y_m and z_m of the matrix b_m :

$$-z_m = z_m^T + \tilde{J}_m \tag{6.32}$$

$$x_m = By_m + \mathfrak{F}z_m \tag{6.33}$$

$$-Bz_m + z_m B - B\tilde{J}_m = J_m^{(\Delta T)} - x_m \mathfrak{F} - \mathfrak{F}x_m \tag{6.34}$$

$$y_m B - By_m = \mathfrak{F} + z_m \mathfrak{F} + \mathfrak{F}z_m \quad \text{for } m \geq 1 \tag{6.35}$$

$$y_m B - By_m = z_m \mathfrak{F} + \mathfrak{F}z_m \quad \text{for } m = 0 \tag{6.36}$$

Here $\tilde{J}_m = \text{diag}(1, 1, \dots, 1, 0, \dots, 0, 1, 1, \dots, 1)$ where the 0's start at $(m+1, m+1)$ -entry and stop at $(N-(m+1), N-(m+1))$ -entry, and $J_m^{(\Delta T)} = \text{diag}(2T_L, 1, \dots, 1, 0, \dots, 0, 1, \dots, 1, 2T_R)$ where the 0's start at $(m+2, m+2)$ -entry and stop at $(N-(m+2), N-(m+2))$ -entry.

Proof. We consider m s.t. $0 \leq m \leq N$, where b_m solves

$$b_m M + M^T b_m = \Pi_m \quad (6.37)$$

and where

$$\Pi_m = \begin{bmatrix} J_m^{(\Delta T)} & 0 \\ 0 & \tilde{J}_m \end{bmatrix}.$$

From (6.37) and considering that x_m and y_m are symmetric matrices, we get

$$\begin{bmatrix} x_m \mathfrak{F} + \mathfrak{F} x_m + z_m B + B z_m^T & -x_m + \mathfrak{F} z_m + B y_m \\ -x_m + z_m^T \mathfrak{F} + y_m B & -z_m^T - z_m \end{bmatrix} = \begin{bmatrix} J_m^{(\Delta T)} & 0 \\ 0 & \tilde{J}_m \end{bmatrix}.$$

From that we get (6.32) and (6.33) directly, and also that:

$$B z_m^T + z_m B = J_m^{(\Delta T)} - x_m \mathfrak{F} - \mathfrak{F} x_m \quad (6.38)$$

and by applying (6.32) to (6.38) we get (6.34).

Also, using that x_m and y_m are required to be symmetric matrices, from the transposed version of (6.33), we get the equation

$$x_m = y_m B - z_m \mathfrak{F} - \tilde{J}_m \mathfrak{F}$$

which, combined with (6.33), gives (6.35) for $m \geq 1$ and (6.36) for $m = 0$. \square

From now on, we perform all the calculations when the dimension of the block matrices, N , is odd. The same calculations with minor differences hold when N is even as well.

2.6.2 Calculations for $m = 0, 1, 2$

Before we start analyzing the form of the block z_N , we first present in this subsection how each unit in the right hand side of the Lyapunov equation (6.37) for $0 \leq m \leq N$ (that corresponds to the spread of noise on the system), affects the z_m block of the solution b_m . This subsection is only to make it easier for the reader to follow on how perturbing the r.h.s. of the Lyapunov equation affects the solution in each sequential step. Then in the next subsection we analyse the z_N block ($m = N$) which is what we are interested in.

Thus, the reader who is interested only in the proofs, and not in the motivation behind them, might skip this subsection.

For $m = 0$: The unique solution b_0 of

$$b_0 M + M^T b_0 = \text{diag}(2T_L, 0, \dots, 2T_R, 0, \dots, 0)$$

has been computed in [RLL67], where they found exactly the elements of $z_0 := (z_{ij}^{(0)})_{1 \leq i, j \leq N}$ when $a = 0, c = 1$, to be

$$z_{1,j}^{(0)} = \frac{\sinh((N-j)\alpha)}{\sinh(N\alpha)} \quad (6.39)$$

for α constant such that $\cosh(\alpha) = 1 + \frac{1}{2\gamma}$. (It was done in the same manner with [Wan45, Section 11] but there the case was $\Delta T = 0$). Here we describe briefly the steps: first we notice that z_0 is antisymmetric since in (6.32) $J_0^{(0)} = 0$, and second, by (6.34) we get that it has a *Toeplitz*-form

$$z_0 = \begin{bmatrix} 0 & z_{1,2}^{(0)} & z_{1,3}^{(0)} & z_{1,4}^{(0)} & \cdots & z_{1,N-1}^{(0)} & z_{1,N}^{(0)} \\ -z_{1,2}^{(0)} & 0 & z_{1,2}^{(0)} & z_{1,3}^{(0)} & \cdots & z_{1,N-2}^{(0)} & z_{1,N-1}^{(0)} \\ -z_{1,3}^{(0)} & -z_{1,2}^{(0)} & 0 & z_{1,2}^{(0)} & \cdots & & \cdots \\ & & & \ddots & & & \\ -z_{1,N-1}^{(0)} & -z_{1,N-2}^{(0)} & & & & 0 & z_{1,2}^{(0)} \\ -z_{1,N}^{(0)} & -z_{1,N-1}^{(0)} & & & & -z_{1,2}^{(0)} & 0 \end{bmatrix} : \quad (6.40)$$

Indeed note that the r.h.s of (6.34) forms a bordered matrix

$$\left[\begin{array}{c|ccc|c} * & * & \cdots & * & * \\ \hline * & 0 & & 0 & * \\ \vdots & & \ddots & & \vdots \\ * & 0 & & 0 & * \\ \hline * & * & \cdots & * & * \end{array} \right]$$

i.e. only the bordered elements are non zero and so the l.h.s of (6.34) should also have this bordered form. Due to the tridiagonal form of B we get a *Toeplitz* matrix: in particular

using that $B = -c\Delta^N + aI$, the l.h.s of (6.34) is

$$z_0(-c\Delta^N + aI) - (-c\Delta^N + aI)z_0 = c(\Delta^N z_0 - z_0\Delta^N) = \begin{bmatrix} * & * & \cdots & * & * \\ * & 0 & & 0 & * \\ \vdots & & \ddots & & \vdots \\ * & 0 & & 0 & * \\ * & * & \cdots & * & * \end{bmatrix} \quad (6.41)$$

and equating the non-boundary entries, due to the symmetry of Δ^N and the antisymmetry of z_0 , we have that the elements of z_0 will be constant along the diagonals: indeed, for $1 < i < N$, for the diagonal's entries of the equation (6.41) we have

$$\begin{aligned} -cz_{i-1,i}^{(0)} - cz_{i+1,i}^{(0)} + 2cz_{i,i}^{(0)} - 2cz_{i,i}^{(0)} + cz_{i,i-1}^{(0)} + cz_{i,i+1}^{(0)} &= 0 \\ \text{or } 2cz_{i,i+1}^{(0)} - 2cz_{i-1,i}^{(0)} &= 0 \quad \text{and so } z_{i,i+1}^{(0)} = z_{i-1,i}^{(0)}. \end{aligned}$$

For the superdiagonal's entries of the equation (6.41)

$$\begin{aligned} -cz_{i-1,i+1}^{(0)} + 2cz_{i,i+1}^{(0)} - cz_{i+1,i+1}^{(0)} + cz_{ii}^{(0)} - 2cz_{i,i+1}^{(0)} + cz_{i,i+2}^{(0)} &= 0 \\ \text{or } -cz_{i-1,i+1}^{(0)} + cz_{i,i+2}^{(0)} &= 0 \quad \text{and so } z_{i-1,i+1}^{(0)} = z_{i,i+2}^{(0)}. \end{aligned}$$

We repeat these calculations through all the non-boundary entries of the matrix, and using the information we get from each one calculation, we end up with the Toeplitz form of z_0 in (6.40).

We can now see that a solution to (6.36) is a symmetric Hankel matrix which is antisymmetric about the cross diagonal and such that $(y_{1,j}^{(0)})_{j=1}^{N-1} = z_{1,j+1}^{(0)}$. Then we apply (6.33) to get a formula for the entries of x_0 and from the bordered entries of x_0 from (6.34), we end up with the linear equation

$$K_0 \cdot \underline{z}_0 = e_1.$$

Here $\underline{z}_0, e_1 \in \mathbb{C}^{N-1}$ are the vectors $\underline{z}_0 = (z_{1,1}^{(0)}, \dots, z_{1,N-1}^{(0)})^T$, $e_1 = (1, 0, \dots, 0)^T$ and K_0 is a $(N-1) \times (N-1)$ symmetric Jacobi matrix whose entries depend on the (dimensionless) friction constant γ and interaction constant c :

$$K_0 = cB + \gamma^{-1}I.$$

We solve the above equation using for example Cramer's rule and we find an explicit formula for the $z_{1,j}^{(0)}$'s: the recurrence formula of the determinant of K_0 is the same formula of the Chebyshev polynomials of the second kind, so using properties of these polynomials and imposing appropriate initial conditions we end up with the form (6.39).

For $m \geq 1$ we use again the equation (6.34). In the first step we get that: For $m = 1$, *i.e.* for the form of the z_1 -block in b_1 , the elements $z_{1,1}^{(1)}, z_{N,N}^{(1)}$ in the main diagonal are $-1/2$. The difference with the $m = 0$ step is that z_1 is not antisymmetric anymore, since $1/2$ is added in the first entry of the diagonal (due to the form of \tilde{J}_1). So from (6.32) we write

$$-z_{i,i}^{(1)} = z_{i,i}^{(1)} + 1 \quad \text{or} \quad z_{i,i}^{(1)} = -1/2 \quad \text{for } i = 1, N.$$

But we still have the bordered form in the r.h.s. of (6.34), so we still have a *Toeplitz*-form for z_1 .

In the next Lemma we give the form of the z_2 block of b_2 .

Lemma 6.4 (For $m = 2$, form of z_2). *For the z_2 -block of b_2 : There exists an antisymmetric matrix z_2^{anti} : $z_2 = z_2^{anti} - \tilde{J}_2$ and*

$$\left\{ \begin{array}{l} z_{1,1}^{(2)} = z_{2,2}^{(2)} = z_{N,N}^{(2)} = z_{N-1,N-1}^{(2)} = -1/2 \text{ and } z_{i,i}^{(2)} = 0 \text{ otherwise} \\ z_{1,2}^{(2)} + z_{N,N-1}^{(2)} = 2 \frac{1+a+2c}{4c}, \quad z_{N,N-2}^{(2)} + z_{1,3}^{(2)} = 1 \\ z_{N-k,N}^{(2)} = z_{1,k+1}^{(2)} \quad \text{for } 3 \leq k \leq N-3. \end{array} \right.$$

The last property is that the *Toeplitz* form is not perturbed in more than 2 diagonals away from the centre.

So we denote by $\mu_{a,c} := \frac{1+a+2c}{4c}$ and we write:

$$z_2 = \begin{bmatrix} -\frac{1}{2} & z_{1,2}^{(2)} & z_{1,3}^{(2)} & z_{1,4}^{(2)} & \cdots & \cdots & z_{1,N-1}^{(2)} & z_{1,N}^{(2)} \\ -z_{1,2}^{(2)} & -\frac{1}{2} & z_{1,2}^{(2)} - \mu_{a,c} & z_{1,3}^{(2)} + \frac{1}{2} & z_{1,4}^{(2)} & \cdots & z_{1,N-2}^{(2)} & z_{1,N-1}^{(2)} \\ -z_{1,3}^{(2)} & -z_{1,2}^{(2)} + \mu_{a,c} & 0 & z_{1,2}^{(2)} - \mu_{a,c} & \cdots & \cdots & & z_{1,N-2}^{(2)} \\ \vdots & & & \ddots & & & & \\ \vdots & & & & \ddots & & & \\ \vdots & & & & & & 0 & -z_{N,N-1}^{(2)} + \mu_{a,c} & -z_{N,N-2}^{(2)} \\ z_{N,2}^{(2)} & z_{N,3}^{(2)} & \cdots & & & z_{N,N-1}^{(2)} - \mu_{a,c} & -\frac{1}{2} & -z_{N,N-1}^{(2)} \\ z_{N,1}^{(2)} & z_{N,2}^{(2)} & \cdots & & & z_{N,N-2}^{(2)} & z_{N,N-1}^{(2)} & -\frac{1}{2} \end{bmatrix}.$$

Proof of Lemma 6.4. z_2 is not antisymmetric but from (6.32) we immediately have that $z_2 = z_2^{anti} - \tilde{J}_2$, where z_2^{anti} is antisymmetric. So we work with z_2^{anti} and due to the antisymmetry we look only at the upper diagonal part of the matrix.

Here, besides that z_2 is not antisymmetric, the r.h.s of (6.34) is not a bordered matrix anymore and also the matrix $B\tilde{J}_2$ affects non boundary entries as well, in particular it adds the (3×2) top-left and bottom-right submatrices of B to the (3×2) respective

submatrices of z_2 :

$$c(\Delta^N z_2 - z_2 \Delta^N) + (c\Delta^N - aI) \text{diag} \left(\frac{1}{2}, \frac{1}{2}, 0, \dots, 0, \frac{1}{2}, \frac{1}{2} \right) = \begin{bmatrix} * & * & * & \cdots & * & * & * \\ * & 1/2 & 0 & & 0 & 0 & * \\ * & 0 & 0 & & 0 & 0 & * \\ \vdots & & & \ddots & & & \vdots \\ * & 0 & 0 & & 0 & 0 & * \\ * & 0 & 0 & & 0 & 1/2 & * \\ * & * & * & \cdots & * & * & * \end{bmatrix}. \quad (6.42)$$

Equating the entries that correspond to the zero-submatrix as drawn above we will have the same calculations as in the step $m = 0$.

From (6.32) we have $z_{1,1}^{(2)} = z_{2,2}^{(2)} = z_{N,N}^{(2)} = z_{N-1,N-1}^{(2)} = -1/2$ and $z_{i,i}^{(2)} = 0$ for $N-1 > i > 2$. Looking at the $(2,2)$ -entry and the $(2,3)$ -entry of the equation (6.42) we have respectively

$$\begin{aligned} -cz_{2,1}^{(2)} + 2cz_{2,2}^{(2)} - cz_{2,3}^{(2)} + cz_{1,2}^{(2)} - 2cz_{2,2}^{(2)} + cz_{3,2}^{(2)} - \frac{(a+2c)}{2} &= \frac{1}{2} \\ -cz_{2,2}^{(2)} + 2cz_{2,3}^{(2)} - cz_{2,4}^{(2)} + cz_{1,3}^{(2)} - 2cz_{2,3}^{(2)} + cz_{3,3}^{(2)} &= 0 \end{aligned}$$

and since $z_{i,j}^{(2)} = -z_{j,i}^{(2)}$ for $j \neq i$ from (6.32), and also $z_{2,2}^{(2)} = -1/2$, $z_{3,3}^{(2)} = 0$, we get

$$z_{2,3}^{(2)} = z_{1,2}^{(2)} - \mu_{a,c} \quad \text{and} \quad z_{2,4}^{(2)} = z_{1,3}^{(2)} + 1/2.$$

Now looking at the entries (i,i) for $3 \leq i \leq N-2$ of equation (6.42), we write (as in the 0-step):

$$-cz_{i,i-1}^{(2)} + 2cz_{i,i}^{(2)} - cz_{i,i+1}^{(2)} + cz_{i-1,i}^{(2)} - 2cz_{i,i}^{(2)} + cz_{i+1,i}^{(2)} = 0$$

which gives

$$z_{i-1,i}^{(2)} = z_{i,i+1}^{(2)}, \quad 3 \leq i \leq N-2.$$

In particular

$$\begin{aligned} z_{i,i+1}^{(2)} &= z_{1,2}^{(2)} - \mu_{a,c} = -z_{N,N-1}^{(2)} + \mu_{a,c} \quad \text{and} \\ z_{i,i+2}^{(2)} &= z_{1,3}^{(2)} + \frac{1}{2} = -z_{N,N-2}^{(2)} - \frac{1}{2} \end{aligned}$$

where the second equations in both lines are proved by looking at the reversed direction (bottom-right to top-left side of the matrix). Also for $k \geq 2$ and $1 \leq i \leq N-k$, look at $(i, i+k)$ entry of the equation (6.42) and get

$$z_{i,i+k+1}^{(2)} = z_{i-1,i+k}^{(2)}.$$

This corresponds to the Toeplitz property that holds for all the diagonals apart from the 5 central ones. Remember that for $m = 0$ we end up with a Toeplitz matrix. \square

In the m -th step of the sequence of these matrix equations, for the z_m - block of b_m , the central $(4m - 3)$ diagonals have a perturbed Toeplitz form: the elements across these diagonals on each line are changed by constants that depend on the coefficients a, c . The resulting matrix z_m is described in the following way, where $\mu_{a,c} := \frac{1+a+2c}{4c}$:

$$\left\{ \begin{array}{ll} z_{1,j}^{(m)} + z_{N,N-(j-1)}^{(m)} = m\mu_{a,c}, & \text{for } j \text{ even, } j \leq m \\ z_{1,j}^{(m)} + z_{N,N-(j-1)}^{(m)} = -m, & \text{for } j \text{ odd, } j \leq m \\ z_{N-j,N}^{(m)} = z_{1,j+1}^{(m)}, & \text{for } m < j < N - 2, \quad (\text{Toeplitz form}) \\ z_{i,i}^{(m)} = -1/2, & \text{for } 1 \leq m \text{ and } i \geq N - m \\ z_{i,i}^{(m)} = 0, & \text{for } m < i < N - m. \end{array} \right.$$

The explanation is the same as in the step $m = 2$ but this holds for an arbitrary $m \leq N$.

2.6.3 Preliminaries: compute the blocks z_N, y_N, x_N of b_N

Lemma 6.5 (Form of z_N block). *The matrix $z_N := (z_{i,j}^{(N)})_{1 \leq i,j \leq N}$ is a real $N \times N$ matrix of the form*

$$z_N = z_N^{anti} - \frac{1}{2}I$$

where $z_N^{anti} = [z_{i,j}^{(N),anti}]$ is an antisymmetric matrix. We denote by $\mu_{a,c} := \frac{1+a+2c}{2c}$. z_N has the following perturbed Toeplitz form: for $2 \leq i \leq N - k$ and $1 \leq k \leq N - 2$,

$$\left\{ \begin{array}{ll} z_{i,i+k}^{(N),anti} - z_{i-1,i+k-1}^{(N),anti} = -\mu_{a,c}, & \text{for } k \text{ odd} \\ z_{i,i+k}^{(N),anti} - z_{i-1,i+k-1}^{(N),anti} = 1, & \text{for } k \text{ even} \end{array} \right. \quad (6.43)$$

and for the second and second-to-last line respectively:

$$\left\{ \begin{array}{ll} z_{2,k}^{(N),anti} - z_{1,k-1}^{(N),anti} = -\mu_{a,c}, & z_{N-1,k}^{(N),anti} - z_{N,k+1}^{(N),anti} = -\mu_{a,c}, \quad \text{for } k \text{ odd} \\ z_{2,k}^{(N),anti} - z_{1,k-1}^{(N),anti} = 1, & z_{N-1,k}^{(N),anti} - z_{N,k+1}^{(N),anti} = 1 \quad \text{for } k \text{ even} \end{array} \right. \quad (6.44)$$

Regarding the 'cross-diagonal' we have, for $1 \leq k \leq N - 2$,

$$\left\{ \begin{array}{ll} z_{i,i+k}^{(N),anti} - z_{N-k-(i-1),N-(i-1)}^{(N),anti} = (N - k - 2i + 1)\mu_{a,c}, & \text{for } k \text{ odd, } 1 \leq i \leq \frac{N-k}{2} \\ z_{i,i+k}^{(N),anti} - z_{N-k-(i-1),N-(i-1)}^{(N),anti} = k - N + 2i - 1, & \text{for } k \text{ even, } 1 \leq i \leq \frac{N-(k+1)}{2}. \end{array} \right. \quad (6.45)$$

We look at the non-bordered entries of the upper triangular part of (6.34). That is the equation

$$c(-\Delta^N z_N^{anti} + z_N^{anti} \Delta^N) - B = \begin{bmatrix} * & * & * & \cdots & * & * \\ * & 1 & 0 & & 0 & * \\ * & 0 & 1 & & 0 & * \\ \vdots & & & \ddots & \vdots & \\ * & 0 & 0 & & 1 & * \\ * & * & * & \cdots & * & * \end{bmatrix}. \quad (6.48)$$

Looking at the diagonal's entries (i, i) for $1 < i < N$ of the above equation (6.48), we write

$$-cz_{i,i-1}^{(N),anti} + 2cz_{i,i}^{(N),anti} - cz_{i,i+1}^{(N),anti} + cz_{i-1,i}^{(N),anti} - 2cz_{i,i}^{(N),anti} + cz_{i+1,i}^{(N),anti} - (2c + a) = 1$$

and using the antisymmetry of the elements of z_N^{anti} , it gives

$$\begin{aligned} z_{i,i+1}^{(N),anti} &= z_{i-1,i}^{(N),anti} - \mu_{a,c} = z_{i-2,i-1}^{(N),anti} - 2\mu_{a,c} \\ &= \cdots = z_{1,2}^{(N),anti} - (i-1)\mu_{a,c}. \end{aligned}$$

Therefore, inductively we get

$$z_{i,i+1}^{(N),anti} = z_{1,2}^{(N),anti} - (i-1)\mu_{a,c}. \quad (6.49)$$

At the same time, looking from bottom-right to top-left, we can write

$$\begin{aligned} z_{i-1,i}^{(N),anti} &= z_{i,i+1}^{(N),anti} + \mu_{a,c} = z_{i+1,i+2}^{(N),anti} + 2\mu_{a,c} \\ &= \cdots = z_{N,N-1}^{(N),anti} + (i-1)\mu_{a,c}. \end{aligned}$$

Then, looking at the super-diagonal's entries, *i.e.* the $(i, i+1)$ -entry, for $1 < i < N-1$, of equation (6.48), we write

$$-cz_{i,i}^{(N),anti} + 2cz_{i,i+1}^{(N),anti} - cz_{i,i+2}^{(N),anti} + cz_{i-1,i+1}^{(N),anti} - 2cz_{i,i+1}^{(N),anti} + cz_{i+1,i+1}^{(N),anti} + c = 0$$

and that gives

$$z_{i,i+2}^{(N),anti} = z_{i-1,i+1}^{(N),anti} + 1 = \cdots = z_{1,3}^{(N),anti} + (i-1)$$

and at the same time (reversed direction, *i.e.* from bottom right to top left)

$$z_{i-1,i+1}^{(N),anti} = -z_{i+2,i}^{(N),anti} - 1 = \cdots = -z_{N,N-2}^{(N),anti} - (N - (i+1)).$$

Similarly, looking at the entries $(i, i + 2)$ for $1 < i < N - 2$:

$$cz_{i-1,i+2}^{(N),anti} - 2cz_{i,i+2}^{(N),anti} + cz_{i+1,i+2}^{(N),anti} - cz_{i,i+1}^{(N),anti} + 2cz_{i,i+2}^{(N),anti} - cz_{i,i+3}^{(N),anti} = 0.$$

Apply (6.49) twice: $z_{i+1,i+2}^{(N),anti} = z_{1,2}^{(N),anti} - i\mu_{a,c}$ and $-z_{i,i+1}^{(N),anti} = -z_{1,2}^{(N),anti} + (i-1)\mu_{a,c}$ and get

$$z_{i-1,i+2}^{(N),anti} - \mu_{a,c} = z_{i,i+3}^{(N),anti}.$$

So inductively,

$$z_{i,i+3}^{(N),anti} = z_{1,4}^{(N),anti} - (i-1)\mu_{a,c}. \quad (6.50)$$

Also, from the reversed direction we get inductively

$$z_{i,i+3}^{(N),anti} = z_{N,N-3}^{(N),anti} - (N-3-i).$$

For the general case, as stated in the Lemma, we prove it by induction in k . For $k = 1, 2, 3$ is true from the above calculations. We do it for k odd. Let it hold for $k-2$, we look at the $(i, i+k-1)$ -entry of equation (6.48) : for $1 < i < N - (k-1)$,

$$\begin{aligned} cz_{i-1,i+k-1}^{(N),anti} - 2cz_{i,i+k-1}^{(N),anti} + cz_{i+1,i+k-1}^{(N),anti} - cz_{i,i+(k-2)}^{(N),anti} + 2cz_{i,i+k-1}^{(N),anti} - cz_{i,i+k}^{(N),anti} &= 0 \quad \text{or} \\ z_{i-1,i+k-1}^{(N),anti} - z_{i,i+k}^{(N),anti} + (z_{i+1,i+1+(k-2)}^{(N),anti} - z_{i,i+(k-2)}^{(N),anti}) &= 0. \end{aligned}$$

Then from the induction hypothesis we end up with the (6.43). The case k even follows similarly.

Now generalise the previous induction formulas for k odd for example and write:

$$z_{i,i+k}^{(N),anti} = z_{1,k+1}^{(N),anti} - (i-1)\mu_{a,c}$$

and from the reversed direction

$$z_{i,i+k}^{(N),anti} = (N-k-i)\mu_{a,c} + z_{N-k,N}^{(N),anti}.$$

From these two equations we have the specific case (6.46). k even is proven similarly. For

(6.45) we write for k odd:

$$\begin{aligned}
z_{i,i+k}^{(N),anti} - z_{N-k-(i-1),N-(i-1)}^{(N),anti} &= z_{i-1,i+k-1}^{(N),anti} - \mu_{a,c} - (z_{N-k-i,N-i}^{(N),anti} + \mu_{a,c}) \\
&= z_{i-1,i+k-1}^{(N),anti} - z_{N-k-i,N-i}^{(N),anti} - 2\mu_{a,c} \\
&= \cdots = z_{1,k+1}^{(N),anti} - z_{N-k,N}^{(N),anti} - 2(i-1)\mu_{a,c} \\
&= (N-k-2i+1)\mu_{a,c}.
\end{aligned}$$

where in the last line we applied (6.46). The case k even is proven in the same way. \square

The above discussion shows that in order to understand the entries of z_N , we need only to understand the vector $\underline{z}_N = (z_{1,2}^{(N)}, z_{1,3}^{(N)}, \dots, z_{1,N}^{(N)})$.

We state now a Lemma that shows the relation between the elements of \underline{z}_N and the entries of the first row and the last column of $x_N = [x_{i,j}^{(N)}]$, concluding a relation between $x_{1,j}^{(N)}$ and $x_{i,N}^{(N)}$ about the 'cross diagonal'.

Lemma 6.6. For $3 \leq k \leq N$,

$$\begin{cases} z_{1,k}^{(N),anti} = 1 + \frac{\gamma}{c}x_{1,k-1}^{(N)} = -\frac{\gamma}{c}x_{N,N-k+2}^{(N)} - (N-k+1), & \text{for } k \text{ odd} \\ z_{1,k}^{(N),anti} = -\mu_{a,c} + \frac{\gamma}{c}x_{1,k-1}^{(N)} = -\frac{\gamma}{c}x_{N,N-k+2}^{(N)} + (N-k+1)\mu_{a,c}, & \text{for } k \text{ even} \end{cases} \quad (6.51)$$

and $z_{1,2}^{(N),anti} = \frac{\gamma}{c}x_{1,1}^{(N)} - \frac{T_L+a+2c}{2c}$ and so for $3 \leq k \leq N$

$$\begin{cases} x_{1,k-1}^{(N)} = -x_{N,N-k+2}^{(N)} - \frac{c}{\gamma}(N-k+2), & \text{for } k \text{ odd} \\ x_{1,k-1}^{(N)} = -x_{N,N-k+2}^{(N)} + \frac{c}{\gamma}(N-k+2)\mu_{a,c}, & \text{for } k \text{ even.} \end{cases} \quad (6.52)$$

Also $x_{1,N}^{(N)} = \frac{c}{2\gamma}\mu_{a,c}$, where $\mu_{a,c} := \frac{1+a+2c}{2c}$.

Proof. We look at the bordered entries of equation (6.34). Let us first look at (N, j) -entry for j even:

$$-cz_{N,j-1}^{(N),anti} + 2cz_{N,j}^{(N),anti} - cz_{N,j+1}^{(N),anti} + cz_{N-1,j}^{(N),anti} - 2cz_{N,j}^{(N),anti} = -\gamma x_{N,j}^{(N)}.$$

Using Lemma 6.5 we write

$$cz_{1,N-j+2}^{(N),anti} + (j-2)c + cz_{1,N-j}^{(N),anti} + jc - cz_{1,N-j}^{(N),anti} - (j-1)c = -\gamma x_{N,j}^{(N)}$$

and after the obvious cancellations we have for j even

$$x_{N,j}^{(N)} = -\frac{c}{\gamma}z_{1,N-j+2}^{(N),anti} - (j-1)\frac{c}{\gamma}. \quad (6.53)$$

Similarly for j odd we have

$$x_{N,j}^{(N)} = -\frac{c}{\gamma} z_{1,N-j+2}^{(N),anti} + (j-1) \frac{c}{\gamma} \mu_{a,c}. \quad (6.54)$$

Moreover, with exactly the same calculations, but looking at the $(1, j)$ -entry of equation (6.34) we get, for $2 \leq j \leq N-1$,

$$x_{1,j}^{(N)} = \frac{c}{\gamma} z_{1,j+1}^{(N),anti} - \frac{c}{\gamma} \text{ for } j \text{ even} \quad \text{and} \quad x_{1,j}^{(N)} = \frac{c}{\gamma} z_{1,j+1}^{(N),anti} + \frac{c}{\gamma} \mu_{a,c} \text{ for } j \text{ odd}. \quad (6.55)$$

Now for $k := N - j + 2$ then $3 \leq k \leq N$. Since N is odd, whenever j is odd, k is even and the opposite. Solving the equations (6.54) and (6.53) for $z_{1,k}^{(N),anti}$, we get the second equations in (6.51), whereas solving (6.55) for $\lambda := j + 1$, for $z_{1,\lambda}^{(N),anti}$, we get the first equations in (6.51) as well. We conclude with (6.52) just by combining the above relations in both cases.

Finally to get this specific value for $x_{1,N}^{(N)}$ we look at the $(1, N)$ -entry of equation (6.34) and perform the same calculations as above. \square

Considering the above Lemma we can write the matrix z_N also as follows:

$$z_N = \begin{bmatrix} -\frac{1}{2} & \frac{\gamma}{c} x_{1,1}^{(N)} - \kappa_L & 1 + \frac{\gamma}{c} x_{1,2}^{(N)} & \cdots & -\mu_{a,c} + \frac{\gamma}{c} x_{1,N-2}^{(N)} & 1 + \frac{\gamma}{c} x_{1,N-1}^{(N)} \\ -\frac{\gamma}{c} x_{1,1}^{(N)} + \kappa_L & -\frac{1}{2} & \frac{\gamma}{c} x_{1,1}^{(N)} - \kappa_L - \mu_{a,c} & \cdots & \frac{\gamma}{c} x_{1,N-3}^{(N)} + 2 & \frac{\gamma}{c} x_{1,N-2}^{(N)} - 2\mu_{a,c} \\ \vdots & & & & \vdots & \\ & & & \ddots & & \\ & \cdots & & \frac{\gamma}{c} x_{N,N}^{(N)} - \kappa_R - \mu_{a,c} & -\frac{1}{2} & \frac{\gamma}{c} x_{1,1}^{(N)} - \kappa_L - (N-2)\mu_{a,c} \\ & & & \cdots & \frac{\gamma}{c} x_{N,N}^{(N)} - \kappa_R & -\frac{1}{2} \end{bmatrix}$$

where $\kappa_L := \frac{T_L + a + 2c}{2c}$ and $\kappa_R := \frac{T_R + a + 2c}{2c}$.

In the following we state a Lemma about the symmetries that hold in y_N -block of b_N , concluding that all the entries of y_N can be written in terms of the vectors $\underline{y}_N := (y_{1,N}^{(N)}, y_{1,N-1}^{(N)}, \dots, y_{1,1}^{(N)})$ and \underline{z}_N .

Lemma 6.7. For $2 \leq i \leq N - (k + 1)$ and $1 \leq k \leq N - 3$,

$$y_{i-1,i+k}^{(N)} - y_{i,i+k-1}^{(N)} + (y_{i+1,i+k}^{(N)} - y_{i,i+k+1}^{(N)}) = 0 \quad (6.56)$$

$$y_{2,k}^{(N)} = y_{1,k-1}^{(N)} + y_{1,k+1}^{(N)} + \frac{\gamma}{c} z_{1,k}^{(N)}, \quad \text{for } 2 \leq k \leq N - 1, \quad (6.57)$$

$$\text{and } y_{2,N}^{(N)} = y_{1,N-1}^{(N)} + \frac{2\gamma}{c} z_{1,N}^{(N)}$$

$$y_{k,N}^{(N)} = \frac{\gamma}{c} (z_{k-1,N}^{(N)} + z_{1,N-(k-2)}^{(N)}) + y_{1,N-(k-1)}^{(N)}, \quad \text{for } 2 \leq k \leq N \quad (6.58)$$

Proof. Due to symmetry of y_N is enough to look at the upper-triagonal part. We look at the entries $(i, i + k)$ of equation (6.35). For $k = 1$ we have

$$-y_{i,i}^{(N)} - y_{i,i+2}^{(N)} + y_{i-1,i+1}^{(N)} + y_{i+1,i+1}^{(N)} = 0$$

which is the equation (6.56). For $1 < k < N - 1$ we prove it by induction in k , like in the proof of Lemma (6.5). Let us now look at the $(1, N)$ - entry of (6.35):

$$-cy_{1,N-1}^{(N)} + 2cy_{1,N}^{(N)} - 2cy_{1,N}^{(N)} + cy_{2,N}^{(N)} = 2\gamma z_{1,N}^{(N),anti}$$

which gives $y_{2,N}^{(N)} = y_{1,N-1}^{(N)} + \frac{2\gamma}{c} z_{1,N}^{(N)}$. For (6.57) we look at $(1, k)$ - entry:

$$-cy_{1,k-1}^{(N)} + 2cy_{1,k}^{(N)} - cy_{1,k+1}^{(N)} - 2cy_{1,k}^{(N)} + cy_{2,k}^{(N)} = \gamma z_{1,k}^{(N),anti}$$

which is

$$-y_{1,k-1}^{(N)} - y_{1,k+1}^{(N)} + y_{2,k}^{(N)} = \frac{\gamma}{c} z_{1,k}^{(N),anti}$$

and this is the desired equation. For (6.58), we look at $(k - 1, N)$ - entry of (6.35) for $k \geq 3$. Performing the same calculations as above we get

$$y_{k,N}^{(N)} = \frac{\gamma}{c} z_{k-1,N}^{(N),anti} - y_{k-2,N}^{(N)} + y_{k-1,N-1}^{(N)}.$$

Then using the relations (6.56) and (6.57) for each of the terms above, we get the stated relation. \square

With the result of the following Lemma we relate the entries of \underline{y}_N with the entries of \underline{z}_N .

Lemma 6.8. *Let B be the matrix (1.7). We have*

$$\underline{y}_N = B^{-1} \underline{\tilde{z}}_N \tag{6.59}$$

where $\underline{\tilde{z}}_N$ is the vector

$$\underline{\tilde{z}}_N = \begin{bmatrix} \gamma z_{1,N}^{(N)} + \frac{c}{2\gamma} \mu_{a,c} \\ \frac{c}{\gamma} z_{1,N}^{(N)} - \frac{c}{\gamma} \\ \frac{c}{\gamma} z_{1,N-1}^{(N)} + \frac{c}{\gamma} \mu_{a,c} \\ \vdots \\ \frac{c}{\gamma} z_{1,N-i}^{(N)} + \frac{c}{\gamma} \mu_{a,c} \\ \frac{c}{\gamma} z_{1,N-(i+1)}^{(N)} - \frac{c}{\gamma} \\ \vdots \\ \frac{c}{\gamma} z_{1,3}^{(N)} - \frac{c}{\gamma} \\ \frac{c}{\gamma} z_{1,2}^{(N)} + \frac{T_L+a+2c}{2\gamma} + \frac{\gamma}{2} \end{bmatrix}$$

where $\mu_{a,c} := \frac{1+a+2c}{2c}$. In particular:

$$\|y_N\|_2 \lesssim \|z_N\|_2 + N^{1/2}. \quad (6.60)$$

Proof. We combine the information for x_{1i} 's we get from two equations: first from (6.33), we remind that equation (6.33) is

$$x_N = By_N + \mathfrak{F}z_N$$

and second from the bordered entries of (6.34), which is

$$-Bz_N + z_N B - B = J_N^{(\Delta T)} - x_N \mathfrak{F} - \mathfrak{F}x_N.$$

We look at the element $x_{1,N}^{(N)}$ and we write:

$$\begin{aligned} x_{1,N}^{(N)} &= (a+2c)y_{1,N}^{(N)} - cy_{2,N}^{(N)} + \gamma z_{1,N}^{(N),anti} = (a+2c)y_{1,N}^{(N)} - cy_{1,N-1}^{(N)} - 2\gamma z_{1,N}^{(N),anti} + \gamma z_{1,N}^{(N),anti} \\ &= (a+2c)y_{1,N}^{(N)} - cy_{1,N-1}^{(N)} - \gamma z_{1,N}^{(N),anti} \end{aligned}$$

and

$$x_{1,N}^{(N)} = \frac{c}{2\gamma} \mu_{a,c}$$

which give

$$(a+2c)y_{1,N}^{(N)} - cy_{1,N-1}^{(N)} = \gamma z_{1,N}^{(N),anti} + \frac{c}{2\gamma} \mu_{a,c}.$$

Moreover

$$\begin{aligned} x_{1,N-1}^{(N)} &= (a+2c)y_{1,N-1}^{(N)} - cy_{2,N-1}^{(N)} + \gamma z_{1,N-1}^{(N),anti} \\ &= (a+2c)y_{1,N-1}^{(N)} - cy_{1,N-2}^{(N)} - cy_{1,N}^{(N)} - \gamma z_{1,N-1}^{(N),anti} + \gamma z_{1,N-1}^{(N),anti} \\ &= (a+2c)y_{1,N-1}^{(N)} - cy_{1,N-2}^{(N)} - cy_{1,N}^{(N)} \end{aligned}$$

and from the proof of Lemma (6.6), see relation (6.55), we have

$$x_{1,N-1}^{(N)} = \frac{c}{\gamma} z_{1,N}^{(N),anti} - \frac{c}{\gamma}.$$

Both of them give

$$(a+2c)y_{1,N-1}^{(N)} - cy_{1,N-2}^{(N)} - cy_{1,N}^{(N)} = \frac{c}{\gamma} z_{1,N}^{(N),anti} - \frac{c}{\gamma}.$$

In general using again Lemma 6.7 and relation (6.55), we have

$$(a + 2c)y_{1,N-i}^{(N)} - cy_{1,N-(i+1)}^{(N)} - cy_{1,N-(i-1)}^{(N)} = \begin{cases} \frac{c}{\gamma}z_{1,N-(i-1)}^{(N),anti} - \frac{c}{\gamma}, & \text{if } i \text{ odd} \\ \frac{c}{\gamma}z_{1,N-(i-1)}^{(N),anti} + \frac{c}{\gamma}\mu_{a,c}, & \text{if } i \text{ even.} \end{cases}$$

For $x_{1,1}^{(N)}$ we use that

$$x_{1,1}^{(N)} = \frac{c}{\gamma}z_{1,2}^{(N),anti} + \frac{c(T_L + a + 2c)}{2\gamma c}$$

from Lemma 6.6, and from (6.33),

$$x_{1,1}^{(N)} = (a + 2c)y_{1,1}^{(N)} - cy_{1,2}^{(N)} - \frac{\gamma}{2}.$$

Putting the above relations in a more compact form we have

$$By_N = \underline{\tilde{z}}_N.$$

We end up with (6.60) considering that $\|B^{-1}\|_2$ is uniformly (in N) bounded, since B has bounded spectral gap. \square

The following Lemma shows, through its proof, that there is one unique solution to the Lyapunov matrix equation (since one can explicitly find the entries of \underline{z}_N , that determine all the rest) and eventually gives the scaling in N of the entries of \underline{z}_N . For $1 \leq k \leq N - 2$, using all the information we have from the block equations in Lemma 6.3, we write all the $z_{1,N-k}^{(N),anti}$ in terms of $z_{1,N}^{(N),anti}$, which we then calculate explicitly. This is presented in the following Lemma.

Lemma 6.9. *For $1 \leq k \leq N - 2$, the order of the entries of \underline{z}_N is given by*

$$\begin{cases} z_{1,N-k}^{(N),anti} = \mathcal{O}\left(R^k z_{1,N}^{(N),anti} + \frac{k}{2}\mu_{a,c}\right), & \text{for } k \text{ odd} \\ z_{1,N-k}^{(N),anti} = \mathcal{O}\left(R^k z_{1,N}^{(N),anti} - \frac{k}{2}\right), & \text{for } k \text{ even} \end{cases} \quad (6.61)$$

and $z_{1,N}^{(N),anti} = \mathcal{O}\left(R^{1-N}\left(\frac{\kappa_R - \kappa_L}{2\gamma}\right)\right)$, where $R := \frac{c}{\gamma^2} + \frac{a+2c}{c}$ and $\mu_{a,c} := \frac{1+a+2c}{2c}$. Therefore

$$|z_{1,i}^{(N),anti}| \lesssim \mathcal{O}\left((\Delta T)R^{-i+1} + (N - i)\right), \quad \text{for } 2 \leq i \leq N$$

where ΔT is the temperature difference at the ends of the chain.

Proof. We look at the equations around $x_{k,N}^{(N)}$ for $2 \leq k \leq N$. First we look at $x_{2,N}^{(N)}$ and from (6.53) we have

$$x_{2,N}^{(N)} = -\frac{c}{\gamma}z_{1,N}^{(N),anti} - \frac{c}{\gamma}$$

while from the $(2, N)$ -entry of (6.33) we have

$$\begin{aligned}
x_{2,N}^{(N)} &= -cy_{1,N}^{(N)} + (a+2c)y_{2,N}^{(N)} - cy_{3,N}^{(N)} \\
&= -cy_{1,N}^{(N)} + (a+2c)y_{1,N-1}^{(N)} + \frac{2\gamma(a+2c)}{c}z_{1,N}^{(N),anti} - \gamma(z_{2,N}^{(N),anti} + z_{1,N-1}^{(N),anti}) - cy_{1,N-2}^{(N)} \\
&= x_{1,N-1}^{(N)} + \frac{2\gamma(a+2c)}{c}z_{1,N}^{(N),anti} - 2\gamma z_{1,N-1}^{(N),anti} + \gamma\mu_{a,c} \\
&= \frac{c}{\gamma}z_{1,N}^{(N),anti} - \frac{c}{\gamma} + \frac{2\gamma(a+2c)}{c}z_{1,N}^{(N),anti} - 2\gamma z_{1,N-1}^{(N),anti} + \gamma\mu_{a,c}.
\end{aligned}$$

Combine them and get

$$z_{1,N-1}^{(N),anti} = Rz_{1,N}^{(N),anti} + \frac{\mu_{a,c}}{2}. \quad (6.62)$$

Then we look at $x_{3,N}^{(N)}$: from (6.54) we have

$$-\frac{c}{\gamma}z_{1,N-1}^{(N),anti} + 2\frac{c\mu_{a,c}}{\gamma}$$

while from the $(3, N)$ -entry of (6.33) we have similarly

$$\begin{aligned}
x_{3,N}^{(N)} &= -cy_{2,N}^{(N)} + (a+2c)y_{3,N}^{(N)} - cy_{4,N}^{(N)} \\
&= x_{1,N-2}^{(N)} - 2\gamma z_{1,N}^{(N),anti} + \frac{2\gamma(a+2c)}{c}z_{1,N-1}^{(N),anti} - 2\gamma z_{1,N-2}^{(N),anti} - \frac{\gamma(a+2c)\mu_{a,c}}{c} - 2\gamma.
\end{aligned}$$

Combine them and get

$$Rz_{1,N-1}^{(N),anti} = z_{1,N}^{(N),anti} + z_{1,N-2}^{(N),anti} + R\frac{\mu_{a,c}}{2} + 1.$$

Then considering (6.62) as well, we have

$$z_{1,N-2}^{(N),anti} = (R^2 - 1)z_{1,N}^{(N),anti} - 1. \quad (6.63)$$

In the same manner, but looking around $x_{4,N}^{(N)}$ and $x_{5,N}^{(N)}$, we get

$$z_{1,N-3}^{(N),anti} = (R^3 - 2R)z_{1,N}^{(N),anti} + \frac{3\mu_{a,c}}{2}, \quad z_{1,N-4}^{(N),anti} = (R^4 - 3R^2 + 1)z_{1,N}^{(N),anti} - 2. \quad (6.64)$$

respectively. Inductively, we have a way to write all the elements of \underline{z}_N in terms of $z_{1,N}^{(N),anti}$, and looking at the leading order in terms of N we have the general formula (6.61) for $1 \leq k \leq N-2$. In particular, for $k = N-3$ (is even by assumption on N) and $k = N-2$

(odd) :

$$z_{1,3}^{(N),anti} \sim R^{N-3} z_{1,N}^{(N),anti} - \frac{N-3}{2}, \quad z_{1,2}^{(N),anti} \sim R^{N-2} z_{1,N}^{(N),anti} + \frac{(N-2)\mu_{a,c}}{2}. \quad (6.65)$$

respectively. Moreover, by looking at $x_{N,N}^{(N)}$ combining (6.33) and (6.34) we have

$$Rz_{1,2}^{(N),anti} = R \frac{(N-2)\mu_{a,c}}{2} - \frac{(3-N)}{2} + \frac{(\kappa_R - \kappa_L)}{2\gamma} + z_{1,3}^{(N),anti}.$$

Plugging in the above equation the relations from (6.65), we write

$$(R^{N-1} + R^{N-3})z_{1,N}^{(N),anti} + \frac{R(N-2)\mu_{a,c}}{2} \sim \frac{R(N-2)\mu_{a,c}}{2} - \frac{(3-N)}{2} + \frac{(\kappa_R - \kappa_L)}{2\gamma} - \frac{(N-3)}{2}$$

which is $z_{1,N}^{(N),anti} \sim R^{1-N} \left(\frac{\kappa_R - \kappa_L}{2\gamma} \right).$

We conclude the last statement by combining the above estimate on $z_{1,N}^{(N),anti}$ with (6.61). \square

Now we estimate the entries \underline{y}_N : from (6.60) and Lemma 6.9,

$$\|\underline{y}_N\|_2 \lesssim \left(\sum_{i=1}^N |z_{1,i}|^2 \right)^{1/2} + N^{1/2} \lesssim N^{3/2} + N^{1/2} \lesssim N^{3/2}.$$

This gives that

$$|y_{1,j}^{(N)}| \lesssim \mathcal{O}(N) \quad (6.66)$$

and then also, since $y_{k,N}^{(N)} = \frac{\gamma}{c}(z_{k-1,N}^{(N)} + z_{1,N-(k-2)}^{(N)}) + y_{1,N-(k-1)}^{(N)}$,

$$|y_{j,N}^{(N)}| \lesssim \mathcal{O}(N). \quad (6.67)$$

Lemma 6.10 (Estimate on the spectral norm of y_N). *For the spectral norm of y_N we have that*

$$\|y_N\|_2 \lesssim \mathcal{O}(N^3).$$

Proof. Let $v = (v_1, v_2, \dots, v_N) \in \mathbb{C}^N$. We write L_i for the i -th row of the matrix y_N and

then calculate

$$\begin{aligned}
|y_N v|_2^2 &= |L_1 \cdot v|^2 + \cdots + |L_N \cdot v|^2 \\
&\leq N \left(|y_{1,1}^{(N)} v_1|^2 + |y_{1,2}^{(N)} v_2|^2 + \cdots + |y_{1,N}^{(N)} v_N|^2 + \quad (\text{from } L_1 \cdot v) \right. \\
&\quad + |y_{2,2}^{(N)} v_2|^2 + |y_{2,2}^{(N)} v_2|^2 + \cdots + |y_{2,N}^{(N)} v_N|^2 + \quad (\text{from } L_2 \cdot v) \\
&\quad \vdots \\
&+ |y_{1, \lfloor \frac{N}{2} \rfloor + 1}^{(N)} v_1|^2 + \cdots + |y_{\lfloor \frac{N}{2} \rfloor + 1, \lfloor \frac{N}{2} \rfloor + 1}^{(N)} v_{\lfloor \frac{N}{2} \rfloor + 1}|^2 + \cdots + |y_{N, \lfloor \frac{N}{2} \rfloor + 1}^{(N)} v_N|^2 + \quad (\text{from } L_{\lfloor \frac{N}{2} \rfloor + 1} \cdot v) \\
&\quad \vdots \\
&\quad \left. + |y_{1,N}^{(N)} v_1|^2 + |y_{2,N}^{(N)} v_2|^2 + \cdots + |y_{N,N}^{(N)} v_N|^2 \right) \quad (\text{from } L_N \cdot v)
\end{aligned}$$

We estimate the terms due to the first half of the matrix, *i.e.* the terms until $L_{\lfloor \frac{N}{2} \rfloor + 1} \cdot v$: from Lemma 6.7 we write all the $y_{i,j}^{(N)}$'s in terms of the entries of \underline{y}_N and \underline{z}_N that, due to the observations above, scale at most like N . In particular for the second line

$$y_{2,k}^{(N)} = y_{1,k-1}^{(N)} + y_{1,k+1}^{(N)} + \frac{\gamma}{c} z_{1,k}^{(N),anti}$$

and more generally

$$y_{i,i+k}^{(N)} = y_{1,1+k}^{(N)} + y_{1,3+k}^{(N)} + \cdots + y_{1,2i+k-1}^{(N)} + \frac{\gamma}{c} \left(z_{1,2+k}^{(N),anti} + \cdots + z_{1,2i+k-2}^{(N),anti} \right).$$

Then, from (6.66):

$$\begin{aligned}
|L_1 \cdot v|^2 + \cdots + \left| L_{\lfloor \frac{N}{2} \rfloor + 1} \cdot v \right|^2 &\lesssim N \left(N^2 |v_1|^2 + \cdots + N^2 |v_N|^2 + \right. & (6.68) \\
&\quad + N^2 |v_1|^2 + 3^2 N^2 |v_2|^2 + \cdots + 3^2 N^2 |v_{N-1}|^2 + N^2 |v_N|^2 + \\
&+ N^2 |v_1|^2 + 3^2 N^2 |v_2|^2 + 5^2 N^2 |v_3|^2 + 5^2 N^2 |v_4|^2 + \cdots + 5^2 N^2 |v_{N-2}|^2 + 3^2 |v_{N-1}|^2 + N^2 |v_N|^2 \\
&\quad \vdots \\
&+ N^2 |v_1|^2 + 3^2 N^2 |v_2|^2 + \cdots + \left(2 \left\lfloor \frac{N}{2} \right\rfloor + 1 \right)^2 N^2 \left| v_{\lfloor \frac{N}{2} \rfloor + 1} \right|^2 + \left(2 \left\lfloor \frac{N}{2} \right\rfloor - 1 \right)^2 N^2 \left| v_{\lfloor \frac{N}{2} \rfloor + 2} \right|^2 + \\
&\quad \left. \cdots + N^2 |v_N|^2 \right).
\end{aligned}$$

So the highest order is due to $\left|L_{\lfloor \frac{N}{2} \rfloor + 1} \cdot v\right|^2$ for which we estimate

$$\left|L_{\lfloor \frac{N}{2} \rfloor + 1} \cdot v\right|^2 \lesssim \left(2N^2 \sum_{i=1}^{\lfloor \frac{N}{2} \rfloor + 1} (2i-1)^2\right) |v|_2^2.$$

The terms $(2i-1)$ in the sum above, denote the number of the entries of $\underline{y}_N, \underline{z}_N$ that each $y_{i,j}^{(N)}$ is given by.

Regarding the terms due to the second half of the matrix, we use again Lemma 6.7, equations (6.56). This way we write the elements $y_{i,j}^{(N)}$'s in terms of $y_{N,j}^{(N)}$'s and then from relation (6.58), we have all the $y_{i,j}^{(N)}$'s in terms of the entries of \underline{y}_N and \underline{z}_N , that scale at most like N . So in the end we have

$$|y_N v|_2^2 \lesssim N \left(N^3 N^2\right) |v|_2^2 = N^6 |v|_2^2.$$

Then

$$\frac{|y_N v|_2}{|v|_2} \lesssim \mathcal{O}(N^3) \quad \text{and so} \quad \|y_N\|_2 \lesssim \mathcal{O}(N^3).$$

Before we finish the proof, we give more details on the estimates (6.68) above: For the first inequality we apply iteratively Lemma 6.7. Regarding the row L_2 :

$$y_{2,2}^{(N)} = y_{1,3}^{(N)} + y_{1,1}^{(N)} + \frac{\gamma}{c} z_{1,2}^{(N),anti}.$$

So $y_{2,2}^{(N)}$ is given by the sum of 3 terms whose absolute value is of order not more than $\mathcal{O}(N)$. The same holds (from Lemma 6.7) for each $y_{2,j}^{(N)}$ for $j \leq N-2$, *i.e.* until we reach the 'cross-diagonal'. After the 'cross-diagonal': $y_{2,N}^{(N)} = y_{1,N-1}^{(N)} + \frac{2\gamma}{c} z_{1,N}^{(N)}$, and $|y_{1,N-1}^{(N)}|, |z_{1,N}^{(N)}|$ have order less than N .

Regarding the row L_3 :

$$y_{3,2}^{(N)} = y_{1,2}^{(N)} + y_{1,4}^{(N)} + \frac{\gamma}{c} z_{1,3}^{(N),anti}$$

is given by the sum of 3 terms whose absolute value has order less than N , while for $y_{3,3}^{(N)}$, by applying Lemma 6.7 twice, *i.e.* until we end up only with elements of \underline{y}_N and \underline{z}_N , we get

$$y_{3,3}^{(N)} = y_{1,3}^{(N)} + y_{1,1}^{(N)} + y_{1,5}^{(N)} + \frac{\gamma}{c} \left(z_{1,2}^{(N),anti} + z_{1,4}^{(N),anti} \right).$$

So $y_{3,3}^{(N)}$ is given by the sum of 5 terms whose absolute value has order less than N . For $y_{3,j}^{(N)}$, $j \leq N-2$ (until the 'cross-diagonal'), apply Lemma 6.7 twice: the value of $y_{3,j}^{(N)}$ is

given by the sum of 5 such terms, while for $N - 1 \leq j \leq N$,

$$\begin{aligned} y_{3,N-1}^{(N)} &= y_{1,N-3}^{(N)} + y_{1,N-1}^{(N)} + \frac{\gamma}{c} z_{1,N-2}^{(N),anti} \\ y_{3,N}^{(N)} &= \frac{\gamma}{c} \left(z_{2,N}^{(N)} + z_{1,N-1}^{(N)} \right) + y_{1,N-2}^{(N)} = \frac{2\gamma}{c} z_{1,N-1}^{(N)} - \frac{\gamma\mu_{a,c}}{c} + y_{1,N-2}^{(N)} \end{aligned}$$

and so they are given by 3 terms with absolute value of order at most N .

In general, the same holds for the row L_i , $i \leq \lfloor \frac{N}{2} \rfloor + 1$ from applications of Lemma 6.7 inductively. For all $y_{i,j}^{(N)}$ we apply Lemma 6.7 until we have written each $y_{i,j}^{(N)}$ only in terms of entries of y_N and z_N .

For $j \leq i$, *i.e.* until the main diagonal, $y_{i,j}^{(N)}$ is given by the sum of ν terms, whose order is less than N , and

$$\nu = 1, 3, 5, \dots, (2i - 1) \quad \text{for } y_{i,1}^{(N)}, y_{i,2}^{(N)}, \dots, y_{i,i}^{(N)}, \text{ respectively.}$$

For that we apply Lemma 6.7 and write

$$y_{i,j}^{(N)} = y_{j,i}^{(N)} = y_{1,i-j+1}^{(N)} + y_{1,i-j+3}^{(N)} + \dots + y_{1,j+i-1}^{(N)} + \frac{\gamma}{c} \left(z_{1,i-j+2}^{(N),anti} + \dots + z_{1,i+j-2}^{(N),anti} \right).$$

This formula gives that $y_{i,j}^{(N)}$ is the sum of $(2j - 1)$ terms whose absolute value has order less than $\mathcal{O}(N)$.

The same holds for $j > N - (i - 1)$, *i.e.* after the 'cross-diagonal', considering also (6.67). As for the rest terms in L_i , for $i \leq j \leq N - (i - 1)$: $y_{i,j}^{(N)}$ is given by the sum of $(2i - 1)$ terms whose order is less than $\mathcal{O}(N)$. \square

Now, from (6.33) we can see that the entries of x_N can be written in terms of entries of z_N as well:

$$\begin{aligned} x_{i,j}^{(N)} &= \sum_{k=1}^N \beta_{i,k} y_{k,j}^{(N)} + \gamma \sum_k (\delta_{(i=1,k=1)} + \delta_{(i=N,k=N)}) z_{k,j}^{(N)} \\ &= \sum_{\substack{k=1, \\ k+j \leq N}}^N \beta_{i,k} z_{1,j+k}^{(N)} + \sum_{\substack{k=1, \\ k+j > N}}^N \beta_{i,k} z_{N,j+k-N-1}^{(N)} + \gamma \sum_k (\delta_{(i=1,k=1)} + \delta_{(i=N,k=N)}) z_{k,j}^{(N)} \end{aligned}$$

where β_{ij} are the elements of the matrix B , (1.7), and the entries of y_N are split into two sums regarding their position about the cross diagonal.

We write

$$\|x_N\|_2 \leq \|B\|_2 \|y_N\|_2 + \|\mathfrak{F}az_N\|_2 \lesssim \|y_N\|_2 + N \lesssim N^3.$$

Proof of Proposition 1.1. We are ready now to bound from above $\|b_N\|_2$. We write for

some positive constant $C_{a,c}^1$

$$\|b_N\|_2 \leq \|x_N\|_2 + \|y_N\|_2 \leq C_{a,c}^1 N^3$$

where for the first inequality: since b_N is positive definite, decomposing b_N in its square root matrices:

$$\begin{aligned} b_N &= \begin{bmatrix} \chi & \zeta \\ \zeta^T & \psi \end{bmatrix} \begin{bmatrix} \chi & \zeta \\ \zeta^T & \psi \end{bmatrix} = \begin{bmatrix} \chi & 0 \\ \zeta^T & 0 \end{bmatrix} \begin{bmatrix} \chi & \zeta \\ 0 & 0 \end{bmatrix} + \begin{bmatrix} 0 & \zeta \\ 0 & \psi \end{bmatrix} \begin{bmatrix} 0 & 0 \\ \zeta^T & \psi \end{bmatrix} \\ &=: X^*X + Y^*Y. \end{aligned}$$

And since X^*X and XX^* are unitarily congruent and the same holds for Y^*Y and YY^* (from polar decomposition for example), there are unitary matrices $U, V \in \mathbb{C}^{N \times N}$ so that:

$$b_N = X^*X + Y^*Y = UXX^*U^* + VYY^*V^* = U \begin{bmatrix} x_N & 0 \\ 0 & 0 \end{bmatrix} U^* + V \begin{bmatrix} 0 & 0 \\ 0 & y_N \end{bmatrix} V^*.$$

Then it is clear that for the spectral norm (which is unitarily invariant):

$$\left\| \begin{bmatrix} x_N & z_N \\ z_N^T & y_N \end{bmatrix} \right\|_2 \leq \|x_N\|_2 + \|y_N\|_2.$$

Regarding the last part of the statement that $\|b_N^{-1}\|_2$ is bounded from above: Let us first state some facts about the spectrum of the matrix b_0 that solves

$$b_0 M + M^T b_0 = \text{diag}(2T_L, 0, \dots, 2T_R, 0, \dots, 0) := \tilde{\Theta}.$$

It is known that b_0 is the covariance matrix that determines the stationary solution of the Liouville equation in the harmonic chain (and it has been found explicitly in [RLL67], see a description of their approach in the beginning of the proof of Lemma 6.5). From [JPS17, Lemma 5.1], we know that b_0 is bounded below and above:

$$T_R \begin{bmatrix} I & 0 \\ 0 & B^{-1} \end{bmatrix} \leq b_0 \leq T_L \begin{bmatrix} I & 0 \\ 0 & B^{-1} \end{bmatrix}.$$

Thus $\|b_0\|_2$ and $\|b_0^{-1}\|_2$ are uniformly bounded in terms of N : from Remark 6.2 we write $B = -c \Delta^N + \sum_{i=1}^N \alpha \delta_i$. Even though here we will only use that $\|b_0^{-1}\|_2$ is finite, in fact when $a > 0$, B possesses a spectral gap uniformly in N . Moreover, $b_N \geq b_0$: since $\Pi_N > \tilde{\Theta}$, for every $t > 0$,

$$e^{-tM^T} \Pi_N e^{-tM} > e^{-tM^T} \tilde{\Theta} e^{-tM}$$

and since $-M$ is stable (all the characteristic roots have negative real part) we have

$$b_N = \int_0^\infty e^{-tM^T} \Pi_N e^{-tM} dt > \int_0^\infty e^{-tM^T} \tilde{\Theta} e^{-tM} dt = b_0.$$

So $b_N^{-1} \leq b_0^{-1}$ and so $\|b_N^{-1}\|_2 \leq \|b_0^{-1}\|_2$ which is less than a finite constant (because of the spectrum of the discrete Laplacian). Therefore there exists positive and finite constant $C_{a,c}^2$ so that $\|b_N^{-1}\|_2 \leq C_{a,c}^2$. Conclude the Proposition by taking $C_{a,c} := \min(C_{a,c}^1, C_{a,c}^2)$. \square

To sum up: for the homogeneous weakly anharmonic chain, the method described in Section 3 with the modified Bakry-Emery criterion, gives a lower bound on the spectral gap that is of order N^{-3} (see the exponential rate in the main Theorems). For the purely harmonic chain, since we know that it always decays with N from Proposition 6.1, this lower bound shows that the spectral gap in this case can not decay at an exponential rate in N , it is at most polynomial.

In the next Proposition, exploiting the estimates on $\|b_N\|_2$ from the above matrix analysis, we get alternatively the lower bound on the spectral gap of the *harmonic* chain.

Proof of Proposition 1.2. We remind that $\|b_N\|_2 \leq C_{a,c} N^3$ by Proposition 1.1 and that the spectral gap divided by $\inf\{\operatorname{Re}(\mu) : \mu \in \sigma(M)\}$ is bounded below and above in terms of N , by Proposition 6.1. From [Ves03, Inequality (13)], [GKK], we have an estimate for the decay of e^{-Mt} :

$$\|e^{-Mt}\|^2 \leq \|b_N\| \|b_N^{-1}\| e^{-t/\|b_N\|}$$

So, for u be the (normalised) eigenvector corresponding to an eigenvalue of M , $\mu > 0$, we write

$$e^{-2\operatorname{Re}(\mu)t} = \|e^{-2\operatorname{Re}(\mu)t} u\|^2 = \|e^{-Mt} u\|^2 \leq \|b_N\| \|b_N^{-1}\| e^{-t/\|b_N\|}$$

and therefore we write $-2\operatorname{Re}(\mu) \leq -\frac{1}{\|b_N\|}$ which means

$$\operatorname{Re}(\mu) \geq \frac{1}{2\|b_N\|}.$$

Taking the infimum over the real parts of the eigenvalues of M , we conclude that

$$\inf\{\operatorname{Re}(\mu) : \mu \in \sigma(M)\} \geq C_{a,c}^{-1} N^{-3}.$$

\square

Eventually, from the whole procedure in this note we have that the scaling of the spectral gap of the homogeneous harmonic chain is in between N^{-3} and N^{-1} . In [BM22, Proposition 9.1] it is proven that this lower bound is the sharp one, *i.e.* an upper bound of order

N^{-3} is provided.

From a simple numerical simulation in Matlab on the spectral gap of the matrix M , the true value is indeed N^{-3} . In particular calculating the real part of the smallest eigenvalue of the matrix M and multiplying the result by N^3 we get the following behaviour in Figure 2.2, which shows that then the spectral gap converges for large N :

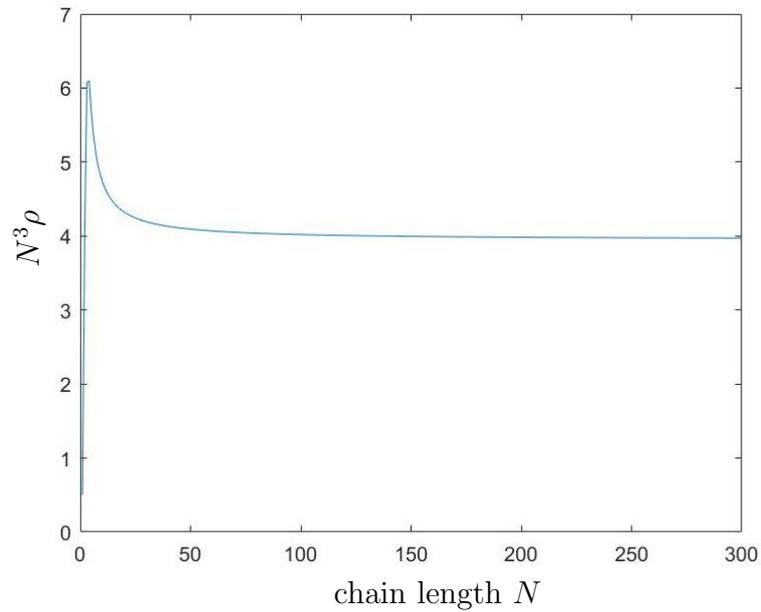


Figure 2.2: Scaled spectral gap as a function of the chain size for pinning coefficient $a = 0$, interaction coefficient $c = 1$ and friction constant $\gamma = 1$. We denote by ρ the spectral gap of the harmonic chain.

Chapter 3

The optimal spectral gap for regular and disordered harmonic networks of oscillators

This chapter is the article published in [BM22] and it is a joint work with Simon Becker.

We consider one-dimensional chains and multi-dimensional networks of harmonic oscillators coupled to two Langevin heat reservoirs at different temperatures. Each particle interacts with its nearest neighbors by harmonic potentials and all individual particles are confined by harmonic potentials, too. In this article, we provide, for the first time, the sharp N dependence of the spectral gap of the associated generator under various physical assumptions and for different spatial dimensions. Our method of proof relies on a new approach to analyze a non self-adjoint eigenvalue problem involving low-rank non-hermitian perturbations of auxiliary discrete Schrödinger operators.

3.1 Introduction

We analyze the dependence of the L^2 -spectral gap of the full Fokker-Planck operator for a classical heat conduction model from non-equilibrium statistical mechanics by using novel ideas from scattering [SZ89] and random matrix theory [FKS97] to reduce it to a non self-adjoint eigenvalue problem involving discrete Schrödinger operators. Even though non self-adjoint eigenvalue problems are often subtle to analyze using perturbative methods, we show that the low-rank nature of the non self-adjoint perturbation allows us to exhibit precise estimates on the behaviour of the spectral gap.

3.1.1 Description of the model

In this article we study the so-called *chain of oscillators*, which is a multi-dimensional model¹ describing heat transport through a configuration of N^d interacting particles, where d is the spatial dimension.

We consider particles labelled according to the sites of a d -dimensional square lattice $[N]^d$, where $[N] := \{1, \dots, N\}$, with *quadratic* nearest neighbour interaction and pinning potentials confining the particles of mass m_i to a lattice structure. Let $\mathbf{m}_{[N]^d} := \text{diag}(m_1, \dots, m_{N^d})$ be the mass matrix, containing the masses m_i of particles $i \in [N]^d$ on the diagonal, and let q_i be the displacement of each particle with respect to their equilibrium position and p_i its momentum. The energy of the oscillator chain is described by a Hamilton function $H : T^*\mathbb{R}^{dN^d} \rightarrow \mathbb{R}$, where $T^*\mathbb{R}^{dN^d}$ is the cotangent bundle denoting physical phase space and can, of course, be identified with \mathbb{R}^{2dN^d} ,

$$\begin{aligned}
 H(\mathbf{q}, \mathbf{p}) &= \frac{\langle \mathbf{p}, \mathbf{m}_{[N]^d}^{-1} \mathbf{p} \rangle}{2} + V_{\eta, \xi}(\mathbf{q}) \quad \text{where} \\
 V_{\eta, \xi}(\mathbf{q}) &= \sum_{i \in [N]^d} \eta_i |q_i|^2 + \sum_{i \sim j} \xi_{ij} |q_i - q_j|^2.
 \end{aligned}
 \tag{1.1}$$

By the symbol \sim , we indicate nearest neighbors on the $[N]^d \subset \mathbb{Z}^d$ lattice and $\eta_i, \xi_{ij} > 0$. The above form of the potential describes particles that are fixed by a quadratic *pinning* potential $U_{\text{pin}, i}(q) = \eta_i |q_i|^2$ and interact through a quadratic *interaction* potential $U_{\text{int}, i \sim j}(q) = \xi_{ij} |q_i - q_j|^2$ for i, j such that $\|i - j\|_\infty = 1$. The quadratic potential models the leading order interaction that pushes the particle back to its equilibrium position. Constants η_i and ξ_{ij} then correspond to twice the *spring constant* in our normalization. The dynamics of this model is such that (some) particles at the boundary on $[N]^d$ are coupled to heat baths at (possibly) different temperatures β^{-1} . Moreover, some particles

¹although in higher dimensions the model is no longer a *chain* of oscillators, but rather a *network*, we shall still use the expression *chain of oscillators* to refer to the model as it was first considered in one dimension and the name *chain of oscillators* has been used pars pro toto.

$i \in \mathcal{F} \subset \partial\{1, \dots, N\}^d$ are subject to friction and we denote by $\gamma_i > 0$, the friction strength at the i -th particle. However, at least for the mathematical analysis of this model, these particles do not have to coincide with the particles that are in contact with the heat bath.

The time evolution is then for particles $i \in \{1, \dots, N\}^d$ described by a coupled system of SDEs:

$$\begin{aligned} dq_i(t) &= \nabla_{p_i} H dt \text{ and} \\ dp_i(t) &= (-\nabla_{q_i} H - \gamma_i p_i \delta_{i \in \mathcal{F}}) dt + \delta_{i \in \mathcal{F}} \sqrt{2m_i \gamma_i \beta_i^{-1}} dW_i \end{aligned} \quad (1.2)$$

where β_i is the inverse temperature at the boundary of the network of oscillators, W_i with $i \in \mathcal{F}$ are iid Wiener processes, $\gamma_i > 0$ a friction parameter, and $\mathcal{F} \subset \{1, \dots, N\}^d$ the set of the particles subject to friction.

For the analysis of one-dimensional chains, we mainly consider friction at both terminal ends, *i.e.* $\mathcal{F} = \{1, N\}$, in which case β_1 and β_N correspond to actual physical inverse temperatures. Our analysis also allows us to study a chain with zero friction at a single end of the chain, this is a scenario that has been considered by Hairer in [Hai09]. In this case, the frictionless end is interpreted to be in contact with an environment at infinite temperature. Thus, the inverse temperature at the frictionless end no longer corresponds to a physical temperature.

The solution to the above system of SDEs (1.2) forms a Markov process, and can thus be equivalently described by a strongly continuous semigroup $P_t f(z) := \mathbb{E}_z(f(p_t, q_t))$ where $(p_t, q_t) \in \mathbb{R}^{2N^d}$ solve the system of SDEs (1.2). Its generator is given by

$$\mathcal{L}f(z) = -\langle z, M_{[N]^d} \nabla_z f(z) \rangle + \langle \nabla_p, \Gamma \mathbf{m}_{[N]^d} \vartheta \nabla_p f(z) \rangle \quad (1.3)$$

where $M_{[N]^d} \in \mathbb{C}^{2N^d \times 2N^d}$, the matrix in the drift part of the above generator, and $\Gamma \in \mathbb{R}^{N^d \times N^d}$, the matrix containing the friction parameters, are matrices of the form

$$\begin{aligned} M_{[N]^d} &:= \begin{pmatrix} \Gamma & -\mathbf{m}_{[N]^d}^{-1} \\ B_{[N]^d} & 0 \end{pmatrix} \text{ and} \\ \Gamma &= \text{diag}(\gamma_{(1,\dots,1)} \delta_{(1,\dots,1) \in \mathcal{F}}, \gamma_{(2,1,\dots,1)} \delta_{(2,1,\dots,1) \in \mathcal{F}}, \dots, \gamma_{(N,\dots,N)} \delta_{(N,\dots,N) \in \mathcal{F}}). \end{aligned}$$

The matrix ϑ containing the temperatures is of the form

$$\vartheta = \text{diag}(\beta_{(1,\dots,1)}^{-1} \delta_{(1,\dots,1) \in \mathcal{F}}, \dots, \beta_{(N,\dots,N)}^{-1} \delta_{(N,\dots,N) \in \mathcal{F}}).$$

Defining for $i, j \in [N]^d$ self-adjoint operators $\langle u, L_{i,j} u \rangle_{\ell^2([N]^d; \mathbb{C})} := |u(i) - u(j)|^2$ that

decompose the negative weighted Neumann Laplacian on $\ell^2([N]^d; \mathbb{C})$ as

$$-\Delta_{[N]^d} = \sum_{i \sim j} \xi_{ij} L_{i,j},$$

we can identify the matrix $B_{[N]^d} \in \mathbb{R}^{N^d \times N^d}$ appearing in $M_{[N]^d}$ with a Schrödinger operator

$$B_{[N]^d} = -\Delta_{[N]^d} + \sum_{i \in [N]^d} \eta_i \delta_i \tag{1.4}$$

where $(\delta_i(u))(j) = u(i)\delta_{ij}$. The operator $B_{[N]^d}$ reduces in one dimension, i.e. $d = 1$, to the Jacobi (tridiagonal) matrix

$$(B_{[N]}f)_n = -\xi_{n,n+1}f_{n+1} - \xi_{n-1,n}f_{n-1} + (\eta_n + \xi_{n,n+1} + \xi_{n-1,n})f_n.$$

with the convention that $\xi_{0,1} = \xi_{N,N+1} = 0$.

3.1.2 State of the art and motivation

The (multi-dimensional) chain of oscillators is a non-equilibrium statistical mechanics model initially introduced to study heat transport in media. It was first introduced for the rigorous derivation of Fourier's law, or a rigorous proof of its breakdown: this is well described in several overview articles on the subject: [BLRB00], [Lep16, Dha08] and [FB19]. The linear (harmonic) case was the first to be studied in [RLL67], where the non equilibrium steady state (NESS) was explicitly constructed and the behavior of the heat flux analyzed as well, leading (as expected) to the breakdown of Fourier's law. For results regarding on chains with anharmonic potentials, we refer the reader to [EPRB99a, EPRB99b, EH00] where existence and uniqueness of stationary states was studied and to [RBT02, Car07] where exponential convergence towards the NESS has been proved. Regarding the existence, uniqueness of a NESS and exponential convergence towards it in more complicated anharmonic d -dimensional networks of oscillators (not only for square lattices) see [CEHRB18]. In [Raq19, Men20] bounded perturbations of the harmonic chain are discussed. Note also that short chains of rotors with Langevin thermostats have been studied in [CP17, CEP15]. In the articles [HM09, Hai09] some negative results are presented, *i.e.* lack of spectral gap, in cases where the pinning potential is stronger than the coupling one.

The main motivation of this article is to find the exact scaling of the spectral gap of the associated generator of the dynamics as defined above, in terms of the number of the particles. Quantitative results in this sense are missing from the literature and even in the simplest cases for the chain of oscillators, *i.e.* the linear (harmonic) chains, the dependence on the dimension of the spectral gap has been open. Attempts have been made

through hypocoercive techniques to get N -dependent estimates under certain assumptions on the potentials: see the discussion in [Vil09a, Section 9.2] where this question was first raised. The techniques discussed in Villani’s monograph however only yield rather far from optimal estimates on the spectral gap in terms of the system size. To the authors’ knowledge, the only relevant result so far that gives a polynomial lower bound on the spectral gap for the same model (homogeneous with a weak N -dependent anharmonicity) is [Men20]. Hypocoercive techniques used in that article provide a polynomial lower bound on the spectral gap and upper bounds on the prefactors in front of the exponential that determine the exponential rate of the convergence.

Here we give the sharp upper and lower bounds on the scaling of the spectral gap. In this article we not only cover homogeneous networks of oscillators, but also randomly perturbed pinning potentials or pinning potentials perturbed by single impurities. In addition, our techniques also apply to other scenarios apart from the classical one-dimensional model, in particular it gives scalings for d -dimensional square network cases. These results seem to be the first of their kind.

Microscopic properties and heat transport. Before stating our main results, we want to mention results on the macroscopic heat transport of the chain of oscillators, *e.g.* heat conductivity, and how such properties are determined from microscopic properties of the system. In particular, we would like to highlight which microscopic properties affect the heat transport and which determine the asymptotic behaviour of the spectral gap.

It has been suggested by [CL71] that, for an infinite one-dimensional chain the absolutely continuous part of the spectrum of the Schrödinger operator (1.4), *i.e.* the *metallic part* of the spectrum, leads to infinite conductivity. In the specific example of the homogeneous chain, where there is only absolutely continuous spectrum in the limit, it is well-known that the conductivity is infinite (Fourier’s law doesn’t hold) [RLL67]. Note also that the behavior of the flux does not depend on the dimensionality of the system, see [R.H71] for 2 dimensions. However, in disordered harmonic chains (DHC) with random masses, where all eigenstates of the discrete Schrödinger operator are localized, the heat flux vanishes as $N \rightarrow \infty$ almost surely, see [CL71, RG71, OL74].

First studies of the behaviour of the heat currents in a one-dimensional DHC were done in [CL71, RG71]. In particular, in [RG71] the heat baths are semi infinite harmonic chains distributed according to their equilibrium Gibbs measures at temperatures T_L, T_R (free boundaries). In this case, $\mathbb{E}(J_N) \gtrsim N^{-1/2}$, where $\mathbb{E}(\cdot)$ denotes the expectation over the masses. That $\mathbb{E}(J_N) \sim N^{-1/2}$ was proved a bit later in [Ver79], showing that Fourier’s law does not hold in this model of DHC. Results regarding heat baths coupled at both ends with Ornstein-Uhlenbeck terms with fixed boundaries, *i.e.* $q_0 = q_{N+1} = 0$, was first done in [CL71]. A rigorous proof of $\mathbb{E}(J_N) \sim (\Delta T)N^{-3/2}$ was given in [AH11]. The limiting

behaviour of the heat flux in both of these models is also discussed in [Dha01]. Localization effects of the discrete Schrödinger operator enter also in the study of mean-field limits for the harmonic chain [BHO19].

Our new approach shows that the spectral gap of the generator to (1.2) is determined by the decay rate of eigenstates of the discrete Schrödinger operator (1.4), under a constraint on the level-spacing between its eigenvalues. The Schrödinger operator is given as

$$(B_{[N]^d}f)_i = (-\Delta_{[N]^d}f)_i + \eta_i f_i, \text{ where } f = (f_i)_{i \in [N]^d},$$

and fully defined in terms of masses and the potential strengths. In particular, our results indicate that the presence of exponentially localized eigenstates in the discrete Schrödinger operator, *i.e.* the *insulating part* of the spectrum, causes an exponentially fast closing of the spectral gap. In contrast to this, if the discrete Schrödinger operator possesses only extended states, the spectral gap again decays to 0 as N tends to infinity but this time only at a polynomial rate. Both results only hold under a pressure condition on the eigenvalues.

The above results show that single impurities which correspond to rank one perturbations in the discrete Schrödinger operator should not affect the heat conductivity but do affect the spectral gap. Put differently, heat transport is an effect that is governed by all the modes of the system whereas the spectral gap is -in general- only determined by a single extremizing mode of the Schrödinger operator.

3.1.3 Main results

We study the spectral gap for three scenarios describing fundamentally different physical settings:

- For a homogeneous model with the same physical parameters for every particle (the associated Schrödinger operator possesses only extended states in the limit $N \rightarrow \infty$), Fig. 3.1,
- for a model with a sufficiently strong impurity in the pinning potential of a single particle (the Schrödinger operator possesses both extended and exponentially localized states in the limit $N \rightarrow \infty$), Fig. 3.2, and
- for a model with disordered pinning potential (the Schrödinger operator has only exponentially localized eigenstates in the limit $N \rightarrow \infty$ for $d = 1$, this is also conjectured to be true for $d = 2$, and is conjectured to have both exponentially localized and extended states in dimensions $d \geq 3$), Fig. 3.3. In this article, however, we only use the existence of some localized states.

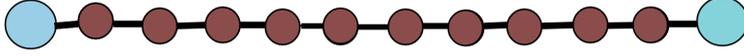


Figure 3.1: Homogeneous chain: Spectral gap $\mathcal{O}(N^{-3})$.

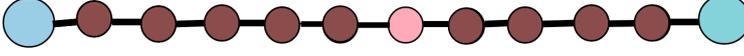


Figure 3.2: Chain with impurity: Spectral gap $\mathcal{O}(e^{-cN})$.

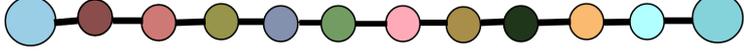


Figure 3.3: Disordered chain: Spectral gap $\mathcal{O}(e^{-cN})$.

Figure 3.4: The one-dimensional chain of oscillators connected to heat baths (big discs) and with various pinning potentials (differently coloured discs indicate different pinning strengths).

Our main results on the N -dependence of the spectral gap of the d -dimensional harmonic chain are summarized in the following theorem:

Theorem 1.1. *Let the positive masses and interaction strengths of all oscillators coincide, N^d be the number of oscillators, placed in a square grid with N oscillations on each side, and d the dimension of the network. If all the friction parameters for all oscillators does not grow faster than the number of boundary particles, i.e. $\sup_{i \in \mathcal{F} \subset \partial[N]^d} \gamma_i \leq \mathcal{O}(N^{d-1})$, the spectral gap of the chain of oscillators decays always as a function of N . In particular,*

- (Homogeneous chain): *Let the pinning strength be the same for all oscillators, then*
 1. *if two particles located at the corners $(1, \dots, 1), (N, \dots, N)$, see Fig. 3.6, are exposed to the same non-zero friction and non-zero diffusion, the spectral gap of the generator satisfies*

$$\lambda_S = \mathcal{O}(N^{-3d}).$$

In particular for the one-dimensional chain of oscillators $\lambda_S = \mathcal{O}(N^{-3})$.

2. *if the same non-zero friction and non-zero diffusion for particles located at the center of two opposite edges of the network*

$$(1, \lceil N/2 \rceil, \dots, \lceil N/2 \rceil), (N, \lceil N/2 \rceil, \dots, \lceil N/2 \rceil),$$

see Fig. 3.7, the spectral gap of the generator satisfies $\lambda_S = \mathcal{O}(N^{-3-(d-1)})$.

3. *if $d = 2$ and the particles exposed to the same non-zero friction are located at opposite edges of the network, the spectral gap satisfies $\lambda_S = \mathcal{O}(N^{-5/2})$.*

- (Chain with impurity): *Let N be even. We assume that all masses and interaction parameters are positive and coincide and the friction parameters γ_i of the boundary*

articles

$$\partial[N]^d := \{i \in [N]^d; \exists i_n : i_n \in \{1, N\}\} \text{ of } [N]^d := \{1, \dots, N\}^d$$

satisfy $\sup_{i \in \partial[N]^d} \gamma_i \in (0, c)$ where c is independent of N and the friction is non-zero on at least one boundary edge. Then, if the pinning strength $\eta_{c_d(N)}$ at the center point $c_d(N) = (N/2, \dots, N/2)$ of the network is sufficiently small compared to the pinning strength of all other oscillators, then the spectral gap λ_S of the generator closes exponentially fast in the number of oscillators, for all $d \geq 1$.

- (Disordered chain): We assume that all masses and interaction parameters are positive and coincide and the friction parameters γ_i of the particles at the boundary

$$\partial[\pm N]^d := \{i \in [\pm N]^d; \|i\|_\infty = N\} \text{ of the network } [\pm N]^d := \{-N, \dots, N\}^d$$

satisfy $\sup_{i \in \partial[\pm N]^d} \gamma_i \in (0, c)$ where c is independent of N and the friction is non-zero on at least one boundary edge. Then, if the pinning strengths are iid random variables according to some compactly supported density $\rho \in C_c(0, \infty)$, the spectral gap λ_S of the generator decays exponentially fast in the number of oscillators, for all $d \geq 1$ for all but finitely many N .

Our findings in Theorem 1.1 are illustrated in one spatial dimension in Figure 3.5.

Open questions.

- While we fully settle the scaling of the spectral gap for one-dimensional oscillator chains, and for many grid-type configurations in higher dimensions, the scaling of the spectral gap for many physically relevant configurations in higher dimensions remains open. Although our method of proof still applies to such configurations as well, the necessary estimates seem to become rather intricate, cf. the discussion below Proposition 3.6.
- It would be interesting to study the behavior of the spectral gap in terms of the dimension of the system in the oscillator chains for more general classes of pinning and interaction potentials, *i.e.* for example for potentials, as studied in [EH00, Ass. 1 and 2]. As a first step, one might consider quartic corrections to the potential in (1.1). While this analysis cannot be reduced to a Schrödinger operator in that case, we still believe the connection between decay properties of (generalized) eigenstates of the symmetric part of the operator and the scaling of the spectral gap to persist.
- Moreover, apart from considering different kinds of potentials, one can study different kind of noises as well, [Raq19, NR], where quantitative rates of convergence are not available, so far.

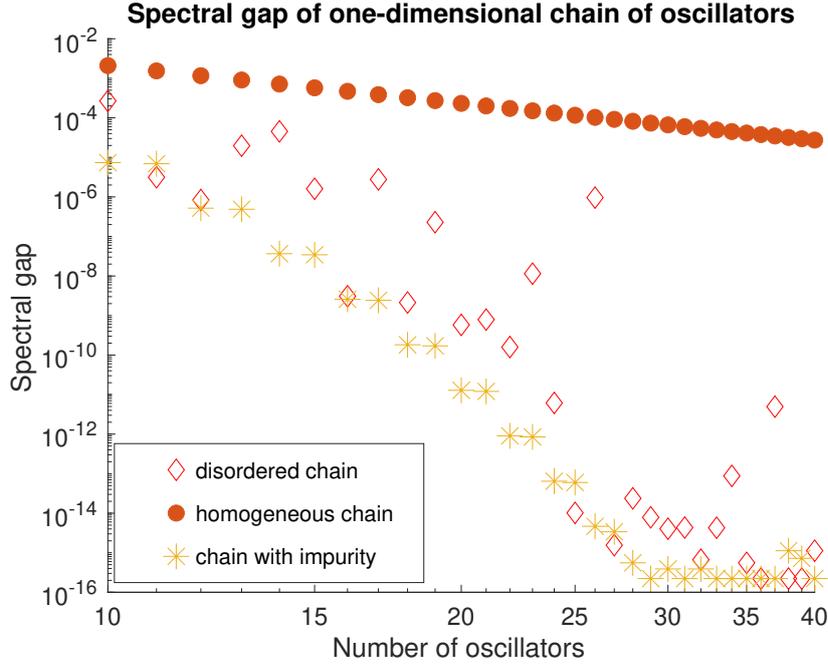


Figure 3.5: Log-log plot of the spectral gap for the one-dimensional chain of oscillators for all three cases considered in Theorem 1.1. The impurity is modeled by choosing a pinning strength $\eta_i = 10$ for all oscillators i apart from the one in the center for which we choose $\eta_{N/2} = 5$. The disorder potential is of the form $V_\omega(n) = 1 + X_n$ where $X_n \sim U(0, 1)$ are i.i.d. uniformly distributed.

- It would also be interesting to extend our analysis to more complicated geometries such as different lattice structures. We expect comparable bounds to the integer lattice, but due to the non-explicit structure of the spectral decomposition of the Laplacian, the analysis of such geometries is presumably more intricate.

Notation. We write $f(z) \leq \mathcal{O}(g(z))$ to indicate that there is $C > 0$ such that $|f(z)| \leq C|g(z)|$ and $f(z) = \mathcal{o}(g(z))$ for $z \rightarrow z_0$ if there is for any $\varepsilon > 0$ a neighbourhood U_ε of z_0 such that $|f(z)| \leq \varepsilon|g(z)|$. Instead of writing $f(z) \leq \mathcal{O}(g(z))$, we sometimes also write $f(z) \lesssim g(z)$. Finally, we introduce the notation $[N] := \{1, \dots, N\}$ and

$$\partial[N]^d := \left\{ i = (i_1, \dots, i_d) \in [N]^d; \|i\|_\infty = N \text{ or } \min_{n \in [d]} i_n = 1 \right\}.$$

The eigenvalues of a self-adjoint matrix A shall be denoted by $\lambda_1(A) \leq \dots \leq \lambda_N(A)$. We also employ the Kronecker delta where $\delta_{n \in I} = 1$ if $n \in I$ and zero otherwise. The inner product of two vectors $x, y \in \mathbb{R}^m$ is denoted by $\langle x, y \rangle$.

3.2 Mathematical preliminaries

For our purposes, it is sometimes favorable to consider also another form, which we obtain upon performing the following change of variables

$$\tilde{p} = \mathbf{m}_{[N]^d}^{-1/2} p, \quad \tilde{q} := \sqrt{B_{[N]^d} q}.$$

This is an isomorphic change of variables if and only if all masses and interaction strength are strictly positive. In the new coordinates, the generator becomes

$$\begin{aligned} \mathcal{L} &= \langle \tilde{p}, \mathbf{m}_{[N]^d}^{-1/2} B_{[N]^d}^{1/2} \nabla_{\tilde{q}} \rangle - \langle \tilde{q}, B_{[N]^d}^{1/2} \mathbf{m}_{[N]^d}^{-1/2} \nabla_{\tilde{p}} \rangle - \langle \tilde{p}, \Gamma \nabla_{\tilde{p}} \rangle + \langle \nabla_{\tilde{p}}, \Gamma \Theta \nabla_{\tilde{p}} \rangle \\ &= -\langle \tilde{z}, \Omega_{[N]^d} \nabla_{\tilde{z}} \rangle + \langle \nabla_{\tilde{p}}, \Gamma \Theta \nabla_{\tilde{p}} \rangle \end{aligned} \quad (2.5)$$

where

$$\Omega_{[N]^d} := \begin{pmatrix} \Gamma & -\mathbf{m}_{[N]^d}^{-1/2} B_{[N]^d}^{1/2} \\ B_{[N]^d}^{1/2} \mathbf{m}_{[N]^d}^{-1/2} & 0 \end{pmatrix}. \quad (2.6)$$

The following Proposition identifies the optimal exponential rate of convergence, and thus the spectral gap, to the NESS for Ornstein–Uhlenbeck operators. This result was first proved, to our knowledge by [MPP02]. Here we state a version given in [AE, Mon19]:

Proposition 2.1 (Proposition 13 in [Mon19], Theorems 4.6 and 6.1 in [AE], Theorem 2.16 in [AAS15]). *Let the generator of an Ornstein-Uhlenbeck process given by*

$$Lf(z) = -\langle (Bz), \nabla_z f(z) \rangle + \operatorname{div}(D\nabla_z f)(z), \quad z \in \mathbb{R}^d \quad (2.7)$$

under the assumptions that

1. *There is no non-trivial subspace of $\ker D$ that is invariant under B^T*
2. *All eigenvalues of the matrix B have positive real part (B is positively stable).*

Let $\rho := \inf\{\operatorname{Re}(\lambda) : \lambda \in \operatorname{Spec}(B)\} > 0$ and let m , that possibly depends on N , be the maximal dimension of the Jordan block of B that corresponds to an eigenvalue λ of B such that $\operatorname{Re}(\lambda) = \rho$.

Then there is a unique invariant measure μ and constant $c > 0$ so that, regarding the long time behaviour of the process with generator (2.7),

$$c^{-1}(1 + t^{2(m-1)})e^{-2\rho t} \leq \|P_t - \mu\|^2 \leq ce^\rho(1 + t^{2(m-1)})e^{-2\rho t}, \quad t \geq 1$$

where $\|P_t - \mu\| := \sup_{\|f\|_{L^2(\mu)}=1} \|(P_t - \mu)f\|_{L^2(\mu)}$.

Therefore, both the exponential rate given by ρ is and the power $(1 + t^{2(m-1)})$ are

optimal. Now if we define for every $\epsilon \in (0, \rho)$,

$$C_{\epsilon, N} := \sup_{t>0} e^{-2\epsilon t} (1 + t^{2(m-1)})$$

we have

$$(1 + t^{2(m-1)})e^{-2\rho t} \leq C_{\epsilon, N}e^{-2(\rho-\epsilon)t}.$$

Note that since m can depend on N , $C_{\epsilon, N}$ depends on N , too. The exponential rate and more generally the estimates of the relaxation time, is due to the drift part of the operator, whereas the hypoellipticity condition is used to ensure us for the existence of a unique invariant measure μ (in [AE, Lemma 3.2] it is established that the invariant measure is in general a non-isotropic Gaussian measure. See also [RLL67] where they find an explicit form of this stationary measure having as motivation to study properties of the NESS of the harmonic oscillators chains.)

We finally would like to mention that such a result holds in relative entropy as well [Mon19].

The above Proposition 2.1 applies to the chain of oscillators as well, where B is just $\Omega_{[N]^d}^T$ in (2.5). Conditions (1) and (2) are satisfied, once we assume there is diffusion and friction, i.e. $\mathcal{F} \neq \emptyset$, since this condition is equivalent to the hypoellipticity of $\partial_t - L$ [Hö7, §1]. Also $\Omega_{[N]^d}$ satisfies condition (ii), see [JPS17, Lemma 5.1], for more details see the Appendix 3.A. Since we don't know if our matrix $\Omega_{[N]^d}$ is diagonalizable, $C_{\epsilon, N}$ here depends possibly on N and when considering the worst case we have a dependence of order $t^{2(N-1)}$ on the right hand side. Then applying Proposition 2.1 in our case we get

$$2c^{-1}e^{-2\rho t} \leq \|P_t - \mu\|^2 \leq ce^\rho(1 + t^{2(N^d-1)})e^{-2\rho t}.$$

To summarize the discussion of this Section: The spectral gap λ_S of the generator of the N -particle dynamics (2.5) is precisely given by

$$\lambda_S := \inf\{\operatorname{Re}(\lambda) : \lambda \in \operatorname{Spec}(\Omega_{[N]^d})\} = \inf\{\operatorname{Re}(\lambda) : \lambda \in \operatorname{Spec}(M_{[N]^d})\}.$$

We record some simple observations about the behaviour of the spectral gap in the following Proposition:

Proposition 2.2. *For the harmonic network of oscillators the following properties hold:*

1. *The characteristic polynomial of $M_{[N]^d}$ satisfies $\det(M_{[N]^d} - \lambda \operatorname{id}) = \det(\lambda^2 - \lambda\Gamma + \mathbf{m}_{[N]^d}^{-1}B_{[N]^d}) = 0$. In particular, the matrix $M_{[N]^d}$ is invertible if and only if $B_{[N]^d}$ is invertible.*

2. If there is the same non-zero friction at every oscillator, i.e. $\Gamma = \gamma \text{id}_{[N]^d}$, $\mathcal{F} = [N^d]$, and $\inf_{N \in \mathbb{N}} \inf_{\lambda \in \text{Spec}(\mathbf{m}_{[N]^d}^{-1} B_{[N]^d})} \lambda > 0$ then the chain of oscillators has a spectral gap that is uniform in the number of oscillators. In particular, if all masses and coupling strength η, ξ coincide and are non-zero, then we have $\inf_{N \in \mathbb{N}} \inf_{\lambda \in \text{Spec}(\mathbf{m}_{[N]^d}^{-1} B_{[N]^d})} \lambda > 0$.
3. The spectral gap of the generator (1.3) decays at least with rate $\mathcal{O}(N^{-1})$ if the friction parameters at particles on the boundary $\partial[N]^d$ of the particle configuration $[N]^d$ does not grow faster than the number of boundary particles, i.e. $\sup_{i \in \mathcal{F} \subset \partial[N]^d} \gamma_i \leq \mathcal{O}(N^{d-1})$.
4. Let $1 \in \mathcal{F} \subset \{1, N\}$ be the left terminal end of a one-dimensional chain, i.e. $d = 1$, with universal (independent of the size of the chain) friction parameters $\gamma_1 > 0, \gamma_N \geq 0$. If all oscillators have the same mass and there are constants $c_1, c_2 > 0$ such that $c_1 < \xi_{i,j}, \eta_i < c_2$ for all N , then the spectral gap of (1.3) does not decay faster than e^{-cN} for some $c > 0$.

Proof. (1): The determinant formula follows from general properties of block matrices. By setting $\lambda = 0$ it follows that $M_{[N]^d}$ is invertible if and only if $\mathbf{m}_{[N]^d}^{-1} B_{[N]^d}$ is invertible.

(2): If $\mathcal{F} = [N^d]$ and $\Gamma = \gamma I$ then $\det(\lambda^2 - \gamma\lambda + \mathbf{m}_{[N]^d}^{-1} B_{[N]^d}) = 0$ is equivalent to solving $\lambda^2 - \gamma\lambda + \mu = 0$ where $\mu \in \text{Spec}(\mathbf{m}_{[N]^d}^{-1} B_{[N]^d})$. Now as the product of two positive definite matrices, $\mathbf{m}_{[N]^d}^{-1} B_{[N]^d}$ has again positive eigenvalues. Thus, all solution to this equation have their real part bounded away from zero.

(3): is a consequence of the identity

$$\sum_{\lambda \in \text{Spec}(M_{[N]^d})} \text{Re}(\lambda) = \text{tr}(M_{[N]^d}) = \text{tr}(\Gamma).$$

Since we have $2N^d$ (counting multiplicity) positive terms that all satisfy $\text{Re}(\lambda) \geq 0$ where $\lambda \in \text{Spec}(M_{[N]^d})$, and by assumption $\text{tr}(\Gamma) \leq \mathcal{O}(N^{d-1})$, we conclude that $\lambda_S \leq \mathcal{O}(N^{-1})$: Indeed we write

$$\sum_{\lambda \in \text{Spec}(M_{[N]^d})} \text{Re}(\lambda) \geq (2N^d) \inf\{\text{Re}(\lambda) : \lambda \in \text{Spec}(M_{[N]^d})\} = \mathcal{O}(N^{d-1})$$

and thus

$$\lambda_S = \inf\{\text{Re}(\lambda) : \lambda \in \text{Spec}(M_{[N]^d})\} \leq \mathcal{O}(N^{-1}).$$

(4): We introduce the transfer matrix [Tes00, (1.29)]

$$A_j(\lambda) = \begin{pmatrix} \frac{\lambda^2 - (\xi_{i,i+1} + \xi_{i+1,i+2} + \eta_{i+1})}{\xi_{i+1,i+2}} & -\frac{\xi_{i,i+1}}{\xi_{i+1,i+2}} \\ 1 & 0 \end{pmatrix}. \quad (2.8)$$

Thanks to the tridiagonal and symmetric form of B_N , the transfer matrix (2.8) allows us to write the solution to $(B_N + \lambda^2)u = 0$ inductively as

$$\begin{pmatrix} u_{i+1} \\ u_i \end{pmatrix} = \prod_{j=i-1}^1 A_j(\lambda) \begin{pmatrix} u_2 \\ u_1 \end{pmatrix}.$$

This way, $\|(u_{i+1}, u_i)^T\| \leq C^{i-1} \|(u_2, u_1)^T\|$ with boundary conditions

$$u_2 = \frac{\eta_1 + \xi_{1,2} - \lambda^2}{\xi_{1,2}} u_1 \text{ and } u_{N-1} = \frac{\eta_N + \xi_{N-1,N} - \lambda^2}{\xi_{N-1,N}} u_N.$$

and where $C = \sup_j \|A_j\|$. The boundary conditions can be obtained from solving $(B_N u)(1) + \lambda^2 u(1) = 0$ and $(B_N u)(N) + \lambda^2 u(N) = 0$.

Let $\lambda \in \text{Spec}(M_{[N]})$ with $\text{Re}(\lambda) = \lambda_S$, then there is u normalized such that

$$(\mathbf{m}_N^{-1} B_N + \lambda^2)u = \lambda \Gamma u.$$

Then, by taking the inner-product with u again:

$$\langle (\mathbf{m}_N^{-1} B_N + \lambda^2)u, u \rangle = \lambda \langle \Gamma u, u \rangle. \quad (2.9)$$

We can assume without loss of generality that $\Im(\lambda) \neq 0$, as

$$\langle \mathbf{m}_N^{-1} B_N u, u \rangle \geq m^{-1} c_1 > 0,$$

where m is the mass of the particles. Thus, there can be no real solution $\lambda = \mathcal{O}(e^{-cN})$ for N sufficiently large to (2.9). Now, since the real and the imaginary parts on both sides should be the same, we write for the imaginary part $\Im(\lambda^2) = \Im(\lambda) \sum_{i \in \mathcal{F}} \gamma_i |u_i|^2$. Writing then $\lambda = \lambda_S + i\Im(\lambda)$ yields

$$\lambda_S = \sum_{i \in \mathcal{F}} \gamma_i \frac{|u_i|^2}{2} \geq \frac{\gamma_1 |u_1|^2}{2}. \quad (2.10)$$

Since u is normalized this implies, using also (2.10), that

$$1 = \sum_{i=1}^N |u_i|^2 \leq C_1^{2N} |u_1|^2 \leq 2 \frac{C_1^{2N}}{\gamma_1} \lambda_S$$

which implies the claim as we assumed that there is friction at the first particle. \square

Remark 2.3. *The artificial case (2), in which we assume friction at every particle, and the result in (3) show that it is the sub-dimensionality of the particles experiencing friction*

that causes the spectral gap to close for almost all configurations of the chain of oscillators.

3.3 Proofs of the main results

3.3.1 Reduction method from scattering theory

In a preliminary step, we harness the low-rank character of the perturbation and reduce the study of the spectral gap to an auxiliary problem.

The following Lemma reduces the dimension of the spectral analysis of $\Omega_{[N]^d} \in \mathbb{C}^{2N^d \times 2N^d}$, which determines the spectral gap of the generator (2.5), to an equivalent problem for a low-dimensional *Wigner matrix* $W_{\mathcal{F}} \in \mathbb{C}^{|\mathcal{F}| \times |\mathcal{F}|}$ and connects the low-dimensional Wigner matrix to the eigenvectors of the off-diagonal blocks of Ω_N . For more background on this method, that originates from scattering theory, we refer to [SZ89]. We apply it here to study the spectra of low-rank perturbations, due to friction at the boundary oscillators, of the Hamiltonian system.

Lemma 3.1 (Low-rank perturbations). *Let B be a self-adjoint matrix on \mathbb{C}^{N^d} with eigenvalues λ_j and eigenvectors v_j and consider the matrix $\mathcal{A} = i\Omega = \mathcal{A}_0 + i\hat{\Gamma}$ with $\hat{\Gamma} := \text{diag}(\Gamma, 0_{\mathbb{C}^{N^d \times N^d}})$ where $\mathcal{A}_0 = \begin{pmatrix} 0 & -iB \\ iB & 0 \end{pmatrix}$. We then have that for $\lambda \in \mathbb{R} \setminus \text{Spec}(B) \cup \text{Spec}(-B)$,*

$$\lambda \in \text{Spec}(\mathcal{A}) \quad \text{if and only if} \quad -i \in \text{Spec}(W_{\mathcal{F}}(\lambda))$$

with

$$W_{\mathcal{F}}(\lambda) = \sum_{\mu \in \pm \text{Spec}(B)} (\lambda - \mu)^{-1} \sum_{i_1, i_2 \in \mathcal{F}} \alpha_{i_1, i_2}(\mu) \pi_{i_1, i_2}^{|\mathcal{F}|} \quad (3.11)$$

for rank one operators $\pi_{i_1, i_2}^{|\mathcal{F}|} := e_{i_1}^{|\mathcal{F}|} \otimes e_{i_2}^{|\mathcal{F}|}$ and matrix-elements

$$\alpha_{i_1, i_2}(\mu = \pm \lambda_j) := \sqrt{\gamma_{i_1} \gamma_{i_2}} \langle V_j^{\pm}, e_{i_1}^{2N^d} \rangle \langle e_{i_2}^{2N^d}, V_j^{\pm} \rangle,$$

with $V_j^{\pm} = \frac{1}{\sqrt{2}}(v_j, \pm i v_j)^T$.

Proof. We introduce matrices $A_{\mathcal{F}} = \left\{ \sqrt{\gamma_a} e_a^{2N^d}(i) \right\}_{i \in [2N^d], a \in \mathcal{F}} \in \mathbb{C}^{2N^d \times |\mathcal{F}|}$ and then have that the friction matrix is given by $\hat{\Gamma} = A_{\mathcal{F}} A_{\mathcal{F}}^*$.

The Wigner $W_{\mathcal{F}}$ -matrix is defined, for $\lambda \notin \pm \text{Spec}(B)$, as

$$W_{\mathcal{F}}(\lambda) := A_{\mathcal{F}}^*(\lambda - \mathcal{A}_0)^{-1} A_{\mathcal{F}} \in \mathbb{C}^{|\mathcal{F}| \times |\mathcal{F}|}.$$

We then obtain from properties of the determinant, and Sylvester's determinant identity,

applied in the second line, that

$$\begin{aligned}
\det(\mathrm{id}_{|\mathcal{F}|} - iW_{\mathcal{F}}(\lambda)) &= \det(\mathrm{id}_{|\mathcal{F}|} - iA_{\mathcal{F}}^*(\lambda - \mathcal{A}_0)^{-1}A_{\mathcal{F}}) \\
&= \det(\mathrm{id}_{\mathbb{C}^{2N^d}} - i(\lambda - \mathcal{A}_0)^{-1}\hat{\Gamma}) \\
&= \det((\lambda - \mathcal{A}_0)^{-1}(\lambda - \mathcal{A}_0 - i\hat{\Gamma})) \\
&= \det((\lambda - \mathcal{A}_0)^{-1}) \det(\lambda - \mathcal{A}).
\end{aligned}$$

Rearranging this identity shows that

$$0 = \det(\lambda - \mathcal{A}) = \det(\lambda - \mathcal{A}_0) \det(\mathrm{id}_{|\mathcal{F}|} - iW_{\mathcal{F}}(\lambda)). \quad (3.12)$$

Thus, all eigenvalues λ of the high-dimensional matrix \mathcal{A} coincide with values λ for which $-i \in \mathrm{Spec}(W_{\mathcal{F}}(\lambda))$. The eigenvectors of \mathcal{A}_0 are given by $V_j^{\pm} = \frac{1}{\sqrt{2}}(v_j, \pm i v_j)^T$ where v_j are eigenvectors of B to eigenvalues λ_j . From spectral decomposition then we write

$$W_{\mathcal{F}}(\lambda) = \sum_{\pm} \sum_{j=1}^{N^d} (\lambda \mp \lambda_j)^{-1} \sum_{i_1, i_2 \in \mathcal{F}} \sqrt{\gamma_{i_1} \gamma_{i_2}} \langle V_j^{\pm}, e_{i_1}^{2N^d} \rangle \langle e_{i_2}^{2N^d}, V_j^{\pm} \rangle e_{i_1}^{|\mathcal{F}|} \otimes e_{i_2}^{|\mathcal{F}|}.$$

This expression coincides with the one given in the statement of the Lemma for $W_{\mathcal{F}}$. \square

Remark 3.2 (Normalization of masses). *In the sequel we assume in our statements that the masses do all coincide and to simplify the notation, we just take them to be equal to one.*

3.3.2 One-dimensional homogeneous chain

We first study the behaviour of a one-dimensional chain of oscillators that consists of particles with the same physical properties. The limiting discrete Schrödinger operator B_{∞} possesses only absolutely continuous spectrum, by standard properties of the discrete Laplacian, and we find a polynomially fast rate for the closing of the spectral gap:

Proposition 3.3 (One-dimensional Homogeneous chain). *Let all pinning and interaction parameters $\eta_i > 0$, $\xi_{ij} > 0$ of the potentials, and masses m_i coincide, respectively and assume that there is at least one particle with non-zero friction $\gamma > 0$ and diffusion at at least one of the terminal ends of the chain. The spectral gap of the harmonic chain of oscillators satisfies $\lambda_S = \mathcal{O}(N^{-3})$.*

Proof. The eigenvectors to the root of the discrete Schrödinger operator $\sqrt{B_N}$, defined in

(1.4), coincide with the eigenvectors to the discrete Laplacian and are just given by

$$v_i(j) = \begin{cases} N^{-\frac{1}{2}} & , i = 1 \\ \sqrt{\frac{2}{N}} \cos\left(\frac{\pi(i-1)(j-\frac{1}{2})}{N}\right) & , \text{otherwise} \end{cases} \quad (3.13)$$

with eigenvalues

$$\lambda_j(\sqrt{B_N}) = \sqrt{4\xi \sin^2\left(\frac{\pi(j-1)}{2N}\right) + \eta}, \text{ for } j \in [N]$$

of $\sqrt{B_N}$. We also define the quantities $\lambda_{-j}(\sqrt{B_N}) := -\lambda_j(\sqrt{B_N})$ and vectors $v_{-j} := v_j$ for $j \in [N]$.

Step 1-Eigenvalue estimates. To start with, we define the differences of all the eigenvalues $\lambda_j(\sqrt{B_N})$ from the largest N -th eigenvalue $\lambda_N(\sqrt{B_N})$:

$$\mu_j := \lambda_j(\sqrt{B_N}) - \lambda_N(\sqrt{B_N}), \quad j \in \pm[N]$$

and we show that the differences μ_j are lower bounded. Indeed we observe that by Taylor expansion we have

$$|\sqrt{4\xi + \eta} - \lambda_j(\sqrt{B_N})| \lesssim |\lambda_N(\sqrt{B_N}) - \lambda_j(\sqrt{B_N})| \quad (3.14)$$

for $j \leq N - 1$, such that by using this estimate in the second line:

$$\begin{aligned} \mu_j^{-1} &= \frac{|\lambda_j(\sqrt{B_N}) + \lambda_N(\sqrt{B_N})|}{|\lambda_j(\sqrt{B_N})^2 - \lambda_N(\sqrt{B_N})^2|} \lesssim |\lambda_j(\sqrt{B_N})^2 - \lambda_N(\sqrt{B_N})^2|^{-1} \\ &\lesssim |\lambda_j(\sqrt{B_N})^2 - (4\xi + \eta)|^{-1}. \end{aligned} \quad (3.15)$$

This yields by combining (3.15) with the explicit expression of the eigenvalues (3.13)

$$\mu_j^{-1} \lesssim \left| \operatorname{sgn}(j) 4\xi \sin^2\left(\frac{\pi(j-1)}{2N}\right) - 4\xi \right|^{-1} \lesssim \left| \cos\left(\frac{\pi(j-1)}{2N}\right) \right|^{-2} \lesssim \mathcal{O}(N^2) \quad (3.16)$$

where the last equality comes from the leading order in Taylor expansion.

Step 2-Wigner matrix. Next, we consider the translated Wigner matrix R that we centre at $\lambda_N \equiv \lambda_N(\sqrt{B_N})$, defined in terms of $W_{\mathcal{F}}$ as in (3.11):

$$R_{\mathcal{F}}(\lambda) := W_{\mathcal{F}}(\lambda + \lambda_N).$$

Since $\cos(\pi k - x) = (-1)^k \cos(x)$, we observe that also $v_j(1) = (-1)^{j-1} v_j(N)$ as

$$\cos\left(\frac{\pi(j-1)}{2N}\right) = \cos\left(\pi(j-1) - \frac{\pi(j-1)(N-\frac{1}{2})}{N}\right) = (-1)^{j-1} \cos\left(\frac{\pi(j-1)(N-\frac{1}{2})}{N}\right).$$

To make the sums on the right of (3.11) more transparent, we define matrices

$$\Gamma_{\{1\}}(j) := 1 \text{ and } \Gamma_{\{1,N\}}(j) := \gamma \begin{pmatrix} 1 & (-1)^{j-1} \\ (-1)^{j-1} & 1 \end{pmatrix}. \quad (3.17)$$

These matrices allow us to rewrite the translated Wigner R -matrix in the more concise form

$$R_{\mathcal{F}}(\lambda) = \sum_{j \in \pm[N]} (\lambda - \mu_j)^{-1} |v_j(1)|^2 \Gamma_{\mathcal{F}}(j). \quad (3.18)$$

Let us now restrict to the case $\mathcal{F} = \{1, N\}$, so that we have friction imposed only on the first and the last particle.

Our aim is to reduce $R_{\mathcal{F}} \in \mathbb{C}^{2 \times 2}$ to a scalar equation². In order to do so, we find that the vectors $u_o = \frac{(1,1)^T}{\sqrt{2}}$, $u_e = \frac{(1,-1)^T}{\sqrt{2}}$ are eigenvectors to the matrices $\Gamma_{\mathcal{F}}$ satisfying

$$\Gamma_{\{1,N\}}(j)(\delta_{j \in 2\mathbb{Z}+1} u_o + \delta_{j \in 2\mathbb{Z}} u_e) = 2\gamma(\delta_{j \in 2\mathbb{Z}+1} u_o + \delta_{j \in 2\mathbb{Z}} u_e).$$

In particular, $u_o \in \ker(\Gamma_{\{1,N\}}(j))$ for $j \in 2\mathbb{Z}$ and $u_e \in \ker(\Gamma_{\{1,N\}}(j))$ for $j \in 2\mathbb{Z} + 1$. **Step 3-Scalar reduction.** Without loss of generality, let N be odd, in which case, we choose $u = u_o$. It follows from the explicit form of the eigenvectors (3.13) and Taylor expansion that $2|v_N(1)|^2 = \mathcal{O}(N^{-3})$. We now use the expansion

$$(\lambda - \mu)^{-1} = -\mu^{-1} \sum_{n=0}^{\infty} (\lambda \mu^{-1})^n = -\mu^{-1} - \mu^{-2} \lambda - \mu^{-2} \lambda^2 (\mu - \lambda)^{-1} \quad (3.19)$$

to rewrite the equation $(R_{\mathcal{F}}(\lambda) + i)u = 0$ in terms of the following scalar functions

$$f(\lambda) = \nu \lambda \quad \text{with} \quad \nu := i - 2\gamma \sum_{j \in \pm[N] \cap 2\mathbb{Z}+1 \setminus \{N\}} \frac{|v_j(1)|^2}{\mu_j} \quad \text{and}$$

$$g(\lambda) = 2\gamma \left(|v_N(1)|^2 - \sum_{j \in \pm[N] \cap 2\mathbb{Z}+1 \setminus \{N\}} \frac{|v_j(1)|^2 \lambda^2}{\mu_j^2} - \sum_{j \in \pm[N] \cap 2\mathbb{Z}+1 \setminus \{N\}} \frac{|v_j(1)|^2}{\mu_j^2} \frac{\lambda^3}{\mu_j - \lambda} \right). \quad (3.20)$$

²if there is friction at one end only, the Wigner R -matrix $R_{\mathcal{F}}$ is already scalar which is why we consider the case of friction at two ends

Indeed, since

$$(R_{\mathcal{F}}(\lambda) + i)u = \left(2\gamma \sum_{j \in \pm[N] \cap 2\mathbb{Z} + 1 \setminus \{N\}} (\lambda - \mu_j)^{-1} |v_j(1)|^2 + i \right) u \quad (3.21)$$

it follows by expanding $(\lambda - \mu_j)^{-1}$, as in (3.19), and multiplying by λ that

$$\lambda(R_{\mathcal{F}}(\lambda) + i)u = (f(\lambda) + g(\lambda))u$$

and thus we reduce our problem to a scalar one, since

$$R_{\mathcal{F}}(\lambda)u = -iu \text{ if and only if } f(\lambda) + g(\lambda) = 0. \quad (3.22)$$

Step 4-Estimation of f, g . Let us now fix a ball

$$K := B(0, r_N) \text{ for some } r_N \text{ to be determined.} \quad (3.23)$$

We then find that for $\lambda \in \partial K$ we have for f

$$r_N = |i\lambda| \leq |f(\lambda)| = \mathcal{O}(r_N). \quad (3.24)$$

Using (3.16) for μ_j^{-2} and also the explicit form of the eigenvectors (3.13), yields that

$$\sum_{j \in \pm[N] \setminus \{N\}} \frac{|v_j(1)|^2}{\mu_j} \lesssim \frac{2}{N} \sum_{j \in \pm[N] \setminus \{N\}} \left| \cos \left(\frac{\pi(j-1)}{2N} \right) \right|^2 \left| \cos \left(\frac{\pi(j-1)}{2N} \right) \right|^{-2} = \mathcal{O}(1). \quad (3.25)$$

We also record that again by (3.16) and (3.13)

$$\begin{aligned} \sum_{j \in \pm[N] \setminus \{N\}} \frac{|v_j(1)|^2}{\mu_j^2} &\lesssim \frac{1}{N} \sum_{j \in \pm[N] \setminus \{N\}} \left| \cos \left(\frac{\pi(j-1)}{2N} \right) \right|^2 \left| \cos \left(\frac{\pi(j-1)}{2N} \right) \right|^{-4} \\ &\lesssim \left| \cos \left(\frac{\pi}{2} - \frac{\pi}{N} \right) \right|^{-2} = \mathcal{O}(N^2) \end{aligned} \quad (3.26)$$

where the last estimate follows by Taylor expanding around $\pi/2$.

Equation (3.26) implies that for $\lambda \in \partial K$ we have for the second term in $g(\lambda)$, as in (3.20), that

$$|\lambda|^2 \left| \sum_{j=1}^{N-1} \frac{|v_j(1)|^2}{\mu_j^2} \right| = \mathcal{O}(N^2 r_N^2).$$

Moreover, if we choose $r_N = \mathcal{O}(N^{-3})$, the the third term of $g(\lambda)$, as in (3.20), can also

be estimated, using (3.26), by

$$\left| \sum_{j \in \pm[N] \setminus \{N\}} \frac{|v_j(1)|^2}{\mu_j^2} \frac{\lambda^3}{\mu_j - \lambda} \right| = |\lambda|^2 \left| \sum_{j \in \pm[N] \setminus \{N\}} \frac{|v_j(1)|^2}{\mu_j^2} \frac{1}{\frac{\mu_j}{\lambda} - 1} \right| \lesssim r_N^2 N^2 N^{-1} = \mathcal{O}(N^{-5}). \quad (3.27)$$

since $\frac{\mu_j}{\lambda} \gtrsim \frac{N^{-2}}{N^{-3}} = \mathcal{O}(N)$ and so $\frac{\lambda}{\mu_j - \lambda} = \mathcal{O}(N^{-1})$.

Combining (3.25), (3.26), and (3.27), this implies that for $\lambda \in \partial K$ we have

$$\begin{aligned} 2\gamma |v_N(1)|^2 - \mathcal{O}(Nr_N^2) - \mathcal{O}(N^2 r_N^2) &\leq |g(\lambda)| \quad \text{and} \\ 2\gamma |v_N(1)|^2 + \mathcal{O}(Nr_N^2) + \mathcal{O}(N^2 r_N^2) &\geq |g(\lambda)|. \end{aligned} \quad (3.28)$$

Step 5-Upper bound. Thus, we choose in (3.23) $r_N := \frac{\alpha}{2} |v_N(1)|^2$ with α large enough, (but independent of N) such that together with (3.24) and the upper bound in (3.28), they imply that on ∂K

$$|g(\lambda)| \lesssim 2\gamma N^{-3} + \frac{\alpha^2 N^{-5}}{4} + \frac{\alpha^2 N^{-4}}{4} = \mathcal{O}(r_N) = \mathcal{O}(|f(\lambda)|)$$

which is the case if

$$2\gamma N^{-3} + \frac{\alpha^2 N^{-5}}{4} + \frac{\alpha^2 N^{-4}}{4} \leq \frac{\alpha}{2} N^{-3} \quad \text{or} \quad 2\gamma + \frac{\alpha^2}{4}(N^{-2} + N^{-1}) \leq \frac{\alpha}{2}.$$

where for large enough α , the last inequality holds true.

Therefore asymptotically with N ,

$$|f(\lambda)| > |g(\lambda)| \quad \text{on } \partial K.$$

By Rouché's Theorem, f and $f + g$ have the same amount of zeros inside K . Since f has precisely one root in K at $\lambda = 0$ so does $f + g$.

This implies by the equivalence (3.22) that $R(\lambda)u = -iu$ has one solution λ with $\lambda \leq \mathcal{O}(N^{-3})$ and so $\lambda_S \leq \mathcal{O}(N^{-3})$ which yields the upper bound on the spectral gap.

Step 6-Lower bound. The lower bound follows analogously. Assuming the modulus of λ would decay faster than $\mathcal{O}(N^{-3})$, i.e. $|\lambda|/|v_N(1)|^2 = o(1)$ then we can select $r_N = |v_N(1)|^2 o(1)$ in (3.23). This way, $g(\lambda)$ does not have a root in $K := B(0, r_N)$ by the lower bound in (3.28), as $|g(\lambda)|$ is lower-bounded by a leading-order term $2\gamma |v_N(1)|^2$. Moreover, by the same lower bound in (3.28) and upper bound in (3.24) we find that on ∂K we have for this choice of r_N

$$|g(\lambda)| > |f(\lambda)| \quad \text{on } \partial K.$$

Thus, since g does not have a root inside K , there is also no root to $f + g$ inside K and thus by (3.22) we necessarily have that $N^{-3} \lesssim \lambda_S$. Now, it could hypothetically happen that it is just the real part of λ , where λ is the solution $\mathcal{O}(N^{-3})$ that causes $\lambda \notin K$, but we argue that the imaginary part in fact decays much faster. In other words, we want to exclude $\Im(\lambda) = \text{Re}(\lambda)\mathcal{O}(1)$.

In order to exclude this scenario, we analyze the imaginary part of $f(\lambda) + g(\lambda) = 0$. This equation reads

$$-\Im(\lambda)2\gamma \sum_{j \in \pm[N] \cap 2\mathbb{Z}+1 \setminus \{N\}} \frac{|v_j(1)|^2}{\mu_j} + \Im(g(\lambda)) = -\text{Re}(\lambda).$$

Since by (3.26) and (3.27), we have $\Im(g(\lambda)) = \mathcal{O}(N^{-4})$ and $2\gamma \sum_{j \in \pm[N] \cap 2\mathbb{Z}+1 \setminus \{N\}} \frac{|v_j(1)|^2}{\mu_j} = \mathcal{O}(1)$, we have by the standing assumption $\Im(\lambda) = \text{Re}(\lambda)\mathcal{O}(1)$, a contradiction since the left hand side is smaller than the right hand side in absolute value. \square

Remark 3.4 (Dependence of λ_S on the friction). *We stress that our proof shows that the spectral gap depends on the friction constant γ , of the two terminal particles. In particular, by carefully analyzing this dependence in the proof, we see that there are constants $c_1, c_2 > 0$ so that*

$$c_1 \left(\frac{\gamma}{1 + \gamma} \right) N^{-3} \leq \lambda_S \leq c_2 \gamma N^{-3}.$$

3.3.3 Higher-dimensional homogeneous networks

We now turn to the d -dimensional homogeneous network of oscillators, on a square network for $d \geq 1$. We will show how we can extend ideas from the one-dimensional setting to the multi-dimensional case, in order to compute the spectral gap, by exploiting the separability of the Neumann Laplacian.

Assuming η and ξ to be constants allows us to perform an analogous reduction of the high-dimensional spectral problem to a scalar problem, as in the one-dimensional case. We have a Schrödinger operator on \mathbb{C}^{N^d} associated to the dynamics, as the first order part of the generator is expressed through the $2N^d \times 2N^d$ -dimensional matrix $\Omega_{[N]^d}$. The multi-dimensional Schrödinger operator has then the following spectral decomposition

$$\sqrt{B_{[N]^d}} = \sum_{j_1=1}^N \cdots \sum_{j_d=1}^N \lambda_{j_1 \dots j_d} (\sqrt{B_{[N]^d}}) v_{j_1 \dots j_d}^{\otimes d} \quad (3.29)$$

where $\lambda_{j_1 \dots j_d} (\sqrt{B_{[N]^d}}) = \left(\eta + \sum_{k=1}^d \lambda_{j_k} \right)^{1/2}$ with $\lambda_j = 4\xi \sin^2 \left(\frac{\pi(j-1)}{2N} \right)$. The eigenvectors

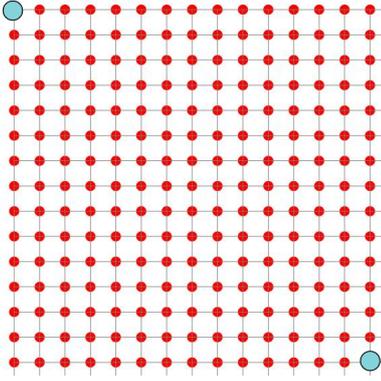


Figure 3.6: Spectral gap $\Theta(N^{-6})$.

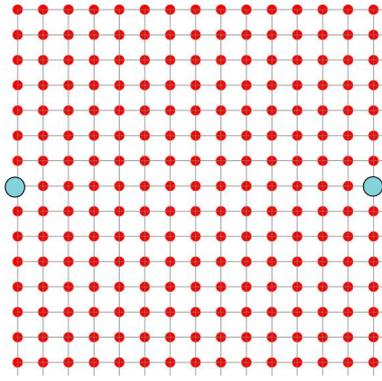


Figure 3.7: Spectral gap $\Theta(N^{-4})$.

Figure 3.8: The \mathbb{Z}^2 -subnetwork with friction at the blue particles

$v_{j_1 \dots j_d}$ are the product states

$$v_{j_1 \dots j_d}(i_1, i_2, \dots, i_d) = v_{j_1}(i_1) \cdots v_{j_d}(i_d) \quad (3.30)$$

such that

$$v_j(i) = \begin{cases} N^{-\frac{1}{2}} & , j=1 \\ \sqrt{\frac{2}{N}} \cos\left(\frac{\pi(j-1)(i-\frac{1}{2})}{N}\right) & , \text{otherwise.} \end{cases} \quad (3.31)$$

Two-particle friction on the d -dimensional network. As a first step we consider friction at two distinguished boundary particles out of the N^d . We now show how the method presented above applies if we consider friction at the two corners of the network, Fig. 3.6, or at the centres of two opposite edges above and below, Fig. 3.7.

We remind the high dimensional version of Lemma 3.1. We consider the matrix

$$i\Omega_{[N]^d} = \begin{pmatrix} 0 & -iB_{[N]^d} \\ iB_{[N]^d} & 0 \end{pmatrix} + i \text{diag}(\Gamma, 0_{\mathbb{C}^{N^d \times N^d}}) \quad (3.32)$$

and reduce the high dimensional spectral problem for $\Omega_{[N]^d}$ to a lower dimensional spectral problem for the Wigner $W_{\mathcal{F}}$ -matrix in $\mathbb{C}^{2 \times 2}$. From this lemma we get the following representation of the $W_{\mathcal{F}}$ -matrix:

$$W_{\mathcal{F}}(\lambda) = \sum_{\pm} \sum_{j=1}^{N^d} (\lambda \mp \lambda_j)^{-1} \sum_{i_1, i_2 \in \mathcal{F}} \sqrt{\gamma_{i_1} \gamma_{i_2}} \langle V_j^{\pm}, e_{i_1}^{2N^d} \rangle \langle e_{i_2}^{2N^d}, V_j^{\pm} \rangle e_{i_1}^{|\mathcal{F}|} \otimes e_{i_2}^{|\mathcal{F}|} \quad (3.33)$$

where $V_j^{\pm} = \frac{1}{\sqrt{2}}(v_j, \pm i v_j)^T$ are of the product form (3.30) with v_j being the eigenvectors of $B_{[N]^d}$.

Proposition 3.5 (Two-particle friction in homogeneous networks). *Let the dimension of the network be $d \geq 1$ and all $\eta_i > 0$, $\xi_{ij} > 0$, and masses m_i coincide, respectively. We*

consider two different scenarios:

- First, we assume that the two particles located at $(1, \dots, 1), (N, \dots, N)$ are subject to non-zero friction $\gamma > 0$ and diffusion. The spectral gap of the harmonic network of oscillators satisfies

$$\lambda_S = \mathcal{O}(N^{-3d}).$$

- Second, we assume the friction with constant $\gamma > 0$ and diffusion acts on the particles located in the centre of two opposite edges of the network at

$$(1, \lceil N/2 \rceil, \dots, \lceil N/2 \rceil), (N, \lceil N/2 \rceil, \dots, \lceil N/2 \rceil).$$

Then the spectral gap of the network of oscillators satisfies

$$\lambda_S = \mathcal{O}(N^{-3-(d-1)}).$$

Proof. To keep the notation simple, we restrict us to stating the proof for $d = 2$. We write that the eigenvalues $\lambda_{i,j}(\sqrt{B_{N^2}}) = (\lambda_i + \lambda_j)^{1/2}$ for $i, j \in [N]$ and that the eigenvectors $v_{i,j}$ are the product states $v_{i,j}(k, l) = v_i(k)v_j(l)$. Here again regarding the couple $(i, j) \in [N]^2$, we define $\lambda_{-i,-j}(\sqrt{B_{N^2}}) := -(\lambda_i + \lambda_j)^{1/2}$ and $v_{-i,-j}(k, l) := v_{i,j}(k, l) = v_i(k)v_j(l)$ when $i, j \in [N]$.

As in the one-dimensional case, we compute first the differences of all the eigenvalues $\lambda_{i,j}(\sqrt{B_{N^2}})$ from the largest eigenvalue $\lambda_{N,N}(\sqrt{B_{N^2}})$:

$$|\lambda_{N,N}(\sqrt{B_{N^2}}) - \lambda_{i,j}(\sqrt{B_{N^2}})| \gtrsim |(8\xi + 2\eta)^{1/2} - \lambda_{i,j}(\sqrt{B_{N^2}})|, \quad (3.34)$$

we define $\mu_{ij} := \lambda_{i,j}(\sqrt{B_{N^2}}) - \lambda_{N,N}(\sqrt{B_{N^2}})$ for $(i, j) \in \pm[N]^2$ so that explicit calculations give

$$\begin{aligned} \mu_{ij}^{-1} &\lesssim |\lambda_{N,N}^2 - \text{sgn}(i)\lambda_{i,j}^2|^{-1} \lesssim |(8\xi + 2\eta) - \lambda_{i,j}^2|^{-1} \\ &\lesssim \left| 8\xi - 4\xi \left(\sin^2 \left(\frac{\pi(j-1)}{2N} \right) + \sin^2 \left(\frac{\pi(i-1)}{2N} \right) \right) \right|^{-1} \\ &\lesssim \left| \cos^2 \left(\frac{\pi(j-1)}{2N} \right) + \cos^2 \left(\frac{\pi(i-1)}{2N} \right) \right|^{-1} \\ &\lesssim \left| \cos^2 \left(\frac{\pi(N-2)}{2N} \right) \right|^{-1} \lesssim \mathcal{O}(N^2) \end{aligned} \quad (3.35)$$

where in the last line we Taylor expanded around $\pi/2$.

Next, we translate the Wigner matrix $R_{\mathcal{F}}(\lambda) = W_{\mathcal{F}}(\lambda + \lambda_{N,N})$ and write

$$R_{\mathcal{F}}(\lambda) := \sum_{(i,j) \in \pm[N]^2} (\lambda - \mu_{ij})^{-1} |v_{i,j}(1,1)|^2 \Gamma_{\mathcal{F}} \in \mathbb{C}^{2 \times 2} \quad (3.36)$$

where

$$\Gamma_{\mathcal{F}} := \begin{pmatrix} \gamma & (-1)^{i+j-2} \gamma \\ (-1)^{i+j-2} \gamma & \gamma \end{pmatrix}$$

since $v_{i,j}(1,1) = (-1)^{i+j-2} v_{i,j}(N,N)$. Note that for $i+j = \text{even}$, the vector $u = 2^{-1/2}(1,1)^T$ is an eigenvector to $\Gamma_{\mathcal{F}}$ in the following sense:

$$\Gamma_{\mathcal{F}} u = 2\gamma \delta_{i+j \in 2\mathbb{Z}} u,$$

where we use the same notation as in the proof for the one dimension. With the above formula and by expanding the term $(\lambda - \mu_{ij})^{-1}$ we are able to rewrite the equation $(R_{\mathcal{F}}(\lambda) + i)u = 0$ in terms of two scalar functions f, g . In particular denoting by \mathcal{A} the set of indices $\mathcal{A} := \{(i,j) \in \pm[N]^2 \setminus (N,N) | i+j \in 2\mathbb{Z}\}$, we have $\lambda(R_{\mathcal{F}}(\lambda) + i)u = f(\lambda) + g(\lambda)$ with

$$\begin{aligned} f(\lambda) &= i\lambda - 2\gamma \sum_{(i,j) \in \mathcal{A}} \lambda \frac{|v_{i,j}(1,1)|^2}{\mu_{ij}} \quad \text{and} \\ g(\lambda) &= 2\gamma \left(|v_{N,N}(1,1)|^2 - \sum_{(i,j) \in \mathcal{A}} \frac{|v_{i,j}(1,1)|^2 \lambda^2}{\mu_{ij}^2} - \sum_{(i,j) \in \mathcal{A}} \frac{|v_{i,j}(1,1)|^2}{\mu_{ij}^2} \frac{\lambda^3}{\mu_{ij} - \lambda} \right). \end{aligned} \quad (3.37)$$

We fix a ball $K := B(0, r_N)$ and we estimate the following terms on the boundary ∂K :

$$\left| \sum_{(i,j) \in \mathcal{A}} \frac{\lambda |v_{i,j}(1,1)|^2}{\mu_{ij}} \right| = |\lambda| \left| \sum_{(i,j) \in \mathcal{A}} \frac{|v_i(1)|^2 |v_j(1)|^2}{\mu_{ij}} \right| \quad (3.38)$$

$$\lesssim \sum_{(i,j) \in \mathcal{A}} N^{-2} \frac{r_N \left| \cos\left(\frac{\pi(i-1)}{2N}\right) \right|^2 \left| \cos\left(\frac{\pi(j-1)}{2N}\right) \right|^2}{\left| \cos\left(\frac{\pi(i-1)}{2N}\right) \right|^2} = \mathcal{O}(r_N) \quad (3.39)$$

after Taylor expansions to estimate the norm of the eigenvectors. Also

$$|\lambda|^2 \left| \sum_{(i,j) \in \mathcal{A}} \frac{|v_{i,j}(1,1)|^2}{\mu_{ij}^2} \right| \lesssim |\lambda|^2 \sum_{(i,j) \in \mathcal{A}} N^{-2} \frac{\left| \cos\left(\frac{\pi(j-1)}{2N}\right) \right|^2}{\left| \cos\left(\frac{\pi(i-1)}{2N}\right) \right|^2} \lesssim \mathcal{O}(N^2 r_N^2) \quad (3.40)$$

and

$$\left| \sum_{(i,j) \in \mathcal{A}} \frac{|v_{i,j}(1,1)|^2}{\mu_{ij}^2} \frac{\lambda^3}{\mu_{ij} - \lambda} \right| = |\lambda|^2 \left| \sum_{(i,j) \in \mathcal{A}} \frac{|v_{i,j}(1,1)|^2}{\mu_{ij}^2} \frac{1}{\frac{\mu_{ij}}{\lambda} - 1} \right| \lesssim \mathcal{O}(N^4 r_N^3) \quad (3.41)$$

since $\frac{\mu_{ij}}{\lambda} \gtrsim N^{-2} r_N^{-1}$. Therefore we collect the following bounds for f, g :

$$|f(\lambda)| \lesssim \mathcal{O}(r_N), \quad |g(\lambda)| \gtrsim (\gamma_{11} + \gamma_{N,N}) |v_{N,N}(1,1)|^2 - \mathcal{O}(N^2 r_N^2) - \mathcal{O}(N^4 r_N^3) \quad (3.42)$$

$$|g(\lambda)| \lesssim (\gamma_{11} + \gamma_{N,N}) |v_{N,N}(1,1)|^2 + \mathcal{O}(N^2 r_N^2) + \mathcal{O}(N^4 r_N^3) \quad (3.43)$$

Choosing $r_N = \frac{\alpha}{2} |v_{N,N}(1,1)|^2 \lesssim \mathcal{O}(N^{-6})$ gives the upper bound for the spectral gap, as at the end of the proof of Proposition 3.3.

The lower bound follows then from choosing $r_N = \mathcal{O}(1)$ in which case

$$\|g(\lambda)\| > \|f(\lambda)\| \text{ on } \partial B(0, r_N).$$

Then, we study the anti-symmetric part of $T(\lambda) := f(\lambda) + g(\lambda)$, i.e. $\langle \frac{T-T^*}{2i} u, u \rangle = 0$, where $u \in \ker(T(\lambda))$ normalized. Writing this out we see that as in the one-dimensional case that $\Im(\lambda) = \text{Re}(\lambda) \mathcal{O}(1)$ cannot hold. This implies the bound on the spectral gap.

As regards the second part of the statement, *i.e.* when the particles subject to friction are located in the centre of the bordered edges, *i.e.* $\mathcal{F} = \{(1, \lceil N/2 \rceil), (N, \lceil N/2 \rceil)\}$, of the network rather than at the corners. The proof follows exactly in the same way as in the first scenario, apart from the last part of it when we fix the radius r_N of the ball K in order to apply Rouché's Theorem. In this case, taking

$$r_N = \frac{\alpha}{2} |v_{N,N}(1, \lceil N/2 \rceil)|^2 \lesssim \mathcal{O}(N^{-3} N^{-1})$$

immediately implies the result. \square

2N-particles exposed to friction on two opposite edges. We consider now a scenario that is perhaps more realistic for two-dimensional systems: We assume the friction to be imposed to all the particles located on the top edge of the network and on the bottom edge as well, cf. Fig. 3.9. We use the same techniques and notation as above and we will show how the same method applies to give an upper bound on the spectral gap. Thus here

$$\mathcal{F} = \{(1, 1), \dots, (1, N), (N, 1), \dots, (N, N)\} \text{ and } |\mathcal{F}| = 2N$$

and the translated (centred at $\lambda_{Nd} = \lambda_{Nd}(\sqrt{B_{[Nd]d}})$) Wigner $R_{\mathcal{F}}$ -matrix in $\mathbb{C}^{2N \times 2N}$ will be

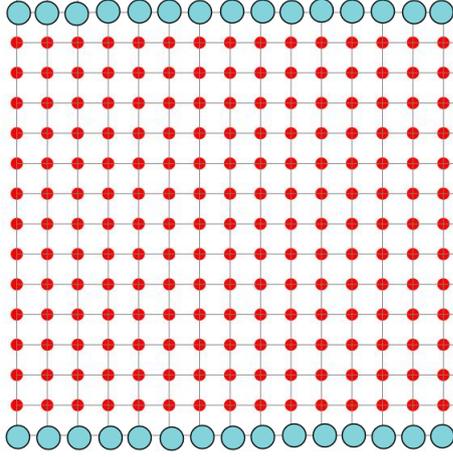


Figure 3.9: The \mathbb{Z}^2 -subnetwork with friction at the blue particles on opposite edges.

$$R_{\mathcal{F}}(\lambda) = \sum_{\mu \in \pm\sqrt{\text{Spec}(B_{[N]^d})} + \lambda_{Nd}} (\lambda - \mu)^{-1} \sum_{i_1, i_2 \in \mathcal{F}} \alpha_{i_1, i_2}(\mu) \pi_{i_1, i_2}^{2N}, \quad (3.44)$$

where

$$\alpha_{i_1, i_2}(\mu = \pm\lambda_j + \lambda_{Nd}) = \sqrt{\gamma_{i_1} \gamma_{i_2}} \langle V_j^\pm, e_{i_1}^{2Nd} \rangle \langle e_{i_2}^{2Nd}, V_j^\pm \rangle, \text{ and } \pi_{i_1, i_2}^{2N} := e_{i_1}^{2N} \otimes e_{i_2}^{2N}$$

with $V_j^\pm = 2^{-1/2}(v_j, \pm i v_j)^T$ and v_j are the eigenvectors of $\sqrt{B_{Nd}}$.

Note that since in this case the Wigner matrix is still high-dimensional $2N \times 2N$ we shall support our analytical findings by some numerics too. In particular we have the following analytical result:

Proposition 3.6 (*2N-particle friction in homogeneous networks*). *Let the two-dimensional square network graph with particles on the N^2 vertices, and all $\eta_i > 0$, $\xi_{ij} > 0$, and masses m_i coincide, respectively. We assume that the 2N particles located at*

$$\{(1, 1), \dots, (1, N), (N, 1), \dots, (N, N)\}$$

are subject to non-zero friction and diffusion. The spectral gap of the harmonic network of oscillators then satisfies

$$\lambda_S \lesssim N^{-5/2}.$$

Proof. We introduce $\lambda_j = \lambda_{j_1, j_2}(\sqrt{B_{N^2}}) = (\lambda_{j_1} + \lambda_{j_2})^{1/2}$ for $j \in [N]^2$ and we define $\lambda_{-j} := -\lambda_j$. The eigenvectors v_j are the product states such that $v_{-j}(k, l) := v_j(k, l) := v_{j_1}(k)v_{j_2}(l)$ when $j \in [N]^2$.

Using the equivalence of Lemma 3.1, we shall study solutions to the equation

$$\det(F(\lambda) + G(\lambda)) = 0 \quad (3.45)$$

where F and G are defined below in terms of the vectors $V_{i,j}^\pm = \frac{1}{\sqrt{2}}(v_{i,j}, \pm i v_{i,j})^T$ and $\mu_j = \lambda_j - \lambda_{N,N}$ for $j \in \pm[N]^2$, where $\mu_j^{-1} = \mathcal{O}(N^2)$ as before in the estimates (3.35). Note that we do not reduce our problem to a scalar one as in the two-particle friction cases above and thus we work with the matrix valued version of Rouché's Theorem stated in Lemma 2.1. The matrices $F(\lambda), G(\lambda)$ are defined, using the notation of Lemma 3.1, as follows:

$$F(\lambda) := i\lambda - \lambda \sum_{j \in \pm[N]^2 \setminus (N,N)} \sum_{i_1, i_2 \in \mathcal{F}} \frac{\alpha_{i_1, i_2}(\lambda_j)}{\mu_j} \pi_{i_1, i_2}^{2N} \quad (3.46)$$

and

$$\begin{aligned} G(\lambda) := & \underbrace{\sum_{i_1, i_2 \in \mathcal{F}} \alpha_{i_1, i_2}(\lambda_{N,N}) \pi_{i_1, i_2}^{2N}}_{=:(I)} \underbrace{-\lambda^2 \sum_{j \in \pm[N]^2 \setminus (N,N)} \sum_{i_1, i_2 \in \mathcal{F}} \frac{\alpha_{i_1, i_2}(\lambda_j)}{\mu_j^2} \pi_{i_1, i_2}^{2N}}_{=:(II)} \\ & - \lambda^3 \underbrace{\sum_{j \in \pm[N]^2 \setminus (N,N)} \sum_{i_1, i_2 \in \mathcal{F}} \frac{\alpha_{i_1, i_2}(\lambda_j)}{\mu_j^2 (\mu_j - \lambda)} \pi_{i_1, i_2}^{2N}}_{=:(III)} \end{aligned} \quad (3.47)$$

so that a solution to (3.45) corresponds to the desired eigenvalue. Before we fix a ball $K = B(0, r_N)$, we want to find an upper bound for the norm $\|\rho_N\|$, where

$$\rho_N := \sum_{i_1, i_2 \in \mathcal{F}} \alpha_{i_1, i_2}(\lambda_{N,N}) \pi_{i_1, i_2}^{2N} \quad (3.48)$$

i.e. is the first term, (I), of G . We will define then, this bound to be the radius r_N of the ball K and we will proceed as in the previous proofs. To understand the dependence of $\|\rho_N\|$ on N we make the following observation:

Due to the symmetries of the eigenvectors, e.g. that $v_{i,j}(1, 1) = (-1)^{i+j-2} v_{i,j}(N, N)$, it suffices to check the scaling of the entries at the columns $1, \dots, \lceil N/2 \rceil$ and only above the main diagonal of the matrix. We estimate them by Taylor expanding, in a similar manner as in the previous proofs. For example for the 3 entries in the corners of the territory that we examine we have

$$\begin{aligned} |v_{N,N}(1, 1)|^2 &\lesssim N^{-6}, & |v_{N,N}(1, \lceil N/2 \rceil)|^2 &\lesssim N^{-4}, \\ v_{N,N}(1, \lceil N/2 \rceil) v_{N,N}(1, 1) &\lesssim N^{-6} + N^{-4} = \mathcal{O}(N^{-4}) \end{aligned}$$

by Young's inequality. So all the entries scale at least like N^{-4} which implies that

$$\|\rho_N\| \leq N^{1/2} \|\rho_N\|_\infty \lesssim N^{1/2} N N^{-4} = \mathcal{O}(N^{-5/2}).$$

We now fix a ball $K = B(0, r_N)$ and choose the radius $r_N := \frac{\alpha}{2} N^{-5/2}$. Therefore

it suffices to find a root of (3.45) inside the ball K and conclude the existence of an eigenvalue by Rouché's theorem. We easily see that for all $v \neq 0$, on ∂K , $\|F(\lambda)v\| \geq |\lambda|\|v\| = r_N\|v\| = \frac{\alpha}{2}N^{-5/2}\|v\|$ since the second term of the right hand side of (3.46) is symmetric. We also collect the estimates for (II)

$$|\lambda|^2 \left| \sum_{(i,j) \in \mathcal{B}} \frac{|v_{i,j}(1,1)|^2}{\mu_{ij}^2} \right| \lesssim r_N^2 = \mathcal{O}(N^{-5}), \quad |\lambda|^2 \left| \sum_{(i,j) \in \mathcal{B}} \frac{|v_{i,j}(1, \lceil N/2 \rceil)|^2}{\mu_{ij}^2} \right| \lesssim r_N^2 = \mathcal{O}(N^{-5})$$

$$|\lambda|^2 \left| \sum_{(i,j) \in \mathcal{B}} \frac{v_{i,j}(1,1)v_{i,j}(1, \lceil N/2 \rceil)}{\mu_{ij}^2} \right| = \mathcal{O}(N^{-5}).$$

Moreover, since $\frac{\lambda}{\mu_{ij} - \lambda} = \mathcal{O}(N^{-1})$, for (III):

$$\left| \sum_{(i,j) \in \mathcal{B}} \frac{|v_{i,j}(1,1)|^2}{\mu_{ij}^2} \frac{\lambda^3}{\mu_{ij} - \lambda} \right| = \mathcal{O}(N^{-5-1}), \quad \left| \sum_{(i,j) \in \mathcal{B}} \frac{|v_{i,j}(1, \lceil N/2 \rceil)|^2}{\mu_{ij}^2} \frac{\lambda^3}{\mu_{ij} - \lambda} \right| = \mathcal{O}(N^{-5-1}),$$

$$\left| \sum_{(i,j) \in \mathcal{B}} \frac{v_{i,j}(1,1)v_{i,j}(1, \lceil N/2 \rceil)}{\mu_{ij}^2} \frac{\lambda^3}{\mu_{ij} - \lambda} \right| = \mathcal{O}(N^{-5-1}).$$

So we can see that all the entries in (II) and (III) of G are bounded by $\mathcal{O}(N^{-5})$ and $\mathcal{O}(N^{-6})$ respectively. Thus, we find the following estimate on the operator norm of terms (II) and (III)

$$\|(\text{II})\| \leq N^{1/2} \|(\text{II})\|_\infty \lesssim N^{1/2} N N^{-5} = N^{1/2} N^{-4} = \mathcal{O}(N^{-7/2}) \quad (3.49)$$

and

$$\|(\text{III})\| \leq N^{1/2} \|(\text{III})\|_\infty \lesssim N^{1/2} N N^{-6} = \mathcal{O}(N^{-9/2}). \quad (3.50)$$

We conclude that

$$\|G\| \lesssim N^{-5/2} + N^{-7/2} + N^{-9/2} = \mathcal{O}(N^{-5/2}). \quad (3.51)$$

We choose α large enough so that we have $\|F(\lambda)v\| > \|G(\lambda)v\|$ on ∂K , for all $v \neq 0$. Since $F(\lambda)$ is not invertible exactly at 0 inside K , we have that there is one point inside K so that $F(\lambda) + G(\lambda)$ is not invertible or in other words there is one root of $(R_{\mathcal{F}}(\lambda) + i)u = 0$ with $\lambda \lesssim N^{-5/2}$. \square

Proposition 3.6 provides *only an upper bound* on the spectral gap. In order to obtain sharp estimates on the spectral gap, one should identify first more precise asymptotics on the scaling of the operator norm, $\|\rho_N\|$, in (3.48). By numerically calculating the operator

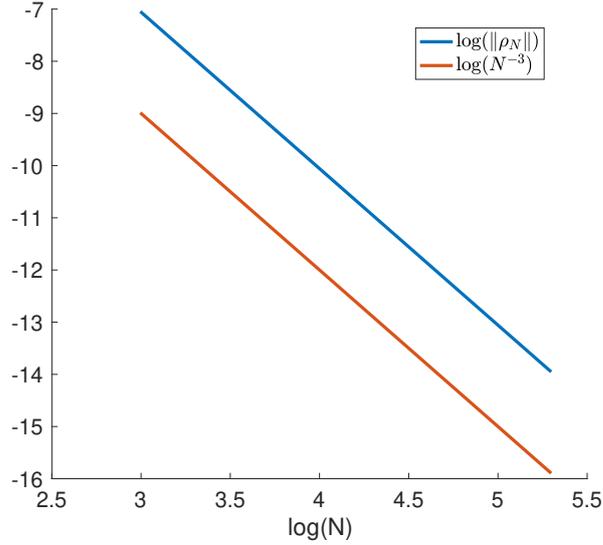


Figure 3.10: Log-log plot of operator norm $\|\rho_N\|$ and reference curve N^{-3} .

norm of $\|\rho_N\|$, we see that the true scaling is $\mathcal{O}(N^{-3})$ instead of $\mathcal{O}(N^{-5/2})$ as provided in the proof of Proposition 3.6.

3.3.4 Single impurities in the chain

An impurity in the chain of oscillators refers to a particle with different physical properties from all the remaining particles. Since certain local impurities such as perturbations of the potential strength for a single particle, are finite-rank perturbations of the discrete Schrödinger operator, they do not effect the essential spectrum, but can lead to additional discrete spectrum in the limiting operator $B_{[\infty]^d}$.

To understand the eigenstates associated to certain points in the discrete spectrum better, we recall a classical result due to Combes and Thomas:

Theorem 3.7. *Let $V \in \ell^\infty(\mathbb{Z}^d)$. Assume there is $u \in \ell^2(\mathbb{Z}^d)$ such that*

$$(-\Delta_{[\infty]^d} + V)u = \lambda u$$

with $\lambda \notin [0, 4d] =: \text{Spec}(-\Delta_{[\infty]^d})$. If $\limsup_{|n| \rightarrow \infty} |V(n)| < \inf_{\mu \in \text{Spec}(-\Delta_{[\infty]^d})} |\mu - \lambda|$, then there is $\nu > 0$ such that

$$u \in \left\{ \varphi \in \ell^2(\mathbb{Z}^d) : \sum_{n \in \mathbb{Z}^d} \exp(2\nu(1 + |n|^2)^{1/2}) |\varphi(n)|^2 < \infty \right\}.$$

The above theorem implies that these eigenstates are exponentially localized in space and -as we show- will cause an exponentially fast closing of the spectral gap. This is in

particular what happens if the pinning strength η of a single particle is *significantly weaker* than the pinning strength of all the other particles (the "flying away" particle). Note that in contrast to a weak pinning potential, a locally vanishing interaction potential would just decouple the chain into two independent pieces.

Let $I_{m_0} := \times_{i=1}^d \{m_0 - \lfloor \frac{N-1}{2} \rfloor e_i, \dots, m_0 + \lceil \frac{N-1}{2} \rceil e_i\}$ be a set of size N^d centred at m_0 . To identify sequences in $\mathbb{R}^{[N]^d}$ with sequences in $\ell^2(\mathbb{Z}^d)$, we define the inclusion map $\iota : \mathbb{R}^{[N]^d} \rightarrow \ell^2(\mathbb{Z}^d)$ by

$$(\iota x)(i) := \begin{cases} x(i), & \text{for } i \in I_{m_0} \\ 0, & \text{otherwise} \end{cases}$$

and define the restriction of the Schrödinger operator by

$$B_{I_{m_0}} x := B_{[\infty]^d}(\iota x).$$

Lemma 3.8. *For some $m_0 \in \mathbb{Z}^d$, let $B_{I_{m_0}}$ be a finite $[N]^d$ -size truncation of a bounded discrete Schrödinger operator $B_{[\infty]^d}$ on $\ell^2(\mathbb{Z}^d)$. Let φ be an eigenfunction to $B_{[\infty]^d}$ with eigenvalue λ_∞ and assume that φ is exponentially localized to a point $m_0 \in \mathbb{Z}^d$ such that*

$$|\varphi(n)| \leq \mathcal{O}(e^{-D|n-m_0|}) \text{ for all } n \in \mathbb{Z}^d. \quad (3.52)$$

We then define the finite $[N]^d$ -size restriction

$$\varphi_{I_{m_0}} := \frac{\varphi|_{I_{m_0}}}{\|\varphi|_{I_{m_0}}\|}.$$

Furthermore, assume that the operator $B_{[N]^d}$ has a unique eigenvalue λ_N , with associated eigenvector ψ_N , such that $\inf_{\lambda \in \text{Spec}(B_{[N]^d})} |\lambda_\infty - \lambda| = d(\lambda_\infty, \lambda_N)$ and a spectral gap of size $\alpha_N > 0$ such that

$$\text{Spec}(B_{[N]^d}) \cap (\lambda_N - \alpha_N, \lambda_N + \alpha_N) = \{\lambda_N\},$$

then

$$\|\psi_N - \varphi_{I_{m_0}}\| \leq \mathcal{O}(e^{-DN} \alpha_N^{-1}).$$

Proof. We first record that (3.52) implies the following exponential tail bound

$$\sqrt{\sum_{|m-m_0| \geq N/2} |\varphi(m)|^2} \leq \mathcal{O}(e^{-DN}). \quad (3.53)$$

We also define the infinite matrix $\widehat{B}_{I_{m_0}}$ given as the direct sum of operators

$$\widehat{B}_{I_{m_0}} := B_{I_{m_0}} \oplus 0$$

with respect to the decomposition $\ell^2(\mathbb{Z}^d) \simeq \ell^2(I_{m_0}) \oplus \ell^2(\mathbb{Z}^d \setminus I_{m_0})$. Thus, we have

$$\begin{aligned} \frac{\|(\widehat{B}_{I_{m_0}} - \lambda_\infty)\iota(\varphi|_{I_{m_0}})\|}{\|\iota(\varphi|_{I_{m_0}})\|} &\leq \frac{\|(\widehat{B}_{I_{m_0}} - B_{[\infty]^d})\iota(\varphi|_{I_{m_0}})\|}{\|\iota(\varphi|_{I_{m_0}})\|} + \frac{\|(B_{[\infty]^d} - \lambda_\infty I)\iota(\varphi|_{I_{m_0}})\|}{\|\iota(\varphi|_{I_{m_0}})\|} \\ &\leq \frac{\|(B_{[\infty]^d} - \lambda_\infty I)(\iota(\varphi|_{I_{m_0}}) - \varphi)\|}{\|\iota(\varphi|_{I_{m_0}})\|} + \frac{\|(B_{[\infty]^d} - \lambda_\infty I)\varphi\|}{\|\iota(\varphi|_{I_{m_0}})\|} \\ &\leq \mathcal{O}(e^{-DN}) \end{aligned}$$

where the first term on the right-hand side of the first line vanishes, up to exponentially small boundary terms, and in the last line we used the estimate (3.53) that holds for the eigenfunctions of B_∞ . Thus, the above bounds show that

$$\frac{\|(B_{I_{m_0}} - \lambda_\infty)\varphi|_{I_{m_0}}\|}{\|\varphi|_{I_{m_0}}\|} \leq \mathcal{O}(e^{-DN}) \quad (3.54)$$

and this implies by self-adjointness that also

$$\inf_{\lambda \in \text{Spec}(B_{I_{m_0}})} |\lambda - \lambda_\infty| = \mathcal{O}(e^{-DN}). \quad (3.55)$$

That $\varphi_{I_{m_0}} := \frac{\varphi|_{I_{m_0}}}{\|\varphi|_{I_{m_0}}\|} \in \mathbb{R}^{N^d}$ is exponentially close to an eigenvector ψ_N with eigenvalue λ_N of $B_{I_{m_0}}$ follows then by the spectral decomposition of $B_{I_{m_0}}$: In particular, let (ψ_i) be an ONB of $B_{I_{m_0}}$ with eigenvalues λ_i then we find by (3.54) that

$$\|(B_{I_{m_0}} - \lambda_\infty)\varphi_{I_{m_0}}\| = \sqrt{\sum_{i=1}^{N^d} |\langle \psi_i, \varphi_{I_{m_0}} \rangle|^2 |\lambda_i - \lambda_\infty|^2} \leq \mathcal{O}(e^{-DN}) =: \varepsilon.$$

This implies that for any $\nu > 0$

$$\sqrt{\sum_{i \in [N^d]: |\lambda_i - \lambda_\infty| \geq \nu \varepsilon} |\langle \psi_i, \varphi_{I_{m_0}} \rangle|^2} \leq \nu^{-1}. \quad (3.56)$$

Now, using that λ_N is a distance α_N apart from the rest of the spectrum of $B_{I_{m_0}}$ and λ_∞ is exponentially close to λ_N by (3.55) with some eigenvector ψ_N of $B_{I_{m_0}}$, we have from (3.56) by setting $\nu := \varepsilon^{-1} c \alpha_N$ that the coefficients of $\varphi_{I_{m_0}}$ in the ONB with respect to all other eigenvectors of $B_{I_{m_0}}$ are exponentially small. Thus, we find that

$$\|\psi_N - \varphi_{I_{m_0}}\| = \mathcal{O}(\nu^{-1}) \leq \mathcal{O}(e^{-DN} \alpha_N^{-1})$$

such that the two vectors are exponentially close to each other. \square

Proposition 3.9 (Impurity). *Without loss of generality, let N be an even number and consider a chain of oscillators with equal masses and unit coupling strength $\xi_{ij} = 1$. In addition, we assume that there is always at least one edge of the grid experiencing friction at the boundary and that the friction of particles is uniformly bounded in N . We define the centre point $c_d(N) = (N/2, \dots, N/2)$ and assume that*

$$\eta_{c_d(N)} + 2d + \varepsilon \leq \eta_i \quad \text{uniformly in } [N]^d$$

for some $\varepsilon > 0$ and all $i \neq c_d(N)$. Then, the spectral gap of the harmonic chain of oscillators described by the operator (2.5) with an impurity as above, decays exponentially fast.

Proof. First we show that the above assumptions imply the existence of an exponentially localized groundstate of $B_{[N]^d}$:

Let $V_{[N]^d} := (\eta_i)_{i \in [N]^d}$, the min-max principle implies for the discrete Schrödinger operator (1.4) that

$$\lambda_1(B_{[N]^d}) \leq \lambda_1(V_{[N]^d}) + \langle e_{c_d(N)}, (-\Delta_{[N]^d})e_{c_d(N)} \rangle = \lambda_1(V_{[N]^d}) + 2d$$

where $e_{c_d(N)}$ is the unit vector that vanishes at every point different from $c_d(N)$. On the other hand, Weyl's inequalities and the assumptions on the coefficients of the pinning potential, imply that

$$\lambda_1(B_{[N]^d}) \leq \|\Delta_{[N]^d}\| + \lambda_1(V_{[N]^d}) \leq \eta_{i \neq c_d(N)} - \varepsilon = \lambda_2(V_{[N]^d}) - \varepsilon \leq \lambda_2(B_{[N]^d}) - \varepsilon$$

where $\|\Delta_{[N]^d}\| \leq 2d$ is the operator norm of the discrete Laplacian. Hence, $B_{[N]^d}$, and thus $\sqrt{B_{[N]^d}}$ has a spectral gap uniformly in N since

$$\lambda_1(B_{[N]^d}) + \varepsilon \leq \lambda_2(B_{[N]^d}) \quad \text{uniformly in } N.$$

Now this implies that for some universal $c > 0$ we have $|v_1(1)|^2, |v_1(N)|^2 \lesssim e^{-cN}$: from Theorem 3.7, cf. also [Tes00, Lemma 2.5], we have that the ground state eigenfunction u of the limiting operator $B_{[\infty]^d}$ is exponentially localized since the operators $B_{[N]^d}$ possess a uniform spectral gap of size at least $\alpha_N := \varepsilon$ and $\lambda_1(B_{[N]^d}) \notin \text{Spec}_{\text{ess}}(B_{[\infty]^d})$.

The previous Lemma 3.8 then implies with $m_0 = c_d(N)$ that there is an eigenstate v_1 to $B_{[N]^d}$

$$\|v_1 - u|_{\varphi_{[N]^d}}\| \leq \mathcal{O}(e^{-DN/2}\varepsilon^{-1}).$$

To conclude the existence of an eigenvalue converging exponentially fast to zero, we shall restrict us again to the case $d = 2$ to keep the notation simple while at the same time

dealing with all technicalities of the multi-dimensional setting.

Using the equivalence of Lemma 3.1, we study the equation

$$\det(F(\lambda) + G(\lambda)) = 0 \quad (3.57)$$

in terms of the vectors $V_j^\pm = \frac{1}{\sqrt{2}}(v_j, \pm iv_j)^T$ and $\mu_j = \lambda_j - \lambda_1$, where v_j are the eigenvectors of the Schrödinger operator $-\Delta_{[N]^d} + V_{[N]^d}$ with eigenvalue λ_j and $\lambda_1 := \lambda_1(\sqrt{B_{[N]^d}})$. Setting $v_{-j} := v_j$ and $\lambda_{-j} := -\lambda_j$, the matrices $F(\lambda), G(\lambda)$ are then defined as follows, using the notation of Lemma 3.1,

$$F(\lambda) := i\lambda - \lambda \sum_{j \in \pm[N^d] \setminus \{1\}} \sum_{i_1, i_2 \in \mathcal{F}} \frac{\alpha_{i_1, i_2}(\lambda_j)}{\mu_j} \pi_{i_1, i_2}^{|\mathcal{F}|} \quad (3.58)$$

and

$$\begin{aligned} G(\lambda) := & \underbrace{\sum_{i_1, i_2 \in \mathcal{F}} \alpha_{i_1, i_2}(\lambda_1) \pi_{i_1, i_2}^{|\mathcal{F}|}}_{=:(I)} - \lambda^2 \underbrace{\sum_{j \in \pm[N^d] \setminus \{1\}} \sum_{i_1, i_2 \in I} \frac{\alpha_{i_1, i_2}(\lambda_j) \pi_{i_1, i_2}^{|\mathcal{F}|}}{\mu_j^2}}_{=:(II)} \\ & - \lambda^3 \underbrace{\sum_{j \in \pm[N^d] \setminus \{1\}} \sum_{i_1, i_2 \in \mathcal{F}} \frac{\alpha_{i_1, i_2}(\lambda_j) \pi_{i_1, i_2}^{|\mathcal{F}|}}{\mu_j^2 (\mu_j - \lambda)}}_{=:(III)} \end{aligned} \quad (3.59)$$

so that a solution to (3.57) corresponds to the desired eigenvalue. Before we fix a ball $K = B(0, r_N)$, we want to find an upper bound on $\|\rho_N\|$, where

$$\rho_N := \sum_{\pm} \sum_{i_1, i_2 \in \mathcal{F}} \alpha_{i_1, i_2}(\mu) \pi_{i_1, i_2}^{|\mathcal{F}|} \quad (3.60)$$

is the first term, (I), of G . From the exponential decay of the eigenstate V_1^\pm it follows that for some $c > 0$ we have

$$\|\rho_N\| = \mathcal{O}(Ne^{-cN}).$$

We now fix a ball $K = B(0, r_N)$ and choose the radius $r_N := \mathcal{O}(Ne^{-cN})$. Therefore it suffices to find a root of (3.45) inside the ball K and conclude the existence of an eigenvalue by Rouché's theorem. We easily see that for all $v \neq 0$, and $\lambda \in \partial K$, $\|F(\lambda)v\| \geq |\lambda|\|v\| = r_N\|v\|$ since the second term of the right hand side of (3.63) is symmetric. On the other hand,

$$\|(II)\| \leq \mathcal{O}(N^2 e^{-2cN}) \text{ and } \|(III)\| \leq \mathcal{O}(N^2 e^{-3cN}).$$

Thus, we have $\|F(\lambda)v\| > \|G(\lambda)v\|$ on ∂K , for all $v \neq 0$. Since $F(\lambda)$ is not invertible

exactly at 0 inside K , we have from Lemma 2.1 that there is one point inside K so that $F(\lambda) + G(\lambda)$ is not invertible or in other words there is one root of $(R_{\mathcal{F}}(\lambda) + i)u = 0$ with $\lambda \lesssim Ne^{-cN}$. \square

3.3.5 Disordered chains

We now study the case of a disordered pinning potential, i.e. we assume that $\eta_i > 0$ are independent identically distributed (i.i.d.) random variables drawn from some bounded density distribution

$$\eta_i \sim \rho \in C_c(0, \infty).$$

Note that additional disorder in the interaction strengths leads to the-somewhat analogous study of random Jacobi operators which is for example discussed in [Tes00, Ch. 5]. In particular, localization for off-diagonal disorder in discrete Schrödinger operators, corresponding to random interactions in the chain of oscillators, is studied in [DKS83, DSS87].

Note that disordered harmonic chains have been studied before [OL74, CL71], even though in these works the randomness is posed in the masses of the particles, rather than the coefficients of the pinning potentials. However, the effect of localization does extend to that setting as well and can be studied- up to some technicalities- along the lines of the proof presented here. We illustrate in Fig. 3.11 that all types of disorder yield an exponentially fast closing of the spectral gap.

The generator of the dynamics is the operator \mathcal{L} given by (2.5). Considering friction and diffusion at at least one end of the chain, cf. Proposition 2.1, the spectral gap is still given as

$$\lambda_S := \inf\{\operatorname{Re}(\lambda) : \lambda \in \operatorname{Spec}(\Omega_{[N]^d})\}.$$

For more details we refer to the Appendix 3.A. From general results stated in Lemma 3.1, studying the spectrum of the matrix $\Omega_{[N]^d}$ is equivalent to studying the points at which the lower dimensional Wigner $W_{\mathcal{F}}$ -matrix is not invertible. The matrix $B_{[N]^d}$, appearing in the matrix entries of $\Omega_{[N]^d}$ (2.5), is the restriction to a finite domain of size N^d of the one-dimensional *discrete Anderson model*. This is explained below.

In the analysis of the disordered case it makes the analysis slightly simpler by labelling particles instead of $[N]^d$ rather by a set

$$[\pm N]^d := \{-N, -N + 1, \dots, N - 1, N\}^d,$$

i.e. we study the scaling of the spectral gap for $(2N + 1)^d$ particles as a function of N where we assume the chain to grow in all directions.

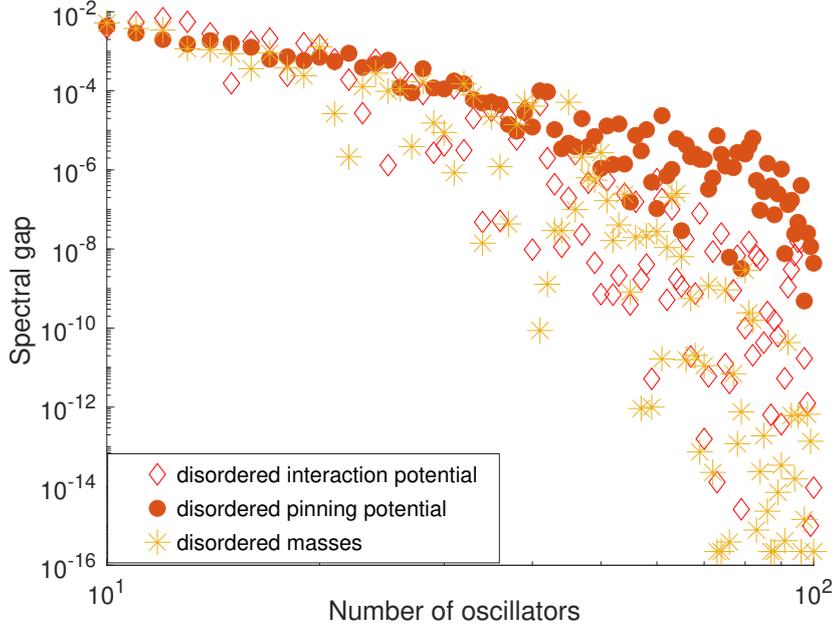


Figure 3.11: Log-log plot of the spectral gap for the one-dimensional chain of oscillators and different types of disorder: Random masses $m_i = \frac{1}{1+X_i}$, random interaction $\xi_{ij} = 1 + X_i$ and random pinning potential $\eta_i = 1 + X_i$ where $X_i \sim U[0, 1]$ are uniform iid.

For disorder in the pinning potential, the limiting discrete Schrödinger operator $B_{[\infty]^d}$ is the multi-dimensional *discrete Anderson model*: the discrete Anderson model is a discrete Schrödinger operator with random single-site potential introduced by Anderson [And58] to describe the absence of diffusion in disordered quantum systems. It is the random discrete Schrödinger operator on $\ell^2(\mathbb{Z}^d)$

$$H_\omega^{[\infty]^d} = -\Delta_{[\infty]^d} + \lambda V_\omega$$

acting on $\ell^2(\mathbb{Z}^d)$ where $\Delta_{[\infty]^d}$ is the discrete Laplacian on \mathbb{Z}^d , $\lambda > 0$ the coupling constant, and V_ω a random potential $V_\omega = \{V_\omega(n) : n \in \mathbb{Z}^d\}$ consisting of i.i.d. variables with common probability distribution with, for our purposes, bounded density μ on $(0, \infty)$. Here, ω is an element of the product probability space $\Omega = (\text{supp}(\mu))^{\mathbb{Z}^d}$ endowed with the σ -algebra generated by the cylinder sets and the product measure $\mu^{\mathbb{Z}^d}$ consisting of the common probability distribution with compact support. The random potential $V_\omega : \mathbb{Z}^d \rightarrow \mathbb{R}$ is defined as projections $\Omega \ni \omega \mapsto V_\omega(n) = \omega_n$ for $n \in \mathbb{Z}^d$.

We also consider $H_\omega^{[\pm N]^d}$ the restriction to finite domains of size $(2N + 1)^d$, of the operator $H_\omega^{[\infty]^d}$, with Neumann boundary conditions.

So the spectral gap of the d -dimensional disordered network of N^d oscillators coupled at two heat baths at different temperatures, as described above, is given by one of the

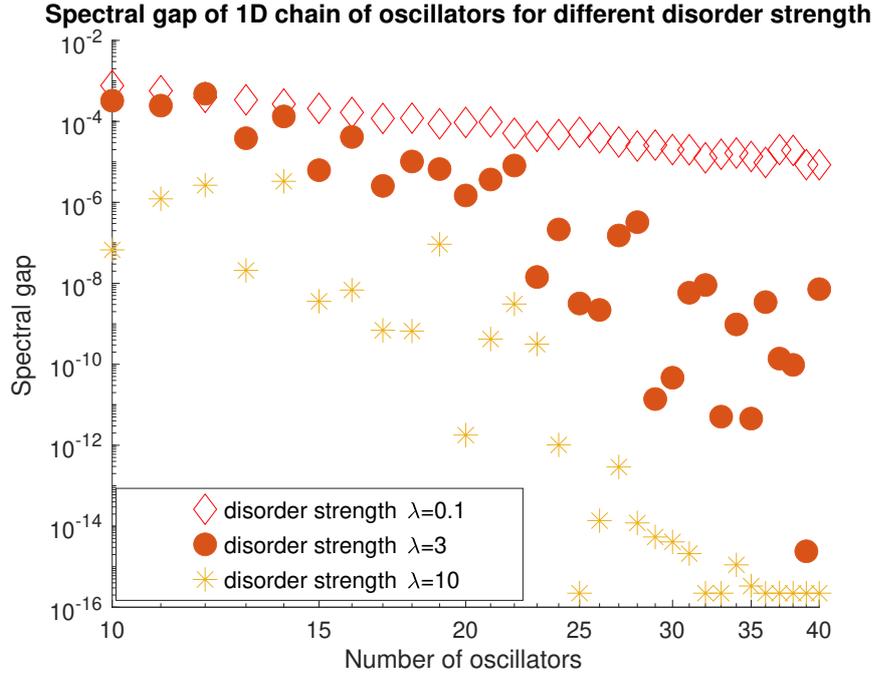


Figure 3.12: Log-log plot of the spectral gap for the one-dimensional chain of oscillators for different disorder strengths when $\eta_i \sim 1 + \lambda U[0, 1]$.

points where the Wigner $W_{\mathcal{F}}$ -matrix is not invertible. Since this lower-dimensional matrix is defined in terms of the eigenvalues and eigenvectors of the matrix $B_{[\pm N]^d}$, see Lemma 3.1, we are interested in the spectrum of $B_{[\pm N]^d}$ which can be identified with $H_{\omega}^{[\pm N]^d}$.

In one dimension, the Anderson model has a.s dense pure point spectrum with exponentially localized eigenstates [FS83, vDK89]. In higher dimensions, $d \geq 2$ this is only known to be true for sufficiently large disorder or low energies and was already shown in [FS83]. From the case of a single impurity we know already that exponentially localized eigenstates should lead to an exponentially fast closing of the spectral gap. However, we have to deal with three additional obstructions in the disordered case:

- The eigenvalues of the Anderson model are not uniformly (in N) bounded away from each other.
- The eigenfunctions of the Anderson model do not obey a rich symmetry as before and can (in general) not be chosen to be even or odd.
- We are studying finite approximations $B_{[\pm N]^d}$ rather than the Anderson model $B_{[\infty]^d} = H_{\omega}^{[\infty]^d}$ itself.

The next Lemma shows that in general eigenvalues will not get any closer than a distance N^{-2d-2} .

Lemma 3.10. *Let $A_N(s([N]^d))$ be the event that for the $(2N + 1)^d$ -size Anderson model $B_{[\pm N]^d}$, there exists an interval of size $s([N]^d)$ that contains (at least) two eigenvalues.*

For the choice $s([\pm N]^d) = N^{-2d-2}$ we have $\mathbb{P}(A_N(s([\pm N]^d))) = 0$ for all but finitely many N .

Proof. The spectrum of $B_{[\pm N]^d}$ is contained in an interval of order one. Thus, we can cover $\text{Spec}(B_{[\pm N]^d})$ by $\mathcal{O}(1/s([\pm N]^d))$ many intervals $(I_n^{[\pm N]^d})_{n \in [\mathcal{O}(1/s([\pm N]^d))]}$ of size $2s([\pm N]^d)$ such that the overlap of each interval $I_n^{[\pm N]^d}$ with its nearest neighbors is another interval of size $s([\pm N]^d)$. This construction implies that if there exists an interval of size $s([\pm N]^d)$ that contains two eigenvalues, these two eigenvalues are also contained in one of the $I_n^{[\pm N]^d}$. We will now use Minami's estimate which bounds from above the probability of two eigenvalues of the finite volume operator being close, see [KM06, (7), App. 2]. More specifically that is

$$\mathbb{P}(|\text{Spec}(B_{[\pm N]^d}) \cap J| \geq 2) \leq \pi^2 \|\rho\|_\infty^2 N^{2d} |J|^2,$$

we write

$$\begin{aligned} \mathbb{P}(A_N(s([\pm N]^d))) &\leq \sum_{n \in [\mathcal{O}(1/s([\pm N]^d))]} \mathbb{P}\left(|I_n^{[\pm N]^d} \cap \text{Spec}(B_{[\pm N]^d})| \geq 2\right) \\ &\leq \sum_{n \in [\mathcal{O}(1/s([\pm N]^d))]} \pi^2 \|\rho\|_\infty^2 N^{2d} 4s([\pm N]^d)^2 \\ &= \mathcal{O}(N^{2d} s([\pm N]^d)) < \infty. \end{aligned} \tag{3.61}$$

We now choose $s([\pm N]^d) = N^{-2d-2}$, such that by the Borel-Cantelli lemma $A_N(s([\pm N]^d))$ happens at most finitely many times a.s. and otherwise eigenvalues of $B_{[\pm N]^d}$ are a.s. at least N^{-2d-2} apart. \square

With this Lemma at hand, we can now give the proof of the exponential decay of the spectral gap.

Proposition 3.11. *Consider the network of oscillators with equal masses, unit interaction strength. In addition, we assume that there is always at least one edge subject to friction at the boundary and that the friction of particles is uniformly bounded in N . Let the pinning constants be iid $\eta \sim \rho \in C_c(0, \infty)$. Then the spectral gap of the chain of oscillators decays, for almost every realization of the disorder in the pinning potential, exponentially fast³.*

Proof. For almost every realization of disorder we can find by general results on the Anderson model [FS83, vDK89] an eigenfunction φ of the operator $B_{[\infty]^d}$, corresponding to an eigenvalue λ_∞ such that

$$\sup_{i; \|\cdot\|_\infty = N} |\varphi(i)| \leq \mathcal{O}(e^{-DN}) \text{ and } \sum_{m \notin [\pm N]^d} |\varphi(m)|^2 \leq \mathcal{O}(e^{-DN}).$$

³The decay of the spectral gap will in general depend on the disorder but is a.s. exponentially fast.

By using Lemma 3.8 with $m_0 = 0$ and Lemma 3.10 it follows that for all but finitely many N the distance between any two eigenvalues is at least $\alpha_N := N^{-2(d+1)}$ and we find an eigenvector $\psi|_{[\pm N]^d}$ to $B|_{[\pm N]^d}$ with eigenvalue λ_1 that approximates φ with eigenvalue λ_∞ . Thus, for all but finitely many N

$$\|\psi|_{[\pm N]^d} - \varphi|_{[\pm N]^d}\| \leq \mathcal{O}(e^{-DN} N^{2(d+1)}).$$

As before, we shall restrict us again to the case $d = 2$ for simplicity and study solutions of the equivalent problem equation

$$\det(F(\lambda) + G(\lambda)) = 0 \quad (3.62)$$

that will be defined in terms of the eigenvectors v_j and eigenvalues λ_j for $j \in [(2N+1)^2]$ of $B|_{[\pm N]^2}$ with λ_1 as above. Then, we define $\mu_j = \lambda_j - \lambda_1$ and setting $v_{-j} := v_j$ and $\lambda_{-j} := -\lambda_j$, the matrices $F(\lambda), G(\lambda)$ are then defined as follows

$$F(\lambda) := i\lambda - \lambda \sum_{j \in \pm[(2N+1)^2] \setminus \{1\}} \sum_{i_1, i_2 \in \mathcal{F}} \frac{\alpha_{i_1, i_2}(\lambda_j)}{\mu_j} \pi_{i_1, i_2}^{|\mathcal{F}|} \quad (3.63)$$

and

$$\begin{aligned} G(\lambda) := & \underbrace{\sum_{i_1, i_2 \in \mathcal{F}} \alpha_{i_1, i_2}(\lambda_1)^{\mathcal{F}} \pi_{i_1, i_2}^{|\mathcal{F}|}}_{=:(I)} \underbrace{-\lambda^2 \sum_{j \in \pm[(2N+1)^2] \setminus \{1\}} \sum_{i_1, i_2 \in I} \frac{\alpha_{i_1, i_2}(\lambda_j) \pi_{i_1, i_2}^{|\mathcal{F}|}}{\mu_j^2}}_{=:(II)} \\ & \underbrace{-\lambda^3 \sum_{j \in \pm[(2N+1)^2] \setminus \{1\}} \sum_{i_1, i_2 \in \mathcal{F}} \frac{\alpha_{i_1, i_2}(\lambda_j) \pi_{i_1, i_2}^{|\mathcal{F}|}}{\mu_j^2 (\mu_j - \lambda)}}_{=:(III)} \end{aligned} \quad (3.64)$$

so that a solution to (3.62) corresponds to the desired eigenvalue. Before we fix a ball $K = B(0, r_N)$, we again want to find an upper bound for the $\|\rho_N\|$, where

$$\rho_N := \sum_{i_1, i_2 \in \mathcal{F}} \alpha_{i_1, i_2}(\lambda_1)^{\mathcal{F}} \pi_{i_1, i_2}^{|\mathcal{F}|} \quad (3.65)$$

i.e. is the first term, (I), of G . Using exponential decay of the eigenstate v_1 it follows that for $c > 0$ we have

$$\|\rho_N\| \leq \mathcal{O}(N e^{-cN}).$$

We now fix a ball $K = B(0, r_N)$ and choose the radius $r_N := \mathcal{O}(N e^{-cN})$. Therefore it suffices to find a root of (3.45) inside the ball K and conclude the existence of an eigenvalue by Rouché's theorem. We easily see that for all $v \neq 0$, and $\lambda \in \partial K$, $\|F(\lambda)v\| \geq$

$|\lambda|\|v\| = r_N\|v\|$ since the second term of the right hand side of (3.63) is symmetric. On the other hand, by Lemma 3.10 we can estimate $\mu_j \geq cN^{-2(2+1)}$ for all but finitely many N and some $c > 0$. Using this lower bound, we have for $\lambda \in \partial K$

$$\|(\text{II})\| \leq \mathcal{O}(N^{2(2+2)}e^{-2cN}) \text{ and } \|(\text{III})\| \leq \mathcal{O}(N^{2(2+2)}e^{-3cN}).$$

Thus, we have $\|F(\lambda)v\| > \|G(\lambda)v\|$ on ∂K , for all $v \neq 0$ for almost all sufficiently large N . Since $F(\lambda)$ is not invertible exactly at 0 inside K , we have from Lemma 2.1 that there is one point inside K so that $F(\lambda) + G(\lambda)$ is not invertible or in other words there is one root of $(R_{\mathcal{F}}(\lambda) + i)u = 0$ with $\lambda \lesssim Ne^{-cN}$. \square

Remark 3.12 (Sharpness of the estimate in $d = 1$). *Note that when $d = 1$ and the friction-sites are $\mathcal{F} \subset \{1, N\}$, with γ_1, γ_N bounded uniformly in N , then we can conclude from item (4) in Proposition 2.2 a lower bounded on the spectral gap (both in the impurity and the disorder case) that is exponentially small in N . In these cases then indeed $\lambda_S = \mathcal{O}(e^{-cN})$.*

Appendix

3.A Proposition 2.1 on the chain of oscillators (2.5)

First we show that $\Omega_{[N]^d}$ given in (2.6) is positively stable. Indeed, as was done in [JPS17], we write

$$\Omega_{[N]^d} - \Omega_{[N]^d}^* = \begin{pmatrix} 0 & -(\mathbf{m}_{[N]^d}^{-1/2} B_{[N]^d}^{1/2} + B_{[N]^d}^{1/2} \mathbf{m}_{[N]^d}^{-1/2}) \\ \mathbf{m}_{[N]^d}^{-1/2} B_{[N]^d}^{1/2} + B_{[N]^d}^{1/2} \mathbf{m}_{[N]^d}^{-1/2} & 0 \end{pmatrix}$$

$$\frac{1}{2}(\Omega_{[N]^d} + \Omega_{[N]^d}^*) = \text{diag}(\Gamma, 0).$$

We denote by $\hat{\Gamma} = \text{diag}(\Gamma, 0)$ and $\hat{\vartheta} = \text{diag}(\vartheta, 0)$. Let $\lambda \in \text{Spec}(\Omega_{[N]^d})$ and u be a non-zero corresponding eigenvector. Hence,

$$\left\langle \frac{1}{2}(\Omega_{[N]^d} + \Omega_{[N]^d}^*)u, u \right\rangle = \text{Re}(\lambda)|u|^2 = |\hat{\Gamma}^{1/2}u|^2 \quad (1.66)$$

which implies that $\text{Re}(\lambda) \geq 0$. If $\text{Re}(\lambda) = 0$ then this implies that u must vanish where $\hat{\Gamma}$ is supported. In other words, if u is an eigenvector to $\Omega_{[N]^d}$ with eigenvalue $\lambda \in i\mathbb{R}$, then it is also, by squaring $\Omega_{[N]^d}$ without the $\hat{\Gamma}$ term, an eigenfunction to

$$S = \begin{pmatrix} -\mathbf{m}_{[N]^d}^{-1} B_{[N]^d} & 0 \\ 0 & -\mathbf{m}_{[N]^d}^{-1} B_{[N]^d} \end{pmatrix}.$$

with eigenvalues $-\lambda^2 \in \mathbb{R}$ and vanishes in addition at the support of $\hat{\Gamma}$. Thus, writing $u = (u_1, u_2)$, both u_1, u_2 have to be eigenfunctions of the Schrödinger operator $\mathbf{m}_{[N]^d}^{-1} B_{[N]^d}$ with eigenvalue λ^2 vanishing where $\hat{\Gamma}$ is supported.

In the homogeneous case, the eigenfunctions are explicit (3.30) and one can verify directly that they do not vanish anywhere on the boundary. Therefore, as long as there is a particle experiencing friction somewhere on the boundary, there does not exist an eigenfunction to the Schrödinger operator that vanishes there.

In the case of the disordered network or the network with an impurity, it suffices to apply a simple unique continuation argument. First observe that the vanishing of an

eigenfunction on an edge implies by directly analyzing $(B_{[N]^d} + \lambda^2)u = 0$ (as in the proof of the item (4) of Prop. 2.2), at the oscillators of the edge, that the eigenfunction also has to vanish on the nearest edge to the boundary edge of oscillators that exhibits friction. Iterating this argument shows that such an eigenfunction has to vanish everywhere.

We also have shown in the last parts of the proofs of the Propositions (3.3), (3.5), by proving an explicit lower bound, that the spectral gap cannot be 0, i.e. $\operatorname{Re}(\lambda) > 0$. Note that another argument that shows that $\operatorname{Re}(\lambda) \neq 0$ can be done by contradiction as then $\hat{\Gamma}^{1/2}u = 0$ and so $\Omega_{[N]^d}^*u = -\Omega_{[N]^d}u = -\lambda u$. Inductively we would have $\hat{\Gamma}^{1/2}\Omega_{[N]^d}^*u = (-\lambda)^{-n}\hat{\Gamma}^{1/2}u = 0$ for all $n \geq 0$. As soon as the interaction coefficient $c > 0$, we have that

$$\bigcap_{n \geq 0} \operatorname{Ker} \left(\hat{\Gamma}^{1/2} \Omega_{[N]^d}^* \right) = \{0\}.$$

This is for example a consequence of the fact that the pair $(\Omega_{[N]^d}, \hat{\Gamma}^{1/2})$ satisfies the Kalman condition when $c > 0$ [Raq19, Lemma 3.2], see also [JPS17, Lemma 5.1 (2)].

Secondly, regarding the condition (1) of Proposition (2.1), the fact that there is no non-trivial subspace of $\operatorname{Ker}(\Gamma\vartheta)$ that is $\Omega_{[N]^d}$ -invariant is equivalent to the hypoellipticity of the operator \mathcal{L} (this is discussed in the first section in [H67]).

For the hypoellipticity, it is sufficient to show that the generator can be written as $\mathcal{L} = X_0 + \sum_{i \in \mathcal{F}} X_i^2$ and that the Lie algebra \mathcal{A} generated by the vector fields

$$\{X_0\}, \{[X_i, X_j]\}_{0 \leq i, j \leq 2dN^d}, \{[X_i, [X_j, X_k]]\}_{i, j, k \geq 0}, \dots$$

satisfies Hörmander's hypoellipticity condition, i.e. \mathcal{A} has full rank. This is true as long as $c > 0$, since for $j = 1, \dots, d$: $[\partial_{p_1^{(j)}}, X_0] = -\frac{1}{2}\partial_{p_1^{(j)}} + \partial_{q_1^{(j)}}$ i.e. $\partial_{q_1^{(j)}} \in \mathcal{A}$. Then calculating $[\partial_{q_1^{(j)}}, X_0]$ we get $\partial_{p_2^{(j)}} \in \mathcal{A}$ when the interaction potential is strictly convex. By the use of successive commutators it is clear that we recover Hörmander's hypoellipticity condition indeed.

3.B Matrix-valued Rouché's theorem

Lemma 2.1 (Matrix-valued Rouché's theorem). *Let $A, B : K \rightarrow \mathbb{C}^{n \times n}$ be two holomorphic functions inside some region K with $\|B(z)v\| < \|A(z)v\|$ for all $v \neq 0$ and $z \in \partial K$. Then, both A and $A + B$ are invertible at an equal number of points inside K .*

Proof. By the argument principle the number of singular points of $A(z) + tB(z)$ in K with $t \in [0, 1]$ is given by

$$N(t) := \frac{1}{2\pi i} \int_{\partial K} \partial_z \log(\det(A(z) + tB(z))) dz$$

and independent of t by continuity of $t \mapsto N(t)$.

□

Chapter 4

Existence of a Non-Equilibrium Steady State for the non-linear BGK equation on an interval

This chapter is a joint work with Josephine Evans and it is published in [EM21].

We show existence of a non-equilibrium steady state for the one-dimensional, non-linear BGK model on an interval with diffusive boundary conditions. These boundary conditions represent the coupling of the system with two heat reservoirs at different temperatures. The result holds when the boundary temperatures at the two ends are away from the equilibrium case, as our analysis is not perturbative around the equilibrium. We employ a fixed point argument to reduce the study of the model with non-linear collisional interactions to the linear BGK.

4.1 Introduction

This work is a contribution to the study of non-equilibrium steady states for non-linear kinetic equations. We study the existence of non-equilibrium steady states for the *non-linear BGK equation* on bounded domains with diffusive boundary conditions. In this paper we look at the 1d case where the velocity variable is in \mathbb{R} and the x variable is in an interval with boundary conditions at different temperatures at each side. We show the existence of a non-equilibrium steady state and explore its properties.

The BGK model of the Boltzmann's equation is a simple kinetic relaxation model introduced by Bhatnagar, Gross and Krook in [BGK54] as a toy model for Boltzmann flows. The evolution problem for the BGK model was first studied in [Per89] and later in [GP89] where global existence was proved and in [PP93] where existence and uniqueness was proved for the initial-value problem in bounded domains.

Here we are interested in non-equilibrium phenomena, that is to say equations with steady states which are not Gibb's states and are induced by effects external to the system of study. In our case these external effects are present as diffusive boundary conditions. We show results which are not derived by perturbations models which have equilibrium states or by models which are close to the hydrodynamic regime. That is to say we work in the regime where the Knudsen number is not considered to be small.

We describe our model in the following subsection.

4.1.1 Description of the model

We consider a gas of particles in the domain $(0, 1)$ where the collisions among the particles are described by the nonlinear BGK operator. The distribution function $f(t, x, v)$ of the gas is the density of the particles at the position $x \in (0, 1)$ with velocity $v \in \mathbb{R}$ at time $t > 0$. We denote by κ the *Knudsen number*¹ and we study the existence of stationary solutions $f(x, v)$ to the following equation

$$\partial_t f + v \partial_x f = \frac{1}{\kappa} (\rho_f \mathcal{M}_{T_f} - f), \quad (1.1)$$

$$f(0, v) = \widetilde{\mathcal{M}}_1(v) \int_{v' < 0} |v'| f(0, v') dv', \quad v > 0, \quad (1.2)$$

$$f(1, v) = \widetilde{\mathcal{M}}_2(v) \int_{v' > 0} |v'| f(1, v') dv', \quad v < 0. \quad (1.3)$$

¹The Knudsen number κ is defined as the ratio between the mean free path and the typical observation length.

Here the *spatial density* $\rho_f(x)$ and the *pressure* $P_f(x) := \rho_f(x)T_f(x)$ are given respectively by

$$\rho_f(x) = \int_{-\infty}^{\infty} f(x, v)dv, \quad \rho_f(x)T_f(x) = \int_{-\infty}^{\infty} v^2 f(x, v)dv \quad (1.4)$$

and then the *local temperature* corresponding to f is T_f . We denote by $\mathcal{M}_{T_f}(v)$ the Maxwellian with temperature T_f i.e.

$$\mathcal{M}_{T_f}(v) = (2\pi T_f)^{-1/2} \exp\left(-\frac{1}{2T_f}v^2\right).$$

Furthermore, $\widetilde{\mathcal{M}}_1, \widetilde{\mathcal{M}}_2$ are Maxwellians at the boundary temperatures T_1, T_2 respectively and they are considered to be renormalised so that, for $i = 1, 2$,

$$\int_0^{\infty} v \widetilde{\mathcal{M}}_i(v)dv = 1. \quad (1.5)$$

This means that

$$\widetilde{\mathcal{M}}_i(v) := \frac{1}{T_i} \exp\left(-\frac{1}{2T_i}v^2\right).$$

In other words we study the steady states of a gas which is coupled to two temperature reservoirs at the two boundaries of the domain $(0, 1)$ and this coupling is implemented through the so-called *diffusive boundary conditions* or *Maxwell boundary conditions*. So that when particles hit one of the boundaries $\{0, 1\}$, they get reflected and re-enter the domain with new velocities drawn from the Maxwellians $\widetilde{\mathcal{M}}_i(v)$ corresponding to temperatures T_1, T_2 at the two ends.

4.1.2 State of the Art

This paper is motivated by [CEL⁺18, CEL⁺19], where they study the non-linear BGK equation on the periodic torus in the presence of scatterers at two different temperatures. There it is straightforward to find one steady state and these papers show that this state is unique under certain conditions. There the non-equilibrium forcing is the same throughout the space. Also for the non-linear BGK equation there is a paper of Ukai [Uka92], about the existence of steady states with prescribed boundary conditions which is a situation similar to that studied here. The boundary conditions we consider here are different, since the paper of Ukai prescribes the density at either side of the interval, whereas in our paper we prescribe diffusive boundary conditions. The techniques are also different.

The majority of the papers investigating non-equilibrium steady states of kinetic equations are in the setting of the Boltzmann equation. We mention first the paper [AN00] which also deals with a non-perturbative setting to show the existence of non-equilibrium

steady states to the Boltzmann equation in the slab. This paper crucially uses the entropy distribution of the equation. There are also a number of papers about similar problems in a perturbative setting either when the difference of the temperatures is small [EGKM13], or when the Knudsen number is small and a hydrodynamic approximation can be used [Ark00, AEMN10, AEMN12]. There have also been works in a spatially homogeneous setting in the presence of scatterers [CLM15] for the Boltzmann equation and [Eva16] for Kac's toy model for the Boltzmann equation. We also mention the preprint [Ber19] which shows exponential convergence towards non-equilibrium steady states for the free transport equation in a domain with Maxwell boundary conditions.

One of the main motivations to study non-equilibrium phenomena, like the one appearing in the model of this note due to non-isothermal boundaries, is the better understanding of the *Fourier's law*, which from a mathematical point of view is a very challenging problem. The Fourier's law, which is well tested for several materials, relates the macroscopic thermal flux $J(t, x)$ to the small variations of the gradient of the temperature $\nabla T(t, x)$:

$$J(t, x) = -K(T)\nabla T(t, x) \tag{1.6}$$

where $0 < K(T) < \infty$ is the thermal conductivity of the material. It is not difficult to see that (1.6) implies the following diffusion equation for the temperature:

$$c(T)\partial_t T = \nabla(K(T)\nabla T)$$

where $c(T)$ is the specific heat of the system per unit volume.

Concerning heat conduction in gases: (1.6) was rigorously proven in [ELM94, ELM95] for the stationary Boltzmann equation in a slab for small Knudsen numbers and when the temperature difference is small. We also refer here again to [EGKM13] where the authors construct solutions to the 3d steady problem with the Boltzmann hard spheres collision operator and diffusive boundaries with different temperatures at the two walls that do not oscillate too much. There the authors work with small temperature difference and they can see mathematically that the Fourier's law does not hold, since they are in the kinetic regime, by combining their result with pre-existing numerical simulations in [OAY89].

The abovementioned works are specific answers to the more general question in Statistical Physics: the mathematically rigorous derivation of Fourier's law or a proof of its breakdown, from microscopic, purely deterministic or stochastic, models. For several overviews on this topic we refer the reader to [BLRB00, Lep16, Dha08, FB19].

An example of such a microscopic heat conduction model, a model of heat reservoirs is the so-called chain of oscillators. For more information on this model we refer to [RLL67, EPRB99b, RBT02, Car07, CEHRB18] where questions of existence and uniqueness of a NESS and exponential approach towards it are addressed, as well as to [Hai09, HM09]

for interesting features of the model: for example cases where there is no spectral gap of the generator of the associated process. Quantitative results concerning the scaling of the spectral gap in terms of the number of the particles, for special cases of the chain, can be found in [Men20, BM22].

4.2 Mathematical Preliminaries

First note that the normalisation (1.5) is chosen so that the equation conserves mass, indeed we record this observation in the following Lemma:

Lemma 2.1. *The equation (1.1) at least formally conserves mass.*

Proof. We write

$$\begin{aligned} \frac{d}{dt} \int f(x, v) dx dv &= - \int v \partial_x f dx dv + \frac{1}{\kappa} \left(\int \rho(x) \mathcal{M}_T(v) dv dx - \int f \right) \\ &= - \int v \partial_x f = \int v f(1, v) dv - \int v f(0, v) dv. \end{aligned}$$

Then we show that each of the boundary terms is zero:

$$\begin{aligned} \int v f(1, v) dv &= \int_{-\infty}^0 v f(1, v) dv + \int_0^{\infty} v f(1, v) dv \\ &= \int_0^{\infty} |v'| f(1, v') dv' \int_{-\infty}^0 \tilde{M}_2(v) v dv + \int_0^{\infty} v f(1, v) dv \\ &= 0. \end{aligned}$$

Similarly we show that the other boundary term is 0 as well, which concludes the proof. \square

4.2.1 Notation

We write $f(x) \leq \mathcal{O}(g(x))$ to denote that there is a constant $C > 0$ such that $|f(x)| \leq C |g(x)|$. We occasionally write $A \lesssim B$ in order to say that $A \leq CB$ for some constant C that only depends on the two temperatures T_1, T_2 . We denote by $\mathcal{B}(A)$ the Borel σ -algebra on A and by n_x the outward unit vector at $x \in \{0, 1\}$. We also write $C_c^\infty(X)$ for the space of the compactly supported smooth functions on X .

4.2.2 Plan of the paper

We introduce the main results in the next Section. In Section 4 we present the proofs of the main results. This is split into subsections showing the different criteria needed to be fulfilled in order to apply the Schauder fixed point Theorem. In particular in subsection

4.3 we present the asymptotic behaviour of the moments in order to get an L^∞ bound on the temperature profile, and then to prove Hölder continuity of it in 4.4. In 4.5 we prove the continuity of the mapping to which we apply Schauder's Theorem in 4.6. Finally, we conclude with Section 5 with a discussion of the results and possible avenues for future research.

4.3 Main Results

We introduce the following condition, under which our main Theorem holds.

Condition 1. *We say that the pair of temperatures T_1, T_2 satisfy this condition when*

$$(C1) \quad \kappa^2 T_1 > \gamma_2 \text{ and}$$

$$(C2) \quad \sqrt{T_2} - \sqrt{T_1} \geq \gamma_1 \kappa^{1/2} T_2^{1/4}$$

where γ_1, γ_2 are positive constants and $\kappa > 0$ is the time renormalizing constant in front of the collision operator in equation (1.1), i.e. the Knudsen number.

Our main results on the steady state of the nonlinear BGK operator with diffusive boundary conditions are summarized in the following Theorem.

Theorem 3.1. *For every two fixed temperatures T_1, T_2 satisfying Condition 1, there exists a steady state which satisfies equation (1.1) with boundary conditions (1.2) and (1.3). Furthermore, this steady state has the following properties:*

- *It has zero momentum uniformly in $x \in (0, 1)$.*
- *It has constant density and pressure equal to $\sqrt{T_1 T_2}$, asymptotically with T_1 . In particular, for all $x \in (0, 1)$,*

$$1 - \gamma_0 \kappa^{-1/2} T_1^{-1/4} \leq \rho_f(x) \leq 1 + \gamma_1 \kappa^{-1/2} T_1^{-1/4}$$

$$\sqrt{T_1 T_2} \lesssim P_f(x) \lesssim \sqrt{T_1 T_2}.$$

- *Its temperature profile is 1/2-Hölder continuous and also it is asymptotically equal to $\sqrt{T_1 T_2}$ with the deviation from $\sqrt{T_1 T_2}$ decreasing as T_1 increases: for all $x \in (0, 1)$,*

$$\sqrt{T_1 T_2} (1 - \gamma_1 \kappa^{-1/2} T_1^{-1/4}) \lesssim T_f(x) \lesssim \sqrt{T_1 T_2} (1 + \gamma_0 \kappa^{-1/2} T_1^{-1/4}),$$

for some constants γ_0, γ_1 and κ the constant in front of the collisional operator in (1.1).

Remark 3.2. *The fact that the steady state of this equation has zero momentum uniformly in x , implies it is also a solution to the similar time independent equation,*

$$v\partial_x f = \rho_f(x)\mathcal{M}_{u_f, T_f}(v) - f,$$

with the boundary conditions (1.2) and (1.3). Here,

$$\mathcal{M}_{u_f, T_f}(v) = (2\pi T_f)^{-1/2} e^{-(v-u_f)^2/T_f},$$

and

$$\rho_f u_f := \int_{\mathbb{R}} f(x, v) v dv.$$

4.4 Proofs

4.4.1 Strategy of Proof

In order to prove the existence of a steady state when T_1, T_2 satisfy condition 1, we perform a fixed point argument. We look at the following linear equation with the same spatially variable diffusive boundary conditions for given temperature profile $T(x)$:

$$\partial_t f + v\partial_x f = \rho(x)\mathcal{M}_{T(x)} - f, \quad (4.7)$$

$$f(0, v) = \widetilde{M}_1(v) \int_{v' < 0} |v'| f(0, v') dv', \quad v > 0, \quad (4.8)$$

$$f(1, v) = \widetilde{M}_2(v) \int_{v' > 0} |v'| f(1, v') dv', \quad v < 0. \quad (4.9)$$

where $\mathcal{M}_{T(x)}$ is the Maxwellian with temperature $T(x)$.

Remark 4.1. *This differs from equation (1.1) since we use a fixed temperature profile in the Maxwellian on the right hand side rather than the temperature profile coming from f .*

We prove the two following facts:

- The PDE (4.7)-(4.8)-(4.9) is the equation on the law of a stochastic process and this stochastic process has a unique equilibrium state. This equilibrium steady state has a temperature profile which we call $\tau(x)$.
- If $T_1 \leq T(x) \leq T_2$ and T_1, T_2 satisfy condition 1 then we have that $T_1 \leq \tau(x) \leq T_2$ and $\tau(x)$ is 1/2-Hölder continuous with modulus of continuity depending on T_1, T_2 .

We define the map $\mathcal{F}(T) = \tau$ which is a map between continuous functions on $(0, 1)$ and thanks to the first fact above, it is well-defined. Then we apply the Schauder fixed point theorem using the second fact above to show that \mathcal{F} has a fixed point. From the

definition of the mapping \mathcal{F} we get that a fixed point implies that the temperature profiles of the nonlinear and the linear model will coincide. Therefore, for T being this fixed point, corresponding to the two temperature profiles, a steady state of the linear model (4.7)-(4.8)-(4.9), will also be a steady state of the nonlinear model (1.1)-(1.2)-(1.3). In the following sections we make it precise how to define the map $\mathcal{F}(T)$, then give bounds on $\mathcal{F}(T)$ which allow us to prove point 2. Finally, we use these to apply the Schauder fixed point theorem.

Note that a similar idea to apply Brouwer fixed point theorem for a finite system of anharmonic crystals coupled to external and self-consistent internal Langevin heat baths can be found in [BLLO09] in order to prove the existence of a stationary self-consistent temperature profile.

4.4.2 Definition of the map $\mathcal{F}(T)$.

In this section we work in the case $\kappa = 1$ in order not to track too many constants and to simplify the presentation, since quantitative bounds in this section do not have impact on our final result. In order to properly define the map $\mathcal{F}(T)$ we need a well defined way of selecting a steady state of the PDE (4.7)-(4.8)-(4.9). In order to do this we define a stochastic process and show that this stochastic process has a unique steady state the law of which is a weak solution to the steady state version of (4.7)-(4.8)-(4.9). First we define what we mean for a weak measure valued solution of (4.7)-(4.8)-(4.9).

Definition 4.2. *A weak solution in the sense of measures to the PDE (4.7)-(4.8)-(4.9) is a triple $\mu_{1,t}, \mu_{2,t}, \mu_t$ with μ_i satisfying that for every test function supported on $\mathbb{R}_i = \mathbb{R}_+$ for $i = 1$ or $\mathbb{R}_i = \mathbb{R}_-$ for $i = 2$*

$$\int_{\mathbb{R}_i} \Phi(v) \mu_i(dv) = \int_{\mathbb{R}-\mathbb{R}_i} |v'| \mu_i(dv') \int_{\mathbb{R}_i} v \widetilde{\mathcal{M}}_i(v) \Phi(\xi, v) dv$$

where $\xi = 0, 1$, the left boundary for $i = 1$ and the right boundary for $i = 2$. Furthermore

$$\begin{aligned} & \int_0^\infty \iint_{(0,1) \times \mathbb{R}} \left(\partial_t \Phi(t, x, v) + v \partial_x \Phi(t, x, v) + \int_{\mathbb{R}} \Phi(t, x, v') \mathcal{M}_{T(x)}(v') dv' - \Phi(t, x, v) \right) \mu_t(dx, dv) dt \\ & + \iint_{(0,1) \times \mathbb{R}} \Phi(0, x, v) \mu_0(dx dv) = \int_0^\infty \int_{\mathbb{R}} \Phi(t, 1, v) \mu_2(dv) dt - \int_0^\infty \int_{\mathbb{R}} \Phi(t, 0, v) \mu_1(dv) dt. \end{aligned}$$

Existence and uniqueness for the linear BGK equation with diffusive boundary conditions. For our purposes we give a probabilistic interpretation of the evolution of the process for the linear BGK. Note also that similar techniques for the free transport equation with diffusive and specular reflective boundary conditions for higher dimensions have been applied in [BF19]. We work on the level of stochastic processes because there

is the possibility of some non-uniqueness occurring at what is known as the ‘grazing set’ which in our case is the two points $(0, 0), (1, 0)$. Defining a stochastic process allows us to set values at these points.

Proposition 4.3. *For every given continuous function $T(x)$ there exists a well defined way in which we can select a triple of measures μ_1, μ_2, μ which is a stationary solution in a weak sense to the linear PDE (4.7)-(4.8)-(4.9).*

We split the proof into two lemmas. We first construct a stochastic process and show that it is well defined and then show that the law of this is a desired weak solution.

Definition 4.4 (Construction of the stochastic process). *Let $(R_i^1)_{i \geq 1}, (R_i^2)_{i \geq 1}$, be two sequences of random variables with R_i^1 having law $v\widetilde{\mathcal{M}}_1$ and R_i^2 having law $|v|\widetilde{\mathcal{M}}_2$. Furthermore let N_i be a set of $N(0, 1)$ random variables and S_i be a sequence of exponential random variables with rate 1. Now we define the deterministic map*

$$\zeta(x, v) = \inf\{s > 0, x + vs \in \{0, 1\}\}$$

which is our first collision with one of the boundaries. Then we define recursively

$$T_{k+1} = T_k + \min\{S_{k+1}, \zeta(X_{T_k}, V_{T_k})\}.$$

Then for $t \in [T_k, T_{k+1})$ we have

$$X_t = X_{T_k} + (t - T_k)V_{T_k}, V_t = V_{T_k}.$$

We jump at the times T_k so that

$$V_{T_{k+1}} = \mathbb{1}_{T_{k+1}-T_k=S_{k+1}}\sqrt{T(X_{T_k})}N_{k+1} + \mathbb{1}_{X_{T_{k+1}}=0}R_{k+1}^1 + \mathbb{1}_{X_{T_{k+1}}=1}R_{k+1}^2$$

where here $T(X_{T_k})$ is the temperature at the position X_{T_k} .

Lemma 4.5 (Non-explosion of the process). *This stochastic process defined in 4.4 is well defined and exists for all $t > 0$.*

Proof. We would like to show that this process is non-explosive i.e. $T_i \rightarrow \infty$ almost surely. Lets look at the event

$$A_k = \{R_{2k+1}^1 < 1, R_{2k+2}^1 < 1, R_{2k+1}^2 < 1, R_{2k+2}^2 < 1, S_{2k+1} > 1, S_{2k+2} > 1\}.$$

The A_k 's are independent events and $\mathbb{P}(A_k) = \mathbb{P}(A_1) = p > 0$. Therefore by Borel-Cantelli A_k happens infinitely often almost surely. On A_k we can see that $T_{2k+2} - T_{2k} > 1$. This is because A_k ensures that $T_{2k+1} - T_{2k} > 1$ or $\zeta(X_{T_{2k}}, V_{T_{2k}}) < 1$, and in the second case

we know that $X_{T_{2k+1}} \in \{0, 1\}$ so the next jump time is defined by R_{2k+1}^1, R_{2k+2}^2 and S_{2k+2} which are all chosen so that $T_{2k+2} - T_{2k+1} > 1$ if $X_{T_{2k+1}} \in \{0, 1\}$. \square

Lemma 4.6. *The law of this stochastic process is a weak solution to the SDE.*

Proof. Here we follow [BF19]. We begin by showing how we can represent the boundary measures: for a set $A \in \mathcal{B}((0, \infty) \times \{0, 1\} \times \Sigma_{\pm})$ with $\Sigma_{\pm} := \{(x, v) \in \{0, 1\} \times \mathbb{R} : \pm v \cdot n_x < 0\}$, we introduce the measures

$$\begin{aligned}\mu_-^i(A) &= \mathbb{E} \left(\mathbb{1}_{(T_i, X_{T_i}, V_{T_i}) \in A} \mathbb{1}_{T_i = \zeta(X_{T_{i-1}}, V_{T_{i-1}})} \right), \\ \mu_+^i(A) &= \mathbb{E} \left(\mathbb{1}_{(T_i, X_{T_i}, V_{T_i-}) \in A} \mathbb{1}_{T_i = \zeta(X_{T_{i-1}}, V_{T_{i-1}})} \right)\end{aligned}$$

i.e. μ_-^i is the law of the triple (T_i, X_{T_i}, V_{T_i}) , *i.e.* after the collision with a boundary, and μ_+^i is the law of the triple (T_i, X_{T_i}, V_{T_i-}) , *i.e.* exactly before the collision with a boundary. Then we have

$$\begin{aligned}\mu_+(A) &= \sum_i \mu_+^i(A) \quad \text{for } A \in \mathcal{B}((0, \infty) \times \Sigma_-), \\ \mu_-(A) &= \sum_i \mu_-^i(A) \quad \text{for } A \in \mathcal{B}((0, \infty) \times \Sigma_+).\end{aligned}$$

These boundary measures satisfy the desired boundary condition. Indeed, we investigate the relationship between these two measures:

$$\begin{aligned}\mu_-^i(A) &= \mathbb{E} \left(\mathbb{1}_{(T_i, X_{T_i}, V_{T_i}) \in A} \mathbb{1}_{T_i = \zeta(X_{T_{i-1}}, V_{T_{i-1}})} \right) \\ &= \mathbb{E} \left(\mathbb{1}_{X_{T_i} = 0} \mathbb{1}_{(T_i, X_{T_i}, R_i^1) \in A} + \mathbb{1}_{X_{T_i} = 1} \mathbb{1}_{(T_i, X_{T_i}, R_i^2) \in A} \right) \\ &= \int \mathbb{E} \left(\mathbb{1}_{X_{T_i} = 0} \mathbb{1}_{(T_i, X_{T_i}, v) \in A} \right) v \widetilde{\mathcal{M}}_1(v) dv + \int \mathbb{E} \left(\mathbb{1}_{X_{T_i} = 1} \mathbb{1}_{(T_i, X_{T_i}, v) \in A} \right) v \widetilde{\mathcal{M}}_2(v) dv.\end{aligned}$$

Therefore,

$$\begin{aligned}\mu_-^i(A) &= \iint_{(0, T) \times (0, \infty)} \int_{-\infty}^0 (\mathbb{1}_{(t, 0, w) \in A}) w \widetilde{\mathcal{M}}_1(w) dw \mu_+^i(dt, dv) \\ &\quad + \iint_{(0, T) \times (0, \infty)} \int_0^{\infty} (\mathbb{1}_{(t, 1, w) \in A}) w \widetilde{\mathcal{M}}_2(w) dw \mu_+^i(dt, dv).\end{aligned}$$

Testing against a test function $\Phi \in C_c^\infty(\mathbb{R}_{\pm})$ we recover the boundary conditions as in the Definition 4.2. Now we would like to show that the tripple will be a weak solution to the PDE. For

$$\mu_1 = \mathbb{1}_{\{x=0\}}(\mu_+ + \mu_-), \quad \mu_2 = \mathbb{1}_{\{x=1\}}(\mu_+ + \mu_-),$$

and $\Phi \in C_c^\infty((0, \infty) \times (0, 1) \times \mathbb{R})$, we Taylor expand around (t, X_t, V_t) and we write

$$\begin{aligned}
& \mathbb{E}(\Phi(t+s, X_{t+s}, V_{t+s}) - \Phi(t, X_t, V_t)) = \\
& \quad \mathbb{E}((\Phi(t+s, X_{t+s}, V_{t+s}) - \Phi(t, X_t, V_t)) \mathbb{1}_{\{X_t+sV_t \in (0,1)\}}) + \\
& \quad \quad + \mathbb{E}((\Phi(t+s, X_{t+s}, V_{t+s}) - \Phi(t, X_t, V_t)) \mathbb{1}_{\{X_t+sV_t \notin (0,1)\}}) = \\
& \mathbb{E} \left(\left(s\partial_t \Phi(t, X_t, V_t) + sV_t \partial_x \Phi(t, X_t, V_t) \right) \mathbb{1}_{\left\{ \begin{array}{l} 0 \text{ jumps in} \\ (t, t+s) \end{array} \right\}} \right) \\
& + \mathbb{E} \left(\int_{-\infty}^{\infty} (\Phi(t, X_t, w) - \Phi(t, X_t, V_t)) (2\pi T(X_t))^{-1/2} \exp\left(-\frac{w^2}{2T(X_t)}\right) dw \mathbb{1}_{\left\{ \begin{array}{l} 1 \text{ jump in} \\ (t, t+s) \end{array} \right\}} \right) + \mathcal{O}(s) \\
& + \mathbb{E} \left(\int_0^{\infty} \Phi(t, X_t, w) w \widetilde{\mathcal{M}}_1(w) dw \mathbb{1}_{\{X_t+sV_t < 0\}} \mathbb{1}_{\{0 \text{ jumps in } (t, t+s)\}} \right) \\
& + \mathbb{E} \left(\int_{-\infty}^0 \Phi(t, X_t, w) w \widetilde{\mathcal{M}}_2(w) dw \mathbb{1}_{\{X_t+sV_t > 1\}} \mathbb{1}_{\{0 \text{ jumps in } (t, t+s)\}} \right).
\end{aligned}$$

Letting s to go to 0, this gives us that

$$\begin{aligned}
& \int (\partial_t \Phi(t, x, v) + v \partial_x \Phi(t, x, v)) \mu_t(dx, dv) + \int \int_w (\Phi(t, x, w) - \Phi(t, x, v)) \mathcal{M}_{T(x)}(w) dw \mu_t(dx, dv) \\
& + \int \int (\Phi(t, 0, w) - \Phi(t, 0, v)) w \widetilde{\mathcal{M}}_1(w) \mu_1(dv) \\
& + \int \int (\Phi(t, 1, w) - \Phi(t, 1, v)) w \widetilde{\mathcal{M}}_2(w) \mu_2(dv) = 0.
\end{aligned}$$

Therefore, μ_t is a weak solution to the PDE according to the Definition 4.2. \square

In order to prove the existence and uniqueness of a steady state for this stochastic process we use Doeblin's Theorem (we can find this in [Hai16] for example). Which is as follows

Condition 2 (Doeblin's condition). *If \mathcal{P} is a stochastic semigroup acting on probability measures over a set Ω then \mathcal{P} satisfies Doeblin's condition if there exists $\alpha \in (0, 1)$ and $\nu \in \mathcal{P}(\Omega)$, a probability measure on Ω such that for every $z \in \Omega$ we have*

$$\mathcal{P}\delta_z \geq \alpha\nu.$$

Theorem 4.7 (Doeblin's Theorem). *If \mathcal{P} satisfies Doeblin's condition then it has a unique steady state.*

Lemma 4.8. *Let \mathcal{P}_t be the stochastic semigroup corresponding to the evolution of the stochastic process defined in 4.4, then there exist a time t_* such that \mathcal{P}_{t_*} satisfies Doeblin's condition 2. In particular, the stochastic process has a unique steady state.*

Proof. We wish to find a lower bound for Doeblin's condition. We apply Duhamel's formula to find that

$$x - vt \in (0, 1), \quad f(t, x, v) = e^{-t} f(0, x - vt, v) + \int_0^t e^{-(t-s)} \rho(x - v(t-s)) \mathcal{M}_{T(x-v(t-s))}(v) ds. \quad (4.10)$$

Similarly,

$$x - vt \leq 0, \quad f(t, x, v) = e^{-x/v} f\left(t - \frac{x}{v}, 0, v\right) + \int_0^{x/v} e^{-(x/v-s)} \rho(vs) \mathcal{M}_{T(vs)}(v) ds, \quad \text{and} \quad (4.11)$$

$$x - vt \geq 1, \quad f(t, x, v) = e^{\frac{(1-x)}{|v|}} f\left(t - \frac{(1-x)}{|v|}, 1, v\right) + \int_0^{\frac{(1-x)}{|v|}} e^{-\left(\frac{-(1-x)}{|v|}-s\right)} \rho(1-vs) \mathcal{M}_{T(1-vs)}(v) ds. \quad (4.12)$$

In light of this, we define

$$R(t, x, v) := \begin{cases} x/v, & \text{for } x/v \leq t \\ t, & \text{for } x/v > t, v > 0 \\ t, & \text{for } v = 0 \\ t, & \text{for } (1-x)/|v| > t, v < 0 \\ (1-x)/|v|, & \text{for } -(1-x)/v \leq t \end{cases}$$

and

$$\pi f(x, v) := \rho_f(x) \mathcal{M}_{T(x)}(v).$$

Then we have the following lower bound

$$f(t, x, v) \geq \int_0^R e^{-R} (\pi f)(s, x - v(R-s), v) ds. \quad (4.13)$$

Regarding the boundary conditions, we substitute in the first term from (4.10):

$$f(t, 0, v) = \widetilde{\mathcal{M}}_1(v) \int_{-\infty}^0 |u| f(t, 0, u) du \geq \widetilde{\mathcal{M}}_1(v) \int_{-1/t}^0 e^{-t|u|} |u| f(0, -ut, u) du$$

and

$$f(t, 1, v) = \widetilde{\mathcal{M}}_2(v) \int_0^{\infty} |u| f(t, 1, u) du \geq \widetilde{\mathcal{M}}_2(v) \int_0^{1/t} e^{-t|u|} |u| f(0, 1-ut, u) du.$$

Now if we consider the initial condition $f(0, x, v) = \delta_{x_0}(x)\delta_{v_0}(v)$, we have

$$f(t, 0, v) \geq e^{-t}\widetilde{\mathcal{M}}_1(v)|v_0|\delta_{x_0}(-v_0t)\mathbb{1}_{|v_0|\leq 1} \quad \text{and}$$

$$f(t, 1, v) \geq e^{-t}\widetilde{\mathcal{M}}_2(v)|v_0|\delta_{x_0}(1-v_0t)\mathbb{1}_{|v_0|\leq 1}.$$

Then we have

$$x - vt \leq 0, \quad f(t, x, v) \geq e^{-t}\widetilde{\mathcal{M}}_1(v)|v_0|\delta_{x_0}\left(-v_0\left(t - \frac{x}{v}\right) \leq 1\right).$$

We need to know the local density and integrate in v . This gives us when $v_0 < 0$,

$$\begin{aligned} \rho(t, x) &\geq \int_{x/t}^{x/(t-1/|v_0|)_+} e^{-t}\widetilde{\mathcal{M}}_1(v)|v_0|\delta_{x_0}\left(-v_0\left(t - \frac{x}{v}\right)\right) dv \\ &\geq \int_0^{\min(|v_0|t, 1)} e^{-t}|v_0|\frac{1}{x|v_0|}\left(\frac{xv_0}{y+v_0t}\right)^2 \widetilde{\mathcal{M}}_1\left(\frac{xv_0}{y+v_0t}\right) \delta_{x_0}(y) dy \\ &\geq \mathbb{1}_{x_0+v_0t \leq 0} e^{-t} \frac{xv_0^2}{(x_0+v_0t)^2} \widetilde{\mathcal{M}}_1\left(\frac{xv_0}{x_0+v_0t}\right). \end{aligned}$$

Also when $v_0 > 0$, we have

$$\begin{aligned} \rho(t, x) &\geq \int_{-\infty}^{(1-x)/|v|} e^{-t}\widetilde{\mathcal{M}}_2(v)|v_0|\delta_{x_0}\left(1-v_0\left(t - \frac{1-x}{|v|}\right)\right) dv \\ &\geq e^{-t}|v_0|\frac{(1-x)v_0}{(x_0-1+v_0t)^2} \widetilde{\mathcal{M}}_2\left(\frac{(1-x)v_0}{1-v_0t-x_0}\right) \mathbb{1}_{x_0+v_0t \geq 1}. \end{aligned}$$

Now in the simplest case where $x_0 + v_0t \in (0, 1)$ we have

$$\rho(t, x) = \delta_{x_0+v_0t}(x).$$

Now we are going to focus on the case where $x - vt \in (0, 1)$ in which case

$$f(t, x, v) \geq \int_0^t e^{-(t-s)} \rho(s, x - v(t-s)) \mathcal{M}_{T(x-v(t-s))}(v) ds.$$

We have

$$\mathcal{M}_{T(x)}(v) \geq \frac{1}{\sqrt{2\pi T_2}} e^{-v^2/2T_1} \geq \sqrt{\frac{T_1}{T_2}} \mathcal{M}_{T_1}(v) := \alpha G(v).$$

Using this we can write

$$f(t, x, v) \geq \alpha G(v) \int_0^t e^{-(t-s)} \rho(s, x - v(t-s)) ds.$$

For a fixed $\epsilon > 0$, we consider the following three cases

1. $v_0 < 0, x_0/|v_0| \leq \epsilon$,
2. $v_0 > 0, (1 - x_0)/v_0 \leq \epsilon$,
3. Neither of these holds.

We observe that in case (1) we know that $t \geq \epsilon$ implies that $x_0 + v_0 t \leq 0$ and in case (2): if $t \geq \epsilon$ then $x_0 + v_0 t \geq 1$.

For the case (1), we have

$$\rho(t, x) \geq e^{-t} \mathbb{1}_{t \geq \epsilon} \frac{xv_0^2}{(x_0 + v_0 t)^2} \widetilde{\mathcal{M}}_1 \left(\frac{xv_0}{x_0 + v_0 t} \right) \geq e^{-t} \mathbb{1}_{t \geq \epsilon} \frac{x}{T_1 t^2} e^{-1/2T_1 \epsilon^2}.$$

Now we can substitute this into (4.13) again to get that

$$\begin{aligned} f(t, x, v) &\geq \alpha e^{-t} G(v) \frac{1}{T_1 t^2} e^{-1/2T_1 \epsilon^2} \int_{\epsilon}^t (x - v(t - s)) ds \\ &= \frac{\alpha e^{-t}}{T_1 t^2} G(v) e^{-1/2T_1 \epsilon^2} (t - \epsilon) \left(x - \frac{v}{2}(t - \epsilon) \right) \mathbb{1}_{t \geq \epsilon}. \end{aligned}$$

If we set $t_* = 2\epsilon$ then we have

$$f(t_*, x, v) \geq \alpha e^{-2\epsilon} G(v) \frac{1}{T_1 \epsilon^2} e^{-1/2T_1 \epsilon^2} \epsilon^2 \mathbb{1}_{x - v\epsilon \in (\epsilon, 1 - \epsilon)}.$$

For the case (2), we work essentially the same as in case (1) to get that

$$f(t, x, v) \geq \frac{\alpha e^{-t}}{T_2 t^2} G(v) e^{-1/2T_2 \epsilon^2} (t - \epsilon) \left(1 - x + \frac{v}{2}(t - \epsilon) \right).$$

Setting $t_* = 2\epsilon$ we have

$$f(t_*, x, v) \geq \alpha e^{-2\epsilon} G(v) \frac{1}{T_2 \epsilon^2} e^{-1/2T_2 \epsilon^2} \epsilon^2 \mathbb{1}_{x - v\epsilon \in (\epsilon, 1 - \epsilon)}.$$

Finally for the third case, we will need further iterations. Initially, we get that

$$\rho(t, x) \geq e^{-t} \delta_{x_0 + tv_0}(x) \mathbb{1}_{t \leq \epsilon}.$$

We substitute this once into (4.13) to get

$$f(t, x, v) \geq e^{-t} \alpha \int_0^t \delta_{x_0 + sv_0}(x - v(t - s)) G(v) \mathbb{1}_{t \leq \epsilon} ds.$$

Integrating in v this, gives

$$\rho(t, x) \geq e^{-t} \mathbb{1}_{t \leq \epsilon} \alpha \int_0^t \int_{-\infty}^{\infty} \delta_{x_0 + sv_0}(x - v(t - s)) G(v) dv ds.$$

After a change of variables, this is bounded below by

$$\rho(t, x) \geq e^{-t} \mathbb{1}_{t \leq \epsilon} \frac{\alpha}{t} \int_0^t G\left(\frac{x - x_0 - v_0 s}{t - s}\right) ds \geq e^{-t} \mathbb{1}_{t \leq \epsilon} \frac{\alpha}{t} \int_0^t G\left(\frac{1}{t - s}\right) ds.$$

We substitute this back into (4.13) to get

$$\begin{aligned} f(t, x, v) &\geq e^{-t} \frac{\alpha^2}{t} G(v) \int_0^t \mathbb{1}_{s \leq \epsilon} \int_0^s G\left(\frac{1}{s - r}\right) dr ds \\ &\geq e^{-t} \frac{\alpha^2}{t} G(v) G(2/\epsilon) \int_\epsilon^t \int_0^\epsilon dr ds \\ &\geq e^{-t} \frac{\alpha^2 \epsilon (t - \epsilon)}{2t} G(v) G(2/\epsilon). \end{aligned}$$

Setting $t_* = 2\epsilon$ we have,

$$f(t_*, x, v) \geq e^{-2\epsilon} \frac{\alpha^2 \epsilon^2}{2\epsilon} G(v) G(2/\epsilon) \mathbb{1}_{x - 2v\epsilon \in (0, 1)}.$$

Now let us set

$$\beta = \alpha e^{-2\epsilon} \min \left\{ \frac{\alpha \epsilon}{2} G\left(\frac{2}{\epsilon}\right), \frac{1}{T_1} e^{-1/2T_1 \epsilon^2}, \frac{1}{T_2} e^{-1/2T_2 \epsilon^2} \right\}.$$

Then in every case we have that

$$f(t_*, x, v) \geq \beta \mathbb{1}_{x - 2v\epsilon \in (\epsilon, 1 - \epsilon)}.$$

□

4.4.3 L^∞ Bounds on $\mathcal{F}(T)$.

As we have uniqueness of a steady state for (4.7)-(4.8)-(4.9), thanks to Lemma 4.8, for f being this solution with temperature profile T , we define the mapping

$$\mathcal{F} : C((0, 1)) \rightarrow C((0, 1)), \quad T \mapsto \frac{\int f(x, v) |v|^2 dv}{\int f(x, v) dv}.$$

In this subsection we first represent the solution to (4.7)- (4.8)- (4.9) in terms of the moments appearing in the boundary conditions. Then we check their asymptotic behaviour concerning the boundary temperatures T_1, T_2 so that we establish the conditions required on these temperatures in order to bound the $\mathcal{F}(T)(x)$ uniformly in x . The goal is to prove the proposition,

Proposition 4.9. *If T_1, T_2 satisfy condition 1, then we have that*

$$T_1 \leq \tau_T(x) \leq T_2$$

uniformly in x .

We begin with the following Lemma.

Lemma 4.10. *For f a solution to (4.7)-(4.8)-(4.9) we have the following representation*

$$f(x, v) = e^{-x/\kappa|v|} f(0, v) + \int_0^x e^{-(x-y)/\kappa|v|} \frac{1}{\kappa|v|} \rho(y) \mathcal{M}_{T(y)} dy \quad v > 0, \quad (4.14)$$

$$f(x, v) = e^{-(1-x)/\kappa|v|} f(1, v) + \int_x^1 e^{-(y-x)/\kappa|v|} \frac{1}{\kappa|v|} \rho(y) \mathcal{M}_{T(y)} dy \quad v < 0. \quad (4.15)$$

Proof. We will use Duhamel's formula to get an exponential formulation for the equation: let $v > 0$

$$\partial_t (e^{t/\kappa} f(vt, v)) = \frac{1}{\kappa} e^{t/\kappa} \rho(vt) \mathcal{M}_{T(vt)}(v).$$

Integrating this gives that

$$e^{t/\kappa} f(vt, v) = f(0, v) + \frac{1}{\kappa} \int_0^t e^{s/\kappa} \rho(vs) \mathcal{M}_{T(vs)}(v) ds.$$

Now we write $x = vt$ and in the integral we make the change of variables $y = vs, dy = vds$.

This gives

$$e^{x/\kappa v} f(x, v) = f(0, v) + \int_0^x e^{y/\kappa v} \frac{1}{\kappa v} \rho(y) \mathcal{M}_{T(y)}(v) dy.$$

Similarly, if $v < 0$ we can write

$$\partial_t (e^{t/\kappa} f(1 + vt, v)) = \frac{1}{\kappa} e^{t/\kappa} \rho(1 + vt) \mathcal{M}_{T(1+vt)}(v),$$

again integrating this yields,

$$e^{t/\kappa} f(1 + vt, v) = f(1, v) + \frac{1}{\kappa} \int_0^t e^{s/\kappa} \rho(1 + vs) \mathcal{M}_{T(1+vs)}(v) ds.$$

Now we make the change of variables $x = 1 + vt, y = 1 + vs$ this gives

$$e^{(1-x)/\kappa|v|} f(x, v) = f(1, v) + \int_x^1 e^{(1-y)/\kappa|v|} \frac{1}{\kappa|v|} \rho(y) \mathcal{M}_{T(y)}(v) dy.$$

□

The above lemma will give us a close form for the moments appearing in the boundary

conditions. We start with the following definitions.

Definition 4.11. *We define the following moments*

$$C_- = \frac{1}{\kappa} \int_0^1 \int_{v<0} e^{-y/\kappa|v|} \rho(y) \mathcal{M}_{T(y)}(v) dv dy, \quad (4.16)$$

$$C_+ = \frac{1}{\kappa} \int_0^1 \int_{v>0} e^{-(1-y)/\kappa|v|} \rho(y) \mathcal{M}_{T(y)}(v) dv dy, \quad (4.17)$$

$$C_1 = \int_{v>0} |v| e^{-1/\kappa|v|} \widetilde{\mathcal{M}}_1(v) dv < 1, \quad (4.18)$$

$$C_2 = \int_{v<0} |v| e^{-1/\kappa|v|} \widetilde{\mathcal{M}}_2(v) dv < 1. \quad (4.19)$$

Lemma 4.12. *The moments appearing in the boundary conditions can be written as*

$$\begin{aligned} \int_{v<0} |v| f(0, v) dv &= \frac{1}{1 - C_1 C_2} (C_- + C_2 C_+), \\ \int_{v>0} |v| f(1, v) dv &= \frac{1}{1 - C_1 C_2} (C_+ + C_1 C_-), \end{aligned}$$

where the quantities C_1, C_2, C_-, C_+ are as in the definition 4.11.

Proof. We use the previous lemma iteratively to get

$$\begin{aligned} \int_{v<0} |v| f(0, v) dv &= \int_{v<0} |v| \left(e^{-1/\kappa|v|} f(1, v) + \int_0^1 \frac{1}{\kappa|v|} e^{-y/\kappa|v|} \rho(y) \mathcal{M}_{T(y)}(v) dy \right) dv \quad (4.20) \\ &= \int_{v<0} |v| e^{-1/\kappa|v|} f(1, v) dv + C_- \\ &= \int_{v<0} |v| e^{-1/\kappa|v|} \widetilde{\mathcal{M}}_2(v) dv \int_{v'>0} |v'| f(1, v') dv' + C_- \\ &= C_2 \int_{v>0} |v| f(1, v) dv + C_-. \end{aligned}$$

Similarly

$$\begin{aligned} \int_{v>0} |v| f(1, v) dv &= \int_{v>0} \left(|v| e^{-1/\kappa|v|} f(0, v) + \frac{1}{\kappa} \int_0^1 e^{-(1-y)/\kappa|v|} \rho(y) \mathcal{M}_{T(y)}(v) dy \right) dv \quad (4.21) \\ &= \int_{v>0} |v| e^{-1/\kappa|v|} f(0, v) dv + C_+ \\ &= \int_{v>0} |v| e^{-1/\kappa|v|} \widetilde{\mathcal{M}}_1(v) dv \int_{v'<0} |v'| f(0, v') dv' + C_+ \\ &= C_1 \int_{v<0} |v| f(0, v) dv + C_+. \end{aligned}$$

Substituting (4.21) into (4.20) gives the result. \square

Combining the previous two Lemmas we get easily the following representation of the solution as stated in the following Lemma.

Lemma 4.13.

$$f(x, v) = e^{-x/\kappa|v|} \widetilde{\mathcal{M}}_1(v) \frac{C_- + C_2 C_+}{1 - C_1 C_2} + \int_0^x \frac{1}{\kappa|v|} e^{-(x-y)/\kappa|v|} \rho(y) \mathcal{M}_{T(y)}(v) dy \quad v > 0, \quad (4.22)$$

$$f(x, v) = e^{-(1-x)/\kappa|v|} \widetilde{\mathcal{M}}_2(v) \frac{C_+ + C_1 C_-}{1 - C_1 C_2} + \int_x^1 \frac{1}{\kappa|v|} e^{-(y-x)/\kappa|v|} \rho(y) \mathcal{M}_{T(y)}(v) dy \quad v < 0. \quad (4.23)$$

We remind here that we are aiming for estimates on $\mathcal{F}(T)$ which is defined as following: if f is a solution to (4.7)-(4.8)-(4.9) with profile T then

$$\mathcal{F}(T)(x) = \frac{\int f(x, v) |v|^2 dv}{\int f(x, v) dv}.$$

In particular, using the following definitions for the *hydrodynamic moments*

$$\begin{aligned} \rho_T(x) &= \int f(x, v) dv, \\ \rho_T(x) u_T(x) &= \int f(x, v) v dv \\ \rho_T(x) (\tau_T(x) + u_T(x)^2) &= P_T(x) = \int f(x, v) v^2 dv, \end{aligned}$$

we would like to show that if $T(x) \in [T_1, T_2]$ then $\tau_T(x) \in [T_1, T_2]$.

Therefore we are interested in the scalings of the different quantities ρ_T, P_T, τ_T in terms of the temperatures $T_1, T_2, T(y) \rightarrow \infty$. These asymptotic behaviours are presented in the following series of Lemmas.

Lemma 4.14. *As $T_1, T_2 \rightarrow \infty$ we have*

$$\frac{1}{1 - C_1 C_2} \sim \sqrt{\frac{2}{\pi}} \frac{\kappa \sqrt{T_1 T_2}}{\sqrt{T_1} + \sqrt{T_2}}.$$

Proof. Let us write $D_1 = 1 - C_1$ and compute that

$$C_1 = \sqrt{\frac{2\pi}{T_1}} \int_0^\infty v e^{-1/\kappa v} (2\pi T_1)^{-1/2} e^{-|v|^2/2T_1} dv = \int_0^\infty u e^{-1/(\kappa\sqrt{T_1}u)} e^{-u^2/2} du.$$

Therefore,

$$D_1 = \int_0^\infty u \left(1 - e^{-1/(\kappa\sqrt{T_1}u)}\right) e^{-u^2/2} du.$$

We can straightforwardly bound this above to get

$$D_1 \leq \int_0^\infty \frac{1}{\kappa\sqrt{T_1}} e^{-u^2/2} du = \frac{1}{\kappa} \sqrt{\frac{\pi}{2T_1}}.$$

In order to bound D_1 below, first Taylor expanding gives us:

$$e^{-1/(\kappa\sqrt{T_1}u)} \leq \max \left\{ 1, 1 - \frac{1}{\kappa\sqrt{T_1}u} + \frac{1}{2\kappa^2 T_1 u^2} \right\}.$$

Therefore,

$$u \left(1 - e^{-1/(\kappa\sqrt{T_1}u)} \right) \geq \frac{1}{\kappa\sqrt{T_1}} \max \left\{ 0, 1 - \frac{1}{2\kappa\sqrt{T_1}u} \right\}.$$

So that for any $\alpha \in (0, 1)$

$$\begin{aligned} D_1 &\geq \frac{1}{\kappa\sqrt{T_1}} \int_0^\infty \max \left\{ 0, 1 - \frac{1}{2\kappa\sqrt{T_1}u} \right\} e^{-u^2/2} du = \frac{1}{\kappa\sqrt{T_1}} \int_{\frac{1}{2\kappa\sqrt{T_1}}}^\infty \left(1 - \frac{1}{2\kappa\sqrt{T_1}u} \right) e^{-u^2/2} du \\ &\geq \frac{1}{\kappa\sqrt{T_1}} \int_{1/(2\kappa\sqrt{T_1}\alpha)}^\infty \left(1 - \frac{1}{2\kappa\sqrt{T_1}u} \right) e^{-u^2/2} du \\ &\geq \frac{1}{\kappa\sqrt{T_1}} (1 - \alpha) \left(2\sqrt{\pi} - \frac{1}{2\alpha\kappa\sqrt{T_1}} \right) \\ &= 2\frac{1}{\kappa} \sqrt{\frac{\pi}{T_1}} - \frac{1}{2\alpha\kappa^2 T_1} - 2\alpha \frac{1}{\kappa} \sqrt{\frac{\pi}{T_1}} + \frac{1}{2\kappa^2 T_1}. \end{aligned}$$

Optimising over α , for $\kappa^2 T_1 > 1/2\pi$, gives

$$D_1 \geq 2\frac{1}{\kappa} \sqrt{\frac{\pi}{T_1}} + \frac{1}{2\kappa^2 T_1} - 2 \left(\frac{\pi}{\kappa^6 T_1^3} \right)^{1/4}.$$

Symmetrically we find that for $T_2 > 1/2\pi$,

$$2\frac{1}{\kappa} \sqrt{\frac{\pi}{T_2}} + \frac{1}{2\kappa^2 T_2} - 2 \left(\frac{\pi}{\kappa^6 T_2^3} \right)^{1/4} \leq D_2 \leq \sqrt{\frac{\pi}{2\kappa^2 T_2}}.$$

We can rewrite

$$1 - C_1 C_2 = D_1 + D_2 - D_1 D_2.$$

Lets write

$$E_i := -\frac{1}{\kappa} \frac{1}{\sqrt{2\pi T_i}} + \left(\frac{8}{\pi\kappa^2 T_i} \right)^{1/4} \sim A\kappa^{-1/2} T_i^{-1/4}$$

Therefore our upper and lower bounds give

$$1 - C_1 C_2 \leq \sqrt{\frac{\pi}{2}} \left(\frac{1}{\kappa\sqrt{T_1}} + \frac{1}{\kappa\sqrt{T_2}} - \sqrt{\frac{\pi}{2\kappa^4 T_1 T_2}} (1 - E_1)(1 - E_2) \right).$$

and

$$1 - C_1 C_2 \geq \sqrt{\frac{\pi}{2}} \left(\frac{1}{\kappa\sqrt{T_1}}(1 - E_1) + \frac{1}{\kappa\sqrt{T_2}}(1 - E_2) - \sqrt{\frac{\pi}{2\kappa^4 T_1 T_2}} \right).$$

Therefore we have

$$1 - K_1 \leq \frac{1 - C_1 C_2}{\sqrt{\frac{\pi}{2}} \left(\frac{1}{\kappa\sqrt{T_1}} + \frac{1}{\kappa\sqrt{T_2}} \right)} \leq 1,$$

where

$$K_1 = \frac{\kappa\sqrt{T_2}E_1 + \kappa\sqrt{T_1}E_2 + 1}{\kappa\sqrt{T_1} + \kappa\sqrt{T_2}} \leq E_1 + E_2 + \frac{1}{\kappa(\sqrt{T_1} + \sqrt{T_2})}.$$

So we end up with

$$\sqrt{\frac{2}{\pi}} \frac{\kappa\sqrt{T_1 T_2}}{\sqrt{T_1} + \sqrt{T_2}} \leq \frac{1}{1 - C_1 C_2} \leq \sqrt{\frac{2}{\pi}} \frac{\kappa\sqrt{T_1 T_2}}{\sqrt{T_1} + \sqrt{T_2}} \frac{1}{1 - E_1 - E_2 - 1/(\kappa(\sqrt{T_1} + \sqrt{T_2}))}.$$

We can also straightforwardly check that if $\kappa^2 T_1 \geq \gamma_2$, for some constant $\gamma_2 > 0$, then we can use the approximation $1/(1 - z) \leq 1 + z$ to get that

$$\frac{1}{1 - E_1 - E_2 - 1/(\kappa(\sqrt{T_1} + \sqrt{T_2}))} \leq 1 + 2 \left(\frac{8}{\pi\kappa^2 T_1} \right)^{1/4} + 2 \left(\frac{8}{\pi\kappa^2 T_2} \right)^{1/4}.$$

□

Lemma 4.15. *If $T_1 \leq T(y)$ then we have that*

$$\frac{1}{\kappa} \left(1 - 2 \left(\frac{2}{\pi\kappa^2 T_1} \right)^{1/4} \right) \leq 2C_-, 2C_+ \leq \frac{1}{\kappa}.$$

Proof. We just show this for C_- , the proof for C_+ is almost identical.

$$\kappa C_- = \int_0^1 \rho(y) \int_{v<0} e^{-y/\kappa|v|} \mathcal{M}_{T(y)}(v) dv dy.$$

The bound $e^{-y/\kappa|v|} \leq 1$ gives us the upper bound immediately.

For the lower bound we look at $D(y) = 1 - C_-$, and wish to bound this above.

$$D = \int_0^1 \rho(y) \int_{v<0} (1 - e^{-y/\kappa|v|}) \mathcal{M}_{T(y)}(v) dv dy.$$

We look at the integral first in v and change variables

$$\int_{v<0} (1 - e^{-y/\kappa|v|}) \mathcal{M}_{T(y)}(v) dv = \int_0^\infty \left(1 - e^{-y/(\kappa\sqrt{T(y)v})} \right) \mathcal{M}_1(v) dv.$$

For any $\alpha \in (0, 1)$ we use the bounds

$$1 - e^{-y/(\kappa\sqrt{T(y)v})} \leq 1, \quad |v| \leq \frac{y}{\alpha\kappa\sqrt{T(y)}},$$

and

$$1 - e^{-y/(\kappa\sqrt{T(y)v})} \leq \alpha, \quad |v| > \frac{y}{\alpha\kappa\sqrt{T(y)}}.$$

This gives us

$$\int_{v<0} (1 - e^{-y/\kappa|v|}) \mathcal{M}_{T(y)}(v) dv \leq \frac{y}{\alpha\sqrt{2\pi\kappa T(y)}} + \frac{\alpha}{2}.$$

We optimise over α to get

$$\int_{v<0} (1 - e^{-y/\kappa|v|}) \mathcal{M}_{T(y)}(v) dv \leq 2 \left(\frac{2y^2}{\pi\kappa^2 T(y)} \right)^{1/4} \leq 2 \left(\frac{2}{\pi\kappa^2 T_1} \right)^{1/4}.$$

We then use the fact that ρ integrates to one to conclude. \square

Combining the above two lemmas gives us the scaling of the quantity appearing in the first term of the representation (4.22). Note that similar calculations will give same scaling regarding (4.23).

Lemma 4.16. *We have*

$$F_1(T_1, T_2) \sqrt{\frac{2}{\pi} \frac{\sqrt{T_1 T_2}}{\sqrt{T_1} + \sqrt{T_2}}} \leq \frac{C_- + C_2 C_+}{1 - C_1 C_2} \leq F_2(T_1, T_2) \sqrt{\frac{2}{\pi} \frac{\sqrt{T_1 T_2}}{\sqrt{T_1} + \sqrt{T_2}}}$$

where

$$F_1(T_1, T_2) := 1 + \left(\frac{\pi}{2\kappa^6 T_1^3} \right)^{1/4} - 2 \left(\frac{2}{\pi\kappa^2 T_1} \right)^{1/4} - \frac{1}{2} \sqrt{\frac{\pi}{2\kappa^2 T_1}} \quad (4.24)$$

and

$$F_2(T_1, T_2) := 1 + \frac{1}{4\kappa^2 T_2} - \sqrt{\frac{\pi}{\kappa^2 T_2}} - \left(\frac{\pi}{\kappa^6 T_2^3} \right)^{1/4}. \quad (4.25)$$

Proof. We just put together the previous two Lemmas. \square

We would now like to get a sense of the different quantities using these results. Let us start with the pressure P_T .

Lemma 4.17. *We have for all $x \in (0, 1)$,*

$$G_1(T_1, T_2) \sqrt{T_1 T_2} \leq P_T(x) \leq G_2(T_1, T_2) \sqrt{T_1 T_2}, \quad (4.26)$$

where

$$G_1(T_1, T_2) = F_1(T_1, T_2) \left(1 - \sqrt{\frac{2}{\pi}} \frac{1}{\kappa(\sqrt{T_1} + \sqrt{T_2})} \right),$$

$$G_2(T_1, T_2) = F_2(T_1, T_2) + \sqrt{\frac{1}{2\pi\kappa^2 T_1}}$$

and F_1, F_2 are functions of the temperatures T_1, T_2 and they are defined in Lemma 4.16. In particular,

$$\sqrt{T_1 T_2} \lesssim P_T(x) \lesssim \sqrt{T_1 T_2}.$$

Proof. Let us first note that the pressure is constant in x . Indeed, from the equation we can easily see that

$$\partial_x(\rho(x)u_T(x)) = 0$$

and from the boundary conditions we have

$$\rho(0)u_T(0) = \rho(1)u_T(1) = 0,$$

hence $u_T(x) = 0$. Since we have that $\partial_x P_T(x) = -\frac{1}{\kappa}\rho(x)u(x) = 0$, we know that $P_T(x)$ is constant.

Now in order to quantify it in terms of the temperatures, we need two further quantities:

$$\int_{v>0} |v|^2 \widetilde{\mathcal{M}}_i(v) dv = \sqrt{\frac{\pi T_i}{2}},$$

which is straightforward to compute. We also show that

$$\sqrt{\frac{T_1}{2\pi}} - \frac{1}{2\kappa} \leq \int_0^1 \rho(y) \int_0^\infty |v| e^{-y/\kappa|v|} \mathcal{M}_{T(y)}(v) dv dy \leq \sqrt{\frac{T_2}{2\pi}}.$$

The upper bound comes from bounding $e^{-y/\kappa|v|}$ by one, the lower bound comes from bounding it below by $1 - y/\kappa|v|$.

More precisely, for v positive, using the representation of the solution in (4.22) for the upper bound we write

$$\int_0^\infty |v|^2 f(x, v) dv = \int_0^\infty v^2 e^{-x/\kappa v} \widetilde{\mathcal{M}}_1(v) dv \left(\frac{C_- + C_2 C_+}{1 - C_1 C_2} \right) + \frac{1}{\kappa} \int_0^\infty \int_0^x \rho(y) |v| e^{-(x-y)/\kappa v} \mathcal{M}_{T(y)}(v) dy dv$$

and since the pressure is constant, for $x = 1$, the above quantity is bounded above by

$$\int_0^\infty |v|^2 f(1, v) dv \leq \sqrt{T_1} \frac{\sqrt{T_1 T_2}}{\sqrt{T_1} + \sqrt{T_2}} F_2(T_1, T_2) + \sqrt{\frac{T_2}{2\pi}}.$$

while the lower bound similarly is found to be

$$\left(\sqrt{\frac{\pi T_1}{2}} - 1 \right) \sqrt{\frac{2}{\pi}} \frac{\kappa \sqrt{T_1 T_2}}{\sqrt{T_1} + \sqrt{T_2}} F_1(T_1, T_2)$$

For v negative, using the representation (4.23), we have

$$\int_{-\infty}^0 |v|^2 f(1, v) dv = \int_{-\infty}^0 |v|^2 \widetilde{\mathcal{M}}_2(v) \frac{C_+ + C_1 C_-}{1 - C_1 C_2} dv.$$

Therefore we can bound it above by,

$$\sqrt{T_2} \frac{\sqrt{T_1 T_2}}{\sqrt{T_1} + \sqrt{T_2}} F_2(T_1, T_2)$$

and below by,

$$\sqrt{T_2} \frac{\sqrt{T_1 T_2}}{\sqrt{T_1} + \sqrt{T_2}} F_1(T_1, T_2).$$

Summing over positive and negative velocities gives us that

$$P_T(x) = P_T(1) \leq \sqrt{T_1 T_2} \left(F_2(T_1, T_2) + \sqrt{\frac{1}{2\pi \kappa^2 T_1}} \right).$$

Similarly, we get the lower bound,

$$P_T(x) = P_T(1) \geq \sqrt{T_1 T_2} F_1(T_1, T_2) \left(1 - \sqrt{\frac{2}{\pi}} \frac{1}{\kappa(\sqrt{T_1} + \sqrt{T_2})} \right)$$

□

The following Lemma concerns the asymptotics of the density ρ .

Lemma 4.18. *We have, uniformly in x ,*

$$1 - \gamma_0 \kappa^{-1/2} T_1^{-1/4} \leq \rho_T(x) \leq 1 + \gamma_1 \kappa^{-1/2} T_1^{-1/4}.$$

for some constants γ_0, γ_1 .

Proof. Looking at the formulae (4.22) and (4.23), we have

$$\begin{aligned} \int_0^\infty f(x, v) dv &= \int_{v>0} e^{-x/\kappa v} \widetilde{\mathcal{M}}_1(v) \frac{C_- + C_2 C_+}{1 - C_1 C_2} + \int_0^x \rho(y) \int_0^\infty \frac{1}{\kappa v} e^{-(x-y)/\kappa v} \mathcal{M}_{T(y)}(v) dv dy \\ &\leq F_2(T_1, T_2) \frac{\sqrt{T_1 T_2}}{\sqrt{T_1} + \sqrt{T_2}} \int_{v>0} \widetilde{\mathcal{M}}_1(v) dv + \int_0^x \rho(y) \int_0^\infty \frac{1}{\kappa v} e^{-(x-y)/\kappa v} \mathcal{M}_{T(y)}(v) dv dy \\ &:= I_1 + I_2 \end{aligned}$$

where we remind that F_2 is given by (4.25). For I_1 applying the above estimates we get

$$I_1 \leq F_2(T_1, T_2) \sqrt{\frac{\pi}{2}} \frac{\sqrt{T_2}}{\sqrt{T_1} + \sqrt{T_2}}.$$

For the second term I_2 : first we notice that

$$\frac{1}{z} e^{-(x-y)/z} \leq \max \left\{ \frac{e^{-1}}{x-y}, \frac{1}{z} \right\}.$$

Therefore

$$\begin{aligned} \int_0^\infty \frac{1}{\kappa v} e^{-(x-y)/\kappa v} \mathcal{M}_{T(y)}(v) dv &= \int_0^\infty \frac{1}{\kappa \sqrt{T(y)} v} e^{-(x-y)/\kappa \sqrt{T(y)} v} \mathcal{M}_1(v) dv \\ &\leq \int_0^a e^{-1} \frac{1}{x-y} \mathcal{M}_1(v) dv + \int_a^\infty \frac{1}{a \kappa \sqrt{T(y)}} \mathcal{M}_1(v) dv \\ &\leq \frac{a}{e^1 (x-y) \sqrt{2\pi}} + \frac{1}{2a \kappa \sqrt{T(y)}}. \end{aligned}$$

Optimising over a gives that

$$\int_0^\infty \frac{1}{\kappa v} e^{-(x-y)/\kappa v} \mathcal{M}_{T(y)}(v) dv \leq e^{-1/2} \left(\frac{2}{\pi \kappa^2 T(y)} \right)^{1/4} \sqrt{\frac{1}{x-y}}.$$

Therefore,

$$I_2 = \int_0^x \rho(y) \int_0^\infty \frac{1}{v} e^{-(x-y)/v} \mathcal{M}_{T(y)}(v) dv dy \leq 2e^{-1/2} \left(\frac{2}{\pi \kappa^2 T_1} \right)^{1/4} \|\rho\|_\infty$$

We can do the same thing for negative v and put it together to get that

$$\|\rho\|_\infty \leq 2e^{-1/2} \left(\frac{2}{\pi \kappa^2 T_1} \right)^{1/4} \|\rho\|_\infty + F_2.$$

Rearranging gives

$$\|\rho\|_\infty \left(1 - \gamma_1 \kappa^{-1/2} T_1^{-1/4} \right) \leq F_2.$$

Hence,

$$\|\rho\|_\infty \leq F_2 (1 - \gamma_1 \kappa^{-1/2} T_1^{-1/4})^{-1}.$$

For a lower bound on ρ we can completely ignore the term where we integrate in y in the formula (4.22). So we just need to bound below terms like

$$\int_0^\infty e^{-1/\kappa v} \widetilde{\mathcal{M}}_1(v) dv.$$

We have already treated terms of this type we bound the integrand below by $1 - \alpha$ for $v \geq 1/\alpha\sqrt{T_1}$ and optimise over α to get

$$\int_0^\infty e^{-1/\kappa v} \widetilde{\mathcal{M}}_1(v) dv \geq \sqrt{\frac{\pi}{2\kappa^2 T_1}} \left(1 - 2 \left(\frac{2}{\pi\kappa^2 T_1} \right)^{1/4} \right).$$

Therefore, we write

$$\int_{v>0} f(x, v) dv \gtrsim \sqrt{\frac{\pi}{2\kappa^2 T_1}} \left(1 - 2 \left(\frac{2}{\pi\kappa^2 T_1} \right)^{1/4} \right) \frac{\sqrt{T_1 T_2}}{\sqrt{T_1} + \sqrt{T_2}} F_1(T_1, T_2)$$

Summing over positive and negative v gives

$$\rho(x) \geq 1 - \gamma_0 \kappa^{-1/2} T_1^{-1/4}.$$

□

Now given the scalings in terms of the temperatures for $P_T(x)$ and $\rho_T(x)$ and the fact that $P_T(x) = \rho_T(x)\tau_T(x)$ for every x we have that

Lemma 4.19. *We have that for all $x \in (0, 1)$, asymptotically with T_1 ,*

$$\sqrt{T_1 T_2} (1 - \gamma_1 \kappa^{-1/2} T_1^{-1/4}) \lesssim \tau_T(x) \lesssim \sqrt{T_1 T_2} (1 + \gamma_0 \kappa^{-1/2} T_1^{-1/4}).$$

Proof. This is simply a matter of piecing together the previous lemmas. □

Proof of Proposition 4.9. This follows immediately from the previous lemma, since from the the second item of condition 1, (C2), we indeed have that

$$\sqrt{T_1 T_2} (1 + \gamma_0 \kappa^{-1/2} T_1^{-1/4}) \leq T_2$$

and

$$\sqrt{T_1 T_2} (1 - \gamma_1 \kappa^{-1/2} T_1^{-1/4}) \geq T_1.$$

□

4.4.4 Hölder continuity of $\mathcal{F}(T)(x)$.

In this Section we show Hölder continuity of order $1/2$ for the map $\mathcal{F}(T) = \tau$. This will allow us to use Schauder fixed point theorem, see Theorem 4.22, to get the desired fixed point for \mathcal{F} . Again in this section the precise constants do not matter for the final result so we work with $\kappa = 1$.

Proposition 4.20. *If $T(x) \in [T_1, T_2]$ then there exists a constant $C(T_1, T_2)$ such that*

$$|\tau(x_1) - \tau(x_2)| \leq C(T_1, T_2) \sqrt{|x_1 - x_2|}.$$

Proof. For $x_1 \leq x_2$ in $(0, 1)$ we write

$$\begin{aligned} |\tau_T(x_1) - \tau_T(x_2)| &= \left| \frac{P}{\rho_T(x_1)} - \frac{P}{\rho_T(x_2)} \right| = |P| \left| \frac{\rho_T(x_2) - \rho_T(x_1)}{\rho_T(x_1)\rho_T(x_2)} \right| \\ &\leq C(T_1, T_2) |\rho_T(x_2) - \rho_T(x_1)| \end{aligned} \quad (4.27)$$

where $P = P_T(x)$ is the constant pressure we got from Lemma 4.17 and $C(T_1, T_2)$ a constant that depends only on the two temperatures and comes from the upper bound on P , Lemma 4.17, and the, uniform in x , lower bound on the density as well, see Lemma 4.18.

Thus, in order to conclude we need to prove Hölder continuity for $\rho(x)$. We need to estimate:

$$\int_0^\infty (f(x_2, v)) - f(x_1, v) dv.$$

We can split this into two terms

$$I_1 = \frac{C_- + C_2 C_+}{1 - C_1 C_2} \sqrt{\frac{2\pi}{T_1}} \int_0^\infty e^{-x_2/v} (1 - e^{-(x_1-x_2)/v}) \mathcal{M}_{T_1}(v) dv,$$

and

$$I_2 = \int_0^{x_2} \frac{1}{|v|} e^{-(x_2-y)/|v|} \rho(y) \mathcal{M}_{T(y)}(v) dy - \int_0^{x_1} \frac{1}{|v|} e^{-(x_1-y)/|v|} \rho(y) \mathcal{M}_{T(y)}(v) dy.$$

In order to bound I_1 from above, we use Lemma 4.16 to write

$$I_1 \leq \theta(T_1, T_2) \int_0^\infty (1 - e^{-(x_2-x_1)/v}) \mathcal{M}_{T_1}(v) dv$$

for some constant $\theta(T_1, T_2)$. Now proceeding as in the proofs of the Lemmas in the previous subsection, we split into $v \leq (x_2 - x_1)/\alpha$ and bound the integrand by 1 for small v and by α for large v :

$$I_1 \lesssim \int_0^{(x_2-x_1)/\alpha} \mathcal{M}_{T_1}(v) dv + \alpha \int_{(x_2-x_1)/\alpha}^\infty \mathcal{M}_{T_1}(v) dv \lesssim \frac{x_2 - x_1}{\alpha \sqrt{2\pi T_1}} + \frac{\alpha}{2}.$$

Optimising over α gives

$$I_1 \leq \theta'(T_1, T_2) \sqrt{(x_2 - x_1)}.$$

Here the constant $\theta'(T_1, T_2)$ depends only on T_1, T_2 . Now we turn to I_2 . We can rewrite it

as

$$I_2 = I_3 + I_4,$$

with

$$I_3 = \int_0^{x_1} \int_{v>0} \frac{1}{v} \rho(y) \mathcal{M}_{T(y)}(v) (e^{-(x_2-y)/v} - e^{-(x_1-y)/v}) \, dv dy,$$

and

$$I_4 = \int_{x_1}^{x_2} \int_{v>0} \frac{1}{v} \rho(y) \mathcal{M}_{T(y)}(v) e^{-(x_2-y)/v} \, dv dy.$$

Looking first at I_4 we show that

$$I_4 \leq \|\rho\|_\infty \sqrt{\frac{T_2}{T_1}} \int_{x_1}^{x_2} \frac{1}{v} e^{-(x_2-y)/v} \mathcal{M}_{T_2}(v) \, dv dy.$$

Integrating in y gives

$$I_4 \leq \text{Const.} \int_{v>0} (1 - e^{-(x_2-x_1)/v}) \mathcal{M}_{T_2}(v) \, dv \leq \text{Const.} \sqrt{x_2 - x_1}.$$

Now,

$$I_3 \leq \|\rho\|_\infty \sqrt{\frac{T_2}{T_1}} \int_0^{x_1} \int_{v>0} \frac{1}{v} \mathcal{M}_{T_2}(v) e^{-(x_1-y)/v} (1 - e^{-(x_2-x_1)/v}) \, dv dy.$$

Integrating this in y gives

$$I_3 \leq \|\rho\|_\infty \sqrt{\frac{T_2}{T_1}} \int_{v>0} \mathcal{M}_{T_2}(v) (1 - e^{-x_1/v}) (1 - e^{-(x_2-x_1)/v}) \, dv.$$

We can bound this by

$$I_3 \leq \text{Const.} \int_{v>0} \mathcal{M}_{T_2}(v) (1 - e^{-(x_2-x_1)/v}) \, dv \leq \text{Const.} \sqrt{x_2 - x_1}.$$

So we can repeat this for $v < 0$ to get

$$|\rho(x_2) - \rho(x_1)| \leq C(T_1, T_2) \sqrt{x_2 - x_1}.$$

This gives uniform Hölder continuity for ρ . Now we get Hölder continuity for the $\tau(x)$ by combining this with (4.27):

$$|\tau_T(x_1) - \tau_T(x_2)| \leq C(T_1, T_2) \sqrt{x_2 - x_1}.$$

□

4.4.5 Continuity of the map \mathcal{F}

In this subsection we are going to prove the continuity of the map \mathcal{F} which is the second main ingredient in order to apply Schauder's fixed point Theorem. Here we continue to work with $\kappa = 1$.

Proposition 4.21. *The map \mathcal{F} is continuous from $C((0, 1))$ to $C((0, 1))$ with the L^∞ norm.*

Proof. Let $T(x), \tilde{T}(x)$ be two different continuous functions satisfying the bounds, *i.e.* are bounded below and above by T_1, T_2 respectively where T_1, T_2 satisfy condition (1). In order to conclude the continuity of \mathcal{F} , we want to estimate the quantity $|\mathcal{F}(T)(x) - \mathcal{F}(\tilde{T})(x)|$ and bound it in terms of the difference of the two temperatures $|T(x) - \tilde{T}(x)|$ for all $x \in (0, 1)$. In what follows we write $\tilde{P} := P_{\tilde{T}}, \tilde{\rho} := \rho_{\tilde{T}}$ and we have

$$\begin{aligned} |\mathcal{F}(T)(x) - \mathcal{F}(\tilde{T})(x)| &= \left| \frac{P}{\rho}(x) - \frac{\tilde{P}}{\tilde{\rho}}(x) \right| \\ &\leq \frac{|P - \tilde{P}|}{\rho}(x) + \frac{P\tilde{P}|\rho - \tilde{\rho}|}{\rho\tilde{\rho}}(x). \end{aligned}$$

Therefore we need to estimate the differences between the two densities and the two pressures that correspond to the two different temperatures. We proceed as in the proofs of the Lemmas in subsection 4.4.3, using Lemma 4.13. We recall the result of Lemma 4.13

$$\begin{aligned} f(x, v) &= e^{-x/|v|} \tilde{\mathcal{M}}_1(v) \frac{C_- + C_2 C_+}{1 - C_1 C_2} + \int_0^x \frac{1}{|v|} e^{-(x-y)/|v|} \rho(y) \mathcal{M}_{T(y)}(v) dy \quad v > 0, \\ f(x, v) &= e^{-(1-x)/|v|} \tilde{\mathcal{M}}_2(v) \frac{C_+ + C_1 C_-}{1 - C_1 C_2} + \int_x^1 \frac{1}{|v|} e^{-(y-x)/|v|} \rho(y) \mathcal{M}_{T(y)}(v) dy \quad v < 0. \end{aligned}$$

First note that the constants C_1, C_2 do not depend on whether we use T or \tilde{T} . However C_-, C_+ depend on this. In this case we would like to look at the differences between two different realisations. We recall

$$C_- = \int_0^1 \rho(y) \int_{-\infty}^0 e^{-y/|v|} \mathcal{M}_{T(y)}(v) dv dy.$$

Here we first look at the integral in v ,

$$\int_{-\infty}^0 e^{-y/|v|} \mathcal{M}_{T(y)}(v) dv = \int_0^\infty e^{-y/\sqrt{T(y)v}} \mathcal{M}_1(v) dv := F\left(y, \sqrt{T(y)}\right).$$

We calculate

$$\begin{aligned}\frac{d}{dt}F(y, t) &= \int_0^\infty \frac{y}{t^2 v} e^{-y/tv} \mathcal{M}_1(v) dv \\ &= \int_0^\infty \frac{1}{t} \frac{d}{dv} (e^{-y/tv}) v \mathcal{M}_1(v) dv \\ &= \int_0^\infty \frac{1}{t} e^{-y/tv} (v^2 - 1) \mathcal{M}_1(v) dv \leq \frac{2}{t}.\end{aligned}$$

Therefore,

$$\left| F\left(y, \sqrt{T(y)}\right) - F\left(y, \sqrt{\tilde{T}(y)}\right) \right| \leq \frac{2}{\sqrt{T_1}} \left| \sqrt{T(y)} - \sqrt{\tilde{T}(y)} \right|.$$

This means that

$$|C_- - \tilde{C}_-| \leq \frac{2}{\sqrt{T_1}} \|\sqrt{T} - \sqrt{\tilde{T}}\|_\infty + \int_0^1 |\rho(y) - \tilde{\rho}(y)| \int_0^\infty (1 - e^{-y/v\sqrt{\tilde{T}(y)}}) \mathcal{M}_1(v) dv dy.$$

Then we can use our bounds from earlier to get that

$$|C_- - \tilde{C}_-| \leq \frac{2}{\sqrt{T_1}} \|\sqrt{T} - \sqrt{\tilde{T}}\|_\infty + \sqrt{\frac{\pi}{2T_1}} \|\rho - \tilde{\rho}\|_\infty.$$

Exactly the same result is true for C_+ .

Now in order to bound the difference of the densities, we write

$$B_1(x) = \int_0^\infty e^{-x/v} \tilde{\mathcal{M}}_1(v) dv \approx \sqrt{\frac{\pi}{2T_1}},$$

and

$$B_2(x) = \int_{-\infty}^0 e^{-(1-x)/|v|} \tilde{\mathcal{M}}_2(v) dv \approx \sqrt{\frac{\pi}{2T_2}}.$$

These quantities don't depend on T, \tilde{T} . Let us also write

$$A_1(x) = \int_0^x \int_0^\infty \frac{1}{v} e^{-(x-y)/|v|} \rho(y) \mathcal{M}_{T(y)}(v) dv,$$

and $A_2(x)$ defined symmetrically. Then we have that

$$\rho(x) = \frac{B_1(x)(C_- + C_2 C_+)}{1 - C_1 C_2} + \frac{B_2(x)(C_+ + C_1 C_-)}{1 - C_1 C_2} + A_1 + A_2. \quad (4.28)$$

Therefore,

$$|\rho(x) - \tilde{\rho}(x)| \leq \frac{2(B_1(x) + B_2(x))}{1 - C_1C_2} \left(|C_- - \tilde{C}_-| + |C_+ - \tilde{C}_+| \right) + |A_1 - \tilde{A}_1| + |A_2 - \tilde{A}_2|. \quad (4.29)$$

We know from Lemma 4.14 that

$$(1 - C_1C_2)^{-1} \approx \sqrt{\frac{2}{\pi}} \frac{\sqrt{T_1T_2}}{\sqrt{T_1} + \sqrt{T_2}}.$$

Therefore,

$$\frac{2(B_1(x) + B_2(x))}{1 - C_1C_2} \leq 2.$$

Therefore we can bound the first term in the rhs of (4.29) by

$$4(2 + \sqrt{\pi/2}) \frac{1}{\sqrt{T_1}} \left(\|\sqrt{T} - \sqrt{\tilde{T}}\|_\infty + \|\rho - \tilde{\rho}\|_\infty \right).$$

Regarding the differences between the A_i 's, we look only at A_1 , since the other case is the same. Let us write

$$G(y, t) = \int_0^\infty \frac{1}{vt} e^{-(x-y)/vt} \mathcal{M}_1(v) dv.$$

By our earlier calculations, for example in the proof of the Lemma 4.18, we know that

$$G(y, t) \leq e^{-1/2} \left(\frac{2}{\pi t^2} \right)^{1/4}.$$

Then we can differentiate to see

$$\frac{d}{dt} G(y, t) = \int_0^\infty \left(-\frac{1}{vt^2} + \frac{x-y}{v^2t^3} \right) e^{-(x-y)/vt} \mathcal{M}_1(v) dv \leq \frac{2}{t} G(y, t) \leq Ct^{-3/2}.$$

This last inequality only holds for $t \geq 1$. Now we have,

$$A_1(x) - \tilde{A}_1(x) \leq \int_0^1 \left(\rho(y) \left| G\left(y, \sqrt{T(y)}\right) - G\left(y, \sqrt{\tilde{T}(y)}\right) \right| + (\rho(y) - \tilde{\rho}(y)) G\left(y, \sqrt{\tilde{T}(y)}\right) \right) dy.$$

Therefore,

$$|A_1(x) - \tilde{A}_1(x)| \leq CT_1^{-3/4} \|\sqrt{T} - \sqrt{\tilde{T}}\|_\infty + CT_1^{-1/4} \|\rho - \tilde{\rho}\|_\infty.$$

Therefore overall,

$$\|\rho - \tilde{\rho}\|_\infty \leq CT_1^{-1/4} \|\rho - \tilde{\rho}\|_\infty + CT_1^{-1/2} \|\sqrt{T} - \sqrt{\tilde{T}}\|_\infty.$$

Hence,

$$\|\rho - \tilde{\rho}\|_\infty \leq CT_1^{-1/2} \|\sqrt{T} - \sqrt{\tilde{T}}\|_\infty. \quad (4.30)$$

Regarding the estimation of the difference of the pressures we define the following.

$$D_1(x) = \int_0^\infty |v|^2 e^{-x/v} \tilde{\mathcal{M}}_1(v) dv, \quad D_2(x) = \int_{-\infty}^0 |v|^2 e^{-(1-x)/v} \tilde{\mathcal{M}}_2(v) dv.$$

These quantities do not depend on T or \tilde{T} and we have that

$$D_1 \approx \sqrt{T_1}, \quad D_2 \approx \sqrt{T_2}.$$

Furthermore, we have

$$E_1(x) = \int_0^x \int_0^\infty |v| e^{-(x-y)/v} \rho(y) \mathcal{M}_{T(y)}(v) dv dy,$$

and

$$E_2(x) = \int_x^1 \int_{-\infty}^0 |v| e^{-(y-x)/|v|} \rho(y) \mathcal{M}_{T(y)}(v) dv dy.$$

Then the formula for the pressure can be rewritten as follows

$$P = \frac{D_1(C_- + C_2 C_+) + D_2(C_+ + C_1 C_-)}{1 - C_1 C_2} + E_1 + E_2.$$

Therefore,

$$|P - \tilde{P}| \leq \frac{2(D_1 + D_2)}{1 - C_1 C_2} \left(|C_- - \tilde{C}_-| + |C_+ - \tilde{C}_+| \right) + |E_1 - \tilde{E}_1| + |E_2 - \tilde{E}_2|.$$

So we can bound,

$$\frac{2(D_1 + D_2)}{1 - C_1 C_2} \leq 2(\sqrt{T_1} + \sqrt{T_2}) \frac{\sqrt{T_1 T_2}}{\sqrt{T_1} + \sqrt{T_2}} = 2\sqrt{T_1 T_2}.$$

Then we want to bound the first term by

$$C\sqrt{T_2} \|\sqrt{T} - \sqrt{\tilde{T}}\|_\infty.$$

In general we can see that,

$$|P - \tilde{P}| \leq C\sqrt{T_2} \|\sqrt{T} - \sqrt{\tilde{T}}\|_\infty. \quad (4.31)$$

Finally about the difference in temperatures, we use the results from Lemmas 4.18 and

4.17: that $\rho, \tilde{\rho} \sim 1$, and $P \sim \sqrt{T_1 T_2}$. Combining (4.30) and (4.31) with the calculations in the beginning of this proof, we have for all x

$$\begin{aligned} \left| \mathcal{F}(T)(x) - \mathcal{F}(\tilde{T})(x) \right| &\leq \frac{C\sqrt{T_2}}{1 + \kappa_1 T_1^{-1/4}} \|\sqrt{T} - \sqrt{\tilde{T}}\|_\infty + \frac{(T_1 T_2)C}{(1 + \kappa_1 T_1^{-1/4})^2} \|\sqrt{T} - \sqrt{\tilde{T}}\|_\infty \\ &\leq \Lambda(T_1, T_2) \|\sqrt{T} - \sqrt{\tilde{T}}\|_\infty \end{aligned}$$

for a constant $\Lambda(T_1, T_2)$ that depends only on the temperatures T_1, T_2 . Since T, \tilde{T} are bounded below by T_1 this gives the required continuity. □

4.4.6 Fixed Point Argument

In this subsection we show how an application of Schauder's fixed point theorem yields the main result. First, for completeness we remind here the Schauder's Theorem, which can be found for example in [Sma74, Theorem 2.3.7].

Theorem 4.22 (Schauder Fixed Point Theorem). *Let S be a non-empty, convex closed subset of a Hausdorff topological vector space and F a mapping of S into itself so that $F(S)$ is compact then F has a fixed point.*

Proof of Theorem 3.1. We apply Schauder's Theorem to get a fixed point for \mathcal{F} :

Firstly by Proposition 4.21 we know that the map $\mathcal{F} : C(0, 1) \rightarrow C(0, 1)$ is a continuous map. For T_1, T_2 fixed temperatures satisfying condition 1, we have that $T(x) \in [T_1, T_2]$ implies $\tau \in [T_1, T_2]$, in other words if we define the set

$$S_{T_1, T_2} := \{T \in C([0, 1]) : T_1 \leq T(x) \leq T_2\},$$

then

$$\mathcal{F}(S_{T_1, T_2}) \subset S_{T_1, T_2}.$$

Also, from Proposition 4.20, we have that $\mathcal{F}(S_{T_1, T_2})$ satisfies a Hölder condition of order $1/2$ with a constant depending only on the two fixed temperatures. Since moreover $\mathcal{F}(S_{T_1, T_2})$ is uniformly bounded, we conclude by Arzela-Ascoli, the compactness of the set.

The existence of a fixed point for this mapping ensures us that the steady state for the linear BGK model with temperature profile $T(x)$ is a steady state for the original non-linear model (1.1)-(1.2)-(1.3) as well since $T(x) = T_f(x)$. The properties of this non-equilibrium steady state listed in the statement are proved in Lemmas 4.18, 4.19 and Proposition 4.21 respectively. □

4.5 Discussion of the results and future work

First we look at how Fourier's law applies in this specific context. The heat flux associated to the NESS is constant along the interval: Recall that the temperature that corresponds to the stationary solution f is given by

$$T_f(x) = \frac{1}{\rho_f(x)} \int |v - u(x)|^2 f(x, v) dv$$

and the heat flux is the vector field

$$J(x) := \int (v - u(x)) |v - u(x)|^2 f(x, v) dv.$$

Here we have $u(x) = 0$ everywhere (see beginning of proof of Lemma 4.17). We easily get that

$$\partial_x J(x) = 0 \quad \text{for } x \in (0, 1),$$

i.e. the heat flux is constant. This means that if Fourier's law (1.6) holds, then $\kappa(T_f) \partial_x T_f(x)$ is constant. Note that this conclusion can be also found in [EGKM13, proof of Theorem 1.5] for the full Boltzmann operator and for temperatures close to equilibrium. There, through comparison with numerical simulations indicating that the temperature is a nonlinear function, one can see that indeed Fourier's law is violated in the kinetic regime.

In our setting $T_f(x)$ is close to the constant function $\sqrt{T_1 T_2}$ as $T_1 \rightarrow \infty$, as described in the main Theorem 3.1. So for large boundary temperatures T_1 , the function $T_f(x)$ is constant in the bulk of the domain $(0, 1)$ which is reminiscent to the behaviour of the heat flux in the harmonic atom networks.

Comparison with the heat flux in the microscopic harmonic atom chains. In the case of harmonic oscillator chains the temperature profile is close to being constant, and in particular in the centre of the chain it is the linear average $(T_1 + T_2)/2$ as shown in [RLL67], at least in the case of small temperature difference. The temperature is paradoxically lower than the average very close to the hot reservoir. This purely harmonic system of atoms is ballistic (Fourier's law does not hold) and this is what causes the flat temperature profile there.

In contrast to this, we expect the BGK model we consider here to be the kinetic limit of the heat conduction microscopic model of harmonic atom chains perturbed by a conservative stochastic dynamics as considered in [BO05] where Fourier's law holds. We prove for the BGK model that the temperature gets close to the constant $\sqrt{T_1 T_2}$ for T_1 large. This behaviour of the temperature profile however does not contradict the expected diffusivity of our system, i.e. the fact that the conductivity in the hydrodynamic regime is finite, since our result here does not hold on the hydrodynamic regime.

As regards the connection of microscopic oscillator chains with the Boltzmann equation for phonons, it has been shown that one can derive a phonon Boltzmann equation as a kinetic limit (high frequency limit) starting from infinite chain of harmonic oscillators with a small anharmonicity. We refer to [Spo06] for that and to [BOS10] for a stochastically perturbed version of it. Another very interesting work analyzing the kinetic limit in the case of an infinite linear chain of oscillators coupled to a single Langevin thermostat at the boundary is [KORS20].

Possible directions. The most natural and important question arising from these results is uniqueness of the steady state given here. A less ambitious question in the same direction is whether the steady state found here is stable under small perturbations, this is done in the Boltzmann equation setting in [AEMN10, AEMN12] and in the BGK setting in [CEL⁺18, CEL⁺19]. This would also be an interesting question in terms of the study of hypocoercivity as there are only a small number of works showing hypocoercivity for equations on bounded domains and these are generally in the context of the Boltzmann equation initiated by [Guo10]. Showing hypocoercivity for equations with non-explicit non-equilibrium states is also a significant challenge.

Another possible angle for future work is to investigate similar problems in higher dimensions. This would involve looking at the non-linear BGK equation where $x \in \Omega \subset \mathbb{R}^d$ and Ω is a smooth bounded domain. In this case getting L^∞ estimates on the solution from the Langrangian expansion of the steady state becomes much more challenging.

Chapter 5

A quantitative perturbative approach to hydrodynamic limits

This chapter is a joint work with Daniel Marahrens and Clément Mouhot and has not been published yet.

We present a new unified method for proving the hydrodynamic limit of several interacting particle systems on a lattice, and obtaining explicit bounds on the rate of convergence to the hydrodynamic limit. In the case of the diffusive scaling, for the first time in the literature, the convergence is proven to be uniform in time. We employ a ‘consistency-stability’ method with modulated Wasserstein-1 distance and a cost being a microscopic ℓ_1 distance. We compare the law of the stochastic process to the law of a process built to have the desired hydrodynamic behavior, the local Gibbs measure. The method is a simplification compared to existing unified methods as it avoids the use of the One and Two Block Estimates.

5.1 Introduction

We consider the hydrodynamic limits of interacting particle systems on a lattice. The problem is to show that under an appropriate scaling of time and space, the local particle densities of a stochastic lattice gas converge to the solution of a macroscopic partial differential equation. The goal of this work is to provide a general framework for proving a hydrodynamic limit with an explicit rate of convergence which is also uniform in time under parabolic scaling. We will present our method in a general way first and then we will apply our general framework to three processes: the zero-range process, simple-exclusion process and Ginzburg Landau process with Kawasaki dynamics. Note that the hydrodynamic limit for all these is well-known and the limit equation is given by a nonlinear diffusion equation under parabolic scaling and by a nonlinear hyperbolic equation under hyperbolic (Eulerian) scaling, see a review in [KL99, Rez91].

Let us introduce some notation. Denote the discrete torus $\mathbb{T}_N^d \cong (\mathbb{Z}/N\mathbb{Z})^d \cong \{1, \dots, N\}^d$ and consider particle configurations in $X_N := \mathbb{N}^{\mathbb{T}_N^d}$ or $\mathbb{R}^{\mathbb{T}_N^d}$, the state space for the jump process and a diffusion process. The lattice \mathbb{T}_N^d can be thought of as a discrete approximation of the d -dimensional Torus $\mathbb{T}^d = \mathbb{R}^d/\mathbb{Z}^d$ with periodic boundary conditions $x + e \equiv x$ for all $x \in \mathbb{T}^d$ and $e \in \mathbb{Z}^d$. Variables in the discrete torus \mathbb{T}_N^d are called *microscopic* and denoted by x, y, z , whereas variables in the continuous torus \mathbb{T}^d are called *macroscopic* and denoted by u . We embed \mathbb{T}_N^d in \mathbb{T}^d via

$$\mathbb{T}_N^d \rightarrow \mathbb{T}^d, \quad x \mapsto \frac{x}{N}.$$

This embeds the microscopic variables $x \in \mathbb{T}_N^d$ into the macroscopic ones $u \in \mathbb{T}^d$. Hence the macroscopic distance between sites of the lattice is N^{-1} . In general, we will denote particle configurations in X_N by the letter η . The interacting particle system evolves through a stochastic process and is described by a time-dependent probability (Radon) measure $\mu_t^N \in P(X_N)$.

Consider $p : \mathbb{T}_N^d \times \mathbb{T}_N^d \rightarrow \mathbb{R}_+$ so that $p(x, y) = p(0, y - x) := p(y - x)$, $\sum_{z \in \mathbb{Z}^d} p(z) = 1$ and its support $\{z \in \mathbb{Z}^d : p(z) > 0\}$ is finite, i.e. $p(z) = 0$ for $|z| > A$ for some $A \in \mathbb{R}$. These are the finite range, translation invariant, irreducible transition probabilities. We also denote by γ the mean transition rate:

$$\gamma = (\gamma_1, \dots, \gamma_d) := \sum_{z \in \mathbb{Z}^d} zp(z).$$

For any initial measure $\mu_0^N \in P(X_N)$ we obtain a unique measure $\mu_t^N \in P(X_N)$ describing the state of the process at a later time t . This also yields a semigroup $(S_t^N)_{t \geq 0}$ on $P(X_N)$, which is given by $\mu_t^N = S_t^N \mu_0^N$ for all $t \geq 0$. The semigroup S_t^N is a Feller-semigroup uniquely determined by its generator, see [Lig85, Chapter 1]. The generator is

a linear operator $\mathcal{L}_N : C_b(X_N) \rightarrow C_b(X_N)$ and satisfies

$$\frac{d}{dt} \langle \mu_t^N, f \rangle = \langle \mu_t^N, \mathcal{L}_N f \rangle, \quad (1.1)$$

where we have denoted by $\langle \cdot, \cdot \rangle$ the integral of a continuous function with respect to a measure. Equivalently, this is the duality pairing between (Radon) measures and bounded continuous functions. Thus \mathcal{L}_N can also be thought of as the generator of the dual semigroup on $C_b(X_N)$, which is the set of bounded continuous functions on X_N .

Let us make precise the notion of convergence of the particle process. Given a particle configuration $\eta \in X_N$, the particle densities are given by the *empirical measure*

$$\alpha_\eta^N := \frac{1}{N^d} \sum_{x \in \mathbb{T}_N^d} \eta(x) \delta_{\frac{x}{N}} \in \mathcal{M}_+(\mathbb{T}^d). \quad (1.2)$$

where $\mathcal{M}_+(\mathbb{T}^d)$ is the space of positive Radon measures on the torus. Let $f_t \in H$ be the solution to the hydrodynamical equation given initial data f_0 . The goal is to show that the empirical measure (1.2) possesses an asymptotic in N density profile $f_t(\cdot)$: for any smooth function $\varphi : \mathbb{T}^d \rightarrow \mathbb{R}$,

$$\text{for all } t \geq 0, \quad \lim_{N \rightarrow \infty} \mathbb{P}_{\mu_t^N} (|\langle \alpha_\eta^N, \varphi \rangle - \langle f_t, \varphi \rangle| > \epsilon) = 0 \quad (1.3)$$

and to estimate the rate of convergence. Here $\mathbb{P}_{\mu^N}(A)$ denotes the probability corresponding to the (measurable) event A under the probability measure $\mu^N \in P(X_N)$:

$$\mathbb{P}_{\mu^N}(A) = \int_{X_N} \chi_A(\eta) \mu(d\eta),$$

where χ_A denotes the characteristic function of A . We denote the expectation of a measurable function f with respect to a probability measure $\mu^N \in P(X_N)$ by

$$\mathbb{E}_{\mu^N}[f(\eta)] = \langle \mu^N, f \rangle = \int_{X_N} f(\eta) \mu^N(d\eta).$$

A measure μ^N is called *invariant* (or equilibrium) measure, if

$$\langle \mu^N, \mathcal{L}_N f \rangle = 0 \quad \text{for all } f \in C_b(X_N),$$

cf. equation (1.1).

We shall show that as the number N of sites in the lattice \mathbb{T}_N^d approaches infinity, the empirical measure converges to the solution of the limit partial differential equation

$$\partial_t f_t = L f_t \quad (1.4)$$

where L is a diffusion operator whose diffusion coefficient will be specified for each model separately.

We consider the space of microscopic variables X_N equipped with a (Gibbs) probability measure

$$\nu_\lambda^N(\eta) = Z^{-1} e^{\sum_{x \in \mathbb{T}_N^d} \eta(x) \lambda_x}, \quad (1.5)$$

where Z is a normalizing constant to ensure $\nu_\lambda^N(X_N) = 1$, the microscopic variables $\eta(x) \in \mathbb{N}$ or $\in \mathbb{R}$ depending on the process, and λ_x are coefficients varying on the macroscopic scale.

We assume the following Hypotheses:

(H1) Microscopic stability / Lyapunov condition. We assume that we can define a coupling between two processes (η_t, ζ_t) evolving according to the same law, with a density denoted by G_t^N that satisfies

$$\partial_t G_t^N(\eta, \zeta) = \tilde{\mathcal{L}}_N^* G_t^N(\eta, \zeta).$$

The coupling operator $\tilde{\mathcal{L}}_N$ is such that each marginal of G_t^N w.r.t. a reference measure $d\nu_\alpha^N$ with $\alpha \geq 0$, i.e. $\int_{X_N} G_t^N(\eta, \zeta) d\nu_\alpha^N(\eta)$, is evolving according to the Kolmogorov equation

$$\partial_t f_t^N(\eta) = \mathcal{L}_N^* f_t^N(\eta), \quad \text{where } f_t^N(\eta) = \frac{d\mu_t^N}{d\nu_\alpha^N}. \quad (1.6)$$

For every $f_t \in H$ solution to the limit partial differential equation (1.4), we introduce the *local Gibbs measure* $\nu_{f_t(\cdot)}^N$, i.e. the Gibbs measure with slowly varying parameters $\lambda_x = \lambda(f_t(x/N))$ in (1.5), associated to f_t . The density then $\psi_t^N = \frac{d\nu_{f_t(\cdot)}^N}{d\nu_\alpha^N}$, for $\alpha \geq 0$, takes the form

$$\psi_t^N(\zeta) = \frac{1}{Z_t} e^{\sum_{x \in \mathbb{T}_N^d} \zeta(x) \lambda(f_t(\frac{x}{N}))}, \quad (1.7)$$

and satisfies for some rate function $E^N(t, \zeta) \rightarrow 0$ as $N \rightarrow \infty$,

$$\partial_t \psi_t^N(\zeta) - \mathcal{L}_N^* \psi_t^N(\zeta) = E^N(t, \zeta). \quad (1.8)$$

Then the coupling density $G^N(\eta, \zeta)$ on X_N^2 , solves the equation

$$\partial_t G_t^N(\eta, \zeta) - \tilde{\mathcal{L}}_N^* G_t^N(\eta, \zeta) = S^N(t, \eta, \zeta) := \frac{d\nu_\alpha^N}{d\nu_\alpha^N}(\eta) \otimes E^N(t, \zeta) \quad (1.9)$$

and we choose the initial data $G_0^N(\eta, \zeta)$ to be the *optimal coupling* between the law of the stochastic process, f_t^N , and the local Gibbs density ψ_t^N .

We say that our model satisfies Hypothesis **(H1)** if

$$\tilde{\mathcal{L}}_N \left(\frac{1}{N^d} \sum_x |\eta(x) - \zeta(x)| \right) \leq 0.$$

Note that the evolution equation (1.9) is introduced so that taking the first marginal in the coupled Kolmogorov equation we recover the equation (1.6) and taking the second marginal we recover (1.8). Indeed we write

$$\partial_t \int_{\zeta \in X_N} G_t^N(\eta, \zeta) d\nu_\alpha^N(\zeta) - \tilde{\mathcal{L}}_N^* \int_{\zeta \in X_N} G_t^N(\eta, \zeta) d\nu_\alpha^N(\zeta) = \int_{\zeta \in X_N} E^N(t, \zeta) d\nu_\alpha^N(\zeta) = 0 \quad (1.10)$$

where the last equality is due to the conservation of mass: the fact that

$$\int_{X_N} \mathcal{L}_N^* \psi_t^N(\zeta) d\nu_\alpha^N(\zeta) = 0.$$

This yields (1.6) on the first marginal, whereas we have

$$\partial_t \int_{\eta \in X_N} G_t^N(\eta, \zeta) d\nu_\alpha^N(\eta) - \tilde{\mathcal{L}}_N^* \int_{\eta \in X_N} G_t^N(\eta, \zeta) d\nu_\alpha^N(\eta) = E^N(t, \zeta) \int_{\eta \in X_N} d\nu_\alpha^N(\eta) \quad (1.11)$$

on the second marginal, which yields (1.8).

(H2) Macroscopic stability. Let $(H, \|\cdot\|_H)$ be the space of solutions to the limit PDE. Typically $H = L^\infty(\mathbb{T}^d)$ will do for our purposes. We assume that for every solution $f_t \in H$, there is $K > 0$, $T \in (0, \infty]$, so that

$$\|D^k f_t\|_H \leq K, \text{ for all } t \in [0, T]$$

and multi-indices k so that $|k| \leq 4$.

When $T = \infty$, there is $R(t) \xrightarrow{t \rightarrow \infty} 0$ so that

$$\|D^k(f_t - f_\infty)\|_H \lesssim_{\|f_0\|_H} R(t), \text{ and } R(t) \in L^1((0, \infty))$$

for $f_\infty \in H$.

(H3) Consistency estimate. We assume that the local Gibbs measure has the following property: There exists a rate function \mathcal{E}^N vanishing as N goes to infinity, so that

$$\iint_{X_N^2} \frac{1}{N^d} \sum_x |\eta(x) - \zeta(x)| (\partial_t - \mathcal{L}_N^*) \psi_t^N(\zeta) d\nu_\alpha^N(\eta) d\nu_\alpha^N(\zeta) \lesssim \mathcal{E}^N \max_{k \in \{1, \dots, 4\}} \|D^k(f_t - f_\infty)\|_H.$$

Our main general result on the hydrodynamic limit is stated in the following Theorem:

Theorem 1.1. *Let $F \in \text{Lip}(\mathbb{R})$ and $\phi \in C_c^\infty(\mathbb{T}^d)$. Let f_0 be the initial data to the hydrodynamical equation (1.4) and μ_0^N be the initial distribution of the stochastic process.*

We also consider the density of the local Gibbs measure ψ_t^N given in (1.7), and the coupling G_t^N between ψ_t^N and $f_t^N := d\mu_t^N/d\nu_\lambda^N$. We assume that for $C_0 < \infty$ independent of N , there exists $\mathcal{R}^N \rightarrow 0$ as $N \rightarrow \infty$ so that

$$\begin{aligned} \int_{X_N} \left| N^{-d} \sum_x \eta(x) \phi\left(\frac{x}{N}\right) - \int f_0(u) \phi(u) du \right| d\mu_0^N(\eta) &\leq C_0 \mathcal{R}^N, \\ \int_{X_N^2} \sum_x |\eta(x) - \zeta(x)| G_0^N(d\eta, d\zeta) &\leq C_0 \mathcal{R}^N. \end{aligned} \quad (1.12)$$

Then, under the Assumptions **(H1)**-**(H2)**-**(H3)**, there are constants $0 < C_1, C_2 < \infty$ independent of N, t and

$$r(t) = \begin{cases} \in L^1((0, \infty)) & \text{if } T = \infty, \\ tK & \text{if } T < \infty. \end{cases}$$

such that for all $t \geq 0$

$$\left| \int_{X_N} F\left(N^{-d} \sum_{x \in \mathbb{T}_N^d} \eta(x) \phi\left(\frac{x}{N}\right)\right) - F\left(\int_{\mathbb{T}^d} f_t(u) \phi(u) du\right) d\mu_t^N(\eta) \right| \leq C_1 r(t) \mathcal{E}^N + \mathcal{R}^N + C_2 N^{-\frac{d}{d+2}} \quad (1.13)$$

where \mathcal{E}^N is the rate function from **(H3)** and where $f_t(\cdot)$ solves the hydrodynamical equation (1.4).

Remark 1.2. If f_0 is continuous, one can construct an initial particle distribution μ_0^N for which the initial assumptions hold: namely the local Gibbs measure $\mu_0^N = \nu_{f_0(\cdot)}^N$.

Remark 1.3. Note that this convergence in distribution of the random variable $J_N := \langle \alpha_\eta^N, \phi \rangle$ to the deterministic object $\langle f_t, \phi \rangle$ implies convergence in probability. This can be done by choosing the function F to be an approximation of an indicator function with support on a translation of $(-\delta, \delta)$ for $\delta > 0$. Indeed, let $\delta > 0$, and $F_\delta, \tilde{F}_\delta$ to be smooth approximations from above of the indicator functions on $[x + \delta, \infty), (-\infty, x - \delta]$, respectively and they are so that $F_\delta(J) = \tilde{F}_\delta(J) = 0$. Then

$$\begin{aligned} \mathbb{P}_{\mu_t^N}(|J_N - J| > \delta) &\leq \mathbb{P}_{\mu_t^N}(J_N > J + \delta) + \mathbb{P}_{\mu_t^N}(J_N < J - \delta) \\ &\leq \mathbb{E}_{\mu_t^N}(F_\delta(J_N)) + \mathbb{E}_{\mu_t^N}(\tilde{F}_\delta(J_N)) \rightarrow 0 \end{aligned}$$

as $N \rightarrow \infty$.

Here we will apply our result to three prototypical models, the *zero-range processes*, the *simple exclusion processes* and the *Ginzburg-Landau* model.

5.1.1 Zero-Range process

Here the state space is given by $X_N = \mathbb{N}^{\mathbb{T}_N^d}$ as there is no restriction on the number of the particles per site $x \in \mathbb{T}_N^d$ and the generator is given by

$$\text{for all } f \in C_b(X_N), \quad \mathcal{L}_N f(\eta) = \sum_{x, y \sim x} p(y-x) g(\eta(x)) [f(\eta^{x,y}) - f(\eta)] \quad (1.14)$$

where $\eta^{x,y}$ is the configuration of the particle system after one particle has jumped from site x to a neighboring site $y \in \mathbb{T}_N^d$:

$$\eta^{x,y}(z) = \begin{cases} \eta(x) - 1 & \text{if } z = x, \\ \eta(y) + 1 & \text{if } z = y, \\ \eta(z) & \text{otherwise.} \end{cases} \quad (1.15)$$

In order for the process to remain in the state space X_N , we always assume $g(0) = 0$. Since the jump rate on a given site only depends on the number of particles at that particular site, this process is called *zero range process*. The *jump rate* $g : \mathbb{N} \rightarrow [0, \infty)$ can be thought of as describing the interactions of particles occupying the same site. A special case is the case of linear g , where the particles perform independent random walks on the lattice.

A convenient family of invariant measures is given by the *grand-canonical* or *Gibbs* measures, given by

$$\nu_\rho^N(\eta) = \prod_{x \in \mathbb{T}_N^d} \frac{\sigma(\rho)^{\eta(x)}}{g(\eta(x))! Z(\sigma(\rho))}, \quad (1.16)$$

where Z is the *partition function* of the zero range process and $\rho \geq 0$. Furthermore we used the notation $g(n)! := g(1) \cdot g(2) \cdots g(n)$ and $g(0)! := 1$. The partition function is defined as

$$Z(\phi) = \sum_{n=0}^{\infty} \frac{\phi^n}{g(n)!}. \quad (1.17)$$

The function $\sigma(\rho)$ is chosen such that

$$\langle \nu_\rho^N, \eta(0) \rangle = \rho.$$

We shall elaborate on the construction of σ in a later Section. Since the number of particles is conserved and the process has no other conserved quantities, another important set of invariant measure is given by the *canonical measures*

$$\nu^{N,K}(\eta) = \nu_\rho^N(\eta \mid \sum_x \eta(x) = K), \quad (1.18)$$

which are the grand-canonical measures conditioned on hyperplanes of constant number of particles. Note that this definition is independent of ρ . Since the equilibrium ν_ρ^N is made up of independent random variables, we expect the convergence (1.3) to hold if we can show that the process is locally at $u \in \mathbb{T}^d$ in equilibrium $\nu_{f_t(u)}^N$ with average density $f_t(u)$.

Diffusive scaling. We accelerate the zero-range process $(\eta_t)_t$ by a factor N^2 , *i.e.* the microscopic spatial variables scale like N and time like N^2 , and we assume that the mean $\gamma = 0$. The generator in this case is

$$\text{for all } f \in C_b(X_N), \quad \mathcal{L}_N f(\eta) = N^2 \sum_{x, y \sim x} p(y-x) g(\eta(x)) [f(\eta^{x,y}) - f(\eta)].$$

Under diffusive scaling, the empirical measure of the zero range process converges to the solution f_t to the *nonlinear diffusion equation*

$$\partial_t f_t = \Delta_c \sigma(f_t). \tag{1.19}$$

for the nonlinearity $\sigma : [0, \infty) \rightarrow [0, \infty)$ appearing in (1.16). We denote by $c = (c_{i,j})_{1 \leq i, j \leq d}$ the correlations matrix

$$c_{i,j} := \sum_{x \in \mathbb{Z}^d} p(x) x_i x_j$$

and the diffusion operator is given by

$$\Delta_c = \sum_{1 \leq i, j \leq d} c_{i,j} \partial_{u_i} \partial_{u_j}.$$

Hydrodynamic limit under hyperbolic scaling. We accelerate the zero-range process $(\eta_t)_t$ by a factor N , *i.e.* both the microscopic spatial variables and the time scale with N , and we assume that the mean $\gamma \neq 0$. The generator in this case is

$$\text{for all } f \in C_b(X_N), \quad \mathcal{L}_N f(\eta) = N \sum_{x, y \sim x} p(y-x) g(\eta(x)) [f(\eta^{x,y}) - f(\eta)].$$

Under the hyperbolic scaling, the empirical density of the zero-range process converges to the solution f_t to the *conservation law*

$$\partial_t f_t = \gamma \cdot \nabla \sigma(f_t). \tag{1.20}$$

When σ is not linear, the solution of (1.25) may develop discontinuities (shocks) in which case is not differentiable and it is then understood in the sense of distributions. Moreover, in the case of shocks, the solutions are not determined uniquely by their initial data. We therefore seek for the relevant solutions under some criteria so that we have

uniqueness, the so-called entropy solutions. Nevertheless, up to a finite time T of the appearance of the first shock, there is a smooth solution to the equation.

Let us make the following assumptions on the rate function $g : \mathbb{N} \rightarrow [0, \infty)$.

Assumption 2 (Assumptions on the jump rate on the Zero-Range process). *We assume the following*

(ZR1) Non-degeneracy: Assume that g satisfies $g(0) = 0$ and $g(n) > 0$ for all $n > 0$.

(ZR2) Lipschitz-property: Furthermore we require that g is Lipschitz continuous with

$$0 \leq |g(n+1) - g(n)| \leq g^* < +\infty$$

for all $n \in \mathbb{N}$.

(ZR3) Spectral gap: We also assume that there exists $n_0 > 0$ and $\delta > 0$ such that

$$g(n) - g(j) \geq \delta$$

for any $j \in \mathbb{N}$ and $n \geq j + n_0$.

(ZR4) Attractivity: Let the jump rate g be monotonously increasing, i.e.

$$g(n+1) \geq g(n)$$

for all $n \in \mathbb{N}$.

As before $(\eta_t)_t$ is the Markov process generated by \mathcal{L}_N , with initial distribution μ^N . We assume $\mu^N \leq \nu_\rho^N$ for some $\rho \geq 0$.

Corollary 1.4 (Hydrodynamic limit for the Zero-Range process under diffusive scaling).

Let $d = 1$, $F \in Lip(\mathbb{R})$ and $\phi \in C_c^\infty(\mathbb{T}^d)$. Let f_0 be the initial data to the diffusion equation (1.19) and μ^N be the initial distribution of the zero-range process. We assume that for $C_0 < \infty$ independent of N ,

$$\int_{X_N} \left| N^{-d} \sum_x \eta(x) \phi\left(\frac{x}{N}\right) - \int f_0(u) \phi(u) du \right| d\mu^N(\eta) \leq C_0 N^{-\frac{d}{d+2}}. \quad (1.21)$$

For $t > 0$, under Assumption 2, there exists constant $0 < C < \infty$ independent of N, t such that

$$\left| \int_{X_N} F \left(N^{-d} \sum_{x \in \mathbb{T}_N^d} \eta(x) \phi\left(\frac{x}{N}\right) \right) - F \left(\int_{\mathbb{T}^d} f_t(u) \phi(u) du \right) d\mu_t^N(\eta) \right| \leq CN^{-\frac{d}{2+d}} \quad (1.22)$$

where $f_t(\cdot)$ solves the equation

$$\partial_t f_t = \Delta_c \sigma(f_t)$$

for the nonlinearity $\sigma : [0, \infty) \rightarrow [0, \infty)$ appearing in (1.16).

Remark 1.5. Note that the restriction on the dimension $d = 1$ is here only because the main Hypothesis **(H2)** is proved for the nonlinear diffusion equation only in the case $d = 1$ in the Appendix 6.6.2.

5.1.2 Simple Exclusion model

In contrast with the zero-range process, the simple exclusion process allows at most one particle per site. The jump is suppressed if it leads to an already occupied site. The state space therefore is $X_N = \{0, 1\}^{\mathbb{T}_N^d}$ and the generator of the process is given by

$$\text{for all } f \in C_b(X_N), \quad \mathcal{L}_N f(\eta) = \sum_{x, y \sim x} p(y-x) (\eta(x)(1-\eta(y)) [f(\eta^{x,y}) - f(\eta)]) \quad (1.23)$$

where $\eta^{x,y}$ is the configuration of the particle system after one particle has jumped from site x to a neighboring site y , given by (1.15).

A family of invariant measures is given by, for $0 < \alpha < 1$ the Bernoulli product measures with parameter α , i.e.

$$\nu_\alpha^N(\eta) = \prod_{x \in \mathbb{T}_N^d} \alpha^{\eta(x)} (1-\alpha)^{1-\eta(x)}.$$

Diffusive scaling. We assume that the mean $\gamma = 0$ and we accelerate the process $(\eta_t)_t$ by a factor N^2 , i.e. the microscopic x -variables scale with N , while the time with N^2 . The generator then is

$$\text{for all } f \in C_b(X_N), \quad \mathcal{L}_N f(\eta) = N^2 \sum_{x, y \sim x} p(y-x) \eta(x)(1-\eta(y)) [f(\eta^{x,y}) - f(\eta)].$$

Under diffusive scaling, the empirical densities of the simple exclusion process converges to the solution f_t to the *diffusion equation*

$$\partial_t f_t = \Delta_c f_t, \quad \text{where } \Delta_c = \sum_{1 \leq i, j \leq d} c_{i,j} \partial_{u_i} \partial_{u_j} \quad (1.24)$$

and $c = (c_{i,j})_{1 \leq i, j \leq d}$ is the correlations matrix

$$c_{i,j} := \sum_{x \in \mathbb{Z}^d} p(x) x_i x_j.$$

Hydrodynamic limit under hyperbolic scaling. We accelerate the process $(\eta_t)_t$ by a factor N , *i.e.* both the microscopic spatial variables and the time scale like N , and we assume that the mean $\gamma = \sum_z p(z) \neq 0$. The generator is

$$\text{for all } f \in C_b(X_N), \quad \mathcal{L}_N f(\eta) = N \sum_{x,y \sim x} p(y-x) \eta(x)(1-\eta(y)) [f(\eta^{x,y}) - f(\eta)].$$

Under the hyperbolic scaling, the empirical density of the zero-range process converges to the solution f_t to the *conservation law*

$$\partial_t f_t = \gamma \cdot \nabla \sigma(f_t) \quad (1.25)$$

where $\sigma(f_t) = f_t(1 - f_t)$. Due to the nonlinearity, the solution of (1.25) can develop shocks (depending on the monotonicity of f_0) even for smooth initial data [Daf16, Chapter 4]. Therefore, up to the time T of the appearance of the first discontinuity, we have a hydrodynamic limit, as there is a smooth solution to the equation.

Corollary 1.6 (Hydrodynamic limit for the Symmetric Simple Exclusion process under diffusive scaling). *Let $d \geq 1$, $F \in Lip(\mathbb{R})$ and $\phi \in C_c^\infty(\mathbb{T}^d)$. Let f_0 be the initial data to the diffusion equation (1.24) and μ_0^N be the initial distribution of the simple exclusion process. We assume that at $t = 0$ there exists $C_0 < \infty$ independent of N ,*

$$\int_{X_N} \left| N^{-d} \sum_x \eta(x) \phi\left(\frac{x}{N}\right) - \int f_0(u) \phi(u) du \right| d\mu_0^N(\eta) \leq C_0 N^{-\frac{d}{d+2}}. \quad (1.26)$$

For $t > 0$ there exists constant $0 < C < \infty$ independent of N, t such that

$$\left| \int_{X_N} F \left(N^{-d} \sum_{x \in \mathbb{T}_N^d} \eta(x) \phi\left(\frac{x}{N}\right) \right) - F \left(\int_{\mathbb{T}^d} f_t(u) \phi(u) du \right) d\mu_t^N(\eta) \right| \leq C N^{-\frac{1}{1+2d}} \quad (1.27)$$

where $f_t(\cdot)$ solves the diffusion equation

$$\partial_t f_t = \Delta_c f_t.$$

5.1.3 Ginzburg-Landau type models

Let $T_N = \mathbb{Z}/(N\mathbb{Z})$, $N \in \mathbb{N}^*$. be the one-dimensional periodic integer lattice. To each lattice site $x \in \mathbb{T}_N$ we associate the continuous variable $\eta(x) \in \mathbb{R}$ which represents a charge at this site and $\eta = (\eta(x))_{x \in \mathbb{T}_N} \in \mathbb{R}^{\mathbb{T}_N}$ is then a field configuration. At $t > 0$ the configuration is $\eta_t = (\eta_t(x))_{x \in \mathbb{T}_N}$. The charges evolve randomly according to a diffusion process to adjacent sites. We apply the diffusive scaling in space and time, *i.e.* speed up

the time by N^2 and shrink the space between charges by N so that we obtain a system of spins (charges) located at points x/N with $x = 1, \dots, N$ of the circle $\mathbb{S} = \mathbb{R}/\mathbb{Z}$.

The Ginzburg-Landau dynamics for η is described by the set of stochastic differential equations, for $x \in \mathbb{T}_N$,

$$d\eta_t(x) = \frac{N^2}{2} \left(V'(\eta(x+1)) - 2V'(\eta(x)) + V'(\eta(x-1)) \right) dt + N(dW_t(x) - dW_t(x+1)), \quad (1.28)$$

where $W_t(x)$, $x = 1, \dots, N$ are independent Brownian motions and $V : \mathbb{R} \rightarrow \mathbb{R}$, $V \in C^2(\mathbb{R})$ is the external single-site potential.

Assumption 3 (Assumptions on the single-site potential of the Ginzburg-Landau model).
We assume

(GL1) $V(u) = V_0(u) + V_1(u)$ and there exist $C, \lambda > 0$ so that

$$V_0''(u) \geq \lambda \text{ and } \|V_1\|_{L^\infty(\mathbb{T})} \leq C, \quad \|V_1'\|_{L^\infty(\mathbb{T})} \leq C.$$

This assumption can be directly compared with the one-body non-convex potentials considered in [GOVW09, DMOWa, Fat13] as well. One can take for example the double-well potential.

The infinitesimal generator of the diffusion process $\eta(x)$ is the operator

$$\begin{aligned} \mathcal{L}_N := & \frac{N^2}{2} \sum_{x \sim y \in \mathbb{T}_N} \left(\frac{\partial}{\partial \eta(x)} - \frac{\partial}{\partial \eta(y)} \right)^2 \\ & - \frac{N^2}{2} \sum_{x \sim y \in \mathbb{T}_N} \left(\frac{\partial V}{\partial \eta(x)} - \frac{\partial V}{\partial \eta(y)} \right) \left(\frac{\partial}{\partial \eta(x)} - \frac{\partial}{\partial \eta(y)} \right). \end{aligned} \quad (1.29)$$

The generator \mathcal{L}_N is symmetric with respect to the invariant (Gibbs) product measure

$$d\nu^N(\eta) := \prod_{i \in \mathbb{T}_N} e^{-V(\eta(x_i))} d\eta(x_i) \quad \text{on } \mathbb{R}^{\mathbb{T}_N}.$$

Consider the Radon-Nikodym derivative f_0^N of the initial state of the process, μ_0^N , with respect to the reference measure $d\nu^N$. Then at time $t > 0$, $f_t^N := d\mu_t^N/d\nu^N$ and solves

$$\partial_t f_t^N = \mathcal{L}_N f_t^N.$$

Given a charge configuration η , we define the empirical measure

$$\alpha_\eta^N = \frac{1}{N} \sum_x \eta(x) \delta_{x/N} \quad \text{on } \mathbb{S}.$$

In order to describe the hydrodynamical equation in this case, let us introduce some notation. Let $M(\lambda)$ the function defined in assumption (A3) above and consider

$$\text{for all } \lambda \in \mathbb{R}, \quad p(\lambda) = \log M(\lambda), \quad h(y) := \sup_{\lambda \in \mathbb{R}} (\lambda y - p(\lambda)).$$

Then $h(\cdot)$ and $p(\cdot)$ are a pair of conjugate convex functions and

$$h'(y) = \lambda \quad \text{iff} \quad y = p'(\lambda)$$

where

$$p'(\lambda) = \frac{M'(\lambda)}{M(\lambda)} = \frac{\int u e^{\lambda u - V(u)} du}{M(\lambda)}$$

i.e. h' and p' are the inverse of each other. Moreover h' and p' are smooth and strictly increasing functions.

We prove in the next statement that the empirical measure of the Ginzburg-Landau dynamics has a macroscopic profile f_t that solves the diffusion equation

$$\partial_t f_t(u) = \partial_{uu} h'(f_t(u)), \quad (t, u) \in (0, \infty) \times \mathbb{S}. \quad (1.30)$$

Corollary 1.7 (Hydrodynamic limit for Ginzburg-Landau type models under diffusive scaling). *Let $d = 1$, $F \in \text{Lip}(\mathbb{R})$ and $\phi \in C_c^\infty(\mathbb{T})$. Let f_0 be the initial data to the diffusion equation (1.30) and μ_0^N be the initial distribution of the Ginzburg-Landau process. We assume that at $t = 0$ there exists $C_0 < \infty$ independent of N ,*

$$\int_{X_N} \left| N^{-d} \sum_x \eta(x) \phi\left(\frac{x}{N}\right) - \int f_0(u) \phi(u) du \right| d\mu_0^N(\eta) \leq C_0 N^{-\frac{1}{3}}. \quad (1.31)$$

For $t > 0$, under Assumption 3, there exists constant $0 < C < \infty$ independent of N, t such that

$$\left| \int_{X_N} F\left(N^{-d} \sum_{x \in \mathbb{T}_N} \eta(x) \phi\left(\frac{x}{N}\right)\right) - F\left(\int_{\mathbb{T}} f_t(u) \phi(u) du\right) d\mu_t^N(\eta) \right| \leq C N^{-\frac{1}{3}} \quad (1.32)$$

where f_t solves the nonlinear diffusion equation

$$\partial_t f_t = \partial_{uu} h'(f_t).$$

Remark 1.8. *When the potential is convex, as we assume here, the rate $N^{-1/3}$ matches the one in [DMOWa], which is the only fully quantitative result in the literature so far.*

5.1.4 State of the art

The hydrodynamic limit under diffusive scaling for the Ginzburg-Landau process was obtained first by Fritz in [Fri89]. Motivated by the work in [Fri89] then Guo, Papanicolaou and Varadhan introduced in [GPV88] a more general method, applicable to several reversible models under diffusive scaling, which is based on martingale convergence and estimates of the entropy. Apart from the *entropy method*, [GPV88], see Theorem 1.9 below, one can identify one more important method which is due to Yau [Yau91], the so-called *relative entropy method*, see Theorem 1.10 below. This is based on a Grönwall-type estimate for a relative entropy functional. Yau's method, even though it needs stronger assumptions on the initial data, i.e. closeness to hydrodynamic behavior in the sense of relative entropy rather than in the sense of macroscopic observables, it is simpler and gives stronger results. For an extensive account of these methods we refer to the book [KL99].

In order to state the following theorems, we need one more definition. Let $\mu, \nu \in P(X_N)$ be two probability measures. Then the entropy of μ relative to ν is defined as

$$H^N(\mu|\nu) = \int_{X_N} \log\left(\frac{d\mu}{d\nu}\right) d\mu \quad (1.33)$$

whenever μ is absolutely continuous with respect to ν . The relative entropy is connected to the Fisher information

$$\mathcal{D}_N(\mu|\nu) = \int_{X_N} \sqrt{\frac{d\mu}{d\nu}} \mathcal{L}_N \sqrt{\frac{d\mu}{d\nu}} d\nu. \quad (1.34)$$

The entropy method for the zero-range process can be summarized in the following theorem, [KL99, Chapter 5, Theorem 1.1]. Note that in the following theorems, we have not tried to optimize the assumptions. The proofs under the given assumptions can be found in [KL99].

Theorem 1.9 (Guo-Papanicolaou-Varadhan for the Zero-Range Process). *Assume (ZR1) and (ZR2) of Assumption 2 as well as $g(n) \geq g_0 n$ for some $g_0 > 0$ and let $\mu_0^N \in P(X_N)$ and $f_0 \in L^\infty(\mathbb{T}^d)$ such that*

$$\text{for all } \varphi \in C(\mathbb{T}^d), \delta > 0, \quad \lim_{N \rightarrow \infty} \mathbb{P}_{\mu_0^N}(|\langle \alpha_\eta^N, \varphi \rangle - \langle \varphi, f_0 \rangle| > \delta) = 0.$$

Furthermore we assume that the initial data satisfy the bounds

$$\frac{1}{N^d} H(\mu_0^N | \nu_\rho^N) \leq C \quad \text{and} \quad \left\langle \mu_0^N, \frac{1}{N^d} \sum_{x \in \mathbb{T}_N^d} \eta(x)^2 \right\rangle \leq C$$

for some $\rho > 0$ and a constant $C < +\infty$.

Then, for $t > 0$, it holds that

$$\text{for all } \varphi \in C(\mathbb{T}^d), \delta > 0, \quad \lim_{N \rightarrow \infty} \mathbb{P}_{\mu_t^N} (|\langle \alpha_\eta^N, \varphi \rangle - \langle \varphi, f_t \rangle| > \delta) = 0,$$

where f_t is the unique weak solution to (1.19) and μ_t^N solves (1.1) with Cauchy datum μ_0^N .

Thus the entropy method yields propagation in time of the hydrodynamic profile. The relative entropy method by Yau, on the other hand, concerns the conservation of a stronger notion. In analogy to (1.16), we define a local Gibbs measure with macroscopic profile $f_t \in L^\infty(\mathbb{T}^d)$ by

$$\nu_{f_t(\cdot)}^N(\eta) = \prod_{x \in \mathbb{T}_N^d} \frac{\sigma(f_t(\frac{x}{N}))^{\eta(x)}}{g(\eta(x))! Z(\sigma(f_t(\frac{x}{N})))} \quad (1.35)$$

where $\sigma(\rho)$ is chosen such that $\langle \nu_\rho^N, \eta(0) \rangle = \rho$ as discussed in subsection 5.1.1.

This measure has the property that it is locally (in infinitesimal macroscopic neighborhoods where f_t is constant) in equilibrium with a non-equilibrium profile f_t as $N \rightarrow \infty$. The relative entropy method then yields for the zero-range process, [KL99, Chapter 6, Theorem 1.1]:

Theorem 1.10 (Yau for the Zero-Range Process). *Assume (i) and (ii) of Assumption 2 as well as that the partition function Z is finite on all $[0, \infty)$, e.g. $g(n) \geq g_0 n$ for some $g_0 > 0$. Let $\mu_t^N \in P(X_N)$ that solve (1.1) and $f_t \in C^2(\mathbb{T}^d)$ solve (1.19). Furthermore assume that initially the rescaled relative entropy $N^{-d} H^N(\mu_0^N | \nu_{f_0(\cdot)}^N)$ vanishes in the limit, i.e.*

$$\lim_{N \rightarrow \infty} \frac{1}{N^d} H^N(\mu_0^N | \nu_{f_0(\cdot)}^N) = 0.$$

Then for all $t \geq 0$,

$$\lim_{N \rightarrow \infty} \frac{1}{N^d} H^N(\mu_t^N | \nu_{f_t(\cdot)}^N) = 0. \quad (1.36)$$

Note that the convergence of the relative entropy (1.36) implies that μ_t^N has profile f_t :

$$\lim_{N \rightarrow \infty} \mathbb{P}_{\mu_t^N} (|\langle \alpha_\eta^N, \varphi \rangle - \langle \varphi, f_t \rangle| > \delta) = 0.$$

Thus the convergence of the relative entropy is stronger notion of hydrodynamic limit. Yau's relative entropy method shows that this stronger notion is conserved by the evolution.

Regarding quantitative estimates of the convergence in the hydrodynamic limit, a first step was achieved by the method introduced by N. Grunewald, F. Otto, C. Villani, and M. Westdickenberg in [GOVW09] for the Ginzburg-Landau model with Kawasaki dynamics, when the potential is not necessarily convex. There, the authors prove a logarithmic Sobolev inequality and the hydrodynamic limit based on a coarse-graining of the state-space. In a more recent work [DMOWa, DMOWa] the quantitative theory is

further developed for the Ginzburg-Landau model where the authors establish exact error estimates to the limit.

Another question that can be asked in this setting is the convergence of the microscopic entropy to the hydrodynamic entropy, which has been answered by [Kos01, Fat13] at a qualitative level. We discuss about it in the work in progress-section 5.7.

5.2 Quantitative Local Law of Large Numbers

Let f_t be a solution to the limit partial differential equation (1.4). We denote by $\overline{\eta(x)}^\ell$ for $0 < \ell < N$, the ℓ -averages given by

$$\overline{\eta(x)}^\ell = \frac{1}{\ell_*^d} \sum_{|y-x| \leq \ell} \eta(y)$$

where $\ell_* = 2\ell + 1$.

We give the proof of two lemmas concerning the exact rates of the law of large numbers of the product Gibbs measure, for the sake of completeness. Lemma 2.2 is used to show that choosing the initial data to be the product Gibbs measure with varying coefficient $f_0(\cdot)$, we recover indeed the desired hydrodynamical equation.

Lemma 2.1 (Quantitative Local Law of large numbers). *Let f_t be a solution to the limit PDE (1.4) satisfying **(H2)**. We consider $0 < \ell < N, \alpha \geq 0$,*

$$\psi_t^N(\zeta) = d\nu_{f_t(\cdot)}^N(\zeta) / d\nu_\alpha^N(\zeta).$$

Let $\theta : X \rightarrow [0, \infty)$, where $X = \mathbb{R}$ or \mathbb{N} , so that its average with respect to the local Gibbs measure $\vartheta : \mathbb{R} \rightarrow \mathbb{R}_+$,

$$\vartheta(f_t(x/N)) := \int_{X_N} \theta(\zeta(x)) \psi_t^N(\zeta) d\nu_\alpha^N(\zeta) = \mathbb{E}_{\nu_{f_t(\cdot)}^N}(\theta(\zeta(x)))$$

is Lipschitz. Assume that there exists a weight function $\mathcal{W} : X_N^2 \rightarrow \mathbb{R}_+$ so that for fixed $x \in \mathbb{T}_N^d$,

$$\int_{X_N} \zeta(x)^k \psi_t^N(\zeta) d\nu_\alpha^N(\zeta) < \infty \quad \text{and} \quad \iint_{X_N^2} \mathcal{W}(\eta(x), \zeta(x))^2 \psi_t^N(\zeta) d\nu_\alpha^N(\zeta) d\nu_\alpha^N(\eta) < \infty$$

for $|k| \leq 2$. We then have

$$N^{-d} \sum_{x \in \mathbb{T}_N^d} \iint_{X_N \times X_N} \mathcal{W}(\eta(x), \zeta(x)) \left| \overline{\theta(\zeta(x))}^\ell - \vartheta(\zeta(x)^\ell) \right| \psi_t^N(\zeta) d\nu_\alpha^N(\zeta) d\nu_\alpha^N(\eta) \lesssim \frac{1}{\ell^{d/2}} + \frac{\ell}{N}. \quad (2.37)$$

Proof. The proof takes advantage of the independency of the variables under the law $\nu_{f_t(\cdot)}^N$. We first apply a Cauchy-Schwarz inequality and we use the hypothesis on the second moment of the weight \mathcal{W} , so that we need to estimate

$$N^{-d} \sum_{x \in \mathbb{T}_N^d} \left(\int_{X_N} \left| \overline{\theta(\zeta(x))}^\ell - \vartheta(\overline{\zeta(x)}^\ell) \right|^2 \psi_t^N(\zeta) d\nu_\alpha^N(\zeta) \right)^{1/2}.$$

We write for fixed $x \in \mathbb{T}_N^d$ and $|y_i| \leq \ell$:

$$\begin{aligned} & \left(\int_{X_N} \left| \frac{1}{\ell_*^d} \sum_{i=1}^{\ell_*^d} (\theta \circ \zeta)(x + y_i) - \vartheta(\overline{\zeta(x)}^\ell) \right|^2 d\nu_{f_t(\cdot)}^N(\zeta) \right)^{1/2} \lesssim \\ & \left(\int_{X_N} \left| \frac{1}{\ell_*^d} \sum_{i=1}^{\ell_*^d} \left((\theta \circ \zeta)(x + y_i) - \vartheta \left(f_t \left(\frac{x + y_i}{N} \right) \right) \right) \right|^2 + \right. \\ & \quad \left. + \left| \frac{1}{\ell_*^d} \sum_{i=1}^{\ell_*^d} \left(\vartheta \left(f_t \left(\frac{x + y_i}{N} \right) \right) - \vartheta(\overline{\zeta(x + y_i)}^\ell) \right) \right|^2 + \right. \\ & \quad \left. + \left| \frac{1}{\ell_*^d} \sum_{i=1}^{\ell_*^d} \left(\vartheta(\overline{\zeta(x + y_i)}^\ell) - \vartheta(\overline{\zeta(x)}^\ell) \right) \right|^2 d\nu_{f_t(\cdot)}^N(\zeta) \right)^{1/2} := (I) + (II) + (III). \end{aligned} \tag{2.38}$$

As for the first term

$$\begin{aligned}
(I) &\leq \int_{X_N} \left| \frac{1}{\ell_*^d} \sum_{i=1}^{\ell_*^d} \left((\theta \circ \zeta)(x + y_i) - \mathbb{E}_{\nu_{f_t(\cdot)}^N} \left((\theta \circ \zeta)(x + y_i) \right) \right) \right|^2 d\nu_{f_t(\cdot)}^N(\zeta) = \\
&\frac{1}{\ell_*^{2d}} \sum_{i \neq j} \int_{X_N} \left(\theta(\zeta(x + y_i)) - \mathbb{E}_{\nu_{f_t(\cdot)}^N} \left(\theta(\zeta(x + y_i)) \right) \right) \left(\theta(\zeta(x + y_j)) - \mathbb{E}_{\nu_{f_t(\cdot)}^N} \left(\theta(\zeta(x + y_j)) \right) \right) d\nu_{f_t(\cdot)}^N(\zeta) \\
&\quad + \int_{X_N} \frac{1}{\ell_*^{2d}} \sum_i \left(\theta(\zeta(x + y_i)) - \mathbb{E}_{\nu_{f_t(\cdot)}^N} \left(\theta(\zeta(x + y_i)) \right) \right)^2 d\nu_{f_t(\cdot)}^N(\zeta) \\
&= \frac{1}{\ell_*^{2d}} \sum_{i \neq j} \left[\int_{X_N} \left(\theta(\zeta(x + y_i)) - \mathbb{E}_{\nu_{f_t(\cdot)}^N} \left(\theta(\zeta(x + y_i)) \right) \right) d\nu_{f_t(\cdot)}^N(\zeta) \right] \times \\
&\quad \times \left[\int_{X_N} \theta(\zeta(x + y_j)) - \mathbb{E}_{\nu_{f_t(\cdot)}^N} \left(\theta(\zeta(x + y_j)) \right) d\nu_{f_t(\cdot)}^N(\zeta) \right] \\
&+ \int_{X_N} \frac{1}{\ell_*^{2d}} \sum_{i=1}^{\ell_*^d} \left(\theta(\zeta(x + y_i)) - \mathbb{E}_{\nu_{f_t(\cdot)}^N} \left(\theta(\zeta(x + y_i)) \right) \right)^2 d\nu_{f_t(\cdot)}^N(\zeta) \\
&= \frac{1}{\ell_*^{2d}} \sum_{i=1}^{\ell_*^d} \int_{X_N} \left(\theta(\zeta(x + y_i)) - \mathbb{E}_{\nu_{f_t(\cdot)}^N} \left(\theta(\zeta(x + y_i)) \right) \right)^2 d\nu_{f_t(\cdot)}^N(\zeta) = \mathcal{O}(\ell_*^{-d})
\end{aligned} \tag{2.39}$$

where we have used the form of the product measure $\nu_{f_t(\cdot)}^N$ and in the last line the uniform in N upper bounds of the moments (up to the second moment) since f_t is bounded.

As for the second term

$$\begin{aligned}
(II) &\lesssim \int_{X_N} \frac{1}{\ell_*^d} \sum_{i=1}^{\ell_*^d} \left| f_t \left(\frac{x + y_i}{N} \right) - \overline{\zeta(x + y_i)}^\ell \right|^2 d\nu_{f_t(\cdot)}^N(\zeta) \\
&\leq \int_{X_N} \frac{1}{\ell_*^d} \sum_{i=1}^{\ell_*^d} \left(\frac{1}{\ell_*^d} \sum_{j=1}^{\ell_*^d} \left| f_t \left(\frac{x + y_i + y_j}{N} \right) - f_t \left(\frac{x + y_i}{N} \right) \right|^2 + \right. \\
&\quad \left. + \frac{1}{\ell_*^d} \sum_{j=1}^{\ell_*^d} \left| f_t \left(\frac{x + y_i + y_j}{N} \right) - \zeta(x + y_i + y_j) \right|^2 \right) \lesssim \left(\frac{\ell}{N} \right)^2 + \frac{1}{\ell^d}
\end{aligned} \tag{2.40}$$

due to the smoothness of f_t and for the last estimate we just repeat the calculations as we did for the first term. As for the third term, using that ϑ is Lipschitz we need to estimate:

$$\begin{aligned}
(III) &\lesssim \int_{X_N} \frac{1}{\ell_*^d} \sum_{i=1}^{\ell_*^d} \left| \overline{\zeta(x)}^\ell - \overline{\zeta(x+y_i)}^\ell \right|^2 d\nu_{f_t(\cdot)}^N(\zeta) \\
&\leq \int_{X_N} \frac{1}{\ell_*^d} \sum_{i=1}^{\ell_*^d} \left| \overline{\zeta(x)}^\ell - \mathbb{E}_{\nu_{f_t(\cdot)}^N} \left(\overline{\zeta(x)}^\ell \right) \right|^2 d\nu_{f_t(\cdot)}^N(\zeta) + \\
&\quad + \int_{X_N} \frac{1}{\ell_*^d} \sum_{i=1}^{\ell_*^d} \left| \overline{\zeta(x+y_i)}^\ell - \mathbb{E}_{\nu_{f_t(\cdot)}^N} \left(\overline{\zeta(x+y_i)}^\ell \right) \right|^2 d\nu_{f_t(\cdot)}^N(\zeta) \\
&\quad + \int_{X_N} \frac{1}{\ell_*^d} \sum_{i=1}^{\ell_*^d} \left| \mathbb{E}_{\nu_{f_t(\cdot)}^N} \left(\overline{\zeta(x)}^\ell \right) - \mathbb{E}_{\nu_{f_t(\cdot)}^N} \left(\overline{\zeta(x+y_i)}^\ell \right) \right|^2 d\nu_{f_t(\cdot)}^N(\zeta) \\
&\lesssim \frac{1}{\ell^d} + \left| \int_{X_N} \left(\overline{\zeta(x+y_i)}^\ell - \overline{\zeta(x)}^\ell \right) d\nu_{f_t(\cdot)}^N(\zeta) \right|^2 \lesssim \frac{1}{\ell^{d/2}} + \left| f_t \left(\frac{x+y_i}{N} \right) - f_t \left(\frac{x}{N} \right) \right|^2 \lesssim \frac{1}{\ell^d} + \left(\frac{\ell}{N} \right)^2
\end{aligned} \tag{2.41}$$

where the sums in the last line are neglected as they are normalized and thus they are of order 1. Gathering therefore all our error estimates together and taking account of the square root, we have a total error of order $\ell^{-d/2} + \ell/N$. \square

Lemma 2.2 (Sampling rate). *Let $t \geq 0$ and $\phi \in C_c^\infty(\mathbb{T}^d)$ a test function. Under the law $\nu_{f_t(\cdot)}^N$, the term $\int_{\mathbb{T}^d} \alpha_\eta^N(u) \phi(u) du$, where $\alpha_\eta^N(u)$ is the empirical measure $N^{-d} \sum_x \eta(x) \delta_{x/N}(u)$ associated to a configuration $\eta \in X_N$, converges in mean to $\int_{\mathbb{T}^d} f_t(u) \phi(u) du$ and moreover*

$$\int_{X_N} \left| \frac{1}{N^d} \sum_x \eta(x) \phi \left(\frac{x}{N} \right) - \int_{\mathbb{T}^d} f_t(u) \phi(u) du \right| d\nu_{f_t(\cdot)}^N(\eta) \leq CN^{-\frac{d}{d+2}}. \tag{2.42}$$

Proof. Given $0 < \ell < N$, we first compare the expression in (2.42) to the same formula where η is replaced by its local ℓ -average $\overline{\eta(x)}^\ell$ and we write, with the same manipulations as in the previous lemma:

$$\begin{aligned}
&\int_{X_N} \left| \frac{1}{N^d} \sum_{x \in \mathbb{T}_N^d} \eta(x) \phi \left(\frac{x}{N} \right) - \int_{\mathbb{T}^d} f_t(u) \phi(u) du \right| d\nu_{f_t(\cdot)}^N(\eta) \leq \\
&\int_{X_N} \left| \frac{1}{N^d} \sum_{x \in \mathbb{T}_N^d} \overline{\eta(x)}^\ell \phi \left(\frac{x}{N} \right) - \int_{\mathbb{T}^d} f_t(u) \phi(u) d\nu_{f_t(\cdot)}^N(\eta) \right| d\nu_{f_t(\cdot)}^N(\eta) + \frac{\ell}{N} \lesssim \\
&\int_{X_N} \left| \frac{1}{N^d} \sum_{x \in \mathbb{T}_N^d} \overline{\eta(x)}^\ell \phi \left(\frac{x}{N} \right) - \mathbb{E}_{\nu_{f_t(\cdot)}^N} \left(\overline{\eta(x)}^\ell \right) \phi \left(\frac{x}{N} \right) \right| d\nu_{f_t(\cdot)}^N(\eta) + \\
&\quad + \left| \frac{1}{N^d} \sum_{x \in \mathbb{T}_N^d} f_t \left(\frac{x}{N} \right) \phi \left(\frac{x}{N} \right) - \int_{\mathbb{T}^d} f_t(u) \phi(u) du \right| + \frac{\ell}{N} \lesssim \frac{1}{\ell^{d/2}} + \frac{1}{N^d} + \frac{\ell}{N}.
\end{aligned} \tag{2.43}$$

Optimizing now over ℓ we find that for $\ell = \ell(N) \sim N^{\frac{2}{d+2}}$, we get the stated rate. \square

5.3 Proof of the main abstract Theorem

Proof of the Theorem 1.1. For $F \in \text{Lip}(\mathbb{R})$ and $\phi \in C_c^\infty(\mathbb{T}^d)$, we write

$$\begin{aligned} & \int_{X_N} \left| F \left(\frac{1}{N^d} \sum_x \eta(x) \phi \left(\frac{x}{N} \right) \right) - F(\langle f_t, \phi \rangle) \right| d\mu_t^N(\eta) \\ & \leq \|F\|_{\text{Lip}} \left| \int_{X_N} \frac{1}{N^d} \sum_x \eta(x) \phi \left(\frac{x}{N} \right) d\mu_t^N(\eta) - \int_{\mathbb{T}^d} f_t(u) \phi(u) du \right| \end{aligned} \quad (3.44)$$

Then we bound the right-hand side as follows:

$$\begin{aligned} & \mathbb{E}_{\mu_t^N} \left(\frac{1}{N^d} \sum_x \eta(x) \phi \left(\frac{x}{N} \right) - \langle f_t(u), \phi(u) \rangle_{L^2(\mathbb{T}^d)} \right) \\ & \leq \iint_{X_N^2} \left| \frac{1}{N^d} \sum_x \eta(x) \phi \left(\frac{x}{N} \right) - \int_{\mathbb{T}^d} f_t(u) \phi(u) du \right| G_t^N(\eta, \zeta) d\nu_\lambda^N(\eta) d\nu_\lambda^N(\zeta) \\ & \leq \iint_{X_N^2} \left| \frac{1}{N^d} \sum_x (\eta(x) - \zeta(x)) \phi \left(\frac{x}{N} \right) \right| G_t^N(\eta, \zeta) d\nu_\lambda^N(\eta) d\nu_\lambda^N(\zeta) \\ & \quad + \int_{X_N} \left| \frac{1}{N^d} \sum_x \zeta(x) \phi \left(\frac{x}{N} \right) - \int_{\mathbb{T}^d} f_t(u) \phi(u) du \right| d\nu_{f_t(\cdot)}^N(\zeta) \\ & \leq C_1 \iint_{X_N^2} \frac{1}{N^d} \sum_x |\eta(x) - \zeta(x)| G_t^N(\eta, \zeta) d\nu_\lambda^N(\eta) d\nu_\lambda^N(\zeta) + C_2 \frac{1}{N^{d/(d+2)}} \end{aligned} \quad (3.45)$$

where in the last line we applied Lemma 2.2 for the second term. Regarding the first term, we calculate

$$\begin{aligned} & \frac{d}{dt} \iint_{X_N^2} \frac{1}{N^d} \sum_x |\eta(x) - \zeta(x)| G_t^N(\eta, \zeta) d\nu_\lambda^N(\eta) d\nu_\lambda^N(\zeta) \\ & \stackrel{(H3)}{\leq} \iint_{X_N^2} \frac{1}{N^d} \sum_x |\eta(x) - \zeta(x)| \tilde{\mathcal{L}}_N^* G_t^N(\eta, \zeta) d\nu_\lambda^N(\eta) d\nu_\lambda^N(\zeta) + \max_k \|D^k(f_t - f_\infty)\|_H \mathcal{E}^N \\ & \stackrel{(H1)}{\leq} \max_k \|D^k(f_t - f_\infty)\|_H \mathcal{E}^N. \end{aligned} \quad (3.46)$$

Integrating then in time we get

$$\begin{aligned} & \iint_{X_N^2} \frac{1}{N^d} \sum_x |\eta(x) - \zeta(x)| G_t^N(\eta, \zeta) d\nu_\lambda^N(\eta) d\nu_\lambda^N(\zeta) \\ & \leq \iint_{X_N^2} \frac{1}{N^d} \sum_x |\eta(x) - \zeta(x)| G_0^N(\eta, \zeta) d\nu_\lambda^N(\eta) d\nu_\lambda^N(\zeta) + \mathcal{E}^N \int_0^t \max_k \|D^k(f_s - f_\infty)\|_H ds. \end{aligned} \quad (3.47)$$

Finally, the assumptions on the initial coupling G_0^N imply that the first term of the right-hand side vanishes as \mathcal{R}^N and the second term, due to assumption **(H2)** equals to $\mathcal{E}^N Kt$ if $T < \infty$, while in the case of $T = \infty$, the second term equals $\mathcal{E}^N \int_0^t R(s) ds$ which is integrable in time. These conclude the statement of the main Theorem. \square

5.4 Proof of (H1)-(H2)-(H3) for the Zero-Range Process

We recall that the generator is, (1.23):

$$\text{for all } f \in C_b(X_N), \quad \mathcal{L}_N f(\eta) = \sum_{x, y \sim x} p(y-x) g(\eta(x)) [f(\eta^{x,y}) - f(\eta)] \quad (4.48)$$

where the jump rate satisfies Assumption 2. We also recall that the function $\sigma(\rho)$, which is the nonlinearity appearing in limit equation, is chosen so that $\langle \nu_\rho^N, \eta(0) \rangle = \rho$. We give some details now on the construction of σ .

Let $Z : [0, \phi^*) \rightarrow \mathbb{R}$ be the *partition function* of the zero range process given by (1.17), with ϕ^* denoting the radius of convergence of Z . An important consequence of Assumption 2, (iii) on the jump rate, is that $\phi^* = +\infty$, since the assumption implies $g(n) \geq \tilde{\delta}n$ for some $\tilde{\delta} \leq \delta/n_0$.

The *density function* as a function of the *fugacity* ϕ is given by

$$R(\phi) = \phi \partial_\phi \log(Z(\phi)) = \frac{1}{Z(\phi)} \sum_{n \geq 0} \frac{n\phi^n}{g(n)!}. \quad (4.49)$$

This is a smooth function $R : [0, \infty) \rightarrow \mathbb{R}$ and it holds that, [KL99], R is monotonously increasing with $\lim_{\phi \rightarrow \infty} R(\phi) = \infty$. Then $\sigma : [0, \infty) \rightarrow [0, \infty)$ is well-defined as its inverse function, $\sigma = R^{-1}$. Thus $\nu_{\sigma(\rho)}^N$, as defined in (1.16), is an invariant and translation-invariant product measure with density

$$\langle \nu_\rho^N, \eta(x) \rangle = \rho.$$

Furthermore its average jump rate satisfies

$$\langle \nu_\rho^N, g(\eta(x)) \rangle = \sigma(\rho).$$

The Lipschitz continuity of the rate function implies that $\rho \mapsto \sigma(\rho)$ is also Lipschitz continuous with constant g^* , [KL99, Corollary 3.6]. The second assumption implies that $\inf_\rho \sigma(\rho)/\rho > 0$. Note, however, that $g(n) \geq \tilde{\delta}n$ yields $\sigma'(0) > 0$. Therefore it is impossible to obtain a fast diffusion, e.g. $\sigma(\rho) = \rho^m$, $m > 1$, in this limit. Indeed Assumption 2 yields

Lemma 4.1.

$$0 < \inf_{\rho \geq 0} \sigma'(\rho) \leq \sup_{\rho \geq 0} \sigma'(\rho) < +\infty. \quad (4.50)$$

The upper bound extends to higher derivatives as well, i.e.

$$\sup_{\rho \in \mathbb{R}} |\sigma^{(k)}(\rho)| < +\infty \quad (4.51)$$

for all integers $k > 0$.

Sketch of proof. The second order bound follows from

$$\sigma''(\rho) = -\frac{R''(\sigma(\rho))\sigma'(\rho)}{R'(\sigma(\rho))^2},$$

since σ and R are inverse to each other, i.e. $R(\sigma(\rho)) = \rho$. Assumption 2 implies $\delta^j \leq Z^{(j)}(\phi)/Z(\phi) \leq (g^*)^j$ is bounded, and the explicit expressions for R'' and R' then yield a bound on $\sigma''(\rho)$. Higher derivatives are treated analogously. \square

In what follows we discuss about consequences of the attractivity assumption.

Attractivity and moment bounds for Zero-range process.

We take advantage of attractivity, i.e. Assumption 2, (iv). Combined with a *coupling* of two processes, it allows us to prove uniform estimates on the particle moments. This discussion can be found as well in [Lig85, KL99], therefore we simply sketch the results here.

Consider two copies of the zero range process with initial configurations $\eta, \zeta \in X_N$ so that

$$\text{for all } x \in \mathbb{T}_N^d \quad \eta \leq \zeta, \quad \text{i.e.} \quad \eta(x) \leq \zeta(x).$$

Assumption 2, (iv) simply states $g(n+1) \geq g(n)$ for all $n \in \mathbb{N}$ and hence we can always let particles of the process with more particles jump at a higher rate. Specifically at an arbitrary site $x \in \mathbb{T}_N^d$, at time $t = 0$ where we have $\eta(x) \leq \zeta(x)$, we let one particle at $x \in \mathbb{T}_N^d$ of both processes η and ζ jump at the same time with jump rate $g(\eta(x))$ and additionally let just one particles of ζ jump with jump rate $g(\zeta(x)) - g(\eta(x)) \geq 0$. This

coupling almost surely preserves the property $\eta(x) \leq \zeta(x)$ for all $x \in \mathbb{T}_N^d$. It constructs a random particle process (η_t, ζ_t) (which are random variables) with state space $X_N \times X_N$ and whose marginals η_t and ζ_t are both zero range processes with jump rate g , so that

$$\text{for all } t \geq 0, x \in \mathbb{T}_N^d, \quad \eta_t(x) \leq \zeta_t(x)$$

almost surely.

A consequence of this coupling is the preservation of stochastic ordering. Consider $f^N \in C_b(X_N)$ monotonous: $f^N(\eta) \leq f^N(\zeta)$ for all $\eta \leq \zeta$. Two probability measures $\mu, \nu \in P(X_N)$ are said to be ordered, $\mu \leq \nu$, if

$$\langle \mu, f^N \rangle \leq \langle \nu, f^N \rangle \quad \text{for all monotonous } f^N \in C_b(X_N).$$

Suppose now $\mu_0^N, \tilde{\mu}_0^N \in P(X_N)$ are two initial measures of the zero range process such that

$$\tilde{\mu}_0^N \leq \mu_0^N.$$

It can be shown [Lig85, Theorem II.2.4] that this property is equivalent to the existence of a coupling measure on $X_N \times X_N$ with marginals $\tilde{\mu}_0^N$ and μ_0^N that concentrates on $\{\eta \leq \zeta\}$. This coupling is precisely defined and used for hypothesis **(H1)** in Section 5.4.2. As shown above, under the evolution of the coupled process, the support of the coupled probability measure remains within $\{\eta \leq \zeta\}$ and it follows, again by [Lig85, Theorem II.2.4], that $\tilde{\mu}_t^N \leq \mu_t^N$.

Let us now turn to the problem of bounding the moments of the particle system. We define the k -th order moment as

$$M_k[\mu^N] := \left\langle \mu^N, \frac{1}{N^d} \sum_{x \in \mathbb{T}_N^d} \eta(x)^k \right\rangle.$$

Lemma 4.2. *Assume that the initial measure is bounded from above by the invariant measure with fugacity $\phi > 0$, ν_ϕ^N for some $\phi > 0$, i.e. $\mu_0^N \leq \nu_\phi^N$. Then for any $k > 0$, it holds that*

$$M_k[\mu_t^N] \leq M_k[\nu_\phi^N] = C_k < +\infty$$

for all $N > 0$ and $t \geq 0$.

Proof. All moments of ν_ϕ^N are finite and translation-invariant yields

$$M_k[\nu_\phi^N] = \langle \nu_\phi^N, \eta(0)^k \rangle = C_k$$

independent of N . Attractivity yields

$$\mu_t^N \leq \nu_\phi^N,$$

and hence

$$M_k[\mu_t^N] \leq M_k[\nu_\phi^N]$$

since $N^{-d} \sum_{x \in \mathbb{T}_N^d} \eta(x)^k \geq 0$. □

In what follows we consider the diffusive/parabolic scaling in time. The framework however holds also for the hyperbolic scaling but for finite time: for the time interval where our solution to the limit equation is smooth. We discuss this in the Remark 4.6 after the proofs.

We consider f_t to be the unique strong solution to the quasi-linear diffusion equation (1.19). Let us stress here that f_t satisfies Assumption **(H3)** with $H = L^\infty$ as proven in the Appendix 6.6.2. Following the abstract method, we consider the local Gibbs measure with slowly varying coefficient $f_t(\cdot)$ as defined in (1.35) whose density ψ_t^N is

$$\psi_t^N(\zeta) := \frac{d\nu_{f_t(\cdot)}^N(\zeta)}{d\nu_\alpha^N(\zeta)} = e^{\sum_{x \in \mathbb{T}_N^d} \zeta(x) \log\left(\frac{\sigma(f_t(x/N))}{\sigma(\alpha)}\right) - \log\left(\frac{Z(\sigma(f_t(x/N)))}{Z(\sigma(\alpha))}\right)}. \quad (4.52)$$

The last equality is a reformulation based on the form of the product measure $\nu_{f_t(\cdot)}^N$. This corresponds to the density of an artificial process that we consider here because it has the right hydrodynamics. This is proved with an explicit rate for the sake of completeness in the preliminaries-Section 5.2, Lemma 2.2.

5.4.1 Consistency estimate

The density ψ_t^N satisfies

Proposition 4.3. *Let $d = 1$ and $k, \alpha > 0$. There exists $0 < C_0 < \infty$ and $c > 0$ such that*

$$\iint_{X_N^2} N^{-d} \sum_{x \in \mathbb{T}_N^d} |\eta(x) - \zeta(x)|^k (\partial_t \psi_t^N(\zeta) - \mathcal{L}^* \psi_t^N(\zeta)) d\nu_\alpha^N(\eta) d\nu_\alpha^N(\zeta) \leq C_0 e^{-ct} N^{-\frac{d}{2+d}}. \quad (4.53)$$

Proof. We split the proof into several steps.

Step 1: Explicit calculations on the local equilibrium measure. First we compute

$$\begin{aligned}
\mathcal{L}_N^* \psi_t^N(\zeta) &= N^2 \sum_{x \sim y} p(y-x) g(\zeta(x)) \left(e^{\sum_{z \in \mathbb{T}_N^d} \zeta^{x,y}(z) \log\left(\frac{\sigma(f_t(z/N))}{\sigma(\alpha)}\right) - \log\left(\frac{Z(\sigma(f_t(z/N)))}{Z(\sigma(\alpha))}\right)} \right. \\
&\quad \left. - e^{\sum_{z \in \mathbb{T}_N^d} \zeta(z) \log\left(\frac{\sigma(f_t(z/N))}{\sigma(\alpha)}\right) - \log\left(\frac{Z(\sigma(f_t(z/N)))}{Z(\sigma(\alpha))}\right)} \right) \\
&= N^2 \sum_{x \sim y} p(y-x) g(\zeta(x)) e^{\sum_{z \in \mathbb{T}_N^d} \zeta(z) \log\left(\frac{\sigma(f_t(z/N))}{\sigma(\alpha)}\right) - \log\left(\frac{Z(\sigma(f_t(z/N)))}{Z(\sigma(\alpha))}\right)} \times \\
&\quad \times \left(e^{\log\left(\frac{\sigma(f_t(y/N))}{\sigma(\alpha)}\right) - \log\left(\frac{\sigma(f_t(x/N))}{\sigma(\alpha)}\right)} - 1 \right) \\
&= N^2 \sum_{x \sim y} p(y-x) g(\zeta(x)) \psi_t^N(\zeta) \left(\frac{\sigma(f_t(y/N))}{\sigma(f_t(x/N))} - 1 \right).
\end{aligned}$$

Since $\sum_{x \sim y} \sigma(f_t(x/N)) p(y-x) \left(\frac{\sigma(f_t(y/N))}{\sigma(f_t(x/N))} - 1 \right) = 0$, we deduce

$$\mathcal{L}_N^* \psi_t^N(\zeta) = N^2 \psi_t^N(\zeta) \sum_{x \sim y} p(y-x) (g(\zeta(x)) - \sigma(f_t(x/N))) \left(\frac{\sigma(f_t(y/N)) - \sigma(f_t(x/N))}{\sigma(f_t(x/N))} \right).$$

This can be reformulated in terms of the weighted Discrete Laplacian

$$\frac{1}{N^2} \Delta_c^N \phi(x/N) := c_1 \phi((x+1)/N) + c_{-1} \phi((x-1)/N) - (c_1 + c_{-1}) \phi(x/N)$$

where c_i 's are related to the transition probabilities. Then we have

$$\begin{aligned}
N^{-d} \sum_{x \in \mathbb{T}_N^d} |\eta(x) - \zeta(x)|^k \mathcal{L}_N^* \psi_t^N(\zeta) &= \\
N^{-d} \sum_{x \in \mathbb{T}_N^d} |\eta(x) - \zeta(x)|^k \sum_{y \in \mathbb{T}_N^d} (g(\zeta(y)) - \sigma(f_t(y/N))) \frac{\Delta_c^N \sigma(f_t(y/N))}{\sigma(f_t(y/N))} &\quad (4.54) \\
= N^{-d} \sum_x |\eta(x) - \zeta(x)|^k (g(\zeta(x)) - \sigma(f_t(x/N))) \frac{\Delta_c^N \sigma(f_t(x/N))}{\sigma(f_t(x/N))} + R_1
\end{aligned}$$

where we split the sum in y into two sums: $y = x$ and $y \neq x$ and

$$R_1 := N^{-d} \sum_x |\eta(x) - \zeta(x)|^k \sum_{y \neq x} (g(\zeta(y)) - \sigma(f_t(y/N))) \frac{\Delta_c^N \sigma(f_t(y/N))}{\sigma(f_t(y/N))}.$$

On the other hand, calculating $\partial_t \psi_t^N(\zeta)$, we write

$$\partial_t \psi_t^N(\zeta) = \psi_t^N(\zeta) \sum_x \frac{\Delta_c(\sigma(f_t(x/N)))}{\sigma(f_t(x/N))} \sigma'(f_t(x/N)) (\zeta(x) - f_t(x/N))$$

so that

$$\begin{aligned} N^{-d} \sum_x |\eta(x) - \zeta(x)|^k \partial_t \psi_t^N(\zeta) &= \\ N^{-d} \sum_x |\eta(x) - \zeta(x)|^k \frac{\Delta_c(\sigma(f_t(x/N)))}{\sigma(f_t(x/N))} \sigma'(f_t(x/N)) (\zeta(x) - f_t(x/N)) &+ R_2 \end{aligned} \quad (4.55)$$

where

$$R_2 := N^{-d} \sum_x \sum_{y \neq x} |\eta(x) - \zeta(x)|^k \frac{\Delta_c(\sigma(f_t(y/N)))}{\sigma(f_t(y/N))} \sigma'(f_t(y/N)) (\zeta(y) - f_t(y/N)).$$

For the computation of $\partial_t Z(\sigma(f_t(x/N)))$, we have used the relation

$$\sum_{k \geq 0} \frac{k \sigma(f_t(x/N))^k}{g(k)! Z(\sigma(f_t(x/N)))} = \mathbb{E}_{\nu_{f_t(\cdot)}}(\zeta(0)) = f_t\left(\frac{x}{N}\right).$$

We therefore estimate

$$\begin{aligned} N^{-d} \sum_x |\eta(x) - \zeta(x)|^k \frac{(\partial_t - \mathcal{L}^*) \psi_t^N(\zeta)}{\psi_t^N(\zeta)} &\leq \\ N^{-d} \sum_x |\eta(x) - \zeta(x)|^k (g(\zeta(x)) - \sigma(f_t(x/N))) \frac{\Delta_c^N \sigma(f_t(x/N))}{\sigma(f_t(x/N))} & \\ - N^{-d} \sum_x |\eta(x) - \zeta(x)|^k \frac{\Delta_c(\sigma(f_t(x/N)))}{\sigma(f_t(x/N))} \sigma'(f_t(x/N)) (\zeta(x) - f_t(x/N)) &+ R_1 + R_2. \end{aligned} \quad (4.56)$$

Step 2: Replacement with the continuous Laplacian. As a second step, we may replace the discrete Laplacian Δ_c^N with the continuous Laplacian Δ_c to get the error:

$$\mathcal{R}_N := N^{-d} \sum_x |\eta(x) - \zeta(x)|^k \frac{(N^2 \Delta_c^N - \Delta_c)(\sigma(f_t(x/N)))}{\sigma(f_t(x/N))} g(\zeta(x)).$$

This error vanishes as N goes to infinity since

$$\mathcal{R}_N \lesssim N^{-d} \sum_x |\eta(x) - \zeta(x)|^k \frac{\|(\sigma \circ f_t)^{(4)}\|_\infty}{12N^2} |\zeta(x)| \lesssim e^{-ct} N^{-2}.$$

Here we applied Cauchy-Schwarz, Young's Inequality and the boundedness of the moments

from Lemma 4.2. The exponentially fast decay in time of $\|(\sigma \circ f_t)^{(4)}\|_\infty$ is an application of the results proved in the Appendix that hold for $d = 1$. The equation (4.56) is taking then the form

$$\begin{aligned} & \frac{1}{N^d} \sum_x |\eta(x) - \zeta(x)|^k \frac{(\partial_t - \mathcal{L}_N^*) \psi_t^N(\zeta)}{\psi_t^N(\zeta)} = \\ & \frac{1}{N^d} \sum_x |\eta(x) - \zeta(x)|^k \left(g(\zeta(x)) - \sigma \left(f_t \left(\frac{x}{N} \right) \right) - \sigma' \left(f_t \left(\frac{x}{N} \right) \right) \left(\zeta(x) - f_t \left(\frac{x}{N} \right) \right) \right) \times \\ & \quad \times \frac{\Delta_c \sigma \left(f_t \left(\frac{x}{N} \right) \right)}{\sigma \left(f_t \left(\frac{x}{N} \right) \right)} := (I) + e^{-ct} N^{-2} + R_1 + R_2. \end{aligned} \tag{4.57}$$

Multiplying now both sides by $\psi_t^N(\zeta)$ and integrating with respect to $d\nu_\alpha^N(\eta)$ and $d\nu_\alpha^N(\zeta)$:

The first two errors $R_1 \psi_t^N(\zeta)$ and $R_2 \psi_t^N(\zeta)$ when averaged they give 0 due to the conservation of mass, i.e. $\int \mathcal{L}^* \psi_t^N d\nu_\alpha^N = 0$, which means (since the local Gibbs measure is product) that

$$\sum_{x \in \mathbb{T}_N^d} \int_{\zeta(x)} (g(\zeta(x)) - \sigma(f_t(x/N))) \frac{\Delta_c^N \sigma(f_t(x/N))}{\sigma(f_t(x/N))} d\nu_{f_t(\cdot)}^N(\zeta(x)).$$

Then due to the definition of σ

$$\begin{aligned} \iint_{X_N^2} R_1 \psi_t^N(\zeta) d\nu_\alpha^N(\zeta) d\nu_\alpha^N(\eta) &= -N^{-d} \sum_x \int_{\eta(x)} \int_{\zeta(x)} |\eta(x) - \zeta(x)|^k d\nu_{f_t(\cdot)}^1(\zeta(x)) d\nu_{f_t(\cdot)}^1(\eta(x)) \times \\ & \quad \times \int_{\zeta(x)} (g(\zeta(x)) - \sigma(f_t(x/N))) \frac{\Delta_c^N \sigma(f_t(x/N))}{\sigma(f_t(x/N))} d\nu_{f_t(\cdot)}^1(\zeta(x)) = 0. \end{aligned}$$

For R_2 , we have similarly as above:

$$0 = \int_{X_N} \partial_t \psi_t^N(\zeta) d\nu_\alpha^N(\zeta) = \sum_x \int_{\zeta(x)} \frac{\Delta_c(\sigma(f_t(x/N)))}{\sigma(f_t(x/N))} \sigma'(f_t(x/N)) (\zeta(x) - f_t(x/N)) d\nu_{f_t(\cdot)}^1(\zeta(x))$$

so that

$$\begin{aligned} \iint_{X_N^2} R_2 \psi_t^N(\zeta) d\nu_\alpha^N(\zeta) d\nu_\alpha^N(\eta) &= -N^{-d} \sum_x \int_{\eta(x)} \int_{\zeta(x)} |\eta(x) - \zeta(x)|^k d\nu_{f_t(\cdot)}^1(\zeta(x)) d\nu_{f_t(\cdot)}^1(\eta(x)) \times \\ & \quad \times \int_{\zeta(x)} (\zeta(x) - f_t(x/N)) \frac{\Delta_c^N \sigma(f_t(x/N))}{\sigma(f_t(x/N))} d\nu_{f_t(\cdot)}^1(\zeta(x)) = 0. \end{aligned}$$

Step 3: Replacement with the ℓ -averages. This is split into the following steps:

Firstly, for $\ell \in \mathbb{N}$, $0 < \ell < N$, we may replace $\zeta(x)$ and $g(\zeta(x))$ in the above formula by their ℓ -averages around x : $\overline{\zeta(x)}^\ell$ and $\overline{g(\zeta(x))}^\ell$. Indeed, we present the proof here for

$\zeta(x)$ and we denote by $\phi(x/N) := \sigma' \left(f_t \left(\frac{x}{N} \right) \right) \frac{\Delta_c \sigma \left(f_t \left(\frac{x}{N} \right) \right)}{\sigma \left(f_t \left(\frac{x}{N} \right) \right)}$ which is continuous. We then estimate the following difference for $k > 0$:

$$\begin{aligned}
& \iint_{X_N^2} \frac{1}{N^d} \sum_x |\eta(x) - \zeta(x)|^k (\zeta(x) - \overline{\zeta(x)}^\ell) \sigma' \left(f_t \left(\frac{x}{N} \right) \right) \frac{\Delta_c \sigma \left(f_t \left(\frac{x}{N} \right) \right)}{\sigma \left(f_t \left(\frac{x}{N} \right) \right)} d\nu_{f_t(\cdot)}^N(\zeta) d\nu_\alpha^N(\eta) = \\
& \leq \left(\iint_{X_N^2} \left(N^{-d} \sum_x |\eta(x) - \zeta(x)|^k \right)^2 d\nu_{f_t(\cdot)}^N(\zeta) d\nu_\alpha^N(\eta) \right)^{1/2} \times \\
& \quad \times \left(\iint_{X_N^2} \left(\zeta(x) - \overline{\zeta(x)}^\ell \right)^2 \phi^2(x/N) d\nu_{f_t(\cdot)}^N(\zeta) d\nu_\alpha^N(\eta) \right)^{1/2}.
\end{aligned} \tag{4.58}$$

Due to the moment bounds, see Lemma 4.2, the first factor is bounded uniformly in N . We estimate the other factor which equals to

$$C e^{-ct} \left(\iint_{X_N^2} \left(\frac{1}{\ell_*^d} \sum_{|w| \leq \ell} (\zeta(x) - \zeta(x+w)) \right)^2 d\nu_{f_t(\cdot)}^N(\zeta) d\nu_\alpha^N(\eta) \right)^{1/2}.$$

This integral squared equals to:

$$\begin{aligned}
& \int_{X_N} \left(\frac{1}{\ell_*^d} \sum_{i=1}^{\ell_*^d} \left((\zeta(x) - f_t \left(\frac{x}{N} \right)) + \left(f_t \left(\frac{x}{N} \right) - f_t \left(\frac{x+y_i}{N} \right) \right) + \left(f_t \left(\frac{x+y_i}{N} \right) - \zeta(x+y_i) \right) \right) \right)^2 d\nu_{f_t(\cdot)}^N(\zeta) \\
& = \int_{X_N} \left\{ \frac{1}{\ell_*^{2d}} \sum_{i=1}^{\ell_*^d} \left((\zeta(x) - f_t \left(\frac{x}{N} \right))^2 + \left(f_t \left(\frac{x+y_i}{N} \right) - \zeta(x+y_i) \right)^2 + \left(f_t \left(\frac{x}{N} \right) - f_t \left(\frac{x+y_i}{N} \right) \right)^2 \right) \right. \\
& + \frac{2}{\ell_*^{2d}} \sum_{i \neq j}^{\ell_*^d} \left(\zeta(x) - f_t \left(\frac{x}{N} \right) \right) \left(f_t \left(\frac{x+y_i}{N} \right) - \zeta(x+y_i) \right) + \left(\zeta(x) - f_t \left(\frac{x}{N} \right) \right) \left(f_t \left(\frac{x}{N} \right) - f_t \left(\frac{x+y_i}{N} \right) \right) \\
& + \left(f_t \left(\frac{x+y_i}{N} \right) - \zeta(x+y_i) \right) \left(f_t \left(\frac{x}{N} \right) - f_t \left(\frac{x+y_i}{N} \right) \right) \\
& + \left(f_t \left(\frac{x+y_i}{N} \right) - \zeta(x+y_i) \right) \left(f_t \left(\frac{x}{N} \right) - f_t \left(\frac{x+y_j}{N} \right) \right) \\
& + \left(f_t \left(\frac{x+y_i}{N} \right) - \zeta(x+y_i) \right) \left(f_t \left(\frac{x+y_j}{N} \right) - \zeta(x+y_j) \right) \\
& \left. + \left(f_t \left(\frac{x}{N} \right) - f_t \left(\frac{x+y_i}{N} \right) \right) \left(f_t \left(\frac{x}{N} \right) - f_t \left(\frac{x+y_j}{N} \right) \right) \right\} d\nu_{f_t(\cdot)}^N(\zeta)
\end{aligned} \tag{4.59}$$

where for y_i we have $|y_i| \leq \ell$ for all $i = 1, \dots, \ell_*^d$. The first five terms of the second summand are zero due to orthogonality. Regarding the first integral, the first two terms

give an error of order ℓ^{-d} since the moments are bounded and $f_t \in L^\infty$, and the third term gives an error of order $\ell^{-d}(\ell/N)^2$ due to the smoothness of f_t . Finally the term in the last line leaves an error of order $(\ell/N)^2$. Thus overall of this replacement we get an error of order $Ce^{-ct}(\ell^{-d/2} + \ell/N)$. Optimizing now this w.r.t. ℓ , for $\ell = N^{1/(1+d/2)}$, we get an error of order $N^{-d/(d+2)}$.

Then we apply the local law of large numbers, Lemma 2.1 with $X = \mathbb{N}$, $\theta = g$, $\vartheta = \sigma$ and with the weight function for fixed $x \in \mathbb{T}_N^d$, $\mathcal{W}(\eta(x), \zeta(x)) = |\eta(x) - \zeta(x)|^k$. We write therefore (I) up to an error of order $Ce^{-ct}\ell^{-d/2} + Ce^{-ct}\ell/N$ as:

$$\begin{aligned} & \iint_{X_N^2} \frac{1}{N^d} \sum_x |\eta(x) - \zeta(x)|^k \left(\sigma(\overline{\zeta(x)}^\ell) - \sigma\left(f_t\left(\frac{x}{N}\right)\right) - \sigma'\left(f_t\left(\frac{x}{N}\right)\right) \left(\overline{\zeta(x)}^\ell - f_t\left(\frac{x}{N}\right)\right) \right) \\ & \quad \times \frac{\Delta_c \sigma\left(f_t\left(\frac{x}{N}\right)\right)}{\sigma\left(f_t\left(\frac{x}{N}\right)\right)} \psi_t^N(\zeta) d\nu_\alpha^N(\zeta) d\nu_\alpha^N(\eta). \end{aligned}$$

Step 4: From ℓ -averages to the macroscopic profile. For some ρ in between $\overline{\zeta(x)}^\ell$ and $f_t\left(\frac{x}{N}\right)$, we bound the above formula from

$$\begin{aligned} & \iint_{X_N^2} \frac{1}{N^d} \sum_x |\eta(x) - \zeta(x)|^k \frac{\sigma''(\rho)}{2} \left(f_t\left(\frac{x}{N}\right) - \overline{\zeta(x)}^\ell \right)^2 \frac{\Delta_c \sigma\left(f_t\left(\frac{x}{N}\right)\right)}{\sigma\left(f_t\left(\frac{x}{N}\right)\right)} \psi_t^N(\zeta) d\nu_\alpha^N(\zeta) d\nu_\alpha^N(\eta) \\ & \lesssim Ce^{-ct} \iint_{X_N^2} \frac{1}{N^d} \sum_x |\eta(x) - \zeta(x)|^k \left(f_t\left(\frac{x}{N}\right) - \overline{\zeta(x)}^\ell \right)^2 \psi_t^N(\zeta) d\nu_\alpha^N(\zeta) d\nu_\alpha^N(\eta) \end{aligned} \tag{4.60}$$

due to our assumptions on σ and the regularity of the limit PDE. Then by Cauchy-Schwarz,

$$\begin{aligned}
&\lesssim C e^{-ct} \iint_{X_N^2} \left(N^{-d} \sum_x |(\eta - \zeta)|^{2k}(x) \right)^{1/2} \left(N^{-d} \sum_x \left(f_t(x/N) - \overline{\zeta(x)}^\ell \right)^4 \right)^{1/2} \psi_t^N(\zeta) d\nu_\alpha^N(\zeta) d\nu_\alpha^N(\eta) \\
&\lesssim C e^{-ct} \left(\iint_{X_N^2} N^{-d} \sum_x \left(f_t(x/N) - \overline{\zeta(x)}^\ell \right)^4 \psi_t^N(\zeta) d\nu_\alpha^N(\zeta) d\nu_\alpha^N(\eta) \right)^{1/2} \\
&= C e^{-ct} \left(\int_{X_N} N^{-d} \sum_x \left(f_t(x/N) - \overline{\zeta(x)}^\ell \right)^4 d\nu_{f_t(\cdot)}^N(\zeta) \right)^{1/2} \\
&\stackrel{\substack{y_i = x_i + x, \\ |x_i| \leq \ell}}{=} C e^{-ct} \left(\int_{X_N} N^{-d} \sum_x \left(\ell_*^{-d} \sum_{i=1}^{\ell_*^d} \left(f_t\left(\frac{x}{N}\right) - \zeta(y_i) \right) \right)^4 d\nu_{f_t(\cdot)}^N(\zeta) \right)^{1/2} \\
&= C e^{-ct} \left(\int_{X_N} N^{-d} \sum_x \left(\ell_*^{-d} \sum_{i=1}^{\ell_*^d} \left(f_t\left(\frac{x}{N}\right) - f_t\left(\frac{y_i}{N}\right) \right) + \ell_*^{-d} \sum_{i=1}^{\ell_*^d} \left(f_t\left(\frac{y_i}{N}\right) - \zeta(y_i) \right) \right)^4 d\nu_{f_t(\cdot)}^N(\zeta) \right)^{1/2} \\
&\lesssim C e^{-ct} \left(\int_{X_N} N^{-d} \sum_x \left(A_{\ell,N} + B_{\ell,N}(\zeta) \right)^4 d\nu_{f_t(\cdot)}^N(\zeta) \right)^{1/2} = \\
&C e^{-ct} \left(\int_{X_N} N^{-d} \sum_x \left(A_{\ell,N}^4 + B_{\ell,N}^4(\zeta) + 4A_{\ell,N}^3 B_{\ell,N}(\zeta) + 4B_{\ell,N}^3(\zeta) A_{\ell,N} + 6A_{\ell,N}^2 B_{\ell,N}^2(\zeta) \right) d\nu_{f_t(\cdot)}^N(\zeta) \right)^{1/2}. \tag{4.61}
\end{aligned}$$

Now $|A_{\ell,N}^4| \lesssim (\ell/N)^4$ due to the smoothness of f_t and that $|x - y_i| \leq \ell$. Also,

$$\left| \int_{X_N} B_{\ell,N}^4(\zeta) d\nu_{f_t(\cdot)}^N(\zeta) \right| \lesssim C \ell_*^{-2d}$$

since $\mathbb{E}_{\nu_{f_t(\cdot)}^N} \left(f_t\left(\frac{y_i}{N}\right) - \zeta(y_i) \right) = 0$. Indeed

$$\begin{aligned}
\mathbb{E}_{\nu_{f_t(\cdot)}^N} \left(\left(\ell_*^{-d} \sum_{i=1}^{\ell_*^d} f_t\left(\frac{y_i}{N}\right) - \zeta(y_i) \right)^4 \right) &= \mathbb{E}_{\nu_{f_t(\cdot)}^N} \left(\ell_*^{-4d} \sum_{i=1}^{\ell_*^d} \left(f_t\left(\frac{y_i}{N}\right) - \zeta(y_i) \right)^4 \right) + \\
&+ \mathbb{E}_{\nu_{f_t(\cdot)}^N} \left(2\ell_*^{-4d} \sum_{i < j} \left(f_t\left(\frac{y_i}{N}\right) - \zeta(y_i) \right)^2 \left(f_t\left(\frac{y_j}{N}\right) - \zeta(y_j) \right)^2 \right) \leq C \ell_*^{-2d} \tag{4.62}
\end{aligned}$$

where C is the constant coming from the moment bounds up to the fourth moment and the L^∞ bound of f_t . Similarly for the other terms we compute

$$\begin{aligned}
\left| \int_{X_N} 4A_{\ell,N} B_{\ell,N}^3(\zeta) d\nu_{f_t(\cdot)}^N(\zeta) \right| &\lesssim \left(\int A_{\ell,N}^2 d\nu_{f_t(\cdot)}^N(\zeta) \right)^{1/2} \left(\int B_{\ell,N}^6(\zeta) d\nu_{f_t(\cdot)}^N(\zeta) \right)^{1/2} \lesssim (\ell/N) \ell^{-3d} \\
\left| \int_{X_N} 4A_{\ell,N}^3 B_{\ell,N}(\zeta) d\nu_{f_t(\cdot)}^N(\zeta) \right| &\lesssim 0 \\
\left| \int_{X_N} 6A_{\ell,N}^2 B_{\ell,N}^2(\zeta) d\nu_{f_t(\cdot)}^N(\zeta) \right| &\lesssim \left(\int A_{\ell,N}^4 d\nu_{f_t(\cdot)}^N(\zeta) \right)^{1/2} \left(\int B_{\ell,N}^4(\zeta) d\nu_{f_t(\cdot)}^N(\zeta) \right)^{1/2} \lesssim (\ell/N)^2 \ell^{-2d}
\end{aligned}$$

where the above estimates consisted of Cauchy-Schwarz and the moment bounds.

Step 5: Final rate. Gathering all the errors together, we have that

$$(I) + \mathcal{R}_N \lesssim C e^{-ct} \left\{ (\ell/N)^{1/2} \ell^{-3d/2} + \ell^{1-d}/N + \left(\frac{\ell}{N} \right)^2 + \ell^{-d} + (\ell^{-d/2} + \ell/N) + N^{-2} \right\},$$

which in terms of N , choosing $\ell = N^{1/(1+d/2)}$, is of order

$$\mathcal{O}(N^{-3d/2} + N^{-d/(1+d/2)} + N^{-d/(2+d)} + N^{-2}) = \mathcal{O}(N^{-d/(2+d)}).$$

□

5.4.2 Microscopic Stability estimate

We employ the basic coupling, or Wasserstein coupling, discussed in [Lig85], see also [Rez91], which is a coupling of two zero-range processes with generator $\tilde{\mathcal{L}} : C_b(X_N^2) \rightarrow C_b(X_N^2)$ given by

$$\begin{aligned}
\tilde{\mathcal{L}} f(\eta, \zeta) &:= N^2 \sum_{x,y} p(y-x) g(\eta(x)) \wedge g(\zeta(x)) (f(\eta^{xy}, \zeta^{xy}) - f(\eta, \zeta)) \\
&+ N^2 \sum_{x,y} p(y-x) \left(g(\eta(x)) - g(\eta(x)) \wedge g(\zeta(x)) \right) (f(\eta^{xy}, \zeta) - f(\eta, \zeta)) \\
&+ N^2 \sum_{x,y} p(y-x) \left(g(\zeta(x)) - g(\eta(x)) \wedge g(\zeta(x)) \right) (f(\eta, \zeta^{xy}) - f(\eta, \zeta)).
\end{aligned} \tag{4.63}$$

Note that indeed when both η and ζ are zero-range processes, their coupled law satisfies exactly the forward Kolmogorov equation, i.e. each marginal corresponds to a zero-range process at the respective rate of jump. The generator of this coupled process is defined like above so that the particles in processes η, ζ are jumping simultaneously as much as possible.

We are interested in the coupled process, since we want to estimate the discrete L^1 -distance between two solutions in the microscopic level and in particular the distance among the density of a ‘true’ zero-range process f_t^N and the density of the artificial process

ψ_t^N as given in (4.52). We have the following energy estimate on the law of the coupled process.

Lemma 4.4. *Let G_t^N be the coupling density on X_N^2 evolving according to (1.9). The first marginal of it is the evolution of the density ψ_t^N , relative to the reference measure $d\nu_\alpha^N$, of an artificial process considered so that it has the desired hydrodynamical behavior, while the second marginal gives us the density of a zero-range process f_t^N . For $\phi \in C_c^\infty(\mathbb{T}^d)$ we have that*

$$\begin{aligned} & \iint_{X_N^2} N^{-d} \sum_x |\eta(x) - \zeta(x)| \phi\left(\frac{x}{N}\right) G_t^N(\eta, \zeta) d\nu_\alpha^N(\eta) d\nu_\alpha^N(\zeta) \\ & \leq \iint_{X_N^2} N^{-d} \sum_x |\eta(x) - \zeta(x)| \phi\left(\frac{x}{N}\right) G_0^N(\eta, \zeta) d\nu_\alpha^N(\eta) d\nu_\alpha^N(\zeta) + CN^{-\frac{d}{2+d}}(1 - e^{-ct}). \end{aligned} \tag{4.64}$$

Proof. We calculate

$$\begin{aligned} & \frac{d}{dt} \iint_{X_N^2} N^{-d} \sum_x |\eta(x) - \zeta(x)| \phi\left(\frac{x}{N}\right) G_t^N(\eta, \zeta) d\nu_\alpha^N(\eta) d\nu_\alpha^N(\zeta) \leq \\ & \iint_{X_N^2} N^{-d} \sum_x |\eta(x) - \zeta(x)| \tilde{\mathcal{L}}_N^* G_t^N(\eta, \zeta) d\nu_\alpha^N(\eta) d\nu_\alpha^N(\zeta) + C_0 e^{-ct} N^{-d/(2+d)} \end{aligned}$$

where the last estimate is due to Proposition 4.3 for $k = 1$. For the first term in the right-hand side we compute

$$\begin{aligned} \tilde{\mathcal{L}}_N(|\eta - \zeta|)(x) &= N^2 \sum_{x \sim y} ((g(\zeta(x)) - g(\eta(x))) - (g(\zeta(y)) - g(\eta(y)))) \mathbb{1}_{\substack{\eta(x) \geq \zeta(x) \\ \eta(y) \geq \zeta(y)}} \\ &+ N^2 \sum_{x \sim y} ((g(\zeta(y)) - g(\eta(y))) - (g(\zeta(x)) - g(\eta(x)))) \mathbb{1}_{\substack{\zeta(x) \geq \eta(x) \\ \zeta(y) \geq \eta(y)}} \\ &- N^2 \sum_{x \sim y} (|g(\zeta(x)) - g(\eta(x))| + |g(\zeta(y)) - g(\eta(y))|) \mathbb{1}_{\{\text{the rest scenarios}\}} \end{aligned}$$

since the last term is non-negative we write

$$\begin{aligned} \tilde{\mathcal{L}}_N \left(N^{-d} \sum_x |\eta - \zeta|(x) \right) &\leq N^{2-d} \sum_{\substack{x \in \mathbb{T}_N^d \\ x \sim y}} \left((g(\zeta(x)) - g(\eta(x))) \mathbb{1}_{\substack{\eta(x) \geq \zeta(x) \\ \eta(y) \geq \zeta(y)}} \right) \\ &- N^{2-d} \sum_{\substack{x \in \mathbb{T}_N^d \\ x \sim y}} \left((g(\zeta(y)) - g(\eta(y))) \mathbb{1}_{\substack{\eta(x) \geq \zeta(x) \\ \eta(y) \geq \zeta(y)}} \right) + N^{2-d} \sum_{\substack{x \in \mathbb{T}_N^d \\ x \sim y}} \left((g(\zeta(y)) - g(\eta(y))) \mathbb{1}_{\substack{\zeta(x) \geq \eta(x) \\ \zeta(y) \geq \eta(y)}} \right) \\ &- N^{2-d} \sum_{\substack{x \in \mathbb{T}_N^d \\ x \sim y}} \left((g(\zeta(x)) - g(\eta(x))) \mathbb{1}_{\substack{\zeta(x) \geq \eta(x) \\ \zeta(y) \geq \eta(y)}} \right). \end{aligned}$$

We exchange x, y to see that the 2nd with the 3rd and the 4th with the 5th are canceled, and thus

$$\frac{1}{N^d} \sum_{x \in \mathbb{T}_N^d} \widetilde{\mathcal{L}}_N(|\eta - \zeta|)(x) \leq 0. \quad (4.65)$$

Therefore we have

$$\begin{aligned} & \iint_{X_N^2} N^{-d} \sum_x |\eta(x) - \zeta(x)| \phi\left(\frac{x}{N}\right) G_t^N(\eta, \zeta) d\nu_\alpha^N(\eta) d\nu_\alpha^N(\zeta) \\ & \leq \iint_{X_N^2} N^{-d} \sum_x |\eta(x) - \zeta(x)| \phi\left(\frac{x}{N}\right) G_0^N(\eta, \zeta) d\nu_\alpha^N(\eta) d\nu_\alpha^N(\zeta) + CN^{-\frac{d}{2+d}} \int_0^t e^{-cs} ds. \end{aligned}$$

□

Remark 4.5 (contraction property for a copy of two zero-range processes). *Note that when both of our processes are zero-range processes, say the evolution of η_t and ζ_t is governed by \mathcal{L}_N with initial distributions μ_1^N, μ_2^N , we consider the coupled process (η_t, ζ_t) on the product space $X_N \times X_N$ with generator $\widetilde{\mathcal{L}}_N$. Then the Lemma 4.4 tells us that the quantity*

$$N^{-d} \sum_x \iint_{X_N^2} |\eta(x) - \zeta(x)| \widetilde{\mu}_t^N(\eta, \zeta)$$

is non-increasing in time, where $\widetilde{\mu}_t^N$ is the coupling measure. In other words, we have a contraction property in Wasserstein-1 distance with the cost being the microscopic ℓ_1 distance $N^{-d} \sum_x |\eta(x) - \zeta(x)|$: for all $t > 0$,

$$W_1(\mu_{t,1}^N, \mu_{t,2}^N) \leq W_1(\mu_{0,1}^N, \mu_{0,2}^N) \quad (4.66)$$

for the appropriate initial data so that we catch the infimum.

Proof of Corollary 1.4. We show that we can apply Theorem 1.1. Indeed the hypotheses **(H3)**, **(H1)** are implied by the Lemmas 4.3 and 4.4 above. The regularity properties for the hydrodynamical equation (1.19) in the Appendix 5.A imply hypothesis **(H2)** with $H = L^\infty(\mathbb{T}^d)$ and $T = \infty$ as we are in the parabolic case (given of course the assumptions on the jump rate (2)). □

Remark 4.6 (Explicit rate for $T < \infty$ under Eulerian scaling). *Note that when one is interested in hyperbolic scaling (Eulerian scaling) to the N -particle system, where we expect our limit PDE to be a conservation law $\partial_t f_t = \gamma \cdot \nabla \sigma(f_t)$, we can still apply our method to get an explicit rate of convergence to the hydrodynamic limit with the disadvantage that the result is valid only up to a finite time T of the appearance of the first discontinuity. In particular for the consistency estimate **(H3)** same manipulations, as shown, can be*

performed with the difference that the bound on the derivatives depends on time. As for the microscopic stability estimate **(H1)** nothing changes.

Similar calculations have been done in [GkS03, section 3] for a multispecies zero-range process leading to a system of conservation laws. The relative entropy method of Yau was applied there up to a finite time as well (up to the appearance of the first shock).

The only result proving the hydrodynamic limit so far under hyperbolic scaling for all times is by Rezakhanlou in [Rez91].

5.5 Proof of (H1)-(H2)-(H3) for the Simple Exclusion process

We consider $H = L^\infty(\mathbb{T}^d)$ the space of solutions to the linear diffusion equation

$$\partial_t f_t = \Delta_c f_t.$$

Here we also have to impose a bound condition on the initial profile, in particular we need a constant $\delta > 0$ to exist so that

$$\delta \leq f_0 \leq 1 - \delta.$$

We consider the *local Gibbs measure*, which here is characterized by the relation

$$\nu_{f_t(\cdot)}^N(\{\eta(x) = 1\}) = f_t\left(\frac{x}{N}\right) = 1 - \nu_{f_t(\cdot)}^N(\{\eta(x) = 0\}).$$

For $\alpha \in (0, 1)$, $f_t \in (0, 1)$, we consider the relative density

$$\psi_t^N(\zeta) := \frac{d\nu_{f_t(\cdot)}^N}{d\nu_\alpha}(\zeta) = e^{\sum_x \zeta(x) \lambda(t, x/N)} e^{\sum_x \log\left(\frac{1-f_t(x/N)}{1-\alpha}\right)} \quad (5.67)$$

where

$$\lambda(t, x/N) := \log\left(\frac{f_t(x/N)(1-\alpha)}{\alpha(1-f_t(x/N))}\right).$$

Inspired again by the relative entropy method of Yau [Yau91], we aim at obtaining a quantitative version of the hydrodynamic limit from the SSEP to the heat equation, without invoking the so-called one-block estimate.

5.5.1 Consistency estimate

Proposition 5.1. *For all $d \geq 1$, for $\eta, \zeta \in \{0, 1\}^{\mathbb{T}_N^d}$ and $\alpha \in (0, 1)$ we have that*

$$\iint_{X_N^2} N^{-d} \sum_{x \in \mathbb{T}_N^d} |\eta(x) - \zeta(x)| (\partial_t \psi_t^N(\zeta) - \mathcal{L}_N^* \psi_t^N(\zeta)) d\nu_\alpha^N(\eta) d\nu_\alpha^N(\zeta) \leq C_0 e^{-ct} N^{-\frac{d}{2+d}}. \quad (5.68)$$

Proof. We compute

$$\begin{aligned} \mathcal{L}_N^* \psi_t^N(\zeta) &= \frac{N^2}{2} \sum_{x \sim y} \zeta(x)(1 - \zeta(y)) \psi_t^N(\zeta) (e^{\lambda(t, y/N) - \lambda(t, x/N)} - 1) \\ &= \psi_t^N(\zeta) \frac{N^2}{2} \sum_x \zeta(x)(1 - \zeta(x+1)) (e^{\lambda(t, (x+1)/N) - \lambda(t, x/N)} - 1) + \\ &\quad + \psi_t^N(\zeta) \frac{N^2}{2} \sum_x \zeta(x+1)(1 - \zeta(x)) (e^{\lambda(t, x/N) - \lambda(t, (x+1)/N)} - 1) \end{aligned} \quad (5.69)$$

where for the second line we considered the process $\tilde{\zeta}(x) := \zeta(x-1)$. We expand then the exponential $e^x = \sum_{k \geq 0} \frac{x^k}{k!}$ to write

$$\begin{aligned} \mathcal{L}_N^* \psi_t^N(\zeta) &= \psi_t^N(\zeta) \frac{N^2}{2} \sum_x \left(\zeta(x)(1 - \zeta(x+1)) \left(\lambda \left(t, \frac{x+1}{N} \right) - \lambda \left(t, \frac{x}{N} \right) \right) + \right. \\ &\quad \left. + \zeta(x+1)(1 - \zeta(x)) \left(\lambda \left(t, \frac{x}{N} \right) - \lambda \left(t, \frac{x+1}{N} \right) \right) \right) + \\ &\quad + \left(\zeta(x)(1 - \zeta(x+1)) + \zeta(x+1)(1 - \zeta(x)) \right) \frac{(\lambda(t, \frac{x+1}{N}) - \lambda(t, \frac{x}{N}))^2}{2} + \\ &\quad + \sum_{\substack{k \geq 3 \\ k: \text{odd}}} \left(\zeta(x) - \zeta(x+1) \right) \frac{(\lambda(t, \frac{x+1}{N}) - \lambda(t, \frac{x}{N}))^k}{k!} + \\ &\quad + \sum_{\substack{k \geq 4 \\ k: \text{even}}} \left(\zeta(x) + \zeta(x+1) - 2\zeta(x)\zeta(x+1) \right) \frac{(\lambda(t, \frac{x+1}{N}) - \lambda(t, \frac{x}{N}))^k}{k!} \\ &= \psi_t^N(\zeta) \frac{N^2}{2} \sum_x \left(\zeta(x) \Delta^N \lambda \left(t, \frac{x}{N} \right) + \theta(\zeta(x)) \left| \nabla^N \lambda \left(t, \frac{x}{N} \right) \right|^2 + \Lambda_N^{k \geq 3} \right) \end{aligned} \quad (5.70)$$

where $\theta(\zeta(x)) := (1/2)(\zeta(x) + \zeta(x+1) - 2\zeta(x)\zeta(x+1))$.

Thus,

$$\begin{aligned}
& \iint_{X_N^2} N^{-d} \sum_{x \in \mathbb{T}_N^d} |\eta(x) - \zeta(x)| \mathcal{L}_N^* \psi_t^N(\zeta) d\nu_\alpha^N(\eta) d\nu_\alpha^N(\zeta) \\
&= \frac{N^{2-d}}{2} \iint_{X_N^2} \sum_{x \in \mathbb{T}_N^d} |\eta(x) - \zeta(x)| \sum_y \left(\zeta(y) \Delta^N \lambda \left(t, \frac{y}{N} \right) + \theta(\zeta(y)) \left| \nabla^N \lambda \left(t, \frac{y}{N} \right) \right|^2 + \right. \\
&\hspace{20em} \left. + \Lambda_N^{k \geq 3} \right) d\nu_\alpha^N(\eta) d\nu_{f_t(\cdot)}^N(\zeta) \\
&= \frac{N^{2-d}}{2} \iint_{X_N^2} \sum_{x \in \mathbb{T}_N^d} |\eta(x) - \zeta(x)| \left(\zeta(x) \Delta^N \lambda \left(t, \frac{x}{N} \right) + \theta(\zeta(x)) \left| \nabla^N \lambda \left(t, \frac{x}{N} \right) \right|^2 + \Lambda_N^{k \geq 3} \right) \\
&\hspace{20em} d\nu_\alpha^N(\eta) d\nu_{f_t(\cdot)}^N(\zeta) \\
&+ \frac{N^{2-d}}{2} \iint_{X_N^2} \sum_{x \in \mathbb{T}_N^d} |\eta(x) - \zeta(x)| \sum_{y \neq x} \left(\zeta(y) \Delta^N \lambda \left(t, \frac{y}{N} \right) + \theta(\zeta(y)) \left| \nabla^N \lambda \left(t, \frac{y}{N} \right) \right|^2 + \right. \\
&\hspace{20em} \left. + \Lambda_N^{k \geq 3} \right) d\nu_\alpha^N(\eta) d\nu_{f_t(\cdot)}^N(\zeta)
\end{aligned} \tag{5.71}$$

where we split the sum in y into two sums: $y = x$ and $y \neq x$. Conservation of mass, i.e. $\int \mathcal{L}_N^* \psi_t^N(\zeta) d\nu_\alpha^N(\zeta) = 0$, now yields that

$$\sum_x \int_{\zeta(x)} \left(\zeta(x) \Delta^N \lambda \left(t, \frac{x}{N} \right) + \theta(\zeta(x)) \left| \nabla^N \lambda \left(t, \frac{x}{N} \right) \right|^2 + \Lambda_N^{k \geq 3} \right) d\nu_{f_t(\cdot)}^1(\zeta(x)) = 0. \tag{5.72}$$

We therefore write

$$\begin{aligned}
& \iint_{X_N^2} N^{-d} \sum_{x \in \mathbb{T}_N^d} |\eta(x) - \zeta(x)| \mathcal{L}_N^* \psi_t^N(\zeta) d\nu_\alpha^N(\eta) d\nu_\alpha^N(\zeta) = \\
& \frac{N^{2-d}}{2} \iint_{X_N^2} \sum_{x \in \mathbb{T}_N^d} |\eta(x) - \zeta(x)| \left(\zeta(x) \Delta^N \lambda \left(t, \frac{x}{N} \right) + \theta(\zeta(x)) \left| \nabla^N \lambda \left(t, \frac{x}{N} \right) \right|^2 + \Lambda_N^{k \geq 3} \right) \\
&\hspace{20em} d\nu_\alpha^N(\eta) d\nu_{f_t(\cdot)}^N(\zeta) \\
& - \frac{N^{2-d}}{2} \iint_{X_N^2} \sum_{x \in \mathbb{T}_N^d} |\eta(x) - \zeta(x)| d\nu_\alpha^1(\eta(x)) d\nu_{f_t(\cdot)}^1(\zeta(x)) \times \\
&\quad \times \int_{\zeta(x)} \left(\zeta(x) \Delta^N \lambda \left(t, \frac{x}{N} \right) + \theta(\zeta(x)) \left| \nabla^N \lambda \left(t, \frac{x}{N} \right) \right|^2 + \Lambda_N^{k \geq 3} \right) d\nu_{f_t(\cdot)}^1(\zeta(x)).
\end{aligned} \tag{5.73}$$

Now we calculate $\partial_t \psi_t^N(\zeta)$:

$$\begin{aligned}
\partial_t \psi_t^N(\zeta) &= \psi_t^N(\zeta) \partial_t \log \psi_t^N(\zeta) = \psi_t^N(\zeta) \sum_{x \in \mathbb{T}_N^d} \partial_t \lambda(t, x/N) (\zeta(x) - f_t(x/N)) \\
&= \psi_t^N(\zeta) \sum_{x \in \mathbb{T}_N^d} \frac{\Delta f_t(x/N)}{2f_t(x/N)(1-f_t(x/N))} (\zeta(x) - f_t(x/N)) \\
&= \psi_t^N(\zeta) \sum_{x \in \mathbb{T}_N^d} \left(\Delta \lambda_t \left(\frac{x}{N} \right) - \vartheta' \left(f_t \left(\frac{x}{N} \right) \right) |\nabla \lambda(t, x/N)|^2 \right) \left(\zeta(x) - f_t \left(\frac{x}{N} \right) \right)
\end{aligned} \tag{5.74}$$

where

$$\vartheta \left(f_t \left(\frac{x}{N} \right) \right) = \mathbb{E}_{\nu_{f_t(\cdot)}^N} [\theta(\zeta(x))] = f_t \left(\frac{x}{N} \right) - f_t \left(\frac{x}{N} \right)^2. \tag{5.75}$$

The last line is implied by the relation

$$\partial_t \lambda_t \left(\frac{x}{N} \right) = \Delta \lambda_t \left(\frac{x}{N} \right) - \vartheta' \left(f_t \left(\frac{x}{N} \right) \right).$$

We also have that

$$0 = \partial_t \int X_N \psi_t^N(\zeta) d\nu_\alpha^N(\zeta) = \sum_{x \in \mathbb{T}_N^d} \int_{\zeta(x)} \partial_t \lambda_t \left(\frac{x}{N} \right) \left(\zeta(x) - f_t \left(\frac{x}{N} \right) \right) d\nu_{f_t(\cdot)}^1(\zeta(x)).$$

Then

$$\begin{aligned}
&\iint_{X_N^2} N^{-d} \sum_{x \in \mathbb{T}_N^d} |\eta(x) - \zeta(x)| (\mathcal{L}_N^* \psi_t^N(\zeta) - \partial_t \psi_t^N(\zeta)) d\nu_\alpha^N(\eta) d\nu_\alpha^N(\zeta) = \\
&\frac{N^{2-d}}{2} \iint_{X_N^2} \sum_{x \in \mathbb{T}_N^d} |\eta(x) - \zeta(x)| \left(\zeta(x) \Delta^N \lambda \left(t, \frac{x}{N} \right) + \theta(\zeta(x)) \left| \nabla^N \lambda \left(t, \frac{x}{N} \right) \right|^2 + \Lambda_N^{k \geq 3} \right) \\
&\quad d\nu_\alpha^N(\eta) d\nu_{f_t(\cdot)}^N(\zeta) = \\
&-\frac{N^{2-d}}{2} \iint_{X_N^2} \sum_{x \in \mathbb{T}_N^d} |\eta(x) - \zeta(x)| d\nu_\alpha^N(\eta) d\nu_{f_t(\cdot)}^N(\zeta) \times \\
&\quad \times \int_{\zeta(x)} \left(\zeta(x) \Delta^N \lambda \left(t, \frac{x}{N} \right) + \theta(\zeta(x)) \left| \nabla^N \lambda \left(t, \frac{x}{N} \right) \right|^2 + \Lambda_N^{k \geq 3} \right) d\nu_{f_t(\cdot)}^1(\zeta(x)) \\
&-\frac{N^{-d}}{2} \iint_{X_N^2} \sum_{x \in \mathbb{T}_N^d} |\eta(x) - \zeta(x)| \left(\Delta \lambda_t \left(\frac{x}{N} \right) - \vartheta' \left(f_t \left(\frac{x}{N} \right) \right) |\nabla \lambda(t, x/N)|^2 \right) \times \\
&\quad \times \left(\zeta(x) - f_t \left(\frac{x}{N} \right) \right) d\nu_{f_t(\cdot)}^N(\zeta).
\end{aligned} \tag{5.76}$$

We replace the discrete Laplacian Δ^N and the discrete derivative $|\nabla^N|^2$ with the continuous

versions up to two errors $\mathcal{R}_{1,N}$ and $\mathcal{R}_{2,N}$:

$$\begin{aligned}
& \iint_{X_N^2} N^{-d} \sum_{x \in \mathbb{T}_N^d} |\eta(x) - \zeta(x)| (\mathcal{L}_N^* \psi_t^N(\zeta) - \partial_t \psi_t^N(\zeta)) d\nu_\alpha^N(\eta) d\nu_\alpha^N(\zeta) = \\
& \frac{N^{-d}}{2} \iint_{X_N^2} \sum_{x \in \mathbb{T}_N^d} |\eta(x) - \zeta(x)| \left(\zeta(x) \Delta \lambda \left(t, \frac{x}{N} \right) + \theta(\zeta(x)) \left| \nabla \lambda \left(t, \frac{x}{N} \right) \right|^2 \right) d\nu_\alpha^N(\eta) d\nu_{f_t(\cdot)}^N(\zeta) \\
& - \frac{N^{-d}}{2} \iint_{X_N^2} \sum_{x \in \mathbb{T}_N^d} |\eta(x) - \zeta(x)| d\nu_\alpha^N(\eta) d\nu_{f_t(\cdot)}^N(\zeta) \times \\
& \quad \times \int_{\zeta(x)} \left(\zeta(x) \Delta \lambda \left(t, \frac{x}{N} \right) + \theta(\zeta(x)) \left| \nabla \lambda \left(t, \frac{x}{N} \right) \right|^2 \right) d\nu_{f_t(\cdot)}^1(\zeta(x)) \\
& - \frac{N^{-d}}{2} \iint_{X_N^2} \sum_{x \in \mathbb{T}_N^d} |\eta(x) - \zeta(x)| \left(\Delta \lambda_t \left(\frac{x}{N} \right) - \vartheta' \left(f_t \left(\frac{x}{N} \right) \right) \left| \nabla \lambda \left(t, \frac{x}{N} \right) \right|^2 \right) \times \\
& \quad \times \left(\zeta(x) - f_t \left(\frac{x}{N} \right) \right) d\nu_{f_t(\cdot)}^N(\zeta) \\
& + \mathcal{R}_{1,N} + \mathcal{R}_{2,N} + \mathcal{R}(\Lambda_N^{k \geq 3}).
\end{aligned} \tag{5.77}$$

Gathering the same terms we write

$$\begin{aligned}
& \iint_{X_N^2} N^{-d} \sum_{x \in \mathbb{T}_N^d} |\eta(x) - \zeta(x)| (\mathcal{L}_N^* \psi_t^N(\zeta) - \partial_t \psi_t^N(\zeta)) d\nu_\alpha^N(\eta) d\nu_\alpha^N(\zeta) = \\
& \frac{N^{-d}}{2} \iint_{X_N^2} \sum_{x \in \mathbb{T}_N^d} |\eta(x) - \zeta(x)| \left\{ \Delta \lambda_t \left(\frac{x}{N} \right) \left(\zeta(x) - f_t \left(\frac{x}{N} \right) - \left(\zeta(x) - f_t \left(\frac{x}{N} \right) \right) \right) \right. \\
& \quad \left. + \left| \nabla \lambda \left(t, \frac{x}{N} \right) \right|^2 \left(\theta(\zeta(x)) - \vartheta \left(f_t \left(\frac{x}{N} \right) \right) - \vartheta' \left(f_t \left(\frac{x}{N} \right) \right) \left(\zeta(x) - f_t \left(\frac{x}{N} \right) \right) \right) \right\} d\nu_\alpha^N(\eta) d\nu_{f_t(\cdot)}^N(\zeta) \\
& - \frac{N^{-d}}{2} \iint_{X_N^2} \sum_{x \in \mathbb{T}_N^d} |\eta(x) - \zeta(x)| d\nu_\alpha^N(\eta) d\nu_{f_t(\cdot)}^N(\zeta) \times \\
& \quad \times \int_{\zeta(x)} \left(\zeta(x) \Delta \lambda \left(t, \frac{x}{N} \right) + \theta(\zeta(x)) \left| \nabla \lambda \left(t, \frac{x}{N} \right) \right|^2 + \Lambda_N^{k \geq 3} \right) d\nu_{f_t(\cdot)}^1(\zeta(x)) \\
& + \frac{N^{-d}}{2} \iint_{X_N^2} \sum_{x \in \mathbb{T}_N^d} |\eta(x) - \zeta(x)| \left(\Delta \lambda_t \left(\frac{x}{N} \right) f_t \left(\frac{x}{N} \right) + \left| \nabla \lambda \left(t, \frac{x}{N} \right) \right|^2 \vartheta \left(f_t \left(\frac{x}{N} \right) \right) \right) d\nu_\alpha^N(\eta) d\nu_{f_t(\cdot)}^N(\zeta) \\
& + \mathcal{R}_{1,N} + \mathcal{R}_{2,N} + \mathcal{R}(\Lambda_N^{k \geq 3}) \\
& = E_1 + E_2 + E_3 + \mathcal{R}_{1,N} + \mathcal{R}_{2,N} + \mathcal{R}(\Lambda_N^{k \geq 3}).
\end{aligned} \tag{5.78}$$

The first line of E_1 vanishes. For the second line of E_1 we apply the same steps as in the consistency estimate of the zero-range process, namely first we replace $\zeta(x)$ with its local ℓ -averages, we then apply Lemma 2.1 in the discrete case, we Taylor expand and use that

ϑ'' is bounded. Finally we estimate by hand. We end up therefore with an error of order $e^{-ct} N^{-\frac{d}{2+d}}$.

For E_3 , we first use that the quantity $|\eta(x) - \zeta(x)|$ is bounded in the SEP and then we add and subtract the term

$$\int_{\mathbb{T}^d} (\Delta\lambda(t, u)f_t(u) + |\nabla\lambda(t, u)|^2 (f_t(u) - f_t(u)^2)) du.$$

E_3 is estimated then as follows

$$\begin{aligned} |E_3| \lesssim & \left| N^{-d} \sum_{x \in \mathbb{T}_N^d} \left(\Delta\lambda\left(t, \frac{x}{N}\right) f_t\left(\frac{x}{N}\right) + \left| \nabla\lambda\left(t, \frac{x}{N}\right) \right|^2 \left(f_t\left(\frac{x}{N}\right) - f_t\left(\frac{x}{N}\right)^2 \right) \right) \right. \\ & \left. - \int_{\mathbb{T}^d} (\Delta\lambda(t, u)f_t(u) + |\nabla\lambda(t, u)|^2 (f_t(u) - f_t(u)^2)) du \right| \\ & + \int_{\mathbb{T}^d} \left(\Delta\lambda(t, u)f_t(u) + \left| \nabla\lambda\left(t, \frac{x}{N}\right) \right|^2 (f_t(u) - f_t(u)^2) \right) du \lesssim e^{-ct} N^{-1}. \end{aligned} \quad (5.79)$$

For the above: Explicit calculations give that the last integral is zero as the integrand is given by $\partial_u \left(\frac{\partial_u f_t(u)}{1-f_t(u)} \right)$ and we are on the \mathbb{T}^d . The first term of the right-hand side is the Riemann differences controlled by $N^{-1} \times \|Q\|_{L^2(\mathbb{T}^d)}$ where $Q(u) := \Delta\lambda_t(u)f_t(u) + |\nabla\lambda(t, \frac{x}{N})|^2 (f_t(u) - f_t(u)^2)$.

E_2 is of order N^{-1} as well, since it consists of the same terms as E_3 .

Regarding the error $\mathcal{R}(\Lambda_N^{k \geq 3})$ we show that it is less than N^{-1} :

$$\begin{aligned} |\mathcal{R}(\Lambda_N^{k \geq 3})| &= \left| \frac{N^{2-d}}{2} \iint_{X_N^2} \sum_{x \in \mathbb{T}_N^d} |\eta(x) - \zeta(x)| \sum_{\substack{k \geq 3 \\ k: \text{odd}}} (\zeta(x) - \zeta(x+1)) \frac{(\lambda(t, \frac{x+1}{N}) - \lambda(t, \frac{x}{N}))^k}{k!} \right. \\ & \quad \left. + \sum_{\substack{k \geq 4 \\ k: \text{even}}} 2\theta(\zeta(x)) \frac{(\lambda(t, \frac{x+1}{N}) - \lambda(t, \frac{x}{N}))^k}{k!} d\nu_\alpha^N(\eta) d\nu_{f_t(\cdot)}^N(\zeta) \right| \\ & \lesssim N^{-d} \sum_x N^2 \sum_{k \geq 3} \|\nabla\lambda^N\|_\infty^k \frac{1}{N^k k!} \lesssim \sum_{k \geq 3} N^{2-k} \frac{C^k}{k!}. \end{aligned} \quad (5.80)$$

The above series is the expansion of the exponential $N^2(e^{C/N} - 1 - (CN)^{-1} - C^2/(2N^2))$. Now expanding around 0 the term in the parenthesis, we see that it is of lower order, i.e. $\mathcal{O}(N^{-3})$. This yields that $|\mathcal{R}(\Lambda_N^{k \geq 3})| \lesssim N^{-1}$. \square

Remark 5.2. *Note that similar calculations are implied by the result presented in the proof of Theorem 3.1 in [GLT09]. The authors there employ Yau's relative entropy method for a class of kinetically constrained lattice gases to show that the macroscopic density is*

evolving according to the porous medium equation.

5.5.2 Microscopic stability estimate

We employ the basic coupling, or Wasserstein coupling, discussed in [Lig85], see also [Rez91], which is a coupling of two copies of simple exclusion processes. We denote by $b : \mathbb{N}^2 \rightarrow \{0, 1\}$ the function $b(n, m) = 1$ when $n = 1, m = 0$ and 0 otherwise. The generator of the coupled process $\tilde{\mathcal{L}}_N : C_b(X_N^2) \rightarrow C_b(X_N^2)$ is given by

$$\begin{aligned} \tilde{\mathcal{L}}_N f(\eta, \zeta) &:= N^2 \sum_{x,y} p(y-x) b(\eta(x), \eta(y)) \wedge b(\zeta(x), \zeta(y)) (f(\eta^{xy}, \zeta^{xy}) - f(\eta, \zeta)) \\ &+ N^2 \sum_{x,y} p(y-x) \left(b(\eta(x), \eta(y)) - b(\eta(x), \eta(y)) \wedge b(\zeta(x), \zeta(y)) \right) (f(\eta^{xy}, \zeta) - f(\eta, \zeta)) \\ &+ N^2 \sum_{x,y} p(y-x) \left(b(\zeta(x), \zeta(y)) - b(\eta(x), \eta(y)) \wedge b(\zeta(x), \zeta(y)) \right) (f(\eta, \zeta^{xy}) - f(\eta, \zeta)). \end{aligned} \tag{5.81}$$

Note that indeed when both η and ζ are simple exclusion processes, their coupled law satisfies exactly the forward Kolmogorov equation, i.e. each marginal corresponds to a simple exclusion process. The generator of this coupled process is defined like above so that the particles in processes η, ζ ‘agree’ as much as possible.

We are interested in the coupled process, since we want to estimate the discrete L^1 -distance between two solutions in the microscopic level and in particular the distance among the density of a ‘true’ simple-exclusion process f_t^N and the density of the artificial process ψ_t^N as given in (5.67). We have the following energy estimate on the law of the coupled process.

Lemma 5.3. *Let G_t^N be the coupling density on X_N^2 evolving according to (1.9). The first marginal of it is the evolution of the density ψ_t^N , relative to the reference measure $d\nu_\alpha^N$, of an artificial process considered so that it has the desired hydrodynamical behavior, while the second marginal gives us the density of a simple exclusion process f_t^N . For $\phi \in C_c^\infty(\mathbb{T}^d)$ we have that*

$$\begin{aligned} &\iint_{X_N^2} N^{-d} \sum_x |\eta(x) - \zeta(x)| \phi\left(\frac{x}{N}\right) G_t^N(\eta, \zeta) d\nu_\alpha^N(\eta) d\nu_\alpha^N(\zeta) \\ &\leq \iint_{X_N^2} N^{-d} \sum_x |\eta(x) - \zeta(x)| \phi\left(\frac{x}{N}\right) G_0^N(\eta, \zeta) d\nu_\alpha^N(\eta) d\nu_\alpha^N(\zeta) + CN^{-\frac{d}{2+d}}(1 - e^{-ct}). \end{aligned} \tag{5.82}$$

Proof. We calculate

$$\begin{aligned} & \frac{d}{dt} \iint_{X_N^2} N^{-d} \sum_x |\eta(x) - \zeta(x)| \phi\left(\frac{x}{N}\right) G_t^N(\eta, \zeta) d\nu_\alpha^N(\eta) d\nu_\alpha^N(\zeta) \leq \\ & \iint_{X_N^2} N^{-d} \sum_x |\eta(x) - \zeta(x)| \tilde{\mathcal{L}}_N^* G_t^N(\eta, \zeta) d\nu_\alpha^N(\eta) d\nu_\alpha^N(\zeta) + C_0 e^{-ct} N^{-\frac{d}{2+d}} \end{aligned}$$

where the last estimate is from Proposition 5.1. For the first term in the right-hand side we compute

$$\begin{aligned} \tilde{\mathcal{L}}_N(|\eta - \zeta|)(x) &= N^2 \sum_{x \sim y} ((b(\eta(x), \zeta(x)) - b(\eta(x), \zeta(x))) - (b(\eta(y), \zeta(y)) - b(\eta(y), \zeta(y)))) \mathbb{1}_{\substack{\eta(x) \geq \zeta(x) \\ \eta(y) \geq \zeta(y)}} \\ &+ N^2 \sum_{x \sim y} ((b(\eta(y), \zeta(y)) - b(\eta(y), \zeta(y))) - (b(\eta(x), \zeta(x)) - b(\eta(x), \zeta(x)))) \mathbb{1}_{\substack{\zeta(x) \geq \eta(x) \\ \zeta(y) \geq \eta(y)}} \\ &- N^2 \sum_{x \sim y} (|b(\eta(x), \zeta(x)) - b(\eta(x), \zeta(x))| + |b(\eta(y), \zeta(y)) - b(\eta(y), \zeta(y))|) \mathbb{1}_{\{\text{the rest scenarios}\}} \end{aligned}$$

since the last term is non-negative we write

$$\begin{aligned} \tilde{\mathcal{L}}_N \left(N^{-d} \sum_x |\eta - \zeta|(x) \right) &\leq N^{2-d} \sum_{\substack{x \in \mathbb{T}_N^d \\ x \sim y}} \left((b(\eta(x), \zeta(x)) - b(\eta(x), \zeta(x))) \mathbb{1}_{\substack{\eta(x) \geq \zeta(x) \\ \eta(y) \geq \zeta(y)}} \right) \\ &- N^{2-d} \sum_{\substack{x \in \mathbb{T}_N^d \\ x \sim y}} \left((b(\eta(y), \zeta(y)) - b(\eta(y), \zeta(y))) \mathbb{1}_{\substack{\eta(x) \geq \zeta(x) \\ \eta(y) \geq \zeta(y)}} \right) \\ &+ N^{2-d} \sum_{\substack{x \in \mathbb{T}_N^d \\ x \sim y}} \left((b(\eta(y), \zeta(y)) - g(\eta(y), \zeta(y))) \mathbb{1}_{\substack{\zeta(x) \geq \eta(x) \\ \zeta(y) \geq \eta(y)}} \right) \\ &- N^{2-d} \sum_{\substack{x \in \mathbb{T}_N^d \\ x \sim y}} \left((b(\eta(x), \zeta(x)) - b(\eta(x), \zeta(x))) \mathbb{1}_{\substack{\zeta(x) \geq \eta(x) \\ \zeta(y) \geq \eta(y)}} \right). \end{aligned}$$

We exchange x, y to see that the 2nd with the 3rd and the 4th with the 5th are canceled, and thus $N^{-d} \sum_{x \in \mathbb{T}_N^d} \tilde{\mathcal{L}}_N(|\eta - \zeta|)(x) \leq 0$. Integrating in time implies the claim of the Lemma. \square

Proof of the Corollary 1.6. We show that we can apply Theorem 1.1: the hypotheses **(H3)**, **(H1)** are implied by the Lemmas 5.1 and 5.3 above. The hypothesis **(H2)** is well known that it is satisfied with $H = L^\infty(\mathbb{T}^d)$, as our limit equation is just the linear heat equation in the symmetric simple exclusion process-case. \square

5.6 Proof of (H1)-(H2)-(H3) for the Ginzburg-Landau process

First we provide a uniform in N bound on the particle moments with respect to the measure ν_ρ^N for $\rho \geq 0$. We shall take advantage of the attractivity of the process, which in this case is provided by the convexity of the potential V .

Lemma 6.1. *Assume that the one-body potential $V : \mathbb{R} \rightarrow \mathbb{R}$ satisfies the Assumption 3 and that there is a $\rho \geq 0$ such that $\mu_0^N \leq \nu_\rho^N$ where $\nu_\rho^N(\zeta) = e^{-\sum_x V(\zeta(x)) + \rho \sum_x \zeta(x)}$. Then for any $k > 0$ we have for the k -th moments:*

$$\int_{X_N} N^{-d} \sum_{x \in \mathbb{T}_N^d} \eta(x)^k d\nu_\rho^N(\eta) = C_k < \infty.$$

Proof. It is enough to show that $\int_{\mathbb{R}} y^k e^{\rho y - V(y)} dy < C_k$. For that we will use the convexity of the potential away from the origin. Indeed take $R > 0$, say $R \geq x_{min}$ if x_{min} is the point at the bottom of the right well if one thinks of the double-well potential. Then

$$\int_0^\infty y^k e^{\rho y - V(y)} dy = \int_0^R y^k e^{\rho y - V(y)} dy + \int_R^\infty y^k e^{\rho y - V(y)} dy \leq (Re^\rho)^k + \int_R^\infty y^k e^{\rho y - V(y)} dy$$

For the second integral: w.l.o.g. we assume that $M := \sup_{x \in (R, \infty)} e^{-V(x)} = e^{-V(R)}$. Due to the convexity, we can find $\alpha \geq R + 1$ so that $V'(\alpha) \geq (\alpha - R)(V(\alpha) - V(R)) > \alpha - R$, which implies that

$$V(x) \geq V(\alpha) + V'(\alpha)(x - \alpha) \geq V(\alpha) + (\alpha - R)(x - \alpha).$$

Then

$$\begin{aligned} \int_\alpha^\infty y^k e^{\rho y - V(y)} dy &\leq e^{-V(\alpha)} \int_\alpha^\infty y^k e^{\rho y} e^{-(\alpha - R)(y - \alpha)} dy \\ &= \frac{e^{-V(\alpha)}}{\alpha - R} \int_0^\infty \left| \frac{y + \alpha^2 - R\alpha}{\alpha - R} \right|^k e^{\rho(y + \alpha^2 - R\alpha)/(\alpha - R)} e^{-y} dy \\ &\lesssim \frac{e^{\rho\alpha}}{(\alpha - R)^{k+1}} \int_0^\infty |y + \alpha^2 - R\alpha|^k e^{-y\rho(1 - 1/(\alpha - R))} dy \\ &\lesssim \frac{e^{\rho\alpha}}{(\alpha - R)^{k+1}} \end{aligned}$$

since $1 \geq 1/(\alpha - R)$. A similar estimate on $(-\infty, 0)$ follows by symmetry. \square

We consider f_t to be the unique strong solution of the quasilinear diffusion equation (1.30).

Lemma 6.2. *There exists $C > 0$ so that*

$$0 < \frac{1}{C} \leq h''(u) \leq C < \infty$$

for all $u \in \mathbb{R}$.

Proof. The proof follows from basic estimates and properties of the Legendre transform; calculations were done in [GOVW09, Lemma 41], see also [DMOWa, Lemma 5.1] accompanied by the paper [DMOWb]. The constant C is then given by $\exp(\text{osc}_{\mathbb{R}} V_1) := \exp(\sup_{\mathbb{R}} V_1 - \inf_{\mathbb{R}} V_1)$ which is bounded by our Assumption 3. \square

This solution satisfies Assumption **(H2)** of the abstract method with $H = L^\infty$ as proven in the Appendix 6.6.2.

Following the abstract method, we consider the local Gibbs measure with slowly varying coefficient $\lambda(t, x)$, as was done (among other works) in [Yau91], where $\lambda : \mathbb{R}_+ \times \mathbb{T} \rightarrow \mathbb{R}_+$ is a smooth function. For every solution to (1.30), we take

$$\lambda(t, u) = h'(f(t, u)).$$

Then the density ψ_t^N , relevant to the Gibbs measure, is given as follows:

$$\psi_t^N(\eta) := \frac{e^{\sum_x \eta(x) \lambda(t, x/N)}}{\prod_{x \in \mathbb{T}_N} M(\lambda(t, x/N))}, \quad M(\lambda(t, x/N)) := \int_{\mathbb{R}} e^{\eta(x) \lambda(t, x/N) - V(\eta(x))} d\eta(x). \quad (6.83)$$

The macroscopic density is given by the relation

$$\frac{dp}{d\lambda}(\lambda(x/N)) = \left. \frac{d \log M(\lambda)}{d\lambda} \right|_{\lambda=\lambda(t, x/N)} = \frac{\int_{\mathbb{R}^{\mathbb{T}_N}} \zeta(x) e^{\sum_y \zeta(y) \lambda(t, y/N) - V(\zeta(y))} d\zeta}{M(\lambda)} = f(t, x/N).$$

Also when the average spin is $f_t(u)$ and the charges are organised according to the Gibbs measure, the average of $V'(x)$ is $h'(f_t(x/N))$:

$$\begin{aligned} \int_{\mathbb{R}^{\mathbb{T}_N}} V'(\zeta(x)) \psi_t^N(\zeta) d\nu^N(\zeta) &= \frac{1}{M(h'(f_t(x/N)))} \int_{\mathbb{R}^{\mathbb{T}_N}} e^{\sum_x \zeta(x) h'(f_t(x/N))} \frac{\partial}{\partial \zeta(x)} (-e^{-V(\zeta(x))}) d\zeta \\ &= h'(f_t(x/N)) \int_{\mathbb{R}^{\mathbb{T}_N}} \psi_t^N(\zeta) d\nu^N(\zeta) = h'(f_t(x/N)) \end{aligned}$$

after an integration by parts in the second equality.

5.6.1 Consistency estimate

Proposition 6.3. *Let $d = 1$, $k > 0$ and two configurations $\eta, \zeta \in \mathbb{R}^{\mathbb{T}^N}$ of the Ginzburg-Landau process. We have*

$$\iint_{X_N^2} N^{-1} \sum_{x \in \mathbb{T}_N} |\eta(x) - \zeta(x)|^k (\partial_t \psi_t^N(\zeta) - \mathcal{L}_N^* \psi_t^N(\zeta)) d\nu^N(\eta) d\nu^N(\zeta) \leq C_0 e^{-ct} N^{-1/3} \quad (6.84)$$

for some C_0, c positive constants.

Proof. When the generator is acting on the local Gibbs measure, explicit calculations give

$$\begin{aligned} \mathcal{L}_N^* \psi_t^N(\zeta) &= \frac{N^2}{2} \sum_{x \in \mathbb{T}_N} \left(\frac{\partial}{\partial \zeta(x)} - \frac{\partial}{\partial \zeta(x+1)} \right)^2 \psi_t^N(\zeta) \\ &\quad - \left(\frac{\partial V}{\partial \zeta(x)} - \frac{\partial V}{\partial \zeta(x+1)} \right) \left(\frac{\partial}{\partial \zeta(x)} - \frac{\partial}{\partial \zeta(x+1)} \right) \psi_t^N(\zeta) \\ &\quad + \left(\frac{\partial}{\partial \zeta(x)} - \frac{\partial}{\partial \zeta(x-1)} \right)^2 \psi_t^N(\zeta) - \left(\frac{\partial V}{\partial \zeta(x)} - \frac{\partial V}{\partial \zeta(x-1)} \right) \left(\frac{\partial}{\partial \zeta(x)} - \frac{\partial}{\partial \zeta(x-1)} \right) \psi_t^N(\zeta) \\ &= N^2 \psi_t^N(\zeta) \sum_{x \in \mathbb{T}_N} \Delta^N h'(f_t(x/N)) \left(h'(f_t(x/N)) - \frac{\partial V}{\partial \zeta(x)} \right). \end{aligned} \quad (6.85)$$

We write $\lambda = h'(f_t(x/N))$ and calculate the time-derivative part:

$$\begin{aligned} \partial_t \psi_t^N(\zeta) &= \psi_t^N(\zeta) \sum_{x \in \mathbb{T}_N} \partial_t \lambda(t, x/N) \zeta(x) - \psi_t^N(\zeta) \frac{\partial_t M(\lambda(t, x/N))}{M(\lambda(t, x/N))} \\ &= \psi_t^N(\zeta) \sum_{x \in \mathbb{T}_N} \partial_t \lambda(t, x/N) (\zeta(x) - f_t(x/N)). \end{aligned} \quad (6.86)$$

Gathering them together, we want then to estimate

$$\begin{aligned} &\int_{\mathbb{R}^{\mathbb{T}^N}} \int_{\mathbb{R}^{\mathbb{T}^N}} N^{-1} \sum_{x \in \mathbb{T}_N} |\eta(x) - \zeta(x)| (\partial_t - \mathcal{L}_N^*) \psi_t^N(\zeta) d\nu^N(\zeta) d\nu^N(\eta) \\ &= \int_{\mathbb{R}^{\mathbb{T}^N}} \int_{\mathbb{R}^{\mathbb{T}^N}} N^{-1} \sum_{x \in \mathbb{T}_N} |\eta(x) - \zeta(x)| \left\{ \partial_t \lambda(t, x/N) (\zeta(x) - f_t(x/N)) \right. \\ &\quad \left. - N^2 \Delta^N \lambda(t, x/N) (V'(\zeta(x)) - \lambda(t, x/N)) \right\} \psi_t^N(\zeta) d\nu^N(\zeta) d\nu^N(\eta) \quad (6.87) \\ &+ N^{-1} \sum_{x \in \mathbb{T}_N} \sum_{y \neq x} \int_{\mathbb{R}^{\mathbb{T}^N}} \int_{\mathbb{R}^{\mathbb{T}^N}} |\eta(x) - \zeta(x)| \left\{ \partial_t \lambda(t, y/N) (\zeta(y) - f_t(y/N)) \right. \\ &\quad \left. - N^2 \Delta^N \lambda(t, y/N) (V'(\zeta(y)) - \lambda(t, y/N)) \right\} \psi_t^N(\zeta) d\nu^N(\zeta) d\nu^N(\eta) \end{aligned}$$

where we have split the first sum into two sums on x and $y \neq x$. Now using that

$\int_{\mathbb{R}^{\mathbb{T}_N}} (\partial_t - \mathcal{L}_N^*) \psi_t^N(\zeta) d\nu^N(\zeta) = 0$, the right hand side equals to

$$\begin{aligned}
& \int_{\mathbb{R}^{\mathbb{T}_N}} \int_{\mathbb{R}^{\mathbb{T}_N}} N^{-1} \sum_{x \in \mathbb{T}_N} |\eta(x) - \zeta(x)| \left\{ \partial_t \lambda(t, x/N) (\zeta(x) - f_t(x/N)) \right. \\
& \quad \left. - N^2 \Delta^N \lambda(t, x/N) \left(V'(\zeta(x)) - \lambda(t, x/N) \right) \right\} \psi_t^N(\zeta) d\nu^N(\zeta) d\nu^N(\eta) \\
& - N^{-1} \sum_x \int_{\mathbb{R}^{\mathbb{T}_N}} \int_{\mathbb{R}^{\mathbb{T}_N} } |\eta(x) - \zeta(x)| \psi_t^N(\zeta) d\nu^N(\zeta) d\nu^N(\eta) \int_{\mathbb{R}^{\mathbb{T}_N}} \left\{ \partial_t \lambda(t, x/N) (\zeta(x) - f_t(x/N)) \right. \\
& \quad \left. - N^2 \Delta^N \lambda(t, x/N) (V'(\zeta(x)) - \lambda(t, x/N)) \right\} \psi_t^N(\zeta) d\nu^N(\zeta).
\end{aligned} \tag{6.88}$$

The second term above is 0. For the first term of the right-hand side, we replace, up to an error of order $Ce^{-ct}N^{-2}$, the discrete Laplacian with the continuous one:

$$\begin{aligned}
& \int_{\mathbb{R}^{\mathbb{T}_N}} \int_{\mathbb{R}^{\mathbb{T}_N}} N^{-1} \sum_x |\eta(x) - \zeta(x)| (\mathcal{L}_N^* - \partial_t) \psi_t^N(\zeta) d\nu^N(\zeta) d\nu^N(\eta) \\
& = \int_{\mathbb{R}^{\mathbb{T}_N}} \int_{\mathbb{R}^{\mathbb{T}_N}} N^{-1} \sum_x |\eta(x) - \zeta(x)| \left\{ -\partial_t \lambda(t, x/N) (\zeta(x) - f_t(x/N)) \right. \\
& \quad \left. + \partial_{uu} \lambda(t, x/N) \left(V'(\zeta(x)) - \lambda(t, x/N) \right) \right\} \psi_t^N(\zeta) d\nu^N(\zeta) d\nu^N(\eta) + Ce^{-ct}N^{-2} \\
& = \iint_{\mathbb{R}^{\mathbb{T}_N} \times \mathbb{R}^{\mathbb{T}_N}} N^{-1} \sum_x |\eta(x) - \zeta(x)| \left\{ -h''(f_t(x/N)) \partial_{uu} h'(f_t(x/N)) (\zeta(x) - f_t(x/N)) \right. \\
& \quad \left. + \partial_{uu} h'(f_t(x/N)) \left(V'(\zeta(x)) - \lambda(t, x/N) \right) \right\} \psi_t^N(\zeta) d\nu^N(\zeta) d\nu^N(\eta) + Ce^{-ct}N^{-2} \\
& = \iint_{\mathbb{R}^{\mathbb{T}_N} \times \mathbb{R}^{\mathbb{T}_N}} N^{-1} \sum_x |\eta(x) - \zeta(x)| \partial_{uu} h' \left(f_t \left(\frac{x}{N} \right) \right) \times \\
& \quad \times \left(V'(\zeta(x)) - h' \left(f_t \left(\frac{x}{N} \right) \right) - h'' \left(f_t \left(\frac{x}{N} \right) \right) \left(\zeta(x) - f_t \left(\frac{x}{N} \right) \right) \right) \psi_t^N(\zeta) d\nu^N(\zeta) d\nu^N(\eta) + Ce^{-ct}N^{-2}.
\end{aligned} \tag{6.89}$$

Now we replace $\zeta(x)$ by its ℓ -averages $\overline{\zeta(x)}^\ell$. We denote by

$$\phi(t, x/N) = \partial_{uu} h'(f_t(x/N)) h''(f_t(x/N)).$$

In order to estimate the error from this replacement, i.e. from the term

$$\iint_{\mathbb{R}^{\mathbb{T}_N} \times \mathbb{R}^{\mathbb{T}_N}} N^{-1} \sum_x |\eta(x) - \zeta(x)| \phi \left(t, \frac{x}{N} \right) \left(\zeta(x) - \overline{\zeta(x)}^\ell \right),$$

we follow the lines of Step 3 in the proof of Prop. 4.3. Since the variables η, ζ are independent under ν^N , we conclude a bound in ℓ, N which is of order $\mathcal{O}(\ell/N + \ell^{-1/2})$.

In the same manner we also replace $V'(\zeta(x))$ by $\overline{V'(\zeta(x))}^\ell$, which leaves the same error

as above. The right-hand side then takes the form

$$\begin{aligned}
& \iint_{\mathbb{R}^{\mathbb{T}_N} \times \mathbb{R}^{\mathbb{T}_N}} N^{-1} \sum_{x \in \mathbb{T}_N} |\eta(x) - \zeta(x)| \partial_{uu} h' \left(f_t \left(\frac{x}{N} \right) \right) \times \\
& \times \left(\overline{V'(\zeta(x))}^\ell - h' \left(f_t \left(\frac{x}{N} \right) \right) - h'' \left(f_t \left(\frac{x}{N} \right) \right) \left(\zeta(x) - f_t \left(\frac{x}{N} \right) \right) \right) \psi_t^N(\zeta) d\nu^N(\zeta) d\nu^N(\eta) \\
& + C e^{-ct} (N^{-2} \ell / N + \ell^{-1/2}).
\end{aligned} \tag{6.90}$$

An application now of Lemma 2.1, using then that $h^{(k)}$ is bounded and that $\|f_t\|_{H^k} \lesssim e^{-ct} \|f_0\|_{H^k}$, the right-hand side is bounded by above from

$$\begin{aligned}
& C e^{-ct} \int_{\mathbb{R}^{\mathbb{T}_N}} \int_{\mathbb{R}^{\mathbb{T}_N}} N^{-1} \sum_{x \in \mathbb{T}_N} |\eta(x) - \zeta(x)| \times \\
& \times \left(h'(\overline{\zeta(x)}^\ell) - h' \left(f_t \left(\frac{x}{N} \right) \right) - h'' \left(f_t \left(\frac{x}{N} \right) \right) \left(\overline{\zeta(x)}^\ell - f_t \left(\frac{x}{N} \right) \right) \right) \psi_t^N(\zeta) d\nu^N(\zeta) d\nu^N(\eta) \\
& + C e^{-ct} (N^{-2} \ell / N + \ell^{-1/2}).
\end{aligned} \tag{6.91}$$

We now find ρ in between $\overline{\zeta(x)}^\ell$ and $f_t \left(\frac{x}{N} \right)$ so that the integrals are bounded by

$$\int_{\mathbb{R}^{\mathbb{T}_N}} \int_{\mathbb{R}^{\mathbb{T}_N}} N^{-1} \sum_{x \in \mathbb{T}_N} |\eta(x) - \zeta(x)| \frac{(h')''(\rho)}{2} \left(f_t(x/N) - \overline{\zeta(x)}^\ell \right)^2 d\nu^N(\zeta) d\nu^N(\eta). \tag{6.92}$$

Under the assumption of boundedness of $h^{(k)}$ for all k 's, we follow now the step 3 of the proof of Prop. 4.3. This will give in total an error of the form

$$C e^{-ct} N^{-1/3},$$

after optimizing over ℓ . □

5.6.2 Microscopic stability estimate

We consider a coupling of two Ginzburg-Landau processes with generator $\tilde{\mathcal{L}}_N : C_b(X_N^2) \rightarrow X_N^2$ given by

$$\begin{aligned} \tilde{\mathcal{L}}_N f(\eta, \zeta) := & \frac{N^2}{2} \sum_{x \sim y} \left(\left[\left(\frac{\partial}{\partial \eta(x)} - \frac{\partial}{\partial \eta(y)} \right)^* \left(\frac{\partial}{\partial \eta(x)} - \frac{\partial}{\partial \eta(y)} \right) \otimes 1 \right] f(\eta, \zeta) \right. \\ & + \left[1 \otimes \left(\frac{\partial}{\partial \zeta(x)} - \frac{\partial}{\partial \zeta(y)} \right)^* \left(\frac{\partial}{\partial \zeta(x)} - \frac{\partial}{\partial \zeta(y)} \right) \right] f(\eta, \zeta) \\ & \left. + (2 + K) \left(\frac{\partial}{\partial \eta(x)} - \frac{\partial}{\partial \eta(y)} \right) \otimes \left(\frac{\partial}{\partial \zeta(x)} - \frac{\partial}{\partial \zeta(y)} \right) f(\eta, \zeta) \right) \end{aligned} \quad (6.93)$$

where K is a constant to be chosen later and the adjoint is taken in $L^2(d\nu^N)$ and so we recover our generator as we have

$$\left(\frac{\partial}{\partial \eta(x)} - \frac{\partial}{\partial \eta(y)} \right)^* \left(\frac{\partial}{\partial \eta(x)} - \frac{\partial}{\partial \eta(y)} \right) = \left(\frac{\partial}{\partial \eta(x)} - \frac{\partial}{\partial \eta(y)} \right)^2 - \left(\frac{\partial V}{\partial \eta(x)} - \frac{\partial V}{\partial \eta(y)} \right) \left(\frac{\partial}{\partial \eta(x)} - \frac{\partial}{\partial \eta(y)} \right)$$

This should be the analogue of the basic coupling implemented for the jump processes in the previous sections, where the last term would correspond to the simultaneous jumps in a jump process.

Lemma 6.4. *Let G_t^N be the coupling density on X_N^2 evolving according to (1.9). When V satisfies the Assumption (GL1), cf. 3, for a test function $\phi \in C_c^\infty(\mathbb{T})$ we have that*

$$\begin{aligned} & \iint_{X_N^2} N^{-1} \sum_{x \in \mathbb{T}_N} |\eta(x) - \zeta(x)|^2 \phi\left(\frac{x}{N}\right) G_t^N(\eta, \zeta) d\nu^N(\eta) d\nu^N(\zeta) \\ & \leq \iint_{X_N^2} N^{-1} \sum_{x \in \mathbb{T}_N} |\eta(x) - \zeta(x)|^2 \phi\left(\frac{x}{N}\right) G_0^N(\eta, \zeta) d\nu^N(\eta) d\nu^N(\zeta) + CN^{-\frac{1}{3}}(1 - e^{-ct}). \end{aligned} \quad (6.94)$$

Proof. We calculate first the time-derivative of the left-hand side:

$$\begin{aligned} & \frac{d}{dt} \iint_{X_N^2} N^{-1} \sum_{x \in \mathbb{T}_N} |\eta(x) - \zeta(x)|^2 \phi\left(\frac{x}{N}\right) G_t^N(\eta, \zeta) d\nu^N(\eta) d\nu^N(\zeta) \\ & = C_0 e^{-ct} N^{-1/3} + \iint_{X_N^2} \tilde{\mathcal{L}}_N \left(N^{-1} \sum_x |\eta(x) - \zeta(x)|^2 \right) G_t^N(\eta, \zeta) d\nu^N(\eta) d\nu^N(\zeta) \end{aligned} \quad (6.95)$$

where the first term is the error from the consistency estimate. Now about the second

term we have

$$\begin{aligned}
& \iint_{X_N^2} \frac{N}{2} \sum_{x \sim y} \left(8 - 2(V_0'(\eta(x)) - V_0'(\eta(y)))(\eta(x) - \zeta(x) - (\eta(y) - \zeta(y))) \right. \\
& + 2(V_0'(\zeta(x)) - V_0'(\zeta(y)))(\eta(x) - \zeta(x) - (\eta(y) - \zeta(y))) \\
& - 2(V_1'(\eta(x)) - V_1'(\eta(y)))(\eta(x) - \zeta(x) - (\eta(y) - \zeta(y))) \\
& \left. + 2(V_0'(\zeta(x)) - V_0'(\zeta(y)))(\eta(x) - \zeta(x) - (\eta(y) - \zeta(y))) - 8 - 4K \right) G_t^N(\eta, \zeta) d\nu^N(\eta) d\nu^N(\zeta).
\end{aligned} \tag{6.96}$$

Using now the strict convexity of the potential V_0 , i.e. $V_0''(x) \geq \lambda > 0$ and the boundedness of V' , i.e. $V_1'(x) \leq C$, we bound it from above by

$$\iint_{X_N^2} \frac{N}{2} \sum_{x \sim y} \left(-\lambda |\eta(x) - \zeta(x)|^2 + C |\eta(x) - \zeta(x)| - 4K \right) G_t^N(\eta, \zeta) d\nu^N(\eta) d\nu^N(\zeta). \tag{6.97}$$

This is negative when $C < 4\sqrt{K\lambda}$. which implies the Lemma. \square

Proof of Corollary 1.7. We show that we can apply Theorem 1.1. Indeed the hypotheses **(H3)**, **(H1)** are implied by the Proposition 6.3 and Lemma 6.4, respectively. The regularity properties for the hydrodynamical equation (1.19) in the Appendix 5.A imply hypothesis **(H2)** with $H = L^\infty(\mathbb{T}^d)$ given Lemma 6.2. \square

5.7 Perspectives-Work in progress

5.7.1 The case of $d \geq 2$ dimensions

So far in our proof of the hydrodynamic limit in the diffusive case, we have assumed $d = 1$. This restriction is there only because of the stability results that we need for the limit PDE, which is a quasi-linear diffusion equation. In particular, as shown in the Appendix 6.6.2 in order to get, by applying only basic estimates, uniform in time propagation of higher regularity we need to restrict to $d = 1$. This implies a spectral gap in $W^{k,\infty}$ -norm where $k : |k| \leq 4$.

Regularity results for uniformly parabolic equations in higher dimensions usually rely on the famous results of Nash, de Giorgi, and Moser. In order to remove this assumption on the dimension in the diffusive case here an idea is to apply the well-known De Giorgi–Nash–Moser iteration technique combined with Schauder estimates, as was done for similar equations for example in [HNP15, Appendix A].

5.7.2 Convergence of the microscopic entropy to the macroscopic entropy

Another important question in the field of statistical mechanics is the convergence of the microscopic entropy $N^{-d}H^N(\mu_t^N|\nu^N)$ towards the macroscopic entropy. The goal of this subsection is to present our work in progress which is to investigate this problem and its relation to entropic chaos. The problem can be thought of independently from the results of the previous sections. We would like to recover the results as in [Kos01, Fat13].

Let us introduce first some notation. Let $(f_t)_{t \in [0, \infty)} \subset H$ be a solution to the limit equation (1.19) and set

$$f_\infty = \int_{\mathbb{T}^d} f_t(u) \, du,$$

which is independent of t . The notation is furthermore justified on noting that we expect $f_t \rightarrow f_\infty$ as $t \rightarrow \infty$ in, cf. Lemma 1.3. Furthermore we denote the pressure by

$$p(\lambda) = \log Z(e^\lambda), \tag{7.98}$$

where Z is the partition function given in equation (1.17). Then we let the macroscopic entropy be given by

$$H^\infty(f_t) := \int_{\mathbb{T}^d} h(f_t(u)) \, du - h(f_\infty), \tag{7.99}$$

where the function is given by

$$h(\rho) = \rho \log \sigma(\rho) - p(\log \sigma(\rho)).$$

Let us find the corresponding macroscopic Fisher information by differentiating in time. It holds that

$$\frac{d}{dt} H^\infty(f_t) = \int_{\mathbb{T}^d} \left(\partial_t f_t \log \sigma(f_t) + f_t \frac{\sigma'(f_t)}{\sigma(f_t)} \partial_t f_t - p'(\log \sigma(f_t)) \frac{\sigma'(f_t)}{\sigma(f_t)} \partial_t f_t \right) \, du.$$

Since σ is the inverse function of $\phi \partial_\phi \log Z(\phi)$, we find that $p'(\lambda) = \sigma^{-1}(e^\lambda)$ and hence

$$\frac{d}{dt} H^\infty(f_t) = - \int_{\mathbb{T}^d} \frac{\sigma'(f_t(u))^2}{\sigma(f_t(u))} |\nabla f_t(u)|^2 \, du =: -\mathcal{D}_\infty(f_t), \tag{7.100}$$

where $\mathcal{D}_\infty(f_t)$ is called the *macroscopic Fisher information*. Next we establish a microscopic analogue of equation (7.100), relating the microscopic entropy $H^N(\mu_t^N|\nu^N)$ and its Fisher information $D_N(\mu_t^N|\nu^N)$, to be defined presently. Let $f_t^N \in C_b(X_N)$ denote the density of $\mu_t^N \in P(X_N)$ with respect to the Gibbs measure $\nu^N \in P(X_N)$, i.e. set

$$f_t^N(\eta) := \frac{d\mu_t^N}{d\nu_{f_\infty}^N}(\eta). \tag{7.101}$$

The microscopic Fisher information is then defined as

$$\mathcal{D}_N(\mu_t^N | \nu_{f_\infty}^N) := \int_{X_N} \sqrt{f_t^N} N^{-2} \mathcal{L}_N \sqrt{f_t^N} d\nu_{f_\infty}^N = \left\langle \sqrt{f_t^N}, N^{-2} \mathcal{L}_N \sqrt{f_t^N} \right\rangle_{L^2(\nu_{f_\infty}^N)}. \quad (7.102)$$

Abusing notation, we shall sometimes refer to $\mathcal{D}_N(\mu_t^N | \nu_{f_\infty}^N)$ by $\mathcal{D}_N(f_t^N | \nu_{f_\infty}^N)$, where f_t^N is the density defined in (7.101). Also note that we have left out a factor of N^2 as opposed to the natural (*macroscopic*) time-scaling, i.e. the time scale of the Fisher information is the *microscopic* time scale.

Firstly we have indeed the equivalence of entropic chaos and convergence of the entropy. For example for the zero-range process we have the following lemma.

Lemma 7.1. *Under the conclusion of Corollary 1.4, i.e. the hydrodynamic limit for the zero-range process, it holds that*

$$N^{-d} H^N(\mu_t^N | \nu_{f_\infty}^N) = H^\infty(f_t) + N^{-d} H^N(\mu_t^N | \nu_{f_t(\cdot)}^N) + C \left(\frac{1}{N} + e^{-ct} N^{-\frac{1}{2+d}} \right).$$

In particular, the microscopic entropy $N^{-d} H^N(\mu_t^N | \nu^N)$ converges to the macroscopic entropy $H^\infty(f_t)$ if and only if there is entropic chaos, i.e. $N^{-d} H^N(\mu_t^N | \nu_{f_t(\cdot)}^N)$ vanishes as $N \rightarrow \infty$.

Proof. It holds that

$$\begin{aligned} \frac{1}{N^d} H^N(\mu_t^N | \nu_{f_\infty}^N) &= \frac{1}{N^d} \int_{X_N} \log \left(\frac{d\mu_t^N}{d\nu_{f_\infty}^N} \right) d\mu_t^N \\ &= \frac{1}{N^d} \int_{X_N} \log \left(\frac{d\mu_t^N}{d\nu_{f_t(\cdot)}^N} \right) d\mu_t^N + \int_{X_N} \log \left(\frac{d\nu_{f_t(\cdot)}^N}{d\nu_{f_\infty}^N} \right) d\mu_t^N. \end{aligned}$$

It holds that

$$\frac{d\nu_{f_t(\cdot)}^N}{d\nu_{f_\infty}^N}(\eta) = \prod_{x \in \mathbb{T}_N^d} \frac{Z(\sigma(f_\infty))}{Z(\sigma(f_t(x/N)))} \left(\frac{\sigma(f_t(x/N))}{\sigma(f_\infty)} \right)^{\eta(x)}, \quad (7.103)$$

Consequently, the second term equals

$$\begin{aligned} &\frac{1}{N^d} \int_{X_N} \log \left(\frac{d\nu_{f_t(\cdot)}^N}{d\nu_{f_\infty}^N} \right) d\mu_t^N \\ &= \frac{1}{N^d} \sum_{x \in \mathbb{T}_N^d} \int_{X_N} \left(\log \frac{Z(\sigma(f_\infty))}{Z(\sigma(f_t(x/N)))} + \eta(x) \log \frac{\sigma(f_t(x/N))}{\sigma(f_\infty)} \right) d\mu_t^N(\eta). \end{aligned}$$

We know that the macroscopic solution f_t is differentiable, and the hydrodynamic limit yields that the right hand side converges to

$$\int_{\mathbb{T}^d} f_t(u) \log \sigma(f_t(u)) du - \int_{\mathbb{T}^d} p(\log \sigma(f_t(u))) du - f_\infty \log \sigma(f_\infty) + p(\log \sigma(f_\infty)),$$

as $N \rightarrow \infty$. Thus, in view of (7.99), we have shown that

$$\frac{1}{N^d} H^N(\mu_t^N | \nu_{f_\infty}^N) = \frac{1}{N^d} H^N(\mu_t^N | \nu_{f_t(\cdot)}^N) + H^\infty(f_t) + C \left(\frac{1}{N} + e^{-ct} N^{-\frac{d}{2+d}} \right).$$

which concludes the proof. □

The main objective is then to show that under the initial assumption

$$\left| \frac{1}{N^d} H^N[\mu_0^N | \nu_{f_\infty}^N] - H^\infty(f_0) \right| \leq r_{H,0}(N)$$

for some rate function $r_{H,0}(N)$, there are rate function $r_1(N, t), r_2(N, t)$ so that

$$\left| \frac{1}{N^d} H^N[\mu_t^N | \nu_{f_\infty}^N] - H^\infty(f_t) \right| \leq r_{H,0}(N) + r_1(N, t),$$

and similarly for the Fisher information at rate $r_2(N, t)$.

Appendix

5.A Regularity properties of the quasilinear diffusion equation

As we saw for our proof of the hydrodynamic limit relies on a stability result for the limit PDE and in particular on estimates on the (uniform) propagation of higher regularity.

For the limit partial differential equation we consider solutions in

$$H := L^\infty(\mathbb{T}^d).$$

Note that in particular $H \subset L^2(\mathbb{T}^d)$. For each $f \in L^2(\mathbb{T}^d)$, define its $H^{-1}(\mathbb{T}^d)$ -norm by

$$\|f\|_{H^{-1}}^2 := - \int_{\mathbb{T}^d} f \Delta^{-1} f \, du$$

where $\Delta^{-1} f = \tilde{f}$ denotes the solution to the Poisson equation with boundary condition

$$\Delta \tilde{f} = f, \quad \text{such that} \quad \int_{\mathbb{T}^d} \tilde{f} \, du = 0.$$

This norm can be extended to $H^{-1}(\mathbb{T}^d)$ by density and is equivalent to the usual H^{-1} -operator norm. Furthermore it holds that

$$\langle f, \tilde{f} \rangle_{L^2} \leq \|\nabla f\|_{L^2} \|\tilde{f}\|_{H^{-1}} \quad \text{and} \quad \|f\|_{H^{-1}} \leq \|f\|_{L^2} \quad (1.104)$$

for all $f \in H^1(\mathbb{T}^d)$, $\tilde{f} \in H^{-1}(\mathbb{T}^d)$. In the almost linear case, when (4.50) holds, the theory of weak solutions to equation (1.19) is given by the following lemma.

Lemma 1.1 (Weak solutions to the quasi-linear diffusion equation). *For every $f_0 \in H$, the diffusion equation (1.19) possesses a unique weak solution $f_t \in H$, $t \in [0, \infty)$, in the sense that*

$$\int_0^\infty \int_{\mathbb{T}^d} (f_t(u) \partial_t \omega(t, u) + \sigma(f_t(u)) \Delta \omega(t, u)) \, dudt + \int_{\mathbb{T}^d} f_0(u) \omega(0, u) \, du = 0$$

for all $\omega \in C^1([0, \infty); C^2(\mathbb{T}^d))$ with compact support in $[0, \infty) \times \mathbb{T}^d$. Uniqueness thus yields a semigroup

$$S_t^\infty f_0 := f_t$$

The solution also has the following regularity properties. The semigroup S_t^∞ satisfies

$$\|S_t^\infty f_0\|_{L^p} \leq \|f_0\|_{L^p}$$

for all $1 \leq p \leq +\infty$. The solution $f = (f_t)_{t \in [0, T]}$ also satisfies

$$f \in L^2(0, \infty; H^1(\mathbb{T}^d)) \cap H^1(0, \infty; H^{-1}(\mathbb{T}^d)) \subset C([0, \infty); L^2(\mathbb{T}^d)).$$

In particular

$$\frac{d}{dt} \langle f_t, \varphi \rangle = \langle \sigma(f_t), \Delta \varphi \rangle \quad (1.105)$$

for all $t \geq 0$ and all $\varphi \in C^2(\mathbb{T}^d)$.

Proof. Starting from smooth solutions in $C^\infty(\mathbb{T}^d)$, c.f. Ladyzhenskaya [LSU68], it is classical to construct a weak solution using the uniform Hölder–continuity following from the results of de Giorgi–Nash–Moser. For an account of this construction, see also [KL99]. The maximum principle shows that the semigroup S_t^∞ conserves the $L^\infty(\mathbb{T}^d)$ –norm, i.e.

$$\|S_t^\infty f_0\|_{L^\infty} \leq \|f_0\|_{L^\infty}.$$

Therefore it holds that $S_t^\infty : H \rightarrow H$. Now, if we let f_t and \tilde{f}_t be two solutions, it holds that

$$\frac{d}{dt} \|f_t - \tilde{f}_t\|_{H^{-1}} = -2 \int_{\mathbb{T}^d} (f_t - \tilde{f}_t)(\sigma(f_t) - \sigma(\tilde{f}_t)) \, du \leq 0.$$

Thus the solutions are unique. Furthermore it holds that

$$\frac{d}{dt} \|f_t\|_{L^2}^2 = -2 \int_{\mathbb{T}^d} \sigma'(f_t) |\nabla f_t|^2 \, du,$$

whence S_t^∞ is a contraction in $L^2(\mathbb{T}^d)$ and

$$\int_0^T \int_{\mathbb{T}^d} |\nabla f_t|^2 \, dudt \leq C \int_0^T \int_{\mathbb{T}^d} \sigma'(f_t) |\nabla f_t|^2 \, dudt \leq C \|f_0\|_{L^2}^2.$$

is bounded. It follows that $f \in L^2(0, T; H^1(\mathbb{T}^d))$. The diffusion equation $\partial_t f_t = \Delta_c \sigma(f_t)$ consequently yields

$$f \in L^2(0, T; H^1(\mathbb{T}^d)) \cap H^1(0, T; H^{-1}(\mathbb{T}^d)).$$

Interpolation, see Theorem 3 in §5.9.2 in [Eva98], then yields $f \in C([0, T]; L^2(\mathbb{T}^d))$. Now

the weak form of the diffusion equation yields equation (1.105) for all $\varphi \in C^2(\mathbb{T}^d)$ and almost all $t \in [0, T]$. Since f is continuous in time with values in $L^2(\mathbb{T}^d)$, this equation indeed extends to all $t \in [0, T]$. Furthermore it holds that

$$\frac{d}{dt} \int_{\mathbb{T}^d} |f_t|^p du \leq -p(p-1) \int_{\mathbb{T}^d} |f_t|^{p-2} \sigma'(f_t) |\nabla f_t|^2 du \leq 0,$$

if f_t is bounded away from zero. The general case follows from approximation of the modulus function $|\cdot|$ by smooth functions, c.f. the book of Vazquez [V07]. \square

We will need an estimate on the conservation of regularity. For any integer $k > 0$ and $f \in H^k(\mathbb{T}^d)$, let $D^k f$ denote the k -th derivative of f (a tensor). Given $f_0 \in H$, consider the solution f_t to the diffusion equation (1.19) with initial datum f_0 .

Lemma 1.2 (Improved Regularity). *For $d = 1$, we have for all $k > 1$ a uniform in time upper bound on all the derivatives of order k*

$$\|D^k f_t\|_{L^2} \leq C \max \left\{ \|D^k f_0\|_{L^2}, \|\nabla f_0\|_{L^2}^{\frac{2k+1}{2}} + 1 \right\}. \quad (1.106)$$

Proof. Let $\mathfrak{k} \in \mathbb{N}^d$ be any multi-index such that $|\mathfrak{k}| = k$. The filtration equation yields that

$$\frac{d}{dt} \int_{\mathbb{T}^d} |D^{\mathfrak{k}} f_t|^2 du = -2 \int_{\mathbb{T}^d} \nabla D^{\mathfrak{k}} f_t D^{\mathfrak{k}} (\sigma'(f_t) \nabla f_t) du$$

By the Leibniz rule, this is bounded by

$$-2 \int_{\mathbb{T}^d} \sigma'(f_t) |\nabla D^{\mathfrak{k}} f_t|^2 du + C(k) \sum_{m; j_i} \int_{\mathbb{T}^d} \sigma^{(m+1)}(f_t) \nabla D^{\mathfrak{k}} f_t \cdot \nabla D^{\mathfrak{k} - \sum_i j_i} f_t \prod_{j=1}^m D^{j_j} f_t \quad (1.107)$$

where the sum is over all integers $m > 0$ and multi-indices $(j_i)_{i=1}^m$ such that $\sum_{i=1}^m j_i \leq \mathfrak{k}$ and $j_i \neq 0$ for all i . Thanks to Lemma 4.1, each summand of this sum is bounded from above by

$$C \|\nabla D^{\mathfrak{k}} f_t\|_{L^2} \|\nabla D^{\mathfrak{k} - \sum_i j_i} f_t \prod_{j=1}^m D^{j_j} f_t\|_{L^2}. \quad (1.108)$$

First we choose any coefficients $p, (p_i)_{i=1}^k$ such that $1/2 = 1/p + \sum_i 1/p_i$ to obtain that

$$\|\nabla D^{\mathfrak{k} - \sum_i j_i} f_t \prod_{j=1}^m D^{j_j} f_t\|_{L^2} \leq \|\nabla D^{\mathfrak{k} - \sum_i j_i} f_t\|_{L^p} \prod_{j=1}^m \|D^{j_j} f_t\|_{L^{p_j}}. \quad (1.109)$$

Note that every order n of the derivatives appearing in this product satisfies $1 \leq n \leq k$.

We recall here the Gagliardo-Nirenberg-Sobolev inequality for a real valued function h on \mathbb{R}^d : for fixed $1 \leq r, q \leq \infty$ and $m \in \mathbb{N}$, we assume that there are $\theta, j \in \mathbb{N}$ to be such

that

$$\frac{d}{p} - j = \left(\frac{d}{r} - m \right) \theta + \frac{d}{q} (1 - \theta), \quad \frac{j}{m} \leq \theta \leq 1.$$

Then

$$\|D^j h\|_{L^p} \leq C \|D^m h\|_{L^r}^\theta \|h\|_{L^q}^{1-\theta}. \quad (1.110)$$

We apply the above inequality for $r = q = 2$ and setting

$$\theta := \frac{-\frac{d}{p} + \frac{d}{2} + |\mathfrak{k} - \sum_i \mathfrak{j}_i|}{k} \quad \text{and} \quad \theta_i := \frac{-\frac{d}{p_i} + \frac{d}{2} + |\mathfrak{j}_i| - 1}{k}.$$

Note that

$$\frac{|\mathfrak{k} - \sum_i \mathfrak{j}_i|}{k} \leq \theta \leq 1 \quad \text{and} \quad \frac{|\mathfrak{j}_i| - 1}{k} \leq \theta_i \leq 1$$

and that

$$\theta + \sum_i \theta_i = 1 - \frac{m(1 - d/2)}{k} \leq 1 - \frac{1}{2k} \quad \text{and} \quad (1 - \theta) + \sum_i (1 - \theta_i) \leq k + \frac{1}{2}$$

since $1 \leq m \leq k$ and $d = 1$. Then the Gagliardo-Nirenberg-Sobolev inequality and the fact that $m \leq k$ yields

$$\begin{aligned} \|\nabla D^{\mathfrak{k} - \sum_i \mathfrak{j}_i} f_t\|_{L^p} \prod_{j=1}^m \|D^{\mathfrak{j}_j} f_t\|_{L^{p_j}} &\leq C \|D^{k+1} f_t\|_{L^2}^{\frac{2k-m}{2k}} \|\nabla f_t\|_{L^2}^{m + \frac{m}{2k}} \\ &\leq C \|D^{k+1} f_t\|_{L^2}^{\frac{2k-1}{2k}} \|\nabla f_t\|_{L^2}^{\frac{2k+1}{2k}} + 1). \end{aligned} \quad (1.111)$$

By the previous lemma, it holds that $\|f_t\|_{L^\infty} \leq \|f_0\|_{L^\infty}$ and $\|\nabla f_t\|_{L^2} \leq C \|\nabla f_0\|_{L^2}$. Therefore we conclude that for all k , there exist constants $0 < c$ and $C < \infty$ such that

$$\frac{d}{dt} \|D^k f_t\|_{L^2}^2 \leq -c \|D^{k+1} f_t\|_{L^2}^2 + C \left(\|D^{k+1} f_t\|_{L^2}^{2 - \frac{1}{2k}} \|\nabla f_0\|_{L^2}^{\frac{2k+1}{2}} + 1 \right). \quad (1.112)$$

Since the integral of the derivative $D^k f_t$ over the torus \mathbb{T}^d vanishes, Poincaré's inequality yields

$$\|D^k f_t\|_{L^2}^2 \leq C \|D^{k+1} f_t\|_{L^2}^2.$$

We can choose therefore $C' > \text{large enough}$ so that the right-hand side of (1.112) is negative when $\|D^k f_t\| \geq C'$. We then deduce that

$$\|D^k f_t\|_{L^2} \leq C \max \left\{ \|D^k f_0\|_{L^2}, \|\nabla f_0\|_{L^2}^{\frac{2k+1}{2}} + 1 \right\},$$

which concludes the proof of the statement. \square

Next provide some large-time decay estimates which will enable us to provide uniform in time bounds in the hydrodynamic limit.

Lemma 1.3 (Spectral gap). *Let $f_0 \in L^\infty(\mathbb{T}^d)$. Furthermore let $f_\infty = \int_{\mathbb{T}^d} f(u) du$ denote the spatial average of f . Then there exist finite, positive constants c, C such that*

$$\begin{aligned} \|f_t - f_\infty\|_{L^p}^p &\leq C e^{-ct} \|f_0 - f_\infty\|_{L^p}^p, \quad \text{for all } 2 \leq p < +\infty, \\ \|f_t - f_\infty\|_{H^{-1}} &\leq C e^{-ct} \|f_0 - f_\infty\|_{H^{-1}}, \\ \|f_t - f_\infty\|_{L^\infty} &\leq C e^{-ct} \|f_0 - f_\infty\|_{H^{-1}}. \end{aligned} \quad (1.113)$$

Proof. Let f_t be a solution to the diffusion equation. First of all, conservation of mass yields $\int f_t(u) du = f_\infty$. Let $\bar{f}_t := f_t - f_\infty$, which solves the equation

$$\partial_t \bar{f}_t = \nabla \cdot (\sigma'(\bar{f}_t + f_\infty) \nabla \bar{f}_t). \quad (1.114)$$

Note that in contrast to f_t , the function \bar{f}_t is no longer non-negative everywhere. The equation for \bar{f}_t yields

$$\frac{d}{dt} \int_{\mathbb{T}^d} |\bar{f}_t|^p du = p \int_{\mathbb{T}^d} |\bar{f}_t|^{p-2} \bar{f}_t \nabla \cdot (\sigma'(\bar{f}_t + f_\infty) \nabla \bar{f}_t) du. \quad (1.115)$$

Now integration by parts yields

$$\frac{d}{dt} \int_{\mathbb{T}^d} |\bar{f}_t|^p du = -p(p-1) \int_{\mathbb{T}^d} \sigma'(\bar{f}_t + f_\infty) |\bar{f}_t|^{p-2} |\nabla \bar{f}_t|^2 du. \quad (1.116)$$

Since

$$|\bar{f}_t|^{p-2} |\nabla \bar{f}_t|^2 = |\bar{f}_t|^{p/2-1} |\nabla \bar{f}_t|^2 = \frac{4}{p^2} |\nabla |\bar{f}_t|^{p/2}|^2, \quad (1.117)$$

it holds that

$$\frac{d}{dt} \int_{\mathbb{T}^d} |\bar{f}_t|^p du = -\frac{4(p-1)}{p} \int_{\mathbb{T}^d} \sigma'(\bar{f}_t + f_\infty) |\nabla |\bar{f}_t|^{p/2}|^2 du \leq -c \int_{\mathbb{T}^d} |\nabla |\bar{f}_t|^{p/2}|^2 du. \quad (1.118)$$

Now Poincaré's inequality in the L^2 -norm applied to $|\bar{f}_t|^{p/2}$ yields

$$\frac{d}{dt} \int_{\mathbb{T}^d} |\bar{f}_t|^p du \leq -c \int_{\mathbb{T}^d} |\bar{f}_t|^p du, \quad (1.119)$$

which yields the decay of the L^p -norms of $\bar{f}_t = f_t - f_\infty$. Note that c, C can be taken to be independent of the choice of $p \geq 2$.

The decay of the H^{-1} -norm follows from

$$\frac{d}{dt} \|f_t - f_\infty\|_{H^{-1}}^2 = -2 \int_{\mathbb{T}^d} \sigma'(f_t(u)) (f_t(u) - f_\infty)^2 du \leq -c \|f_t - f_\infty\|_{H^{-1}}^2 \quad (1.120)$$

by uniform ellipticity and (1.104).

Next, in order to show the exponential convergence with respect to the L^∞ norm we use that for $k > (d + 2)/2$, there exists a bounded embedding $H^{k-1}(\mathbb{T}^d) \hookrightarrow L^\infty(\mathbb{T}^d)$ and therefore

$$\|f_t - f_\infty\|_{L^\infty} \leq C \|f_t - f_\infty\|_{H^{k-1}}.$$

Moreover interpolation yields

$$\|f_t - f_\infty\|_{H^{k-1}} \leq \|f_t - f_\infty\|_{H^k}^{\frac{k}{k+1}} \|f_t - f_\infty\|_{H^{-1}}^{\frac{1}{k+1}}.$$

Since Lemma 1.2 yields uniform-in-time bounds on the higher order H^k -norms of f_t , we have uniform-in-time bounds on the H^k -norms of $(f_t - f_\infty)$ as well. The existence of spectral gap in H^{-1} -norm then implies that

$$\begin{aligned} \|f_t - f_\infty\|_{L^\infty} &\lesssim C e^{-ct} \|f_0 - f_\infty\|_{H^{-1}}^{\frac{1}{k+1}} \left(\max \{ \|D^k f_0\|_{L^2}, \|\nabla f_0\|_{L^2}^{\frac{2k+1}{2}} + 1 \} \right)^{\frac{k}{k+1}} \\ &\leq C e^{-ct} \|f_0 - f_\infty\|_{H^{-1}}. \end{aligned}$$

This ensures us that the semigroup relaxes indeed exponentially fast in L^∞ -norm as well. \square

Chapter 6

Spectral gap in mean-field $\mathcal{O}(n)$ -model

This chapter is a joint work with Simon Becker and it is published in [BM20].

We study the dependence of the spectral gap for the generator of the Ginzburg-Landau dynamics for all $\mathcal{O}(n)$ -models with mean-field interaction and magnetic field, below and at the critical temperature on the number N of particles. For our analysis of the Gibbs measure, we use a one-step renormalization approach and semiclassical methods to study the eigenvalue-spacing of an auxiliary Schrödinger operator.

6.1 Introduction and main results

6.1.1 $\mathcal{O}(n)$ -model

The model we are concerned with in this article is the generator of the Ginzburg-Landau dynamics, or overdamped Langevin dynamics, of the mean-field $\mathcal{O}(n)$ -model in the critical and supercritical regime $\beta \geq n$, as defined precisely in Section 6.2. Our objective is to study the scaling of the spectral gap in terms of the system size N , for all the numbers of components $n \geq 1$, and including the cases with or without external magnetic field, in the low temperature and critical regime, extending the study of the subcritical regime $\beta < n$ in [BB19]. When $\beta < n$, the spectral gap of the generator remains open uniformly in N and for any number of components n , in the full temperature range.

The mean-field $\mathcal{O}(n)$ -model is defined by the energy function

$$H(\sigma) = \frac{1}{2} \sum_{x \in [N]} \sigma(x)(-\Delta_{\text{MF}}\sigma)(x) - \frac{1}{\beta} \sum_{x \in [N]} \langle h, \sigma(x) \rangle \quad (1.1)$$

acting on spin configurations $\sigma : \{1, \dots, N\} \rightarrow \mathbb{S}^{n-1}$ where Δ_{MF} is the mean-field Laplacian and $h \in \mathbb{R}^n$ an external magnetic field. For our study of spectral gaps, we consider the Ginzburg-Landau dynamics associated with the Gibbs measure $d\rho \propto e^{-\beta H(\sigma)}$ with Hamilton function (1.1). The inverse temperature parameter β is such that lower temperatures (higher β) favors alignment of spins. The study of mean-field $\mathcal{O}(n)$ -models is motivated by the fact that their behavior approximates that of the full $\mathcal{O}(n)$ -model on high-dimensional tori [Ell85, LLP].

6.1.2 State of the art and motivation

The study of spectral gaps in $\mathcal{O}(n)$ models is a popular problem that has received a lot of attention over the last decades. The study of logarithmic Sobolev (and other functional) inequalities is a classical and very effective tool to study concentration of measures and to quantify the relaxation rates, *i.e.* the mixing properties, of the dynamics. In particular, the spectral gap (the speed of relaxation) is determined by the constant in the Log-Sobolev inequalities. We define the spectral gap to be the size of the gap between 0 and the rest of the spectrum of the associated generator L , defined in (2.5). The gap then can be also characterized by

$$\lambda_S := \inf_{f \in L^2(d\rho) \setminus \{0\}} \frac{-\langle Lf, f \rangle_{L^2(d\rho)}}{\text{Var}_\rho(f)} \quad (1.2)$$

where Var_ρ is the variance relative to the equilibrium measure ρ . All these quantities will be specified for our setting in the following section. For further background on functional

inequalities see [Gro93, BE85, Led99, Led01, GZ03, ABC+00] and references therein.

There are only few general approaches for the study of spectral gaps of spin systems, using log-Sobolev inequalities, available and many of them rely on an asymptotic study of log-Sobolev inequalities [LY93, SZ92a, SZ92b, SZ92c] or [MO13] for a more recent result in that direction. In the article [BB19], a simpler proof for a log-Sobolev inequality was provided for bounded and unbounded spin systems and sufficiently high temperatures. The novelty of the approach in [BB19] is the combination of the study of log-Sobolev inequalities with a simple renormalization group approach to decompose the stationary measure in a way that makes it accessible to Bakry-Émery techniques.

Inspired by the method in [BB19], we invoke the same one-step renormalization group procedure to reduce the high-dimensional problem to the study of a low-dimensional *renormalized measure* and a *fluctuation measure*. In the subcritical regime $\beta < n$, which is the regime analyzed in [BB19], the renormalization of the equilibrium measure is particularly efficient, since the renormalized potential is strictly convex such that the Bakry-Émery criterion can be directly applied to this measure and implies that the spectral gap remains open. This renormalization group method has recently also been successfully applied in the study of the spectral gap for hierarchical spin models [BBb] and for a lattice discretization of a massive Sine-Gordon model [BBa].

The low temperature regime, which is the regime we are concerned about within this article, has a non-convex renormalized potential. In this regime, after a single renormalization step, the renormalized potential is not convex. This makes the asymptotic analysis much more difficult and requires new methods:

While we analyze the *Ising model*, $n = 1$, without magnetic field, directly using explicit criteria for spectral gap and log-Sobolev inequalities [BG99, BGL14], we heavily use the equivalence between the generator of the Ginzburg-Landau dynamics and a Schrödinger operator to analyze multi-component, $n \geq 2$, $\mathcal{O}(n)$ -models. This analysis builds heavily upon ideas by Simon [Sim83, CFKS87] and Helffer-Sjöstrand [HS85, HS87] who developed effective semiclassical methods to study the low-lying spectrum of Schrödinger operators in the semiclassical limit (which in our case corresponds to $N \rightarrow \infty$). These results are discussed thoroughly in the final chapters of [NH05]. In this article however, we have to study the spectrum of Schrödinger operators beyond the harmonic approximation. In this case, the limiting operator is not explicitly diagonalizable anymore and the spacing between eigenvalues is no longer linear in the semiclassical parameter N , the number of spins.

The mixing time of the Glauber dynamics of the mean-field Ising model ($\mathcal{O}(1)$) *without magnetic field* has been carefully analyzed in [DLP09b, DLP09a]. There it is shown-among others- that the mixing time in the subcritical regime $\beta < 1$ is $N \log(N)$, the scaling at the critical point $N^{3/2}$ for $\beta = 1$ and in the supercritical regime $\beta > 1$ it is exponential

growing in N . This is to be compared to a spectral gap that remains open for $\beta < 1$, closes like $N^{-1/2}$ for $\beta = 1$ and closes exponentially fast also for $\beta > 1$. Thus, the mixing time for the Glauber dynamics are -up to a factor $1/N$ - comparable to our findings on the spectral gap, cf. Theorem 1.1.

Our main result on the mean-field *Ising* model in the supercritical regime $\beta > n$ is stated in the following Theorem:

Theorem 1.1 (Spectral gap–Supercritical Mean-field Ising models, $\beta > 1$). *Let N be the number of spins and n the number of components.*

For the supercritical mean-field Ising model ($n = 1, \beta > 1$), the spectral gap λ_N of the generator

- *for the case of small magnetic fields $|h| < h_c$, closes as $N \rightarrow \infty$ exponentially fast, $\lambda_N = e^{-N\Delta_{\text{small}}(V)(1+o(1))}$. In particular, for magnetic fields $h \in [0, h_c)$*

$$\Delta_{\text{small}}(V) = \int_{\gamma_1(\beta)}^{\gamma_2(\beta)} \beta (\varphi - \tanh(\beta\varphi + h)) d\varphi$$

where $\gamma_1(\beta) \leq \gamma_2(\beta) \in \mathbb{R}$ are the two smallest numbers satisfying the condition

$$\gamma(\beta) = \tanh(\gamma(\beta) \beta + h).$$

- *For critical magnetic fields $|h| = h_c$, the spectral gap does not close faster than $\mathcal{O}(N^{-1/3})$ anymore.*
- *Finally, for strong magnetic fields $|h| > h_c$, it is bounded away from zero uniformly in N .*

where $h_c = \sqrt{\beta(\beta - 1)} - \text{arccosh}(\sqrt{\beta})$.

In the case of supercritical multi-component systems ($n \geq 2, \beta > n$) without magnetic fields, it is the rotational invariance of the model that leads to a decay of the spectral gap as N tends to infinity. To capture this property, we call a function $f : (\mathbb{S}^n)^N \rightarrow \mathbb{R}$ *radial*, if it is only a function of the norm of the mean spin $|\bar{\sigma}|$. Our main results for all multi-component systems in the supercritical regime $\beta > n$ are summarized in the following Theorem:

Theorem 1.2 (Spectral gap–Supercritical Mean-field $\mathcal{O}(n)$ -models, $\beta > n \geq 2$). *Let N be the number of spins and n the number of components.*

For the supercritical mean-field $\mathcal{O}(n)$ -models ($n \geq 2, \beta > n$), the spectral gap λ_N of the generator

- closes as $\lambda_N = \mathcal{O}(N^{-1})$ if there is no external magnetic field $h = 0$, but remains open $\lambda_N = \mathcal{O}(1)$ for radial functions.
- is bounded away from zero uniformly in the number of spins for all $h \in \mathbb{R}^n \setminus \{0\}$.

We also analyze the behavior of the spectral gap at the critical point $\beta = n$ and $h = 0$. Using a discrete Fourier analysis approach implemented in Section 6.6 for the Ising case $n = 1$ and a direct asymptotic analysis for all higher component systems $n \geq 2$, we find a different asymptotic of the spectral gap from both the supercritical $\beta > n$ (exponentially fast closing) and subcritical $\beta < n$ (spectral gap remains open) regimes:

Theorem 1.3 (Spectral gap–Critical Mean-field $\mathcal{O}(n)$ models, $\beta = n$). *For all critical, $\beta = n$, $h = 0$ mean-field $\mathcal{O}(n)$ -models the spectral gap closes as $\lambda_N = \mathcal{O}(N^{-1/2})$. In particular, the rate $N^{-1/2}$ is attained for the magnetization*

$$M(\sigma) = N^{-1/2} \sum_{x \in [N]} \sigma(x).$$

We emphasize that at the critical points ($\beta = n$, $h = 0$), the gap does no longer close once a non-zero magnetic field is present:

Theorem 1.4 (Spectral gap–Mean-field $\mathcal{O}(n)$ models, $\beta = n$, $h \neq 0$). *For all, $\beta = n$ and $h \neq 0$, the spectral gap of all mean-field $\mathcal{O}(n)$ -models remains open.*

The proof of Theorem 1.4 is along the lines of Theorem 1.1 in the regime $h > h_c$ and follows from Proposition 4.2 in the Ising-case, $n = 1$, and in the multi-component case, $n \geq 2$, from Proposition 5.4.

6.1.3 Organization of the chapter

The chapter is organized as follows:

- In Section 6.2 we introduce the mean-field $\mathcal{O}(n)$ -model.
- In Section 6.3 we introduce the renormalized methods.
- In Section 6.4 we analyze the mean-field Ising model in the supercritical regime $\beta > 1$ and prove Theorem 1.1.
- In Section 6.5 we analyze the higher-component mean-field $\mathcal{O}(n)$ -models in the supercritical regime $\beta > n$ and prove Theorem 1.2.
- In Section 6.6 we study the critical regime and prove both Theorems 1.3 and 1.4.

- Our article contains an appendix that contains technical details and further details on numerical methods.

Notation. We write $f(z) \leq \mathcal{O}(g(z))$ to indicate that there is $C > 0$ such that $|f(z)| \leq C|g(z)|$ and $f(z) = o(g(z))$ for $z \rightarrow z_0$ if there is for any $\varepsilon > 0$ a neighbourhood U_ε of z_0 such that $|f(z)| \leq \varepsilon|g(z)|$. The expectation with respect to a measure μ is denoted by $\mathbb{E}_\mu(X)$. The normalized surface measure on the n sphere is denoted as $dS_{\mathbb{S}^n}$. We write $\mathbb{1}$ to denote a vector or matrix whose entries are all equal to one and id for the identity map. Finally, we introduce the notation $[N] := \{1, \dots, N\}$. The eigenvalues of a self-adjoint matrix A shall be denoted by $\lambda_1(A) \leq \dots \leq \lambda_N(A)$.

6.2 The mean-field $\mathcal{O}(n)$ -model

We study the mean-field $\mathcal{O}(n)$ -model with spin configuration $\sigma : [N] \rightarrow \mathbb{S}^{n-1}$ and introduce the mean-field Laplacian $(\Delta_{\text{MF}}\sigma)(x) := \frac{1}{N} \sum_{y \in [N]} (\sigma(y) - \sigma(x))$.

The mean spin is defined as $\bar{\sigma} := \frac{1}{N} \sum_{x \in [N]} \sigma(x)$. The energy of a spin configuration σ is given by the *Curie-Weiss Hamiltonian*

$$\begin{aligned} H(\sigma) &= \frac{1}{2} \sum_{x \in [N]} \sigma(x) (-\Delta_{\text{MF}}\sigma)(x) - \frac{1}{\beta} \sum_{x \in [N]} \langle h, \sigma(x) \rangle \\ &= \frac{1}{4N} \sum_{x, y \in [N]} |\sigma(x) - \sigma(y)|^2 - \frac{1}{\beta} \sum_{x \in [N]} \langle h, \sigma(x) \rangle \\ &= \frac{N}{2} (1 - |\bar{\sigma}|^2) - \frac{N}{\beta} \langle h, \bar{\sigma} \rangle. \end{aligned} \tag{2.3}$$

where the constant vector $h \in \mathbb{R}^n$ represents an external magnetic field and β is the inverse temperature of the system. The energy of the system can thus be written as a function of the mean-spin $\bar{\sigma}$. This is also why the model is called a mean-field model.

The critical temperature for the $\mathcal{O}(n)$ -models is $\beta = n$ and we study both regimes: the supercritical regime $\beta > n$ and the critical regime $\beta = n$.

The dynamics we consider is the continuous-time Ginzburg-Landau dynamics

$$\partial_t f = \sum_{x \in [N]} \left\langle \nabla_{\mathbb{S}^{n-1}}^{(x)}, \beta^{-1} \nabla_{\mathbb{S}^{n-1}}^{(x)} f + f \nabla_{\mathbb{S}^{n-1}}^{(x)} H \right\rangle_{\mathbb{R}^n} \tag{2.4}$$

to the invariant distribution of the mean-field $\mathcal{O}(n)$ -model which is the Gibbs measure $d\rho(\sigma) := e^{-\beta H(\sigma)} / Z dS_{\mathbb{S}^{n-1}}^{\otimes N}(\sigma)$ with normalizing constant Z . The operators $\Delta_{\mathbb{S}^{n-1}}^{(x)}$ defined by $\langle f, -\Delta_{\mathbb{S}^{n-1}}^{(x)} f \rangle := \langle \nabla_{\mathbb{S}^{n-1}}^{(x)} f, \nabla_{\mathbb{S}^{n-1}}^{(x)} f \rangle$ and $\nabla_{\mathbb{S}^{n-1}}^{(x)}$ are the Laplace-Beltrami and gradient operator on \mathbb{S}^{n-1} acting on spin i , respectively. We recall that for the Ising model $n = 0$ and a function $F : \mathbb{S}^0 \rightarrow \mathbb{R}$, the gradient is given by $(\nabla_{\mathbb{S}^0} F)(\sigma) = F(\sigma) - F(-\sigma)$. The $L^2((\mathbb{S}^{n-1})^N)$ -adjoint of the generator of the Kramers-Smoluchowski equation (2.4) is the

generator

$$(L\zeta)(\sigma) := \sum_{x \in [N]} \beta^{-1} (\Delta_{\mathbb{S}^{n-1}}^{(x)} \zeta)(\sigma) - \langle (\nabla_{\mathbb{S}^{n-1}}^{(x)} H)(\sigma), (\nabla_{\mathbb{S}^{n-1}}^{(x)} \zeta)(\sigma) \rangle_{\mathbb{R}^n}. \quad (2.5)$$

Studying the operator L on the weighted space $L^2((\mathbb{S}^{n-1})^N, d\rho)$ makes this generator self-adjoint. The quadratic form of the generator (2.5) is just a rescaled Dirichlet form

$$-\langle Lf, f \rangle_{L^2(d\rho)} = \beta^{-1} \sum_{x \in [N]} \left\| \nabla_{\mathbb{S}^{n-1}}^{(x)} f \right\|_{L^2(d\rho)}^2.$$

6.3 Renormalized measure and mathematical preliminaries

We start with the definition of entropy with respect to probability measures:

Definition 3.1 (Entropy). *For a probability measure μ on some Borel set Ω the entropy $\text{Ent}_\mu(F)$ of a positive measurable function $F : \Omega \rightarrow \mathbb{R}_{\geq 0}$ with $\int_\Omega F(x) \log^+(F(x)) d\mu(x) < \infty$ is defined as*

$$\text{Ent}_\mu(F) := \int_\Omega F(x) \log \left(F(x) / \int_\Omega F(y) d\mu(y) \right) d\mu(x). \quad (3.6)$$

Instead of studying the generator of the dynamics directly, we apply a one step renormalization first [BBS19, Sec. 1.4]:

Definition 3.2 (Renormalized quantities). *The renormalized single spin potential V_n associated with the mean-field $\mathcal{O}(n)$ -model for $\varphi \in \mathbb{R}^n$ is defined as*

$$\begin{aligned} V_n(\varphi) &= -\log \int_{\mathbb{S}^{n-1}} e^{-\frac{\beta}{2} \|\varphi - \sigma\|^2 + \langle h, \sigma \rangle} dS_{\mathbb{S}^{n-1}}(\sigma) \\ &= \frac{\beta}{2} (1 + \|\varphi\|^2) - \log \left(\Gamma \left(\frac{n}{2} \right) \left(\frac{2}{\|\beta\varphi + h\|} \right)^{\frac{n}{2}-1} I_{\frac{n}{2}-1}(\|\beta\varphi + h\|) \right) \end{aligned} \quad (3.7)$$

where I is the modified Bessel function of the first kind. The N -particle renormalized measure is defined for a normalizing constant $\nu_N^{(n)}$ by

$$d\nu_N(\varphi) = \nu_N^{(n)} e^{-NV_n(\varphi)} d\varphi \text{ on } \mathbb{R}^n. \quad (3.8)$$

Definition 3.3 (Fluctuation measure). *For any $\varphi \in \mathbb{R}^n$, there is a probability measure μ_φ , the fluctuation measure, on $(\mathbb{S}^{n-1})^N$ defined as*

$$\mathbb{E}_{\mu_\varphi}(F) = \int_{(\mathbb{S}^{n-1})^N} F(\sigma) e^{NV_n(\varphi)} \prod_{x \in [N]} e^{-\frac{\beta}{2} \|\varphi - \sigma(x)\|_2^2 + \langle h, \sigma(x) \rangle} dS(\sigma(x)). \quad (3.9)$$

A straightforward calculation, [BBS19, Lemma 1.4.3] shows that the stationary measure $d\rho$ can be decomposed into the fluctuation and renormalized measure such that $\mathbb{E}_\rho(F) = \mathbb{E}_{\nu_N}(\mathbb{E}_{\mu_\varphi}(F))$.

Example 1. *In the case of the Ising model ($n = 1$) the renormalized potential is*

$$V_1(\varphi) = \frac{\beta}{2}(1 + \varphi^2) - \log(\cosh(\beta\varphi + h)). \quad (3.10)$$

For the XY model ($n = 2$) the renormalized potential reads

$$V_2(\varphi) = \frac{\beta}{2}(1 + \|\varphi\|^2) - \log(I_0(\|\beta\varphi + h\|)) \quad (3.11)$$

where I is the modified Bessel function of the first kind. For the Heisenberg model ($n = 3$) one finds

$$V_3(\varphi) = \frac{\beta}{2}(1 + \|\varphi\|^2) - \log\left(\frac{\sinh\|\beta\varphi + h\|}{\|\beta\varphi + h\|}\right).$$

We observe that the renormalized potential grows quadratically at infinity such that $\Delta V_n \in L^\infty(\mathbb{R}^n)$.

The Ginzburg-Landau dynamics for the renormalized measure is then given by the self-adjoint operator $L_{\text{ren}} : D(L_{\text{ren}}) \subset L^2(\mathbb{R}^n, d\nu_N) \rightarrow L^2(\mathbb{R}^n, d\nu_N)$, satisfying

$$(L_{\text{ren}}\zeta)(\varphi) = (\Delta_{\mathbb{R}^n}\zeta)(\varphi) - N \langle \nabla_{\mathbb{R}^n} V_n(\varphi), \nabla_{\mathbb{R}^n} \zeta(\varphi) \rangle. \quad (3.12)$$

The renormalized generator L_{ren} satisfies

$$-\langle L_{\text{ren}} f, f \rangle_{L^2(d\nu_N)} = \|\nabla_{\mathbb{R}^n} f\|_{L^2(d\nu_N)}^2. \quad (3.13)$$

The renormalized Schrödinger operator with null space spanned by e^{-NV_n} is the operator defined by conjugation $-\Delta_{\text{ren}} = e^{-NV_n/2} L_{\text{ren}} e^{NV_n/2}$

$$\Delta_{\text{ren}} = -\Delta_{\mathbb{R}^n} + \frac{N^2}{4} |\nabla V_n(\varphi)|^2 - \frac{N}{2} \Delta V_n(\varphi). \quad (3.14)$$

Definition 3.4 (LSI and SGI). *Let μ be a Borel probability measure on \mathbb{R}^n . We say that μ satisfies a logarithmic Sobolev inequality LSI(k) iff*

$$\text{Ent}_\mu(f^2) \leq \frac{2}{k} \|\nabla f\|_{L^2(d\mu)}^2$$

for all smooth functions f . The LSI(k) implies [Led99, Prop. 2.1] that μ satisfies a spectral gap inequality SGI(k)

$$\text{Var}_\mu(f) \leq \frac{1}{k} \|\nabla f\|_{L^2(d\mu)}^2.$$

Thus, in light of the characterisation (1.2), the spectral gap of L_{ren} is by (3.13) precisely

the constant in the SGI of the renormalized measure.

Remark 3.5. *If f vanishes outside a set Ω of measure $\mu(\Omega) < 1$ and if μ satisfies a SGI(k) then*

$$\|f\|_{L^2(d\mu)}^2 \leq \frac{1}{k(1-\mu(\Omega))} \|\nabla f\|_{L^2(d\mu)}^2. \quad (3.15)$$

For Borel probability measures μ on \mathbb{R} there is an explicit characterization of the measures satisfying a LSI [BG99, Theorem 5.3]:

Any such measure μ satisfies a LSI(k) iff there exist absolute constants $K_0 = 1/150$ and $K_1 = 468$ such that the optimal value k in the LSI(k) satisfies

$$K_0(D_0 + D_1) \leq 1/k \leq K_1(D_0 + D_1)$$

for finite D_0 and D_1 . Let m be the median of μ and $p(t) dt$ the absolutely continuous part of μ with respect to Lebesgue measure. The constants D_0 and D_1 are given by

$$\begin{aligned} D_0 &:= \sup_{x < m} \left(-\mu((-\infty, x]) \log(\mu((-\infty, x])) \int_x^m \frac{ds}{p(s)} \right) \text{ and} \\ D_1 &:= \sup_{x > m} \left(-\mu([x, \infty)) \log(\mu([x, \infty))) \int_m^x \frac{ds}{p(s)} \right). \end{aligned} \quad (3.16)$$

For constants

$$B_0 := \sup_{x < m} \left(\mu((-\infty, x]) \int_x^m \frac{ds}{p(s)} \right) \text{ and } B_1 := \sup_{x > m} \left(\mu([x, \infty)) \int_m^x \frac{ds}{p(s)} \right) \quad (3.17)$$

one defines the Muckenhoupt number [Muc72] $B := \max(B_0, B_1)$. The measure μ satisfies then a SGI with optimal constant $c = 1/k$ if and only if B is finite in which case

$$B/2 \leq c \leq 4B \quad (3.18)$$

[BGL14, Theorem 4.5.1].

Remark 3.6. *The proof given in [BG99, Theorem 5.3] shows that the characterization of LSI constants holds true not only by splitting at the median: Instead, there is $\varepsilon > 0$ such that for any ζ for which $\mu((-\infty, \zeta]), \mu([\zeta, \infty)) \in (1/2 - \varepsilon, 1/2 + \varepsilon)$ the above characterization (3.16) holds true when the median m is replaced by ζ . The same is, up to an unimportant adaptation of the lower bound in (3.18), for the SGI as well, cf. [GR01, Prop. 3.2 + 3.3].*

We continue by observing that the fluctuation measures satisfy a LSI($\frac{2}{\gamma_n}$) independent of h or φ . This follows for $n = 1$ with $\gamma_n = 4$ from a simple application of the tensorization principle to the classical bound on the Bernoulli distribution [ABC⁺00, Led01, SC97]. For number of components $n \geq 2$ one can use the results from [ZQM11].

Proposition 3.7. *Let the renormalized measure ν_N satisfy a LSI(λ), then the full equilibrium measure ρ satisfies a LSI*

$$\text{Ent}_\rho(F^2) \leq \frac{2}{\gamma_n} \left(1 + \frac{8N\beta^2}{\lambda}\right) \sum_{x \in [N]} \left\| \nabla_{\mathbb{S}^{n-1}}^{(x)} F \right\|_{L^2(d\rho)}^2$$

and if the renormalized measure ν_N satisfies a SGI(λ), then the equilibrium measure ρ satisfies a SGI

$$\text{Var}_\rho(F) \leq \frac{1}{\gamma_n} \left(1 + \frac{4N\beta^2}{\lambda}\right) \sum_{x \in [N]} \left\| \nabla_{\mathbb{S}^{n-1}}^{(x)} F \right\|_{L^2(d\rho)}^2.$$

Proof. The proof of the SGI is as follows: For the SGI we obtain the decomposition

$$\begin{aligned} \text{Var}_\rho(F) &= \mathbb{E}_{\nu_N}(\text{Var}_{\mu_\varphi}(F)) + \text{Var}_{\nu_N}(\mathbb{E}_{\mu_\varphi}(F)) \\ &\leq \frac{1}{\gamma_n} \sum_{x \in [N]} \left\| \nabla_{\mathbb{S}^{n-1}}^{(x)} F \right\|_{L^2(d\rho)}^2 + \frac{1}{\lambda} \mathbb{E}_{\nu_N} \left(\left| \nabla_\varphi \mathbb{E}_{\mu_\varphi}(F) \right|^2 \right). \end{aligned} \quad (3.19)$$

To bound the second term in the above estimate, we compute using the Cauchy-Schwarz inequality and the spectral gap inequality for fluctuation measures μ_φ on the sphere, defined by (3.9) such that, see [BB19, Theorem 1, (11)-(15)],

$$\nabla_\varphi \mathbb{E}_{\mu_\varphi}(F) = N \nabla V(\varphi) \mathbb{E}_{\mu_\varphi}(F) - \beta \sum_{x \in [N]} \mathbb{E}_{\mu_\varphi}(F(\varphi - \sigma_x)). \quad (3.20)$$

We then use that by the explicit expression (3.7)

$$\nabla V(\varphi) = \beta \frac{\int_{\mathbb{S}^{n-1}} e^{-\frac{\beta}{2} \|\varphi - \sigma_x\|^2} (\varphi - \sigma_x) dS_{\mathbb{S}^{n-1}}(\sigma_x)}{\int_{\mathbb{S}^{n-1}} e^{-\frac{\beta}{2} \|\varphi - \sigma_x\|^2} dS_{\mathbb{S}^{n-1}}(\sigma_x)} = \beta (\varphi - \mathbb{E}_{\mu_\varphi}(\sigma_x)). \quad (3.21)$$

Inserting this into (3.20) we find that

$$\nabla_\varphi \mathbb{E}_{\mu_\varphi}(F) = \beta \sum_{x \in [N]} \mathbb{E}_{\mu_\varphi}(F \sigma_x) - \mathbb{E}_{\mu_\varphi}(F) \mathbb{E}_{\mu_\varphi}(\sigma_x) = \beta \sum_{x \in [N]} \text{cov}_{\mu_\varphi}(F, \sigma_x).$$

Thus, we have using Cauchy-Schwarz that

$$\left| \nabla_\varphi \mathbb{E}_{\mu_\varphi}(F) \right|^2 \leq N \beta^2 \sum_{x \in [N]} |\text{cov}_{\mu_\varphi}(F, \sigma_x)|^2. \quad (3.22)$$

We can then use that by Cauchy-Schwarz again

$$\begin{aligned}
\text{cov}_{\mu_\varphi}(F, \sigma_x) &= \mathbb{E}_{\mu_\varphi} \left((F - \mathbb{E}_{\mu_\varphi}(F))(\sigma - \mathbb{E}_{\mu_\varphi}(\sigma)) \right) \\
&\leq \sqrt{\mathbb{E}_{\mu_\varphi}(F - \mathbb{E}_{\mu_\varphi}(F))^2} \sqrt{\mathbb{E}_{\mu_\varphi}(\sigma - \mathbb{E}_{\mu_\varphi}(\sigma))^2} \\
&\leq 2\sqrt{\text{Var}_{\mu_\varphi}(F)}.
\end{aligned} \tag{3.23}$$

Finally, inserting this into (3.22) and using the LSI for the fluctuation measure, we find

$$\begin{aligned}
\mathbb{E}_{\nu_N} \left(\left| \nabla_\varphi \mathbb{E}_{\mu_\varphi}(F) \right|^2 \right) &\leq 4N\beta^2 \mathbb{E}_{\nu_N} \text{Var}_{\mu_\varphi}(F) \\
&\leq \frac{4N\beta^2}{\gamma_n} \mathbb{E}_\rho \sum_{x \in [N]} \left| \nabla_{\mathbb{S}^{n-1}}^{(x)} F \right|^2
\end{aligned} \tag{3.24}$$

which after inserting this bound into (3.19) implies the claim. To prove the LSI we follow [BB19] and write

$$\begin{aligned}
\text{Ent}_\rho(F^2) &= \mathbb{E}_{\nu_N} (\text{Ent}_{\mu_\varphi}(F^2)) + \text{Ent}_{\nu_N} (\mathbb{E}_{\mu_\varphi}(F^2)) \\
&\leq \frac{2}{\gamma_n} \sum_{x \in [N]} \left\| \nabla_{\mathbb{S}^{n-1}}^{(x)} F \right\|_{L^2(d\rho)}^2 + \frac{2}{\lambda} \mathbb{E}_{\nu_N} \left(\left| \nabla_\varphi \sqrt{\mathbb{E}_{\mu_\varphi}(F^2)} \right|^2 \right).
\end{aligned}$$

For the second term we have from applying the Cauchy-Schwarz inequality:

$$\left| \nabla_\varphi \sqrt{\mathbb{E}_{\mu_\varphi}(F^2)} \right|^2 = \beta^2 \left| \frac{\sum_{x \in [N]} \text{cov}_{\mu_\varphi}(F^2, \sigma_x)}{\sqrt{\mathbb{E}_{\mu_\varphi}(F^2)}} \right|^2 \leq \beta^2 N \frac{\sum_{x \in [N]} |\text{cov}_{\mu_\varphi}(F^2, \sigma_x)|^2}{\mathbb{E}_{\mu_\varphi}(F^2)}.$$

By *doubling the variables* σ_x, σ'_x , we write

$$\begin{aligned}
|\text{cov}_{\mu_\varphi}(F^2(\sigma_x), \sigma_x)| &= \frac{1}{2} \left| \mathbb{E}_{\mu_\varphi} \left((F^2(\sigma_x) - F^2(\sigma'_x))(\sigma_x - \sigma'_x) \right) \right| \\
&\leq \sqrt{\text{Var}_{\mu_\varphi}(F)} \sqrt{\frac{1}{2} \mathbb{E}_{\mu_\varphi \otimes \mu_\varphi} \left((F(\sigma_x) + F(\sigma'_x))^2 (\sigma_x - \sigma'_x)^2 \right)} \\
&\leq \sqrt{\text{Var}_{\mu_\varphi}(F)} \sqrt{8 \mathbb{E}_{\mu_\varphi}(F^2)}
\end{aligned}$$

where in the last two lines we applied CS inequality and used that $|\sigma_x - \sigma'_x| \leq 2$. Then

$$|\text{cov}_{\mu_\varphi}(F^2, \sigma)|^2 \leq 8 \text{Var}_{\mu_\varphi}(F) \mathbb{E}_{\mu_\varphi}(F^2).$$

This gives

$$\left| \nabla_\varphi \sqrt{\mathbb{E}_{\mu_\varphi}(F^2)} \right|^2 \leq 8N\beta^2 \text{Var}_{\mu_\varphi}(F).$$

Overall we have

$$\begin{aligned} \text{Ent}_\rho(F^2) &\leq \frac{2}{\gamma_n} \sum_{x \in [N]} \left\| \nabla_{\mathbb{S}^{n-1}}^{(x)} F \right\|_{L^2(d\rho)}^2 + \frac{16\beta^2 N}{\lambda \gamma_n} \sum_{x \in [N]} \left\| \nabla_{\mathbb{S}^{n-1}}^{(x)} F \right\|_{L^2(d\rho)}^2 \\ &= \frac{2}{\gamma_n} \left(1 + \frac{8\beta^2 N}{\lambda} \right) \sum_{x \in [N]} \left\| \nabla_{\mathbb{S}^{n-1}}^{(x)} F \right\|_{L^2(d\rho)}^2. \end{aligned}$$

□

6.4 The mean-field Ising model

Without loss of generality, we assume $h \geq 0$ when studying the Ising model. We define the critical magnetic field strength in the Ising model

$$h_c(\beta) := \sqrt{\beta(\beta - 1)} - \text{arccosh}(\sqrt{\beta})$$

for temperatures $\beta \geq 1$ as the supremum of all $h > 0$ such that $x = \tanh(\beta x + h)$ has three distinct solutions for $x \in [-1, 1]$. In particular $h_c(\beta)$ is monotone with respect to the inverse temperature β .

The critical magnetic field strength is chosen in such a way that for fields $h < h_c(\beta)$ there are two potential wells in the renormalized potential landscape, see Figure 6.1, whereas for $h \geq h_c(\beta)$ there is only one, see Figure 6.2 in subsection 6.4.3 where this case is discussed.

6.4.1 Lower bound on spectral gap in weak field $h < h_c(\beta)$ regime

We start by showing that the inverse spectral gap in the Ising model in the case of subcritical magnetic fields, i.e. $h < h_c(\beta)$, converges at most exponentially fast to zero as the number of spins, N , increases.

We start by showing a LSI with exponential constant for the renormalized measure. This implies by Prop. 3.7 that such an LSI must also hold for the full many-particle measure $d\rho$.

Proposition 4.1 (LSI for ν_N). *Let $\beta > 1$ and $h < h_c(\beta)$ such that V_1 is a double well potential where the depth of the smaller well is denoted by $\Delta_{\text{small}}(V)$, cf. Fig. 6.1. The mean-field Ising model satisfies a $\text{LSI}(e^{-N\Delta_{\text{small}}(V)(1+\mathcal{O}(1))})^1$*

$$\text{Ent}_{\nu_N}(F^2) \lesssim e^{N\Delta_{\text{small}}(V)(1+\mathcal{O}(1))} \int_{\mathbb{R}} |F'|^2 d\nu_N.$$

¹If the magnetic field is zero, i.e. $h = 0$, both wells are of equal size.

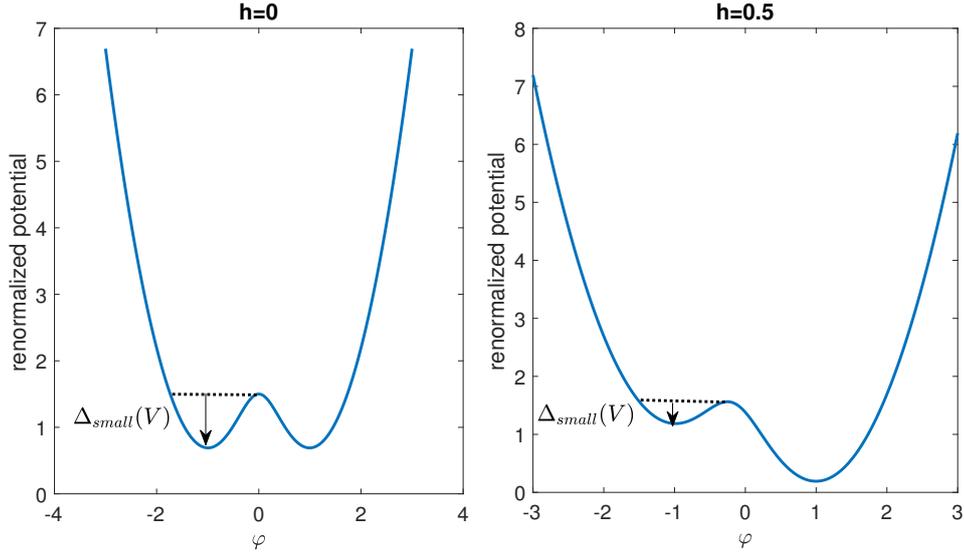


Figure 6.1: *Weak magnetic fields*: Renormalized potentials for the Ising model with $\beta = 3$ and zero $h = 0$ or weak $h = 0.5$ magnetic fields form a double well.

Proof. The renormalized potential V_1 has on $[0, \infty)$ a global minimum with positive second derivative at some φ_{\min} satisfying $\varphi_{\min} = \tanh(\beta\varphi_{\min} + h)$. This follows since the renormalized potential (3.7) reduces to

$$V_1(\varphi) = \frac{\beta}{2}\varphi^2 - \log(\cosh(\beta\varphi + h))$$

and the critical points of this potential are easily found to satisfy $\varphi = \tanh(\beta\varphi + h)$, see also [BBS19, Lemma 1.4.6]. For small temperatures, i.e. $\beta \rightarrow \infty$, one has $\varphi_{\min} = 1 + o(1)$.

We first consider $h = 0$: In this case, the median of the renormalized measure is located precisely at $\varphi = 0$ and $\varphi_{\min} > 0$ is one of the two non-degenerate global minima of the renormalized potential (the other minimum is located at $-\varphi_{\min}$ by axisymmetry).

An application of Laplace's principle, see [Won01, Ch. II, Theorem 1], shows that for all $x > 0$:

$$\begin{aligned} & \lim_{N \rightarrow \infty} \frac{1}{N} \log \left(-\nu_N([x, \infty)) \log(\nu_N([x, \infty))) \int_0^x \frac{e^{NV_1(\varphi)}}{\nu_N^{(1)}} d\varphi \right) \\ &= \lim_{N \rightarrow \infty} \frac{1}{N} \left(\log \int_x^\infty e^{-NV_1(\varphi)} d\varphi + \log(-\log(\nu_N([x, \infty))) + \log \int_0^x e^{NV_1(\varphi)} d\varphi \right) \quad (4.25) \\ &= - \inf_{t \in [x, \infty)} V_1(t) + \sup_{t \in [0, x]} V_1(t). \end{aligned}$$

The supremum of (4.25) is attained at $x = \varphi_{\min}$ such that

$$- \inf_{t \in [x, \infty)} V_1(t) + \sup_{t \in [0, x]} V_1(t) = \Delta_{\text{small}}(V) > 0.$$

Here, we used that for $x > \varphi_{\min}$ we get by Laplace's principle

$$-\log(\nu_N[x, \infty)) = N(V(x) - V(\varphi_{\min}))(1 + o(1))$$

and thus $\lim_{N \rightarrow \infty} \frac{\log(-\log(\nu_N[x, \infty)))}{N} = 0$.

On the other hand, if $x \in (0, \varphi_{\min})$ then, again by Laplace's principle, $-\log(\nu_N[x, \infty)) = -\log(\frac{1}{2}) + o(1)$ and thus $\lim_{N \rightarrow \infty} \frac{\log(-\log(\nu_N[x, \infty)))}{N} = 0$ as well. The case $x = \varphi_{\min}$ can be treated analogously. Hence, we obtain for the constant D_1 as in (3.16)

$$\begin{aligned} D_1 &:= \sup_{x > 0} \left(-\nu_N([x, \infty)) \log(\nu_N([x, \infty))) \int_0^x \frac{e^{NV_1(\varphi)}}{\nu_N^{(1)}} d\varphi \right) \\ &= e^{N\Delta_{\text{small}}(V)(1+o(1))}. \end{aligned} \quad (4.26)$$

The symmetry of the distribution for $h = 0$ implies then that $D_0 = D_1$.

We now consider $h > 0$: The renormalized potential possesses a unique global minimum at some φ_{\min} and the median of the renormalized measure converges to this point φ_{\min} , see Fig. 6.1, as Laplace's principle implies

$$\frac{\int_{\varphi_{\min}}^{\infty} e^{-NV_n(\varphi)} d\varphi}{\int_{-\infty}^{\infty} e^{-NV_n(\varphi)} d\varphi} = \frac{1}{2} + \mathcal{O}(1/N).$$

Hence, it suffices to verify the LSI bounds (3.16) for $m = \varphi_{\min}$ as argued in Remark 3.6.

Arguing as in (4.26) yields for $h > 0$ and $x < \varphi_{\min}$:

$$\begin{aligned} &\lim_{N \rightarrow \infty} \frac{1}{N} \log \left(-\nu_N((-\infty, x]) \log(\nu_N((-\infty, x])) \int_x^m \frac{e^{NV_1(\varphi)}}{\nu_N^{(1)}} d\varphi \right) \\ &= \lim_{N \rightarrow \infty} \frac{1}{N} \left(\log \int_{-\infty}^x e^{-NV_1(\varphi)} d\varphi + \log(-\log(\nu_N([x, \infty)))) + \log \int_x^m e^{NV_1(\varphi)} d\varphi \right) \\ &= - \inf_{t \in (-\infty, x]} V_1(t) + \sup_{t \in [x, m]} V_1(t) \end{aligned} \quad (4.27)$$

which shows $D_0 = e^{N\Delta_{\text{small}}(V)(1+o(1))}$ by taking x to be the minimum of the smaller well of the renormalized potential. For the constant D_1 we get on the other hand for $x > \varphi_{\min}$, since the renormalized potential is monotonically increasing on $[\varphi_{\min}, \infty)$,

$$\begin{aligned} &\lim_{N \rightarrow \infty} \frac{1}{N} \log \left(-\nu_N([x, \infty)) \log(\nu_N([x, \infty))) \int_m^x \frac{e^{NV_1(\varphi)}}{\nu_N^{(1)}} d\varphi \right) \\ &= \lim_{N \rightarrow \infty} \frac{1}{N} \left(\log \int_x^{\infty} e^{-NV_1(\varphi)} d\varphi + \log \int_m^x e^{NV_1(\varphi)} d\varphi + \log(-\log(\nu_N([x, \infty)))) \right) \\ &= - \inf_{t \in [x, \infty)} V_1(t) + \sup_{t \in [m, x]} V_1(t) = 0 \end{aligned} \quad (4.28)$$

such that D_1 is negligible compared with D_0 . \square

6.4.2 Upper bound on spectral gap in weak field $h < h_c(\beta)$ regime.

The upper bound on the spectral gap is obtained by finding an explicit trial function saturating the SGI. For this construction, we use the notation and results of Lemma 2.1.

In order to fix ideas first, we assume $h = 0$. We start by observing that the mean spin $\bar{\sigma}$ can only take values in the set $\mathcal{M} := \{-1, -1 + 2/N, \dots, 1\}$. The weights of the stationary measure $d\rho$ are given by functions $\eta_N : \mathcal{M} \rightarrow \mathbb{R}$

$$\eta_N(i) := \sum_{\sigma; \bar{\sigma}=i} e^{-\beta H(\sigma)} = \binom{N}{N/2(1+i)} e^{-\frac{N\beta}{2}(1-i^2)}. \quad (4.29)$$

where we used (2.3).

We also introduce trial functions $f_N : \{\pm 1\}^N \rightarrow \mathbb{R}$ for the spectral gap inequality given by

$$f_N(\sigma) := \sum_{i \in \mathcal{M}; 0 \leq i \leq \bar{\sigma}} \frac{\mathbb{1}_{\{i \leq \gamma_3(\beta)\}}}{\eta_N(i)} \quad (4.30)$$

with indicator function $\mathbb{1}$ and $\gamma_3(\beta)$ is the largest solution to $\varphi = \tanh(\beta\varphi + h)$. Since f_N depends only on the mean spin, we can identify them with functions $g_N : \mathcal{M} \rightarrow \mathbb{R}$

$$g_N(m) = \sum_{i \in \mathcal{M}; 0 \leq i \leq m} \frac{\mathbb{1}_{\{i \leq \gamma_3(\beta)\}}}{\eta_N(i)} \text{ such that } f_N(\sigma) = g_N(\bar{\sigma}).$$

For the L^2 norm of the f_N we find

$$\|f_N\|_{L^2(d\rho)}^2 = \sum_{i \in \mathcal{M}} \frac{\eta_N(i)}{Z} |g_N(i)|^2 \geq \sum_{i \in \mathcal{M}; i > \gamma_3(\beta)} \frac{\eta_N(i)}{Z} \left(\sum_{j \in \mathcal{M}; 0 \leq j \leq \gamma_3(\beta)} \frac{1}{\eta_N(j)} \right)^2 \quad (4.31)$$

where Z is the normalization constant of the full measure $d\rho$. For the gradient of f_N we find

$$\left| \nabla_{\mathbb{S}^0}^{(i)} f_N(\sigma) \right|^2 = |g_N(\bar{\sigma}) - g_N(\bar{\sigma} \pm 2/N)|^2 \lesssim \eta_N(\bar{\sigma})^{-2}.$$

Hence, for some $C > 0$

$$\sum_{i \in [N]} \left\| \nabla_{\mathbb{S}^0}^{(i)} f_N \right\|_{L^2(d\rho)}^2 \leq \frac{CN}{Z} \sum_{i \in \mathcal{M}; 0 \leq i \leq \gamma_3(\beta)} \frac{1}{\eta_N(i)}. \quad (4.32)$$

Using (3.15) with $\mu(\Omega) = \frac{1}{2}$ implies by comparing (4.31) with (4.32) that the constant γ

in the SGI is bounded from below by

$$\frac{1}{NC} \sum_{i \in \mathcal{M}; i > \gamma_3(\beta)} \eta_N(i) \sum_{i \in \mathcal{M}; 0 \leq i \leq \gamma_3(\beta)} \frac{1}{\eta_N(i)} \leq \frac{1}{2\gamma}. \quad (4.33)$$

We recall from the discussion in Lemma 2.1 that the continuous approximation $\eta_N(i)$ attains its maximum in the limit at $i = \gamma_3(\beta)$ and the summand $\frac{1}{\eta_N(i)}$ in the second sum attains its maximum in the limit at $i = 0$.

Thus it suffices to study the asymptotic of the logarithm of the leading order summands in (4.33) using the asymptotic behaviour of $\zeta_N := \partial_s \log(\eta_N(s))$ given in (2.99)

$$\begin{aligned} \log \left(\frac{\eta_N(\gamma_3(\beta))}{\eta_N(0)} \right) &= N \int_0^{\gamma_3(\beta)} \zeta_N(s) ds = N \int_0^{\gamma_3(\beta)} (\beta s - \operatorname{arctanh}(s)) ds (1 + \mathcal{O}(1)) \\ &= N \left(\frac{\beta \gamma_3(\beta)^2}{2} - \int_0^{\gamma_3(\beta)\beta} \frac{\operatorname{arctanh}(x/\beta)}{\beta} dx \right) (1 + \mathcal{O}(1)) \\ &= -N \int_0^{\gamma_3(\beta)} \beta(x - \tanh(\beta x)) dx (1 + \mathcal{O}(1)) \\ &= N \Delta_{\text{small}}(V)(1 + \mathcal{O}(1)). \end{aligned}$$

Here, we used integration of the inverse function to obtain the last line and (3.10) in the last one. In the case of a positive weak magnetic field $h \in (0, h_c(\beta))$ we choose a trial function $f_{N,h} : \{\pm 1\}^N \rightarrow \mathbb{R}$ given by

$$\begin{aligned} f_{N,h}(\sigma) &:= \sum_{i \in \mathcal{M}; \bar{\sigma} < i < \gamma_3(\beta)} \frac{\mathbb{1}_{\{i \geq \gamma_1(\beta)\}}}{\eta_{N,h}(i)} \text{ where for } i \in \mathcal{M} \\ \eta_{N,h}(i) &:= \binom{N}{N/2(1+i)} e^{-\frac{N\beta}{2}(1-i^2) + hNi}. \end{aligned} \quad (4.34)$$

Proceeding as above in (4.31) we obtain for the L^2 norm the lower bound

$$\|f_{N,h}\|_{L^2(d\rho)}^2 \geq \frac{1}{Z} \sum_{i \in \mathcal{M}; i < \gamma_1(\beta)} \eta_{N,h}(i) \left(\sum_{j \in \mathcal{M}; \gamma_3(\beta) > j \geq \gamma_1(\beta)} \frac{1}{\eta_{N,h}(j)} \right)^2. \quad (4.35)$$

For the Dirichlet form we find, as for (4.32), for some $C > 0$

$$\sum_{x \in [N]} \left\| \nabla_{\mathbb{S}^0}^{(x)} f_{N,h} \right\|_{L^2(d\rho)}^2 \leq \frac{CN}{Z} \sum_{j \in \mathcal{M}; \gamma_3(\beta) > j \geq \gamma_1(\beta)} \frac{1}{\eta_{N,h}(j)}. \quad (4.36)$$

We can apply (3.15) with $\mu(\Omega) = \frac{1}{1-\varepsilon}$ for some $\varepsilon > 0$ since the trial function (4.34) vanishes to the right of the global maximum such that by comparing (4.35) with (4.36) the constant

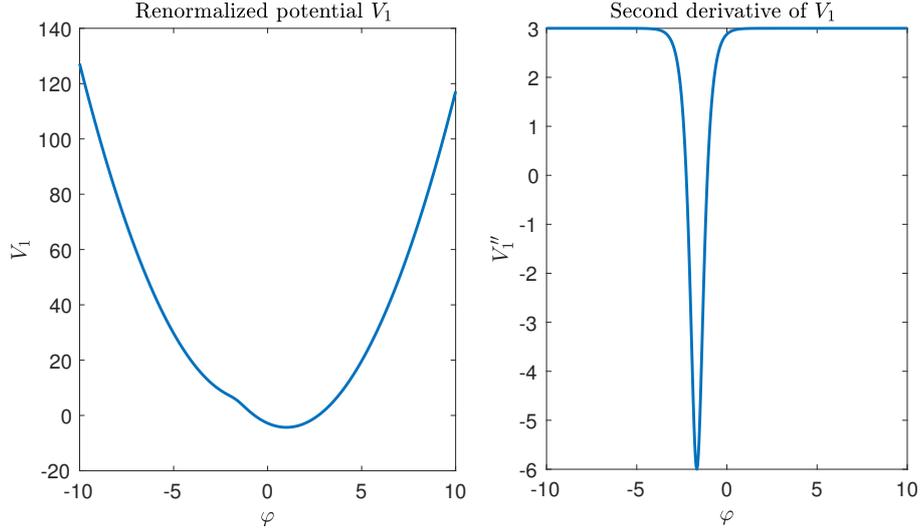


Figure 6.2: *Strong magnetic fields:* The renormalized potential and its second derivative for $h = 5$ for $\beta = 3$. The potential is non-convex even though it is a single well potential. However, it is convex in a neighbourhood of the global minimum.

γ in the SGI is bounded from below by

$$\frac{1}{NC} \sum_{i \in \mathcal{M}; i < \gamma_1(\beta)} \eta_{N,h}(i) \sum_{j \in \mathcal{M}; \gamma_3(\beta) > j \geq \gamma_1(\beta)} \frac{1}{\eta_{N,h}(j)} \leq \frac{1}{\varepsilon\gamma}. \quad (4.37)$$

The weight $\eta_{N,h}(i)$ in the first sum attain their maximum (in the limit) at $i = \gamma_1(\beta)$ and the summands $\frac{1}{\eta_{N,h}(i)}$ in the second sum attain their maximum at $i = \gamma_2(\beta)$.

To explicitly state an upper bound on the spectral gap it suffices to study the asymptotic of the logarithm of the leading order summands

$$\begin{aligned} \log \left(\frac{\eta_{N,h}(\gamma_1(\beta))}{\eta_{N,h}(\gamma_2(\beta))} \right) &= N \int_{\gamma_2(\beta)}^{\gamma_1(\beta)} \zeta_{N,h}(s) ds = \int_{\gamma_2(\beta)}^{\gamma_1(\beta)} (\beta s - \operatorname{arctanh}(s)) ds (1 + o(1)) \\ &= N \left(\frac{\beta(\gamma_1(\beta)^2 - \gamma_2(\beta)^2)}{2} - \int_{\gamma_2(\beta)\beta}^{\gamma_1(\beta)\beta} \frac{\operatorname{arctanh}(x/\beta)}{\beta} dx \right) (1 + o(1)) \\ &= -N \int_{\gamma_2(\beta)}^{\gamma_1(\beta)} \beta(x - \tanh(\beta x)) dx (1 + o(1)) \\ &= N\Delta_{\text{small}}(V)(1 + o(1)). \end{aligned}$$

6.4.3 Spectral gap in strong magnetic field regime $h > h_c(\beta)$.

Next, we study the case of strong magnetic fields for the Ising model, that is V_1' has at most one root, for $\beta > 1$. We also include the case $\beta = 1$ and $h \neq 0$. Unlike in the case of weak magnetic fields, in which case the constant in the LSI for the renormalized measure

is exponentially increasing in the number of spins, the spectral gap of the renormalized measure is now linearly increasing in the number of spins. Responsible for this uniform gap is the local uniform convexity at the minimum of the renormalized potential. More precisely, we have

$$V_1'(\varphi) = \beta(\varphi - \tanh(\beta\varphi + h)) \text{ and } V_1''(\varphi) = \beta(1 - \beta \operatorname{sech}(\beta\varphi + h)^2). \quad (4.38)$$

Thus, $V_1''(\varphi) = 0$ yields $\varphi_{\pm} = \frac{-h \pm \operatorname{arccosh}(\sqrt{\beta})}{\beta}$. Inserting this into $V_1'(\varphi_{\pm}) = 0$ implies that $h_{\pm} = \pm \operatorname{arccosh}(\sqrt{\beta}) \mp \sqrt{\beta(\beta - 1)}$ with $\operatorname{sign} \operatorname{sgn}(h_{\pm}) = \mp 1$ and thus $\varphi_{\pm} = \pm \sqrt{\frac{\beta-1}{\beta}}$. In particular, in the subcritical regime $\beta > 1$ all global minima φ_* have $\operatorname{sign} \operatorname{sgn}(\varphi_*) = \operatorname{sgn}(h)$, such that the renormalized potential satisfies $V_1''(\varphi_*) > 0$. Moreover, for $\beta = 1$ and $h \neq 0$ there are no points at which both the first and second derivative vanish. The third derivative at this point however is always non-zero and given by

$$V_1^{(3)}(\varphi_{\pm}) = \mp 2\sqrt{\beta(\beta - 1)}\beta.$$

Proposition 4.2 (Ising model, strong field). *Let $\beta \geq 1$ and $h > h_c(\beta)$, i.e. V_1 is a single well potential. We obtain for the Ising model a SGI(γ)*

$$\operatorname{Var}_{\nu_N}(F) \leq \frac{1}{\gamma} \int_{\mathbb{R}} |F'|^2 d\nu_N$$

where $\frac{1}{\gamma}$ is uniformly bounded in N .

Proof. Since the renormalized Schrödinger operator and renormalized generator are unitarily equivalent up to a factor, see (3.14), the semiclassical eigenvalue distribution stated in [Sim83, Theo. 1.1] implies the statement of the Proposition:

It follows immediately from the renormalized Schrödinger operator (3.14)

$$\Delta_{\text{ren}} = -\frac{d^2}{d\varphi^2} + \frac{N^2}{4}|V_1'(\varphi)|^2 - \frac{N}{2}V_1''(\varphi). \quad (4.39)$$

that the low-lying eigenfunction of Δ_{ren} accumulate at the unique non-degenerate (the second derivative is non-zero) potential well and the spectral gap of the renormalized measure grows linearly in N . The result then follows from Prop. 3.7. \square

6.4.4 Critical magnetic fields in $n = 1$

Proposition 4.3. *Let $h = h_{\pm}$ and $\beta > 1$. The spectral gap of the radial renormalized Schrödinger operator grows as $\mathcal{O}(N^{2/3})$ and in particular, the spectral gap of the full measure does not close faster than $\mathcal{O}(N^{-1/3})$.*

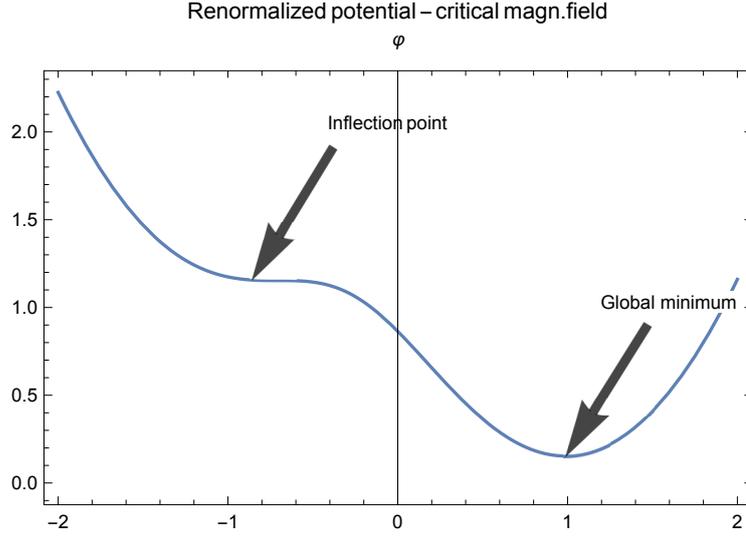


Figure 6.3: *Critical magnetic field for $n = 1$* : Renormalized potential of the Ising model with $\beta = 2$ possesses two critical points, one inflection point and a global minimum.

Proof. Let $\lambda := N/2$ and consider the Schrödinger operator, defined in (3.14),

$$\mathcal{H} := -\partial_x^2 + \lambda^2 |V_1'(x)|^2 - \lambda V_1''(x) \quad (4.40)$$

for the renormalized potential and auxiliary Schrödinger operators, which are obtained as the Taylor expansion of (4.40)

$$\begin{aligned} H_{\varphi_*} &= -\partial_x^2 + \lambda^2 |V_1'(\varphi_*)|^2 (x - \varphi_*)^2 - \lambda V_1''(\varphi_*) \text{ and} \\ H_{\varphi_{\pm}} &= -\partial_x^2 + \lambda^2 \beta^3 (\beta - 1) (x - \varphi_{\pm})^4 \pm \lambda 2\sqrt{\beta(\beta - 1)}\beta (x - \varphi_{\pm}) \end{aligned} \quad (4.41)$$

on $L^2(\mathbb{R})$ localized to the two critical points, the inflection point φ_{\pm} and the global minimum φ_* . We then define $j \in C_c^\infty((-2, 2); [0, 1])$ such that $j(x) = 1$ for $|x| \leq 1$ and from this functions

$$\begin{aligned} J_{\varphi_*}(x) &:= j(\lambda^{2/5}|x - \varphi_*|), \quad J_{\varphi_{\pm}}(x) := j(\lambda^{3/10}|x - \varphi_{\pm}|) \text{ and} \\ J(x) &:= \sqrt{1 - J_{\varphi_{\pm}}(x)^2 - J_{\varphi_*}(x)^2} \text{ with} \\ \|\nabla J_{\varphi_*}\|_{\mathbb{R}^n}^2 &\leq \mathcal{O}(\lambda^{4/5}), \quad \|\nabla J_{\varphi_{\pm}}\|_{\mathbb{R}^N}^2 \leq \mathcal{O}(\lambda^{3/5}). \end{aligned} \quad (4.42)$$

Invoking then unitary maps $U_{\varphi_*}, U_{\varphi_{\pm}} \in \mathcal{L}(L^2(\mathbb{R}))$ defined as

$$(U_{\varphi_*} f)(x) := \lambda^{-1/4} f(\lambda^{-1/2}(x + \varphi_*)) \text{ and } (U_{\varphi_{\pm}} f)(x) := \lambda^{-1/6} f(\lambda^{-1/3}(x + \varphi_{\pm})) \quad (4.43)$$

shows that the two Schrödinger operators in (4.41) are in fact unitarily equivalent, up to

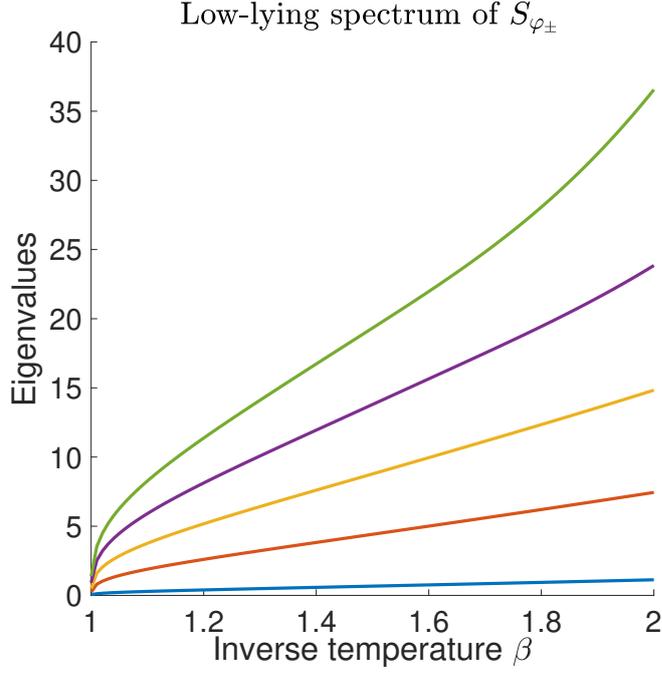


Figure 6.4: The five smallest eigenvalues of the operator $S_{\varphi_{\pm}}$ as a function of β . The smallest eigenvalue is strictly positive.

multiplication by powers of λ , to the λ -independent Schrödinger operators

$$\begin{aligned} S_{\varphi_*} &= -\partial_x^2 + |V_1'(\varphi_*)|^2 x^2 - V_1''(\varphi_*) \\ S_{\varphi_{\pm}} &= -\partial_x^2 + \beta^3(\beta - 1)x^4 \pm 2\sqrt{\beta(\beta - 1)}\beta x, \end{aligned} \quad (4.44)$$

respectively. Both operators have discrete spectrum and that $\inf(\text{Spec}(S_{\varphi_{\pm}})) > 0$ is shown in Section 6.C. We illustrate the behaviour of the smallest eigenvalues of $S_{\varphi_{\pm}}$ in Figure 6.4. More precisely, we have that

$$\lambda U_{\varphi_*}^{-1} S_{\varphi_*} U_{\varphi_*} = H_{\varphi_*} \quad \text{and} \quad \lambda^{2/3} U_{\varphi_{\pm}}^{-1} S_{\varphi_{\pm}} U_{\varphi_{\pm}} = H_{\varphi_{\pm}}. \quad (4.45)$$

Taylor expansion of the potential at the respective critical point and the estimate on the gradient (4.42) imply that

$$|J_{\varphi_*}(\mathcal{H} - H_{\varphi_*})J_{\varphi_*}| \leq \mathcal{O}(\lambda^{4/5}) \quad \text{and also} \quad |J_{\varphi_{\pm}}(\mathcal{H} - H_{\varphi_{\pm}})J_{\varphi_{\pm}}| \leq \mathcal{O}(\lambda^{3/5}). \quad (4.46)$$

Let $0 = e_1 < e_2 \leq \dots$ be the eigenvalues (counting multiplicities) of S_{φ_*} and $0 < f_1 \leq f_2 \leq \dots$ the ones of $S_{\varphi_{\pm}}$ and choose τ such that $\lambda e_{n+1} > \tau > \lambda e_n$ and $\lambda^{2/3} f_{m+1} > \tau > \lambda^{2/3} f_m$ with P_i being the projection onto the eigenspace to all eigenvalues of S_i below τ . The IMS

formula, see [CFKS87, (11.37)] for a version on manifolds, implies that

$$\mathcal{H} = J\mathcal{H}J - |\nabla J|^2 + \sum_{i \in \{\varphi_*, \varphi_\pm\}} (J_i H_i J_i + J_i (\mathcal{H} - H_i) J_i - |\nabla J_i|^2). \quad (4.47)$$

On the other hand, it follows that

$$\begin{aligned} J_{\varphi_*} H_{\varphi_*} J_{\varphi_*} &= J_{\varphi_*} H_{\varphi_*} P_{\varphi_*} J_{\varphi_*} + J_{\varphi_*} H_{\varphi_*} (\text{id} - P_{\varphi_*}) J_{\varphi_*} \\ &\geq J_{\varphi_*} H_{\varphi_*} P_{\varphi_*} J_{\varphi_*} + \lambda e_n J_{\varphi_*}^2 \end{aligned}$$

and also

$$\begin{aligned} J_{\varphi_\pm} H_{\varphi_\pm} J_{\varphi_\pm} &= J_{\varphi_\pm} H_{\varphi_\pm} P_{\varphi_\pm} J_{\varphi_\pm} + J_{\varphi_\pm} H_{\varphi_\pm} (\text{id} - P_{\varphi_\pm}) J_{\varphi_\pm} \\ &\geq J_{\varphi_\pm} H_{\varphi_\pm} P_{\varphi_\pm} J_{\varphi_\pm} + \lambda^{2/3} f_m J_{\varphi_\pm}^2. \end{aligned}$$

In particular, we find

$$\|V_1'\|_{\mathbb{R}^n}^2 \geq c\lambda^{-6/5} \text{ on } J \text{ for some } c > 0.$$

and

$$\|V_1''\|_{\mathbb{R}^n} \geq c\lambda^{-3/10} \text{ on } J \text{ for some } c > 0.$$

This implies for large λ that

$$JHJ \geq \lambda^{2/3} f_m J^2. \quad (4.48)$$

From (4.47) we then conclude that for some $C > 0$

$$\mathcal{H} \geq \lambda^{2/3} f_m J^2 - C\lambda^{4/9} + \sum_{i \in \{\varphi_\pm, \varphi_*\}} J_i H_i P_i J_i = \lambda^{2/3} f_m + \sum_{i \in \{\varphi_\pm, \varphi_*\}} J_i H_i P_i J_i - o(\sqrt{\lambda}).$$

This implies the claim of the Proposition, since

$$\text{rank}(J_0 H_\pm P J_0) \leq n.$$

More precisely, for the eigenvalues $E_1(\lambda) \leq E_2(\lambda) \leq \dots$ of \mathcal{H} we have shown that

$$\liminf_{\lambda \rightarrow \infty} \lambda^{-2/3} E_n(\lambda) \geq f_{n-1} > 0 \text{ for } n \geq 2.$$

In particular, the lowest possible eigenvalue $e_1 = 0$ of the renormalized Schrödinger operator is of course attained as the nullspace of the renormalized Schrödinger operator H_{φ_*} is non-trivial. This shows that the spectral gap of the renormalized Schrödinger operator grows at least proportional to $\lambda^{2/3}$. \square

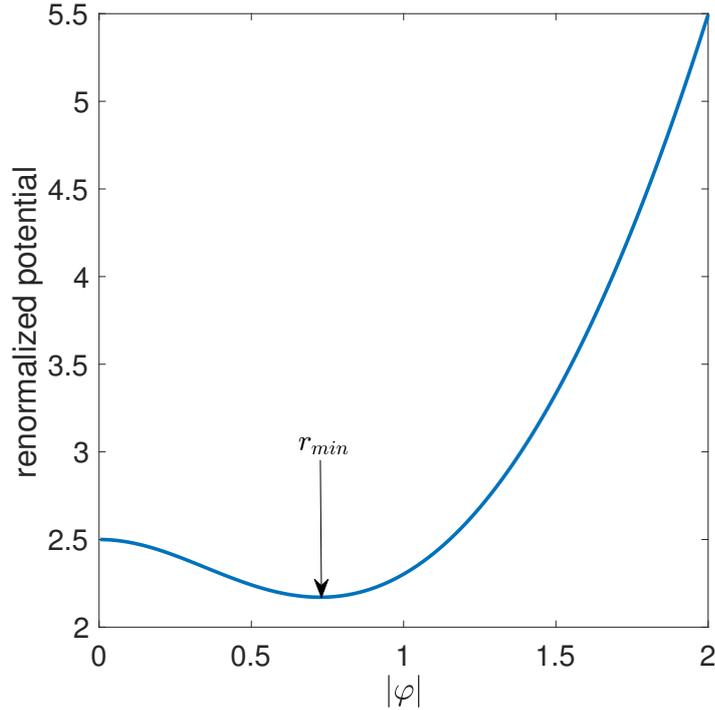


Figure 6.5: *Heisenberg model*, ($n = 3$): The renormalized potential of the Heisenberg model for $h = 0$ and $\beta = 5$.

6.5 Multi-component $\mathcal{O}(n)$ -models

6.5.1 $n \geq 2$: Zero magnetic field, $h = 0$

Let $h = 0$ then the renormalized potential for $n \geq 2$ is radially symmetric and possesses a critical point at $\varphi = 0$. In the supercritical case, i.e. $\beta > n$, the renormalized potential possesses another critical radius $r = \|\varphi\| \in (0, 1)$, see Figure 6.6. To see this, we differentiate the renormalized potential

$$\partial_r V_n(r) = \beta r \left(1 - \frac{I_{n/2}(\beta r)}{r I_{n/2-1}(\beta r)} \right).$$

It is now obvious that $r = 0$ is a critical point of the renormalized potential at which

$$\lim_{r \downarrow 0} \frac{I_{n/2}(\beta r)}{r I_{n/2-1}(\beta r)} = \frac{2}{n} \frac{\beta}{2} > 1 \text{ such that } \partial_r^2 V_n(0) = \beta \left(1 - \frac{\beta}{n} \right) < 0 \quad (5.49)$$

where we used that $\beta > n$ is supercritical. To conclude the existence of precisely one other critical radius r_{\min} at which the renormalized potential attains its global minimum it suffices therefore to show that $\frac{I_{n/2}(\beta r)}{r I_{n/2-1}(\beta r)}$ decays monotonically to zero. We prove this in Lemma 2.2 in the appendix. This implies that also the factor $\left(1 - \frac{I_{n/2}(\beta r)}{r I_{n/2-1}(\beta r)} \right)$ has precisely one root, i.e. the second critical radius.

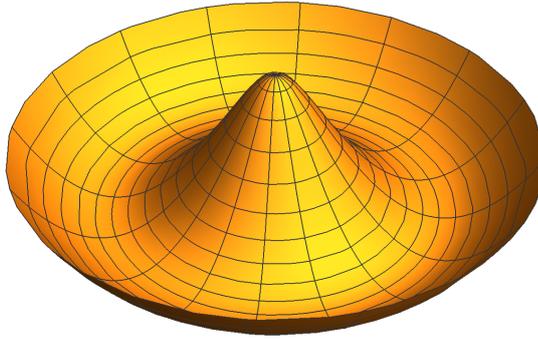


Figure 6.6: *XY-model*: The renormalized potential of the XY-model for $h = 0$ and $\beta = 10$.

6.5.2 Zero magnetic field- A lower bound on the spectral gap

When $h = 0$ and $n \geq 2$, then the renormalized Schrödinger operator (3.14) for $\lambda := N/2$ is the self-adjoint operator

$$\Delta_{\text{ren}} = -\Delta_{\mathbb{R}^n} + \lambda^2 |\nabla_{\mathbb{R}^n} V|^2 - \lambda \Delta_{\mathbb{R}^n} V.$$

This operator is also rotationally symmetric such that by separating (spherical coordinates) the angular part from the radial part, the remaining radial component $\Delta_{\text{ren}}^{\text{rad},\ell}$ of the renormalized Schrödinger operator on $L^2((0, \infty), r^{n-1} dr)$ for $\ell \in \mathbb{N}_0$ reads

$$\Delta_{\text{ren}}^{\text{rad},\ell} = -\left(\partial_r^2 + \frac{n-1}{r}\partial_r - \frac{\ell(\ell+n-2)}{r^2}\right) + \lambda^2 |\partial_r V_n(r)|^2 - \lambda \partial_r^2 V_n(r). \quad (5.50)$$

Here, the term $\ell(\ell+n-2)$ accounts for the eigenvalues of the angular part of the Laplacian. The renormalized potential possesses, when $h = 0$ and $n \geq 2$, exactly two critical radii at which $|\partial_r V_n(r)|^2 = 0$. The radii are $r = 0$ and $r = r_{\min}$, see the beginning of this Section 6.5.1. However, $V_n(r)$ is strictly concave at 0, i.e. $\partial_r^2 V_n(0) < 0$, and by Lemma 2.2 strictly convex at r_{\min} such that $\partial_r^2 V_n(r_{\min}) > 0$. This follows from

$$\partial_r^2 V_n(r_{\min}) = \beta r_{\min} \partial_r |_{r=r_{\min}} \left(1 - \frac{I_{n/2}(\beta r)}{r I_{n/2-1}(\beta r)}\right) > 0,$$

see the beginning of Section 6.5.

The radial symmetry of the renormalized potential implies that the renormalized measure decomposes into $d\nu_N(\varphi) = \nu_N^{(n)} r^{n-1} e^{-NV_n(r)} dr \otimes dS_{\mathbb{S}^{n-1}}$. We study the radial part due to tensorization principle, as the surface measure on \mathbb{S}^{n-1} is known to satisfy a *LSI*(n) [DEKL13, Corollary 2]. Thus the rotational invariance of the renormalized measure implies that the spectral gap inequality for the renormalized measure is at least uniform in N .

In our next Proposition we therefore study the low-lying spectrum of the radial component, $\Delta_{\text{ren}}^{\text{rad},0}$, as $\lambda \rightarrow \infty$.

Proposition 5.1. *Let $h = 0$, $n \geq 2$ and $\beta > n$. The spectral gap of the radial renormalized*

Schrödinger operator $\Delta_{ren}^{rad,0}$ grows linearly in N .

Proof. The proof we present here follows the steps of the proof in [Sim83].

To study the low-lying spectrum of the radial component of the renormalized Schrödinger operator, let $\lambda := N/2$ and consider Schrödinger operators

$$\begin{aligned} H_{\text{osc}}^0(\lambda) &= -\left(\partial_r^2 + \frac{n-1}{r}\partial_r\right) + \lambda^2|\partial_r^2 V_n(0)|^2 r^2 - \lambda \partial_r^2 V_n(0) \text{ and} \\ H_{\text{osc}}^{r_{\min}}(\lambda) &= -\partial_x^2 + \lambda^2 |\partial_r^2 V_n(r_{\min})|^2 (x - r_{\min})^2 - \lambda \partial_r^2 V_n(r_{\min}) \end{aligned} \quad (5.51)$$

where we use the variable x rather than r to emphasize that the last operator is defined on $L^2(\mathbb{R})$, unlike the first one which is an operator on $L^2((0, \infty), r^{n-1} dr)$. Observe that in (5.51) we replaced the gradient term of the Schrödinger operator by its Taylor approximation at the critical point. This explains the occurrence of the second derivative at the critical point in (5.51). Invoking the unitary maps $U_0 \in \mathcal{L}(L^2((0, \infty), r^{n-1} dr))$ and $U_{r_{\min}} \in \mathcal{L}(L^2(\mathbb{R}))$ defined as

$$(U_0 f)(x) = \lambda^{-n/4} f(\lambda^{-1/2} x) \text{ and } (U_{r_{\min}} f)(x) = \lambda^{-1/4} f(\lambda^{-1/2}(x + r_{\min})) \quad (5.52)$$

shows that the two Schrödinger operators in (5.51) are in fact unitarily equivalent, up to multiplication by λ , to the λ -independent Schrödinger operators

$$\begin{aligned} S_{\text{osc}}^0 &= -\left(\partial_r^2 + \frac{n-1}{r}\partial_r\right) + |\partial_r^2 V_n(0)|^2 r^2 - \partial_r^2 V_n(0) \\ S_{\text{osc}}^{r_{\min}} &= -\partial_x^2 + |\partial_r^2 V_n(r_{\min})|^2 x^2 - \partial_r^2 V_n(r_{\min}), \end{aligned} \quad (5.53)$$

respectively. More precisely, we have that

$$U_0^{-1} \lambda S_{\text{osc}}^0 U_0 = H_{\text{osc}}^0(\lambda) \quad \text{and} \quad U_{r_{\min}}^{-1} \lambda S_{\text{osc}}^{r_{\min}} U_{r_{\min}} = H_{\text{osc}}^{r_{\min}}(\lambda). \quad (5.54)$$

Since the bottom of the spectrum of the operator S_{osc}^0 is strictly positive $S_{\text{osc}}^0 \geq -\partial_r^2 V_n(0) > 0$, we conclude from (5.54) that the bottom of the spectrum of $H_{\text{osc}}^0(\lambda)$ increases linearly to infinity as $\lambda \rightarrow \infty$.

To connect the low-energy spectrum of the renormalized Schrödinger operator with the above auxiliary operators, take $j \in C_c^\infty(-\infty, 2)$ such that $j(x) = 1$ for $|x| \leq 1$. Then, we define

$$J_0(x) = j(\lambda^{2/5} |x|), \quad J_{r_{\min}}(x) = j(\lambda^{2/5} |x - r_{\min}|) \text{ with } \|\nabla J_i\|_{\mathbb{R}^n} \leq \mathcal{O}(\lambda^{2/5}) \quad (5.55)$$

for $i \in \{0, r_{\min}\}$ and $J := \sqrt{1 - J_{r_{\min}}^2 - J_0^2}$.

Without loss of generality we can assume that λ is large enough such that J_0 and $J_{r_{\min}}$ are disjoint.

Taylor expansion of the potential at 0 and r_{\min} respectively and the estimate on the gradient (5.55) imply that

$$|J_i(\Delta_{\text{ren}}^{\text{rad},0} - H_{\text{osc}}^i)J_i| \leq \mathcal{O}(\lambda^{4/5}) \text{ for } i \in \{0, r_{\min}\}.$$

Let $0 = e_1 < e_2 \leq \dots$ be the eigenvalues (counting multiplicities) of $S_{\text{osc}}^0 \oplus S_{\text{osc}}^{r_{\min}}$ and choose τ such that $e_{n+1} > \tau > e_n$ with P_i being the projection onto the eigenspace to all eigenvalues of H_{osc}^i below $\tau\lambda$. The IMS (**I**smagilov, **M**organ, and **S**imon/**S**igal) formula, see [Sim83, Lemma 3.1] and [CFKS87, (11.37)] for a version on manifolds, implies that

$$\Delta_{\text{ren}}^{\text{rad},0} = J\Delta_{\text{ren}}^{\text{rad},0}J - |\partial_r J|^2 + \sum_{i \in \{0, r_{\min}\}} (J_i \Delta_{\text{ren}}^{\text{rad},0} J_i - |\partial_r J_i|^2)$$

such that

$$\Delta_{\text{ren}}^{\text{rad},0} = J\Delta_{\text{ren}}^{\text{rad},0}J - |\partial_r J|^2 + \sum_{i \in \{0, r_{\min}\}} (J_i H_{\text{osc}}^i J_i + J_i (\Delta_{\text{ren}}^{\text{rad},0} - H_{\text{osc}}^i) J_i - |\partial_r J_i|^2). \quad (5.56)$$

On the other hand, it follows that

$$J_i H_{\text{osc}}^i J_i = J_i H_{\text{osc}}^i P_i J_i + J_i H_{\text{osc}}^i (\text{id} - P_i) J_i \geq J_i H_{\text{osc}}^i P_i J_i + \lambda e_n J_i^2.$$

By construction, since ∇V_n vanishes linearly on the support of J_i , we have

$$\|\nabla V_n\|_{\mathbb{R}^n}^2 \geq c(\lambda^{-2/5})^2 = c\lambda^{-4/5} \text{ on } J \text{ for some } c > 0.$$

Since ΔV_n is globally bounded anyway, this implies for large λ that

$$J\Delta_{\text{ren}}^{\text{rad},0}J \geq J^2(c\lambda^{6/5} - \lambda) \geq \lambda e_n J^2. \quad (5.57)$$

From (5.56) we then conclude that for some $C > 0$

$$\Delta_{\text{ren}}^{\text{rad},0} \geq \lambda e_n - C\lambda^{4/5} + \sum_{i \in \{0, r_{\min}\}} J_i H_{\text{osc}}^i P_i J_i = \lambda e_n + \sum_{i \in \{0, r_{\min}\}} J_i H_{\text{osc}}^i P_i J_i - o(\lambda).$$

This implies the claim of the Proposition, since

$$\text{rank} \left(\sum_{i \in \{0, r_{\min}\}} J_i H_{\text{osc}}^i P_i J_i \right) \leq n.$$

More precisely, for the eigenvalues $E_1(\lambda) \leq E_2(\lambda) \leq \dots$ of $\Delta_{\text{ren}}^{\text{rad},0}$ we have shown that

$$\liminf_{\lambda \rightarrow \infty} \lambda^{-1} E_n(\lambda) \geq e_n.$$

In particular, the lowest possible eigenvalue $e_1 = 0$ of the renormalized Schrödinger operator is of course attained as the nullspace of the renormalized Schrödinger operator is non-trivial. This shows that the spectral gap of the renormalized Schrödinger operator grows at least linearly in λ in the angular sector $\ell = 0$. \square

Corollary 5.2. *Let $h = 0$, $n \geq 2$ and $\beta > n$. The spectral gap of the full Gibbs measure ρ does not close faster than $\mathcal{O}(N^{-1})$. In particular, for radial functions, i.e. f only depends on $|\bar{\sigma}|$, the spectral gap remains open.*

Proof. Since the spectral gap of the radial component of the renormalized measure grows linearly in N and the spectral gap of the angular component is uniform in N , the tensorization principle implies that the full renormalized measure satisfies a SGI that is uniform in N . Due to Proposition 3.7, the spectral gap of the full measure does therefore not close faster than of order $1/N$.

For radial functions f , the $\mathbb{R}^N \ni \varphi \mapsto E_{\mu_\varphi}(f)$ maps also into radial functions and therefore the spectral gap of the renormalized measure is only determined by the radial renormalized Schrödinger operator in Prop. 5.1. Using Proposition 3.7 and (3.19), this implies that for radial functions, the gap remains open. \square

In the next Proposition we show that the rate N^{-1} in this case is in fact optimal:

Proposition 5.3. *Let $h = 0$, $n \geq 2$ and $\beta > n$. The spectral gap of the full measure ρ of the dynamics decays at least as fast as N^{-1} .*

Proof. We consider the mean-spin $\bar{\sigma} : (\mathbb{S}^n)^N \rightarrow \mathbb{R}^{n+1}$ defined by

$$\bar{\sigma}(\sigma) = \frac{1}{N} \sum_{i=1}^N \sigma_i = (\bar{\sigma}_1(\sigma), \dots, \bar{\sigma}_{n+1}(\sigma)) \in \mathbb{R}^{n+1}. \quad (5.58)$$

In analogy to the spherical harmonics which in cartesian coordinates reads $x_1/\|x\|$, we consider the function:

$$f(\sigma) := \frac{\bar{\sigma}_1(\sigma)}{\|\bar{\sigma}(\sigma)\|} \eta(\|\bar{\sigma}(\sigma)\|). \quad (5.59)$$

where $\eta \in C^\infty(\mathbb{R}; [0, 1])$ is a cut-off function such that for fixed $1 > \delta > 0$:

$$\eta(t) := \begin{cases} 1, & \text{when } t > \delta \text{ and} \\ 0, & \text{when } t \leq \delta/2. \end{cases} \quad (5.60)$$

As we want to compute the covariant derivative $\nabla_{\sigma_1} t(\sigma)$, we consider the parametrisation $\gamma_1(t)$ so that $\gamma_1(0) = \sigma_1$. Then we define $\gamma(t) := (\gamma_1(t), \sigma_2, \dots, \sigma_N)$ and $s(t) := \bar{\sigma}(\gamma(t))$. It is then clear that for $v := \gamma_1'(0)$ we have $s'(0) = v/N$, the first coordinate of which is $s_1'(0) = \langle e_1, v \rangle / N$. We define then

$$s_1(t) := \bar{\sigma}_1(\gamma(t)) = \langle e_1, s(t) \rangle. \quad (5.61)$$

Thus, since $f(\gamma(t)) = \frac{s_1(t)}{\|s(t)\|}$, we find for the derivative

$$\begin{aligned} f'(0) &= \frac{1}{|s(0)|^2} \left(|s(0)| s_1'(0) - s_1(0) \frac{s(0) \cdot s'(0)}{|s(0)|} \right) \eta(|s(0)|) \\ &\quad + \frac{s_1(0)}{|s(0)|} \eta'(|s(0)|) \frac{s(0) \cdot s'(0)}{|s(0)|} \\ &= \frac{1}{N |\bar{\sigma}(\sigma)|^2} \left(|\bar{\sigma}(\sigma)| \langle e_1, v \rangle - \langle e_1, \bar{\sigma}(\sigma) \rangle \frac{\langle \bar{\sigma}(\sigma), v \rangle}{|\bar{\sigma}(\sigma)|} \right) \eta(|\bar{\sigma}(\sigma)|) \\ &\quad + \frac{\bar{\sigma}_1(\sigma)}{|\bar{\sigma}(\sigma)|} \eta'(|\bar{\sigma}(\sigma)|) \frac{\langle \bar{\sigma}(\sigma), v \rangle}{N |\bar{\sigma}(\sigma)|}. \end{aligned} \quad (5.62)$$

Therefore, we see that in terms of

$$\mu(\sigma) := \frac{1}{N} \left(\frac{1}{|\bar{\sigma}(\sigma)|^2} \left(|\bar{\sigma}(\sigma)| e_1 - \bar{\sigma}_1(\sigma) \frac{\bar{\sigma}(\sigma)}{|\bar{\sigma}(\sigma)|} \right) \eta(|\bar{\sigma}(\sigma)|) + \frac{\bar{\sigma}_1(\sigma)}{|\bar{\sigma}(\sigma)|^2} \eta'(|\bar{\sigma}(\sigma)|) \bar{\sigma}(\sigma) \right),$$

the derivative is just

$$\nabla_{\sigma_1} f(\sigma) = \mu(\sigma) - \langle \mu(\sigma), \sigma_1 \rangle \sigma_1.$$

The cut-off function η ensures that $|\bar{\sigma}(\sigma)|$ is not small. Therefore we can bound $|Z(\sigma)| = \mathcal{O}(1)$ which implies that $\mathbb{E}_\rho(|\nabla_{\sigma_1} \bar{\sigma}(\sigma)|^2) \lesssim 1/N^2$ or that

$$\sum_{i \in [N]} \mathbb{E}_\rho(|\nabla_{\sigma_i} \bar{\sigma}(\sigma)|^2) \lesssim 1/N.$$

By rotational symmetry we also know that $\mathbb{E}_\rho(f) = 0$. For the second moment $\mathbb{E}_\rho(f(\sigma)^2)$, we have by rotational invariance again

$$\begin{aligned} 1 &= \sum_{i=1}^{n+1} \mathbb{E}_\rho \left(\frac{\bar{\sigma}_i(\sigma)^2}{|\bar{\sigma}(\sigma)|^2} \right) = \sum_{i=1}^{n+1} \mathbb{E}_\rho \left(\frac{\bar{\sigma}_1(\sigma)^2}{|\bar{\sigma}(\sigma)|^2} \right) \\ &= (n+1) \mathbb{E}_\rho \left(\frac{\bar{\sigma}_1(\sigma)^2}{|\bar{\sigma}(\sigma)|^2} \eta(|\bar{\sigma}(\sigma)|) \right) + (n+1) \mathcal{R}_N \end{aligned} \quad (5.63)$$

where \mathcal{R}_N is the error

$$\mathcal{R}_N := \mathbb{E}_\rho \left(\frac{\bar{\sigma}_1(\sigma)^2}{|\bar{\sigma}(\sigma)|^2} (1 - \eta(|\bar{\sigma}(\sigma)|)) \right).$$

Our aim is now to argue that \mathcal{R}_N is small as N is large.

For $\beta > n$ we know that the renormalized potential attains its minimum at hyperspheres $\partial B_{\mathbb{R}^N}(0, r_{\min})$. This implies that the renormalized measure concentrates at such $\varphi \in \partial B(0, r_{\min})$ with exponential tail bounds, i.e. the probability of φ away from $\partial B(0, r_{\min})$ is exponentially small in N . The fluctuation measure then enforces that also the mean spin $\bar{\sigma}$ has to be outside of a ball of radius $\delta > 0$ with high probability. To see this recall that the fluctuation measure can be rewritten as

$$\mathbb{E}_{\mu_\varphi}(F) = \frac{\int_{(\mathbb{S}^{n-1})^N} F(\sigma) e^{\beta N \langle \varphi, \bar{\sigma} \rangle} dS_{\mathbb{S}^{n-1}}^{\otimes N}(\sigma)}{\int_{(\mathbb{S}^{n-1})^N} e^{\beta N \langle \varphi, \bar{\sigma} \rangle} dS_{\mathbb{S}^{n-1}}^{\otimes N}(\sigma)} = \frac{\int_{(\mathbb{S}^{n-1})^N} F(\sigma) e^{\beta N \langle \varphi, \bar{\sigma} \rangle} dS_{\mathbb{S}^{n-1}}^{\otimes N}(\sigma)}{\mathcal{N}(\varphi)^N}. \quad (5.64)$$

Here, the radial normalizing function

$$\mathcal{N}(\varphi) := \int_{\mathbb{S}^{n-1}} e^{\beta \langle \varphi, \sigma \rangle} dS_{\mathbb{S}^{n-1}}(\sigma) = \Gamma\left(\frac{n}{2}\right) \left(\frac{2}{\|\beta\varphi\|}\right)^{\frac{n}{2}-1} I_{\frac{n}{2}-1}(\|\beta\varphi\|)$$

is a strictly monotonically increasing function of $|\varphi|$ that satisfies $\mathcal{N}(\varphi) \geq 1$ and $\mathcal{N}(\varphi) = 1$ if and only if $\varphi = 0$. This follows directly from the Taylor series of the modified Bessel function.

Hence, we can pick δ such that $e^{\beta \langle \varphi, \bar{\sigma} \rangle} < (1 + \mathcal{N}(\varphi))/2$ for all $\varphi \in \partial B(0, r_{\min})$ and $|\bar{\sigma}| \leq \delta$. Hence, we see that for such φ

$$\mathbb{E}_{\mu_\varphi}(\mathbb{1}_{|\bar{\sigma}| \leq \delta}) = \mathcal{O} \left(\left(\frac{1}{2\mathcal{N}(\varphi)} + \frac{1}{2} \right)^N \right).$$

This shows that $\mathbb{E}_\rho(\mathbb{1}_{|\bar{\sigma}| \leq \delta}) = \mathcal{O} \left(\left(\frac{1}{2\mathcal{N}(\varphi)} + \frac{1}{2} \right)^N \right)$ and hence that \mathcal{R}_N tends exponentially fast to zero as well, as N tends to infinity, under the condition that $\beta > n$. \square

6.5.3 Nonzero magnetic fields for $n \geq 2$

The situation $h \neq 0$ and $n \geq 2$ cannot be reduced to a one-dimensional model due to lack of symmetries. Yet, the renormalized Schrödinger operator provides a very elegant tool to show that the spectral gap of the full generator of the Ginzburg-Landau dynamics remains open as $N \rightarrow \infty$.

In fact, whereas the global minimum for $h = 0$ of the renormalized potential is attained on a hypersphere, the global minimum for $h \neq 0$ is attained at a single point, only.

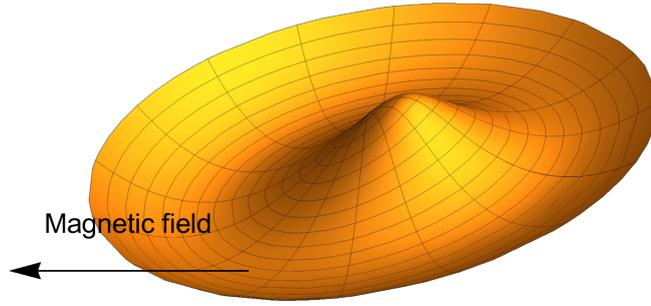


Figure 6.7: *XY-model*: The renormalized potential of the XY-model for $h = (-2, 0)$ and $\beta = 10$. The rotational symmetry is broken.

This allows us to identify the asymptotic of the low-energy spectrum of the renormalized Schrödinger operator directly with the spectrum of a quantum harmonic oscillator.

Let $\varphi_c \in \mathbb{R}^n$ be a critical point of the renormalized potential (3.7). We define the set

$$\Sigma := \left\{ \sum_{i=1}^n (n_i |\lambda_i| + \frac{1}{2} (|\lambda_i| - \lambda_i)) , \text{ with } n_i \in \mathbb{N}_0, \lambda_i \in \sigma(D^2 V_n(\varphi_c)) \right\}$$

where $\lambda_1, \dots, \lambda_n$ comprise the entire spectrum of $D^2 V_n(\varphi_c)$.

Let e_k be the k -th smallest element counting multiplicity in Σ we then have the following Proposition:

Proposition 5.4. *Let $h \neq 0$, $\beta \geq n$, and $n \geq 2$. Let $E_k(\lambda)$ denote the k -th lowest eigenvalue of the renormalized generator then this eigenvalue satisfies the asymptotic law $\lim_{\lambda \rightarrow \infty} \frac{E_k(\lambda)}{\lambda} = e_k$. In particular, the ground state of the renormalized generator in the limit as $\lambda \rightarrow \infty$ is unique and the spectral gap of the renormalized Schrödinger operator remains open and linearly in λ .*

Proof. When $h \neq 0$ then the renormalized potential has a unique non-degenerate minimum. To see this recall that the renormalized potential reads

$$V_n(\varphi, h) = \frac{\beta}{2} (1 + \|\varphi\|^2) - \log \left(\Gamma \left(\frac{n}{2} \right) \left(\frac{2}{\|\beta\varphi + h\|} \right)^{\frac{n}{2}-1} I_{\frac{n}{2}-1}(\|\beta\varphi + h\|) \right).$$

Introducing the new variable $\zeta := \beta\varphi + h$ implies that

$$\begin{aligned} V_n(\varphi(\zeta), h) &= \frac{1}{2\beta} (\beta^2 + \|\zeta - h\|^2) - \log \left(\Gamma \left(\frac{n}{2} \right) \left(\frac{2}{\|\zeta\|} \right)^{\frac{n}{2}-1} I_{\frac{n}{2}-1}(\|\zeta\|) \right) \\ &= \frac{1}{2\beta} (\beta^2 + \|\zeta\|^2 + \|h\|^2 - 2\langle \zeta, h \rangle) - \log \left(\Gamma \left(\frac{n}{2} \right) \left(\frac{2}{\|\zeta\|} \right)^{\frac{n}{2}-1} I_{\frac{n}{2}-1}(\|\zeta\|) \right). \end{aligned} \tag{5.65}$$

Computing the gradient of that expression yields

$$\nabla_{\zeta} V_n(\varphi(\zeta), h) = -\frac{1}{\beta} h + g_{\beta}(\|\zeta\|) \widehat{e}_{\zeta} \quad (5.66)$$

where we introduced the auxiliary function $g_{\beta}(r) := \left(\frac{r}{\beta} - \frac{I_{n/2}(r)}{I_{n/2-1}(r)} \right)$. Thus for the gradient to vanish the vectors h and ζ have to be linearly dependent.

Assuming thus that $\widehat{e}_h = \pm \widehat{e}_{\zeta}$ we obtain from setting the gradient to zero the following equation

$$\frac{\beta I_{n/2}(\|\zeta\|)}{I_{n/2-1}(\|\zeta\|)} = (\|\zeta\| \mp \|h\|).$$

Thus, when h and ζ are aligned, there is precisely one solution, the global minimum of the renormalized potential, satisfying

$$\frac{\beta I_{n/2}(\|\zeta\|)}{I_{n/2-1}(\|\zeta\|)} = (\|\zeta\| - \|h\|)$$

with $g_{\beta}(\|\zeta\|) = \beta^{-1} \|h\| > 0$. That the aligned scenario corresponds to the global minimum is evident from the expression of the renormalized potential (5.65).

The simplicity of the solution follows since the left hand side $\frac{\beta I_{n/2}(\|\zeta\|)}{I_{n/2-1}(\|\zeta\|)}$ is a concave, monotonically increasing function from 0 to β as $\|\zeta\| \rightarrow \infty$.

When h and ζ point in opposite directions, there can, by concavity of the left-hand side, be between zero and two solutions to the equation

$$\frac{\beta I_{n/2}(\|\zeta\|)}{I_{n/2-1}(\|\zeta\|)} = (\|\zeta\| + \|h\|)$$

with $g_{\beta}(\|\zeta\|) = -\beta^{-1} \|h\| < 0$. In particular, for sufficiently low temperatures there exists a local maximum and a saddle point of the renormalized potential as shown in Figure 6.7.

From differentiating (5.66), the Hessian is given by

$$D_{\zeta}^2 V_n(\varphi(\zeta), h) = g'(\|\zeta\|) \frac{\zeta \zeta^T}{\|\zeta\|^2} + g_{\beta}(\|\zeta\|) \left(\frac{\text{id}}{\|\zeta\|} - \frac{\zeta \zeta^T}{\|\zeta\|^3} \right). \quad (5.67)$$

We note that the Hessian has full rank unless at critical points unless $g'_{\beta}(\|\zeta\|) + g_{\beta}(\|\zeta\|)(\|\zeta\| - \|\zeta\|^{-1}) = 0$, since $g_{\beta}(\|\zeta\|) \neq 0$ by (5.66) for non-zero magnetic fields.

In addition, there can be only a saddle point which can only happen at one fixed temperature depending on n .

Finally, if the temperature is sufficiently high, yet still such that $\beta > n$, there may be no critical point if h and ζ point in opposite directions. This is in particular the case when

$\beta = n$ and $h \neq 0$: Taylor expansion at zero yields

$$\frac{\beta I_{n/2}(\|\zeta\|)}{I_{n/2-1}(\|\zeta\|)} = \frac{\beta \Gamma(n/2)}{2\Gamma(1+n/2)} \|\zeta\| + \mathcal{O}(\|\zeta\|^2)$$

where for $\beta = n$ we find $\frac{n\Gamma(n/2)}{2\Gamma(1+n/2)} = 1$ and concavity of the function $\|\zeta\| \mapsto \frac{\beta I_{n/2}(\|\zeta\|)}{I_{n/2-1}(\|\zeta\|)}$ show.

Thus $\|\nabla V_n\|^2$ vanishes at not more than three critical points φ_c on the span of h . In particular, all eigenvalues of $D^2 V_n$ are non-negative only at the global minimum of V_n by (5.67), since we already established that $g'(\|\zeta\|) < 0$ at the other two. To see that they are strictly positive there, it suffices to analyze for $r = \|\zeta\|$

$$\begin{aligned} g'_\beta(\|\zeta\|) &= (\beta^{-1} - \mathcal{I}(\|\zeta\|)^{-1}) + \|\zeta\| \frac{\mathcal{I}'(\|\zeta\|)}{\mathcal{I}(\|\zeta\|)^2} \\ &= \frac{g_\beta(\|\zeta\|)}{\|\zeta\|} + \frac{\|\zeta\| \mathcal{I}'(\|\zeta\|)}{\mathcal{I}(\|\zeta\|)^2} > 0. \end{aligned} \tag{5.68}$$

Hence, we find that

$$g'_\beta(\|\zeta\|) + g_\beta(\|\zeta\|)(\|\zeta\| - \|\zeta\|^{-1}) = g_\beta(\|\zeta\|)\|\zeta\| + \frac{\|\zeta\| \mathcal{I}'(\|\zeta\|)}{\mathcal{I}(\|\zeta\|)^2}. \tag{5.69}$$

In particular, this expression is strictly positive at the global minimum, since $g_\beta(\|\zeta\|) > 0$ and $\mathcal{I}'(\|\zeta\|) > 0$ by general principles, see Lemma 2.2.

The asymptotic behaviour of the spectrum of the renormalized Schrödinger operator has been computed in [Sim83] (which we can directly apply as we satisfy the conditions (A1) – (A4) in [Sim83]) and our above representation of Σ follows by noticing that $\frac{1}{2}D^2 |\nabla V_n|^2(\varphi_c) = (D^2 V_n(\varphi_c))^2 > 0$.

Since the renormalized Schrödinger operator and renormalized generator are unitarily equivalent up to a factor, the semiclassical eigenvalue distribution stated in [Sim83, Theorem 1.1] implies the statement of the Proposition. \square

6.6 The critical regime, Proof of Theo. 1.3

We conclude our analysis by investigating the critical case $\beta = n$ and prove Theorem 1.3. As before, we distinguish between $n = 1$ and multi-component systems $n \geq 2$:

6.6.1 Critical Ising model

It follows from (4.25), which always vanishes for all $x > 0$, that the spectral gap, at the critical point $\beta = n = 1$, does not close exponentially fast in the number of spins. We want to show in this subsection that it closes at least polynomially, though. For a refined analysis in dimension $n = 1$, we recall some basic ideas from discrete Fourier analysis:

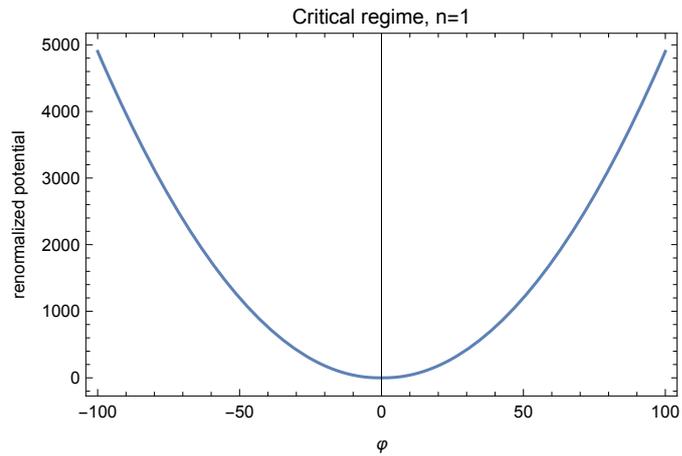


Figure 6.8: The renormalized potential V_1 for $\beta = 1$, $h = 0$ is a symmetric convex function.

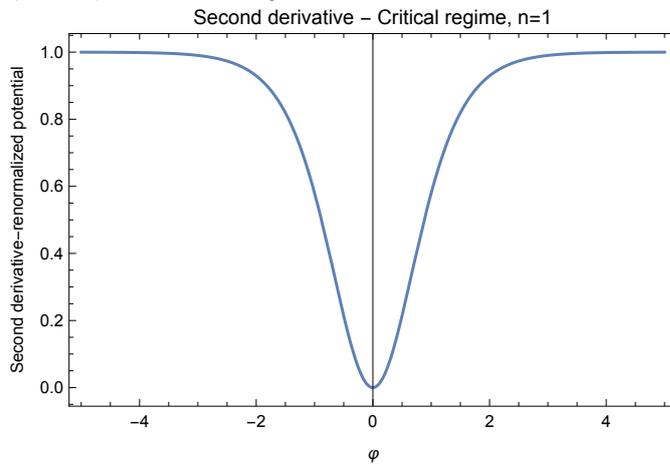


Figure 6.9: Strong convexity of the renormalized potential V_1 fails at the origin, $\varphi = 0$.

Let $f : \{\pm 1\}^N \rightarrow \mathbb{C}$ be an arbitrary function on the hypercube. The $L^2(\{\pm 1\}^N, 2^{-N} d\mu_{\text{count}})$ inner product on the hypercube is defined as

$$\langle f, g \rangle_{\{\pm 1\}^N} := \sum_{x \in \{\pm 1\}^N} 2^{-N} f(x_1, \dots, x_N) \overline{g(x_1, \dots, x_N)}.$$

The characteristic function χ_S for $S \subset [N]$ is defined as $\chi_S(x) := \prod_{i \in S} \sigma_i$ and the family $(\chi_S)_{S \subset [N]}$ forms an orthonormal basis of $L^2(\{\pm 1\}^N)$. In particular, $\chi_\emptyset = 1$. We also define indicator vectors $\mathbf{1}_S \in \mathbb{R}^N$ such that $\mathbf{1}_S(x) = 1$ if $x \in S$ and 0 otherwise.

Every function $f \in L^2(\{\pm 1\}^N)$ admits a unique Fourier decomposition

$$f = \sum_{S \subset [N]} \widehat{f}(S) \chi_S \quad (6.70)$$

where $\widehat{f}(S) := \langle f, \chi_S \rangle$. The variance of the stationary measure is given as the sum of

$$\text{Var}_\rho(f) = \mathbb{E}_{\nu_N}(\text{Var}_{\mu_\varphi}(f)) + \text{Var}_{\nu_N}(\mathbb{E}_{\mu_\varphi}(f)). \quad (6.71)$$

Since the first term on the right-hand side of this equation is always uniformly bounded by the Dirichlet form, as shown in the proof of Proposition 3.7, it suffices to study the behaviour of the second term. Thus, applying the expectation with respect to the fluctuation measure yields by the Fourier decomposition (6.70)

$$\mathbb{E}_{\mu_\varphi}(f) = \sum_{S \subset [N]} \widehat{f}(S) \mathbb{E}_{\mu_\varphi}(\chi_S). \quad (6.72)$$

In particular, using the explicit form of $V_1(\Phi)$, a direct computation yields for all $x \in [N]$

$$\mathbb{E}_{\mu_\varphi}(\sigma(x)) = e^{V_1(\varphi)} \frac{\left(e^{-\frac{\beta}{2}|\varphi-1|^2+h} - e^{-\frac{\beta}{2}|\varphi+1|^2-h} \right)}{2} = \tanh(\beta\varphi + h).$$

Using that μ_φ is a product measure, this implies that the full expression for (6.72) is given by

$$\mathbb{E}_{\mu_\varphi}(f) = \sum_{S \subset [N]} \widehat{f}(S) (\tanh(\beta\varphi + h))^{|S|}. \quad (6.73)$$

Hence, we find for the variance

$$\begin{aligned} \text{Var}_{\nu_N}(\mathbb{E}_{\mu_\varphi}(f)) &= \sum_{S_1, S_2 \subset [N]}^N \widehat{f}(S_1) \widehat{f}(S_2) \left(\mathbb{E}_{\nu_N} \left(\tanh(\beta\varphi + h)^{|S_1|+|S_2|} \right) \right. \\ &\quad \left. - \mathbb{E}_{\nu_N} \left(\tanh(\beta\varphi + h)^{|S_1|} \right) \mathbb{E}_{\nu_N} \left(\tanh(\beta\varphi + h)^{|S_2|} \right) \right) \end{aligned} \quad (6.74)$$

For the Dirichlet form, we find, with $S_1 \Delta S_2$ denoting the symmetric difference of sets S_1 and S_2 ,

$$\begin{aligned}
\sum_{x \in [N]} \mathbb{E}_\rho \left| \nabla_{\mathbb{S}^0}^{(x)} f \right|^2 &= \sum_{x \in [N]} \sum_{S_1, S_2 \subset [N]} \widehat{f}(S_1) \widehat{f}(S_2) \mathbb{E}_\rho (\nabla_{\mathbb{S}^0}^{(x)} \chi_{S_1} \nabla_{\mathbb{S}^0}^{(x)} \chi_{S_2}) \\
&= 4 \sum_{x \in [N]} \sum_{S_1, S_2 \subset [N]} \delta_{x \in S_1} \delta_{x \in S_2} \widehat{f}(S_1) \widehat{f}(S_2) \mathbb{E}_\rho (\chi_{S_1} \chi_{S_2}) \\
&= 4 \sum_{S_1, S_2 \subset [N]} \sum_{x \in S_1 \cap S_2} \widehat{f}(S_1) \widehat{f}(S_2) \mathbb{E}_\rho (\chi_{S_1 \Delta S_2}) \\
&= 4 \sum_{S_1, S_2 \subset [N]} \langle \mathbb{1}_{S_1}, \mathbb{1}_{S_2} \rangle_{\mathbb{R}^N} \widehat{f}(S_1) \widehat{f}(S_2) \mathbb{E}_\rho (\chi_{S_1 \Delta S_2}) \\
&= \mathbb{E}_\rho \left| 2 \sum_{S \subset [N]} \mathbb{1}_S \widehat{f}(S) \chi_S \right|_{\mathbb{R}^N}^2.
\end{aligned} \tag{6.75}$$

Proposition 6.1. *For zero magnetic fields, i.e. $h = 0$, and $\beta \geq 1$, all functions with Fourier support on sets of fixed cardinality $k \in \mathbb{N}$, i.e. for f given as*

$$f = \sum_{S \subset [N]; |S|=k} \widehat{f}(S) \chi_S.$$

satisfy the inequality $\text{Var}_{\nu_N}(\mathbb{E}_{\mu_\varphi}(f)) \leq \frac{N}{4k} \sum_{x \in [N]} \left| \nabla_{\mathbb{S}^{n-1}}^{(x)} f \right|_{L^2(d\rho)}^2$.

In particular, for the magnetization

$$M = \frac{1}{\sqrt{N}} \sum_{x \in [N]} \sigma(x) \tag{6.76}$$

we obtain an inequality

$$\text{Var}_{\nu_N}(\mathbb{E}_{\mu_\varphi}(M)) = \frac{N \mathbb{E}_{\nu_N}(\tanh(\beta\varphi)^2)}{4} \sum_{x \in [N]} \left| \nabla_{\mathbb{S}^{n-1}}^{(x)} M \right|_{L^2(d\rho)}^2.$$

Moreover, the spectral gap for critical $\beta = 1$ closes at least like $\mathcal{O}(N^{-1/2})$.

Proof. When $h = 0$, it suffices to estimate the variance by Jensen's inequality as

$$\begin{aligned}
\text{Var}_{\nu_N}(\mathbb{E}_{\mu_\varphi}(f)) &\leq \mathbb{E}_{\nu_N} \sum_{S_1, S_2 \subset [N]; |S_1|=|S_2|=k} \widehat{f}(S_1) \widehat{f}(S_2) \mathbb{E}_{\mu_\varphi}(\chi_{S_1}) \mathbb{E}_{\mu_\varphi}(\chi_{S_2}) \\
&\leq \mathbb{E}_{\nu_N} \mathbb{E}_{\mu_\varphi} \left| \sum_{S \subset [N]; |S|=k} \widehat{f}(S) \chi_S \right|^2 \\
&= \frac{1}{k^2} \mathbb{E}_\rho \left| \left\langle \sum_{S \subset [N]; |S|=k} \widehat{f}(S) \mathbb{1}_S \chi_S, \mathbb{1}_{[N]} \right\rangle_{\mathbb{R}^N} \right|^2 \\
&\leq \frac{N}{k^2} \mathbb{E}_\rho \left| \sum_{S \subset [N]; |S|=k} \widehat{f}(S) \mathbb{1}_S \chi_S \right|_{\mathbb{R}^N}^2.
\end{aligned} \tag{6.77}$$

Using (6.75) we then obtain the spectral gap inequality

$$\begin{aligned}
\text{Var}_{\nu_N}(\mathbb{E}_{\mu_\varphi}(f)) &\leq \frac{N}{k^2} \mathbb{E}_\rho \left| \sum_{S \subset [N]; |S|=k} \widehat{f}(S) \mathbb{1}_S \chi_S \right|_{\mathbb{R}^N}^2 \\
&= \frac{N}{4k^2} \sum_{x \in [N]} \left| \nabla_{\mathbb{S}^0}^{(x)} f \right|_{L^2(d\rho)}^2.
\end{aligned} \tag{6.78}$$

Turning to the magnetization (6.76), we can write the variance of the magnetization M in terms of the expectation value $\mathbb{E}_{\nu_N}(\tanh(\beta\varphi)^2)$

$$\text{Var}_{\nu_N}(\mathbb{E}_{\mu_\varphi}(M)) = \frac{1}{N} \sum_{x, y \in [N]} \mathbb{E}_{\nu_N}(\tanh(\beta\varphi)^2) = N \mathbb{E}_{\nu_N}(\tanh(\beta\varphi)^2). \tag{6.79}$$

We now recall that $\tanh(\beta\varphi)^2 = \beta^2 \varphi^2 + \mathcal{O}(\varphi^4)$ and for $\beta = 1$

$$V_1(\varphi) = \frac{1}{2} + \frac{\varphi^4}{12} + \mathcal{O}(\varphi^6)$$

by Taylor expanding around 0. It therefore follows from Laplace's principle [Won01, Ch. II, Theorem 1] that

$$\mathbb{E}_{\nu_N}(\tanh(\beta\varphi)^2) \sim N^{1/4} N^{-3/4} = N^{-1/2}. \tag{6.80}$$

On the other hand, we can compute the Dirichlet form of the magnetization using (6.75)

$$\sum_{x \in [N]} \mathbb{E}_\rho \left| \nabla_{\mathbb{S}^0}^{(x)} M \right|^2 = \frac{4}{N} \mathbb{E}_\rho \left| \sum_{x \in [N]} \mathbb{1}_S \chi_S \right|^2 = 4 \mathbb{E}_\rho(1) = 4. \tag{6.81}$$

Thus, comparing (6.79) with (6.81) implies the claim together with the asymptotic (6.80). \square

While Proposition 6.1 shows that the magnetization leads for critical $\beta = 1$ to a spectral gap that closes at least like $\sim N^{-1/2}$, when $h = 0$, the next Proposition shows that the magnetization does not imply a vanishing spectral gap when $h > 0$.

Proposition 6.2. *Let $h > 0$, $\beta \geq 1$, and f a function with Fourier transform supported on sets of cardinality $\leq k$ for some fixed $k \in \mathbb{N}_0$ independent of N , i.e.*

$$f = \sum_{S \subset [N]; |S| \leq k} \widehat{f}(S) \chi_S.$$

Then such functions satisfy an improved inequality with $\varphi_{\min} = \operatorname{argmin}_{\varphi} V_1(\varphi)$

$$\operatorname{Var}_{\nu_N}(\mathbb{E}_{\mu_{\varphi}}(f)) \leq \frac{\beta^2 \operatorname{csch}^2(2(\beta\varphi_{\min} + h))}{2V_1''(\varphi_{\min})} \sum_{x \in [N]} \mathbb{E}_{\rho} \left| \nabla_{\mathbb{S}^0}^{(x)} f \right|_{\mathbb{R}^N}^2 (1 + o(1)) \quad (6.82)$$

with a constant $\frac{\beta^2 \operatorname{csch}^2(2(\beta\varphi_{\min} + h))}{2V_1''(\varphi_{\min})} (1 + o(1))$ that strictly bounded away from zero in the limit $N \rightarrow \infty$. In particular, $V_1''(\varphi_{\min}) > 0$ by the discussion in the beginning of Section 6.4.3.

Proof. Using (4.104), which applies since $V_1''(\varphi_{\min}) > 0$ by the discussion in Subsection 6.4.3, we conclude that

$$\mathbb{E}_{\mu_{\varphi}}(f) = \sum_{S \subset [N]} \widehat{f}(S) (\tanh(\beta\varphi + h))^{|S|} \quad (6.83)$$

implies since

$$\frac{d}{d\varphi} \tanh(\beta\varphi + h) = \beta \operatorname{sech}^2(\beta\varphi + h) = \beta \operatorname{csch}(\beta\varphi + h)^2 \tanh(\beta\varphi + h)^2$$

that

$$\begin{aligned}
& \text{Var}_{\nu_N}(\mathbb{E}_{\mu_\varphi}(f)) \\
&= \frac{1}{2NV_1''(\varphi_{\min})} \left| \sum_{S \subset [N]} \widehat{f}(S) \beta |S| \tanh(\beta\varphi_{\min} + h)^{|S|+1} \text{csch}(\beta\varphi_{\min} + h)^2 \right|^2 (1 + o(1)) \\
&= \frac{\beta^2 \tanh(\beta\varphi_{\min} + h)^2 \text{csch}(\beta\varphi_{\min} + h)^4}{2NV_1''(\varphi_{\min})} \left| \sum_{S \subset [N]} \widehat{f}(S) \tanh(\beta\varphi_{\min} + h)^{|S|} \langle \mathbb{1}_S, \mathbb{1}_{[N]} \rangle_{\mathbb{R}^N} \right|^2 (1 + o(1)) \\
&\leq \frac{2\beta^2 \text{csch}^2(2(\beta\varphi_{\min} + h))}{V_1''(\varphi_{\min})} \left| \sum_{S \subset [N]} \widehat{f}(S) \tanh(\beta\varphi_{\min} + h)^{|S|} \mathbb{1}_S \right|^2 (1 + o(1)) \\
&= \frac{2\beta^2 \text{csch}^2(2(\beta\varphi_{\min} + h))}{V_1''(\varphi_{\min})} \left| \mathbb{E}_\rho \sum_{S \subset [N]} \widehat{f}(S) \chi_S \mathbb{1}_S \right|^2 (1 + o(1)) \\
&\leq \frac{2\beta^2 \text{csch}^2(2(\beta\varphi_{\min} + h))}{V_1''(\varphi_{\min})} \mathbb{E}_\rho \left| \sum_{S \subset [N]} \widehat{f}(S) \chi_S \mathbb{1}_S \right|^2 (1 + o(1)) \\
&= \frac{\beta^2 \text{csch}^2(2(\beta\varphi_{\min} + h))}{2V_1''(\varphi_{\min})} \sum_{x \in [N]} \mathbb{E}_\rho \left| \nabla_{S^0}^{(x)} f \right|_{\mathbb{R}^N}^2 (1 + o(1))
\end{aligned} \tag{6.84}$$

where we used (4.104) in the first line, $|S| = \langle \mathbb{1}_S, \mathbb{1}_{[N]} \rangle$ in the second line, Cauchy-Schwarz and $\text{csch}(x)^4 \tanh(x)^2 = 4 \text{csch}(2x)^2$ in the third line, (4.103) and (6.83) in the fourth line, Jensen's inequality in the fifth line and finally (6.75) in the last line. \square

6.6.2 Critical multi-component systems

In this subsection, we prove the multi-component part of Theorem 1.3:

Proof of Theorem 1.3. The magnetization $M = N^{-1/2} \sum_{x \in [N]} \sigma(x)$ has in the multi-component case always unit Dirichlet norm

$$\sum_{x \in [N]} \mathbb{E}_\rho \left| \nabla_{\mathbb{S}^{n-1}}^{(x)} M \right|^2 = \sum_{x \in [N]} \mathbb{E}_\rho(N^{-1}) = 1. \tag{6.85}$$

On the other hand, we can explicitly calculate using the derivative of the modified Bessel function of the first kind, $\partial_z I_\nu(z) = \frac{\nu}{z} I_\nu(z) + I_{\nu+1}(z)$, and (3.7), the expectation value

$\mathbb{E}_{\mu_\varphi}(\sigma(x))$ that is independent of $x \in [N]$ for $\varphi \neq 0$

$$\begin{aligned} \mathbb{E}_{\mu_\varphi}(\sigma(x)) &= e^{NV_n(\varphi)} e^{-\frac{\beta}{2}(1+\|\varphi\|^2)} \prod_{y \in [N]} \int_{\mathbb{S}^{n-1}} e^{-\beta \langle \varphi, \sigma(y) \rangle} \sigma(x) dS(\sigma(y)) \\ &= \frac{I_{n/2}(\|\beta\varphi\|)}{I_{n/2-1}(\|\beta\varphi\|)} \frac{\varphi}{\|\varphi\|}. \end{aligned} \quad (6.86)$$

Taylor expansion at zero then yields

$$(\mathbb{E}_{\mu_\varphi}(\sigma(x)))^2 = \left(\frac{I_{n/2}(\|\beta\varphi\|)}{I_{n/2-1}(\|\beta\varphi\|)} \right)^2 = \frac{\Gamma(\frac{n}{2})^2}{4\Gamma(1+\frac{n}{2})^2} \|\beta\varphi\|^2 + \mathcal{O}(\|\beta\varphi\|^4).$$

For the renormalized potential we find by Taylor expansion, which we shall already specialize to critical temperatures $\beta = n$, at zero

$$V_n(\varphi) = \frac{n}{2} + \frac{n^3}{8+4n} \|\varphi\|^4 + \mathcal{O}(\|\varphi\|^5).$$

For the magnetization M (6.76), we can write

$$\begin{aligned} \text{Var}_{\nu_N}(\mathbb{E}_{\mu_\varphi}(M)) &= \frac{1}{N} \sum_{x,y \in [N]} \mathbb{E}_{\nu_N} \left(\left(\frac{I_{n/2}(\|\beta\varphi\|)}{I_{n/2-1}(\|\beta\varphi\|)} \right)^2 \right) \\ &= N \mathbb{E}_{\nu_N} \left(\left(\frac{I_{n/2}(\|\beta\varphi\|)}{I_{n/2-1}(\|\beta\varphi\|)} \right)^2 \right). \end{aligned} \quad (6.87)$$

We then have by radial symmetry of both the renormalized potential and the integrand that at critical temperatures $\beta = n$

$$\mathbb{E}_{\nu_N} \left(\left(\frac{I_{n/2}(\|n\varphi\|)}{I_{n/2-1}(\|n\varphi\|)} \right)^2 \right) = \frac{\int_0^\infty e^{-NV_n(r)} r^{n-1} \left(\frac{I_{n/2}(nr)}{I_{n/2-1}(nr)} \right)^2 dr}{\int_0^\infty e^{-NV_n(r)} r^{n-1} dr}.$$

Applying Laplace's principle, cf. [Won01, Ch. II, Theorem 1], with constants $\mu = 4$ and $\alpha = 3 + (n - 1)$ implies that

$$\mathbb{E}_{\nu_N} \left(\left(\frac{I_{n/2}(\|n\varphi\|)}{I_{n/2-1}(\|n\varphi\|)} \right)^2 \right) \sim N^{n/4} N^{-(n+2)/4} = N^{-1/2}.$$

Combining this asymptotic behavior with (6.85) and (6.87) then yields the multi-component claim of Theorem 1.3, *i.e.* the rate $N^{1/2}$ is caught for the trial (mean spin) function M and thus the spectral gap is decaying at least with speed $N^{-1/2}$. \square

The following Proposition shows that the upper bound $N^{-1/2}$ on the spectral gap in

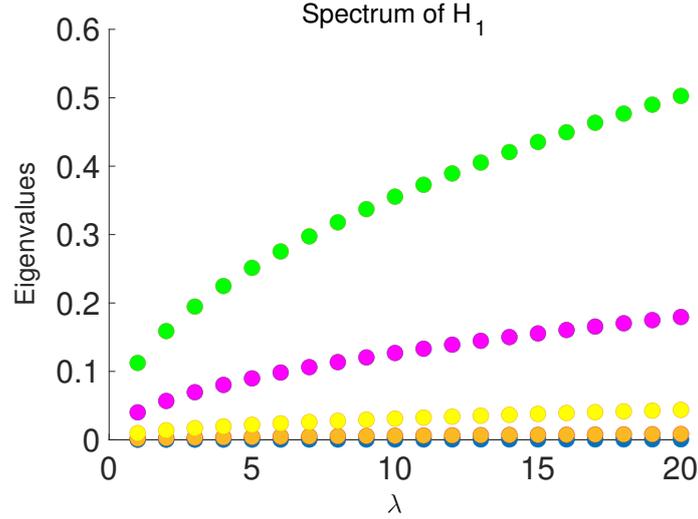


Figure 6.10: The five smallest eigenvalues of the operator H_1 as a function of λ . The smallest eigenvalue stays at zero.

the critical regime $\beta = n$ for all dimensions $n \geq 1$, is in fact sharp:

Proposition 6.3. *Let $h = 0$ and $\beta = n \geq 1$. The spectral gap of the radial renormalized Schrödinger operator grows as $\mathcal{O}(N^{1/2})$ and in particular, the spectral gap of the full measure does not close faster than $\mathcal{O}(N^{-1/2})$.*

Proof. Let $\lambda := N/2$, we then consider the equivalent Schrödinger operators to the renormalized generator

$$\begin{aligned} \mathcal{H}_1 &:= -\partial_x^2 + \lambda^2 |V_1'(x)|^2 - \lambda V_1''(x) \text{ and for } n \geq 2 \\ \mathcal{H}_n^\ell &:= -\left(\partial_r^2 + \frac{n-1}{r} \partial_r\right) + \frac{\ell(\ell+n-2)}{r^2} + \lambda^2 |\nabla V_n|^2 - \lambda \Delta V_n, \quad \ell \in \mathbb{N}_0, \end{aligned} \quad (6.88)$$

where we used that by rotational symmetry of the renormalized potential, for $n \geq 2$, we can decompose the Schrödinger operator into individual angular sectors parametrized by $\ell \in \mathbb{N}_0$. We then introduce auxiliary Schrödinger operators

$$\begin{aligned} H_1 &:= -\partial_x^2 + \lambda^2 \frac{x^6}{9} - \lambda x^2 \text{ and for } n \geq 2 \\ H_n^\ell &:= -\left(\partial_r^2 + \frac{n-1}{r} \partial_r\right) + \frac{\ell(\ell+n-2)}{r^2} + \lambda^2 \frac{n^6}{(2+n)^2} r^6 - \lambda \frac{3n^3}{2+n} r^2, \quad \ell \in \mathbb{N}_0 \end{aligned} \quad (6.89)$$

on $L^2(\mathbb{R})$ and $L^2((0, \infty), r^{n-1} dr)$, respectively. The five first eigenvalues of H_1 are shown in Fig. 6.10. We then define $j \in C_c^\infty(-2, 2)$ such that $j(x) = 1$ for $|x| \leq 1$ and from this

$$J_0(x) = j(\lambda^{2/9} |x|) \text{ and } J := \sqrt{1 - J_0^2} \text{ with } \|\nabla J_0\|_{\mathbb{R}^n} = \mathcal{O}(\lambda^{4/9}). \quad (6.90)$$

Invoking the unitary maps $U_1 \in \mathcal{L}(L^2(\mathbb{R}))$ and $U_n \in \mathcal{L}(L^2((0, \infty), r^{n-1} dr))$ defined as

$$(U_1 f)(x) := \lambda^{-1/8} f(\lambda^{-1/4}(x)) \text{ and } (U_n f)(r) := \lambda^{-n/8} f(\lambda^{-1/4}r) \quad (6.91)$$

shows that the two Schrödinger operators in (6.89) are in fact unitarily equivalent, up to multiplication by $\sqrt{\lambda}$, to the λ -independent Schrödinger operators

$$\begin{aligned} S_1 &= -\partial_x^2 + \frac{1}{9}x^6 - x^2 \text{ and for } n \geq 2 \\ S_n^\ell &= -\left(\partial_r^2 + \frac{n-1}{r}\partial_r\right) + \frac{\ell(\ell+n-2)}{r^2} + \frac{n^6}{(2+n)^2}r^6 - \frac{3n^3}{2+n}r^2, \quad \ell \in \mathbb{N}_0 \end{aligned} \quad (6.92)$$

respectively. That $\inf(\text{Spec}(S_n^0)) = 0$ is shown in Section 6.C. Since $\frac{\ell(\ell+n-2)}{r^2} > 0$ we have consequently that for $\ell > 0$ by monotonicity $\inf(\text{Spec}(S_n^\ell)) \geq \inf(\text{Spec}(S_n^1)) > 0$. More precisely, we have that

$$\lambda^{1/2}U_n^{-1} S_n^\ell U_n = H_n^\ell. \quad (6.93)$$

More precisely, since $(U_n f)(x) := \lambda^{-n/8} f(\lambda^{-1/4}x)$, it follows that

$$\begin{aligned} (S_n^\ell U_n f)(r) &= -\lambda^{-n/8} \left((\lambda^{-1/2} f''(\lambda^{-1/4}r) + \lambda^{-1/4} \frac{n-1}{r} f'(\lambda^{-1/4}r)) + \frac{\ell(\ell+n-2)}{r^2} f(\lambda^{-1/4}r) \right. \\ &\quad \left. + \frac{n^6}{(2+n)^2} r^6 f(\lambda^{-1/4}r) - \frac{3n^3}{2+n} r^2 f(\lambda^{-1/4}r) \right). \end{aligned} \quad (6.94)$$

Then, applying $(U_n^{-1} f)(r) = \lambda^{n/8} f(\lambda^{1/4}r)$ shows that

$$\begin{aligned} (U_n^{-1} S_n^\ell U_n f)(r) &= \lambda^{-1/2} \left(-\left(f''(r) + \frac{n-1}{r} f'(r)\right) + \frac{\ell(\ell+n-2)}{r^2} f(r) \right. \\ &\quad \left. + \lambda^2 \frac{n^6}{(2+n)^2} r^6 f(r) - \lambda \frac{3n^3}{2+n} r^2 f(r) \right). \end{aligned} \quad (6.95)$$

Taylor expansion of the potential at 0 and the estimate on the gradient (6.90) imply that

$$|J_0(\mathcal{H}_n^\ell - H_n^\ell)J_0| = \mathcal{O}(\lambda^{4/9}).$$

Let $0 = e_1 < e_2 \leq \dots$ be the eigenvalues (counting multiplicities) of S_n (over all angular sectors ℓ) and choose τ such that $e_{n+1} > \tau > e_n$ with P being the projection onto the eigenspace to all eigenvalues of H below $\tau\sqrt{\lambda}$. The IMS formula, see [CFKS87, (11.37)]

for a version on manifolds, implies that

$$\mathcal{H}_n = J\mathcal{H}_nJ - |\nabla J|^2 + (J_0\mathcal{H}_nJ_0 - |\nabla J_0|^2)$$

such that

$$\mathcal{H}_n = J\mathcal{H}_nJ - |\nabla J|^2 + (J_0H_nJ_0 + J_0(\mathcal{H}_n - H_n)J_0 - |\nabla J_0|^2). \quad (6.96)$$

On the other hand, it follows that

$$J_0H_nJ_0 = J_0H_nPJ_0 + J_0H_n(\text{id} - P)J_0 \geq J_0H_nPJ_0 + \sqrt{\lambda}e_nJ_0^2.$$

By construction, since ∇V_n vanishes to third order on the support of J_0 , we have

$$\|\nabla V_n\|_{\mathbb{R}^n}^2 \geq c(\lambda^{-2/9})^6 = c\lambda^{-4/3} \text{ on } J \text{ for some } c > 0.$$

Since ΔV_n vanishes to second order

$$\|\Delta V_n\|_{\mathbb{R}^n} \geq c\lambda^{-4/9} \text{ on } J \text{ for some } c > 0.$$

This implies for large λ that

$$JHJ \geq \sqrt{\lambda}e_nJ^2. \quad (6.97)$$

From (6.96) we then conclude that for some $C > 0$

$$\mathcal{H}_n \geq \sqrt{\lambda}e_nJ^2 - C\lambda^{4/9} + J_0H_nPJ_0 = \sqrt{\lambda}e_n + J_0H_nPJ_0 - o(\sqrt{\lambda}).$$

This implies the claim of the Proposition, since

$$\text{rank}(J_0H_nPJ_0) \leq n.$$

More precisely, for the eigenvalues $E_1(\lambda) \leq E_2(\lambda) \leq \dots$ of \mathcal{H}_n we have shown that

$$\liminf_{\lambda \rightarrow \infty} \lambda^{-1/2}E_n(\lambda) \geq e_n.$$

In particular, the lowest possible eigenvalue $e_1 = 0$ of the renormalized Schrödinger operator is of course attained as the nullspace of the renormalized Schrödinger operator is non-trivial. This shows that the spectral gap of the renormalized Schrödinger operator grows at least proportional to $\sqrt{\lambda}$. \square

Appendix

6.A Numerical results

Recall that the eigenfunctions of the operator

$$H_{\text{osc}} := -\frac{\hbar^2}{2\mu} \frac{d^2}{dx^2} + \frac{\mu\omega^2}{2} x^2 \quad (1.98)$$

are given for $n \in \mathbb{N}_0$ by

$$\Psi_n(x) := \frac{1}{\sqrt{2^n n!}} \left(\frac{\mu\omega}{\pi\hbar} \right)^{1/4} e^{-\frac{\mu\omega x^2}{2\hbar}} H_n \left(\sqrt{\frac{\mu\omega}{\hbar}} x \right).$$

Then, it follows that

$$\langle \Psi_n, -\hbar^2 \Psi_m'' \rangle_{L^2(\mathbb{R})} = \begin{cases} \frac{\hbar\mu\omega}{2}(2n+1), & \text{if } n = m \\ -\frac{\hbar\mu\omega}{2}\sqrt{n(n-1)}, & \text{if } n = m+2 \\ -\frac{\hbar\mu\omega}{2}\sqrt{(n+1)(n+2)}, & \text{if } n = m-2. \end{cases}$$

and

$$\langle \Psi_n, x^2 \Psi_m \rangle_{L^2(\mathbb{R})} = \begin{cases} \frac{\hbar}{2\mu\omega}(2n+1), & \text{if } n = m \\ \frac{\hbar}{2\mu\omega}\sqrt{n(n-1)}, & \text{if } n = m+2 \\ \frac{\hbar}{2\mu\omega}\sqrt{(n+1)(n+2)}, & \text{if } n = m-2. \end{cases}$$

Using the annihilation operator $a = 2^{-1/2}(\partial_q + q)$ where $q = \sqrt{\frac{\mu\omega}{\hbar}}x$ and its adjoint we can explicitly compute the matrix elements of all $(\langle \Psi_n, x^n \Psi_m \rangle)$ by writing $q^n = \sqrt{2}(a+a^*)^n$ and using the well-known action of the annihilation operator on eigenstates of (1.98). Using a finite-basis truncation of the above matrices allowed us then to obtain Figures 6.4 and 6.10.

6.B Asymptotic properties of the Ising model

Lemma 2.1. *Let $\beta > 1$ and $h \in [0, h_c)$. The three critical points of $\eta_{N,h} : (-1, 1) \rightarrow \mathbb{R}$*

$$\eta_{N,h}(s) = \frac{\Gamma(N+1)}{\Gamma(N/2(1+s)+1)\Gamma(N/2(1-s)+1)} e^{-\frac{N\beta}{2}(1-s^2)+Nhs}$$

are given by $s_N^c := \gamma(\beta)(1+\mathcal{O}(1))$ where $\gamma(\beta)$ satisfies the critical equation for the continuous renormalized potential

$$\gamma(\beta) = \tanh(\beta\gamma(\beta) + h).$$

Let us order the solutions $\gamma(\beta)$ to that equation by $\gamma_1(\beta) < \gamma_2(\beta) < \gamma_3(\beta)$. For $h = 0$ the function $\eta_{N,0}$ attains (in the limit $N \rightarrow \infty$) its maximum at $\gamma_1(\beta) = -\gamma_3(\beta) < 0$ and minimum at $\gamma_2(\beta) = 0$.

Let $h > 0$, then the function $\eta_{N,h}$ attains (in the limit $N \rightarrow \infty$) its unique global maximum at $\gamma_3(\beta) > 0$ whereas both $\gamma_1(\beta), \gamma_2(\beta) < 0$ and $\gamma_1(\beta), \gamma_2(\beta)$ are local maxima and minima respectively.

The logarithmic derivative $\zeta_{N,h}(s) = \partial_s \log(\eta_{N,h}(s))$ satisfies

$$\zeta_{N,h}(s) = N(\beta s - \operatorname{arctanh}(s) + h)(1 + \mathcal{O}(1)). \quad (2.99)$$

Proof. For $h = 0$ we note that $\eta_{N,0}$ is even and for $h > 0$ the global maxima of $\eta_{N,h}$ must be attained at some $s \geq 0$. Direct computations show by the logarithmic scaling of the digamma function $\Psi_2(s) = \log(\Gamma)'(s) = \log(s) + \mathcal{O}(1/s)$ that the logarithmic derivative $\zeta_{N,h}(s) = \partial_s \log(\eta_{N,h}(s))$ is given by (2.99). Thus, for all critical values s_N^c of $\eta_{N,h}$, i.e. those values that satisfy $\zeta_{N,h}(s_N^c) = 0$, there exists $\gamma(\beta) \in [-1, 1]$ such that $\gamma(\beta) := \lim_{N \rightarrow \infty} s_N^c$ and $\gamma(\beta)$ is any solution to $\gamma(\beta) = \tanh(\gamma(\beta)\beta + h)$.

We then obtain (2.99) directly by differentiating $\log(\eta_{N,h})$ and using the identity

$$\begin{aligned} & -\partial_s \log \left(\Gamma \left(\frac{N(1+s)}{2} + 1 \right) \Gamma \left(\frac{N(1-s)}{2} + 1 \right) \right) \\ &= -\frac{N}{2} \left(\log \left(\frac{1 + N/2(1+s)}{1 + N/2(1-s)} \right) \right) (1 + \mathcal{O}(1)) \\ &= -\frac{N}{2} \left(\log \left(\frac{1 + s \frac{N/2}{1+N/2}}{1 - s \frac{N/2}{1+N/2}} \right) \right) (1 + \mathcal{O}(1)) \\ &= -\frac{N}{2} \left(\log \left(\frac{1+s}{1-s} \right) \right) (1 + \mathcal{O}(1)) \\ &= -N \operatorname{artanh}(s)(1 + \mathcal{O}(1)). \end{aligned} \quad (2.100)$$

Moreover, we read off from (2.99) that

$$\lim_{k \uparrow 1} \zeta_{N,h}(k) = -\infty \text{ and } \lim_{k \downarrow -1} \zeta_{N,h}(k) = \infty.$$

In particular, $\gamma(\beta)$ solves the implicit equation $\gamma(\beta) = \tanh(\beta\gamma(\beta) + h)$. For the second derivative of $\zeta_{N,h}$ which is h -independent, we find the closed-form expression using the derivative of the trigamma function Ψ_3

$$\begin{aligned} \zeta''_{N,h}(s) &= -\frac{N^3}{8} (\Psi'_3(1 + N/2(1 + s)) - \Psi'_3(1 + N/2(1 - s))) \\ &= \frac{N^3}{8} \int_0^\infty z^2 \frac{e^{-z(1+N/2(1+s))} - e^{-z(1+N/2(1-s))}}{1 - e^{-z}} dz. \end{aligned} \quad (2.101)$$

This implies that ζ_N is strictly convex on $[-1, 0)$ and strictly concave on $(0, 1]$. Using the asymptotic of the trigamma function $\Psi_3(s) = 1/s + 1/(2s^2) + \mathcal{O}(1/s^3)$ we find that $\zeta_{N,h}$ is strictly monotone increasing at zero, independent of h ,

$$\zeta'_N(0) = N\beta - \frac{N^2\Psi_3(1 + N/2)}{2} = N \left(\beta - \frac{N/2}{1 + N/2} \right) (1 + o(1)) > 0,$$

since $\beta > 1$. □

Lemma 2.2. *The function $\mathcal{I}(r) := r \frac{I_{n/2-1}(r)}{I_n(r)}$ is strictly monotonically increasing on $(0, \infty)$. In particular $\mathcal{I}'(r) > 0$.*

Proof. By differentiating and using that $I'_\nu(r) = \frac{\nu}{r}I_\nu(r) + I_{\nu+1}(r)$ we find

$$\mathcal{I}'(r) = r \left(1 - \frac{I_{n/2-1}(r)I_{n/2+1}(r)}{I_n(r)^2} \right).$$

Thus, it suffices to record that the product of Bessel functions satisfies $I_{n/2}(z)^2 > (I_{n/2-1}I_{n/2+1})(z)$:

$$\begin{aligned} (I_{n/2-1}I_{n/2+1})(z) &= (z/2)^n \sum_{k=0}^\infty \frac{(n+k+1)_k (z^2/4)^k}{k! \Gamma(n/2 - 1 + k + 1) \Gamma(n/2 + 1 + k + 1)} \\ (I_{n/2}I_{n/2})(z) &= (z/2)^n \sum_{k=0}^\infty \frac{(n+k+1)_k (z^2/4)^k}{k! \Gamma(n/2 + k + 1) \Gamma(n/2 + k + 1)} \end{aligned} \quad (2.102)$$

Hence, the identity follows from

$$\Gamma(n/2 + k + 1)^2 < \Gamma(n/2 - 1 + k + 1) \Gamma(n/2 + 1 + k + 1)$$

which follows itself from logarithmic convexity of the gamma function. □

6.C SUSY Quantum Mechanics

We use ideas from *supersymmetric quantum mechanics*, to show positivity and analyze the ground state of several Schrödinger operators appearing in this article:

In one dimension, we recall that using operators

$$A = \partial_x + W(x) \text{ and } A^* = -\partial_x + W(x)$$

with real-valued and smooth *superpotential* W , we can write

$$A^*A = -\partial_x^2 - W'(x) + W(x)^2 \text{ and } AA^* = -\partial_x^2 + W'(x) + W(x)^2.$$

In particular, $W(x) := \sqrt{\beta(\beta-1)}\beta x^2$ yields operator $S_{\varphi_{\pm}}$ defined in (4.44).

However, solving $A\Psi = 0$ or $A^*\Psi = 0$ shows that $\Psi = Ce^{\pm\sqrt{\beta(\beta-1)}\beta x^3} \notin L^2(\mathbb{R})$. This shows that $\inf(\text{Spec}(AA^*)), \inf(\text{Spec}(A^*A)) > 0$.

We now analyze operators in (6.92). Choosing $W(x) := \frac{x^3}{3}$, yields $A^*A = S_1$ in (6.92), and we find by solving $A\Psi(x) = 0$ that $\Psi(x) \propto e^{-x^4/12}$ which implies that $\inf(\text{Spec}(A^*A)) = 0$.

For radial operators on $L^2((0, \infty), r^{n-1} dr)$, a similar argument applies:

We define operators

$$A = \partial_r + W(r) \text{ and } A^* = -\partial_r + \frac{n-1}{r} + W(r).$$

Choosing then $W(r) := \frac{n^3}{(2+n)}r^3$, such that $A^*A = S_n$ with S_n in (6.92), we find by solving

$$A\Psi = 0 \Rightarrow \Psi(r) \propto e^{-\frac{n^3}{4(n+2)}r^4} \in L^2((0, \infty), r^{n-1} dr).$$

6.D Asymptotic properties

Lemma 4.1. [BBS19, Theo 1.4.10] *Let $V : \mathbb{R} \rightarrow \mathbb{R}$ be smooth with unique global minimum at $\varphi_{min} \in \mathbb{R}$ and $V''(\varphi_{min}) > 0$. Assume that $\int_{\mathbb{R}} e^{-V(\varphi)} d\varphi$ is finite and that $\{\varphi \in \mathbb{R}; V(\varphi) \leq V(\varphi_{min}) + 1\}$ is compact. We also define the probability measure $d\zeta_N(\varphi) = e^{-NV(\varphi)} d\varphi / \int_{\mathbb{R}} e^{-NV(\varphi)} d\varphi$. Then for any bounded smooth function $g : \mathbb{R} \rightarrow \mathbb{R}$*

$$\begin{aligned} \mathbb{E}_{\zeta_N}(g) &= \frac{\int_{\mathbb{R}} g(\varphi) e^{-NV(\varphi)} d\varphi}{\int_{\mathbb{R}} e^{-NV(\varphi)} d\varphi} \\ &= g(\varphi_{min}) + \frac{g''(\varphi_{min})}{2NV''(\varphi_{min})} + \frac{3V'''(\varphi_{min})g'(\varphi_{min})}{4NV''(\varphi_{min})^3} + \mathcal{O}(1/N^2) \end{aligned} \tag{4.103}$$

and for the variance

$$\text{Var}_{\zeta_N}(g) = \frac{g'(\varphi_{min})^2}{NV''(\varphi_{min})} + \mathcal{O}(1/N^2) \quad (4.104)$$

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