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New methods for computer-assisted proofs

(hypo)-elliptic problems, numerical analysis and stochastic dynamics

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Abstract

This thesis is concerned with the treatment of problems, arising from various areas of application of Mathematics — Biology, Fluid Mechanics, Mathematical Physics, Stochastic Dynamics, … — via *computer-assisted proofs*. In particular, we are interested in the application of fundamental ideas in the study of stochastic differential equations and their associated partial differential equations to develop tools in Numerical Analysis and solve new problems with the aid of the computer.

First, taking inspiration from the well-established Functional Analysis of weighted Sobolev spaces associated with gradient diffusion processes, we propose a novel but elementary Numerical Analysis of some differential equations which are naturally well-posed on these topologies. In doing so, we propose an elegant solution to the problem of the construction of *Sobolev orthogonal polynomials* and their use in the resolution of differential equations. Furthermore, we establish a direct link between nonlinear Painlevé recurrence equations and the compactness of embeddings of semi-classically weighted Sobolev spaces. These notions can be applied to both the numerical and rigorous resolution of differential equations via computer-assisted methods: these include Schrödinger-type equations, problems arising from stochastic dynamics and the rigorous computation of (forward) self-similar profiles of semilinear parabolic equations.

Second, we propose a powerful method to give rigorous, tight and explicit bounds on ergodic averages of stochastic flows based on their associated Poisson equation. Our approach is general in the sense that it applies under weak hypoellipticity conditions and outside of perturbative regimes. This allows us to provide a new technique for attacking the fundamental problem of determining the dynamic qualities of a stochastic system via the sign of its Lyapunov exponent. Our method is applied to prove the chaotic nature of both new and classical models, well beyond the prior state-of-the-art.

Declaration of Originality

I hereby declare that the work presented in this thesis is my own unless otherwise stated. To the best of my knowledge the work is original and ideas developed in collaboration with others have been appropriately referenced.

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1

Introduction

In the past decades, computers have played a key role in the settling of major results in Mathematics such as the four-colour theorem [6, 7], the universality of the Feigenbaum constant [160], the Kepler conjecture [131, 132], Smale's 14th problem [211] or more recently the proof of existence of blow-up solutions to Euler's equations with smooth initial data [74]. In nonlinear analysis, much research revolves around the resolution of zero-finding problems of the form

$$F(u) = 0 \tag{1.1}$$

for $F : \mathcal{X} \to \mathcal{X}$, a Banach space mapping. For instance, a solution $u^\star$ to $F(u) = 0$ could be an equilibrium state [10, 59, 217, 234], a periodic solution [117, 215], an invariant manifold [214, 220], a trajectory [147, 216], a particular solution [89, 222] or a self-similar profile [53, 64, 88], etc. of an evolution problem, e.g. a (partial) differential equation, or a discrete dynamical system.

The usual strategy of a *computer-assisted proof* (CAP) to prove the existence of a solution $u^\star \in \mathcal{X}$ to $F(u) = 0$ then usually goes as follows:

1. Find a *numerical solution* $\bar{u} \in \mathcal{X}$ to (1.1) such that $\|F(\bar{u})\|_{\mathcal{X}} \approx 0$.

2. Build a suitable fixed-point operator $T : \mathcal{X} \to \mathcal{X}$ such that fixed points of T are in one-to-one correspondence with zeros of F.

3. Show the self-inclusion $T(\mathcal{U}) \subset \mathcal{U}$ for a closed *small explicit* neighbourhood $\mathcal{U}$ of $\bar{u}$ and compactness or contraction of T on $\mathcal{U}$; therefore establishing the existence of a solution $u^\star \in \mathcal{U}$ to $F(u) = 0$. We may refer to $\mathcal{U}$ as an *enclosure* for $u^\star$.

Such proof of a fixed point for an operator T, can be purely topological [118, 147] or more analytic [139] in nature. A common choice for T is one of a so-called quasi-Newton operator

$$T : \mathcal{X} \longrightarrow \mathcal{X}, \qquad u \longmapsto u - AF(u), \tag{1.2}$$

where $A \approx DF(\bar{u})^{-1}$ such that

$$\|DT(u)\|_{\mathcal{X}\to\mathcal{X}} \approx \|DT(\bar{u})\|_{\mathcal{X}\to\mathcal{X}} = \|\mathrm{id} - ADF(\bar{u})\|_{\mathcal{X}\to\mathcal{X}} \approx 0 \ll 1,$$

for $u \in \mathcal{U}$, making T naturally contracting on $\mathcal{U}$. This construction is made rigorous by the following theorem which is a direct consequence of Banach fixed-point theorem and can be found under various forms in the literature (See [10, 58, 90, 181, 232] and the references therein).

Theorem 1.1 (The Fundamental Theorem)**.** Let $(\mathcal{X}, \|\cdot\|_{\mathcal{X}})$ be a Banach space, let $T : \mathcal{X} \to \mathcal{X}$ be a $\mathcal{C}^1$-map and let $\bar{u} \in \mathcal{X}$ be such that there exist constants $Y, Z_1 \geq 0$ and an increasing continuous function $\mathcal{W} : \mathbb{R}_+ \to \mathbb{R}_+$ such that

$$\|T(\bar{u}) - \bar{u}\|_{\mathcal{X}} \leq Y, \tag{1.3}$$

$$\|DT(\bar{u})\|_{\mathcal{X}\to\mathcal{X}} \leq Z_1, \tag{1.4}$$

$$\|DT(u) - DT(\bar{u})\|_{\mathcal{X}\to\mathcal{X}} \leq \mathcal{W}(\|u - \bar{u}\|_{\mathcal{X}}) \qquad \text{for all } u \in \mathcal{X} \tag{1.5}$$

If there exists $\delta > 0$ such that

$$Y + Z_1\delta + \int_0^\delta \mathcal{W}(s)\mathrm{d}s < \delta, \tag{1.6}$$

$$Z_1 + \mathcal{W}(\delta) < 1, \tag{1.7}$$

then T has a unique fixed point $u^\star$ in $\bar{B}(\bar{u}, \delta)$.

Proof. It suffices to check that (1.6) implies that $T(\bar{B}(\bar{u}, \delta)) \subset \bar{B}(\bar{u}, \delta)$ and that (1.7) implies that $\|DT(u)\|_{\mathcal{X}\to\mathcal{X}} \leq Z_1 + \mathcal{W}(\delta) < 1$ for all $u \in \bar{B}(\bar{u}, \delta)$. See also for instance [58, Theorem 2.1]. □

In the case where T is defined by (1.2), Theorem 1.1 can be seen as some kind of Newton-Kantorovich theorem and (1.3)–(1.5) become respectively

$$\|AF(\bar{u})\|_{\mathcal{X}} \leq Y, \tag{1.8}$$

$$\|\mathrm{id} - ADF(\bar{u})\|_{\mathcal{X}\to\mathcal{X}} \leq Z_1, \tag{1.9}$$

$$\|A(DF(u) - DF(\bar{u}))\|_{\mathcal{X}\to\mathcal{X}} \leq \mathcal{W}(\|u - \bar{u}\|_{\mathcal{X}}) \qquad \text{for all } u \in \mathcal{X} \tag{1.10}$$

Remark 1.2. Note that by construction, if T is as in (1.2), Y is expected to be very close to zero (sometimes of the order of machine epsilon) and Z_1 somewhat close to zero (and thus less than 1, we will see that this is actually linked to "how compact" T is). If $W(\delta) \lesssim \delta^\alpha$ as $\delta \to 0^+$ for some $\alpha > 0$ (e.g. if T is of class $\mathcal{C}^2$, $\alpha = 1$), then (1.4) (or equivalently (1.9)) is the crucial estimate and one can expect δ satisfying conditions (1.6) and (1.7). Furthermore, in this case, one expects to be able to take $\delta \approx Y/(1 - Z_1)$.

In practice, the application of Theorem 1.1 in an infinite dimensional setting requires the combination of functional and numerical analytic arguments. To illustrate the use of this theorem, let us consider the classical example of a (possibly nonlinear) elliptic partial differential on the torus $\mathbb{T}$, which can be regarded through the lens of Fourier series.

Example 1.3 (The classical Fourier example)**.** Consider the simple partial differential equation

$$\Delta u = u + f(x,u), \qquad f \in \mathcal{C}^2(\mathbb{T}\times\mathbb{R}), \tag{1.11}$$

on $\mathbb{T}$ (or equivalently $[0,2\pi)$ with periodic boundary conditions), which can be reformulated as the zero-finding problem

$$F(u) = u + (\mathrm{id}-\Delta)^{-1} f(\cdot,u) = 0, \tag{1.12}$$

say for simplicity on $\mathcal{X} = H^1(\mathbb{T})$ or on $\mathcal{X} = H^2(\mathbb{T})$. Assume that we have found a numerical solution $\bar{u}\in\mathcal{X}$ to (1.12) such that $\|F(\bar{u})\|_{\mathcal{X}} \approx 0$, which should of course be expressed in terms of Fourier series

$$\bar{u} = \sum_{|m|\le n} \bar{u}_m e^{imx}, \qquad \text{for some } n\in\mathbb{N}. \tag{1.13}$$

For both the numerical resolution of the equation and for the analytical pen-and-paper derivation of the bounds (1.3)–(1.5), we should make use of the fact that

$$(\mathrm{id}-\Delta)^{-1} e^{imx} = \frac{1}{1+m^2} e^{imx}, \qquad \text{for all } m\in\mathbb{Z}, \tag{1.14}$$

which should allow us to show and *quantify the compactness* of $(\mathrm{id}-\Delta)^{-1}Df(\cdot,\bar{u}) : \mathcal{X}\to\mathcal{X}$; which holds for instance if $f(x,u)$ is polynomial in u as $\bar{u}\in\mathcal{X}\subset\mathcal{C}^0(\mathbb{T})$. Thus, $(\mathrm{id}-\Delta)^{-1}Df(\cdot,\bar{u})$ is well-approximable in $\mathcal{X}$ by finite rank operators, e.g. by its Fourier *projections*. Furthermore, $DF(\bar{u}) = \mathrm{id} + (\mathrm{id}-\Delta)^{-1}Df(\cdot,\bar{u})$ is a compact perturbation of the identity and we can therefore find a good approximation A to $DF(\bar{u})^{-1}$ such that

$$\|\mathrm{id} - ADF(\bar{u})\|_{\mathcal{X}\to\mathcal{X}} < 1$$

which is the key estimate to prove the contraction of the fixed point operator T defined by (1.2), using Theorem 1.1. For instance, identifying A by its Fourier representation ($\mathcal{X}\simeq\ell^2(\mathbb{Z})$), we could choose $A:\ell^2(\mathbb{Z})\to\ell^2(\mathbb{Z})$ as the block operator

$$A = \begin{pmatrix} \mathrm{id} & & \\ & A_n & \\ & & \mathrm{id} \end{pmatrix}$$

where $A_n \approx (\Pi_n DF(\bar{u})\Pi_n)^{-1}$ and Π_n denotes the projection of $\mathcal{X}$ onto $\mathrm{Span}\{e^{imx}\}_{|m|\le n}$ such that A_n can be seen as an element of $\mathbb{C}^{(2n+1)\times(2n+1)}$. For instance, we can use the computer to rigorously bound $\|\Pi_n(\mathrm{id}-ADF(\bar{u}))\Pi_n\|_{\mathcal{X}\to\mathcal{X}} = \|\Pi_n - A_n\Pi_n DF(\bar{u})\Pi_n\|_{\ell^2\to\ell^2} \approx 0$.

Beyond the possibility of proving new existence results which might be inaccessible by pen-and-paper techniques, CAPs also provide fine and quantitative information on the solution $u^\star$ to the problem (1.1).

By giving guaranteed error bounds on a solution $u^\star$ to $F(u)=0$, CAPs can also be seen as (most) reliable numerical analytic methods. Moreover, a benefit of CAPs which is often omitted is that because of the rigour and suitable numerical and functional analytic setting needed for a

CAP (which is much more demanding than a numerical experiment), they can sometimes lead to new developments in numerical analysis; an aspect which we aim to demonstrate in this thesis.

In particular, as illustrated by Example 1.3, it is clear that a desirable ingredient for the application of Theorem 1.1 is the compactness of $DF(\bar{u}) - \mathrm{id}$. We actually need more than that and further need to be able to *quantify this compactness explicitly*. For instance, the following type of inequality would prove useful for Example 1.3

$$\|u - \Pi_n u\|_{L^2(\mathbb{T})} \leq \frac{1}{n+1}\|u - \Pi_n u\|_{H^1(\mathbb{T})} \qquad \text{for all } u \in H^1(\mathbb{T}), n \in \mathbb{N} \tag{1.15}$$

Such compactness estimates are well-known for classical bases such as finite elements and Fourier, Jacobi, Hermite and Laguerre families. This kind of estimate is often straightforward to obtain when differential operators are diagonal or their inverse is well-behaved with respect to a given explicit basis, e.g. in the case of the Fourier basis, we have (1.14). However, such explicit estimates are more challenging to obtain and use in the resolution of differential equations which are more naturally posed with respect to more exotic bases and functional spaces, such as semiclassical orthogonal polynomials and semiclassically weighted Sobolev spaces. In particular, until recently [53, 54, 67, 88, 218], few general computer-assisted techniques [181, 214] were available to solve elliptic partial differential equations on unbounded domains.

Another setting of interest where such compactness estimates cannot straightforwardly be used is the one of *hypoelliptic equations* and *kinetic models* [49, 134, 224]. While the problem of the computer-assisted resolution of elliptic equations on unbounded domains is likely to be fully resolved in the near future, the treatment of such hypoelliptic/kinetic equations probably constitutes one of the biggest challenges in the domain of computer-assisted proof for the coming years.

In this thesis, we aim to both extend the settings where such explicit compactness estimates can be obtained and give methods to bypass this issue for certain problems using ideas form the Functional Analysis of *diffusion processes*. This leads to the development of both new tools in Numerical Analysis and computer-assisted proofs theory allowing us to solve several new classes of problems.

1.1 A motivation: the Lyapunov exponent for the Hopf normal form with additive noise

Much of the present work was motivated by the computation of the *Lyapunov exponent* λ associated to ergodic stochastic flows $(\varphi_t)_{t\geq 0}$ satisfying a stochastic differential equation of the form

$$\mathrm{d}\varphi_t(\omega, x) = X_0(\varphi_t(\omega, x))\mathrm{d}t + \sigma \mathrm{d}B_t(\omega), \qquad \varphi_0(\omega, x) = x \in \mathcal{M} = \mathbb{T}^{d_1} \times \mathbb{R}^{d_2}, \omega \in (\Omega, \mathbb{P}) \tag{1.16}$$

that is the limit

$$\lambda := \lim_{t\to\infty} \frac{1}{t} \log \|D\varphi_t(\omega, x)v\|, \qquad \text{for almost every } \omega, (x, v) \in \Omega \times T\mathcal{M}, \tag{1.17}$$

which characterises chaos when $\lambda > 0$, or synchronisation when $\lambda < 0$. Therefore, the determination of the sign of the Lyapunov exponent for a given model is a fundamental problem in Stochastic Dynamics [14, 24, 29, 32, 33, 192]. For more details, see Section 1.3 and Chapter 5. In particular, we were interested in proving the positivity of the Lyapunov exponents λ_b for the Hopf normal form with additive noise [24, 73, 94, 97]

$$\mathrm{d}\varphi_t = \left[\begin{pmatrix} \alpha & -\beta \\ \beta & \alpha \end{pmatrix} \varphi_t - \begin{pmatrix} a & b \\ -b & a \end{pmatrix} \varphi_t \|\varphi_t\|^2 \right] \mathrm{d}t + \sigma \mathrm{d} \begin{pmatrix} B_t^1 \\ B_t^2 \end{pmatrix}, \qquad a > 0 \tag{1.18}$$

on $\mathbb{R}^2$, for a shear parameter b large enough, as conjectured in [94, 97]. The challenge of treating this problem via computer assistance led to the development of many ideas and methods exposed in the present thesis. While not all of these ended up being useful for the particular problem of the Hop normal form, it remains a good motivation to introduce some key topics of this thesis.

In this case, λ_b can be written as an integral (see Section 4.1 for a derivation and also [94])

$$\lambda_b = \int_0^{2\pi} \int_0^{\infty} (\alpha - 2ar^2 + \sqrt{a^2+b^2} r^2 \sin 2\vartheta) w(\mathrm{d}r, \mathrm{d}\vartheta) \tag{1.19}$$

where w is the stationary probability density of the process

$$\begin{cases} \mathrm{d}r_t &= \left(\alpha r_t - a r_t^3 + \dfrac{\sigma^2}{2r_t} \right) \mathrm{d}t + \sigma \mathrm{d}\tilde{B}_t^1 \\ \mathrm{d}\vartheta_t &= \left(b r_t^2 + \sqrt{a^2+b^2} r_t^2 \cos(2\vartheta_t) \right) \mathrm{d}t - \dfrac{\sigma}{r_t} \mathrm{d}\tilde{B}_t^2 \end{cases} \tag{1.20}$$

on $\mathbb{R}_+ \times \mathbb{T}$. In principle, if one could compute the stationary density w with rigorous bounds, one would directly be able to enclose λ_b and thus prove its sign. Therefore, one approach to this problem is to obtain w as the solution of the stationary Fokker-Planck equation [189] associated to the diffusion (1.20)

$$-r^2 \frac{\partial}{\partial \vartheta} \left(\left(b + \sqrt{a^2+b^2} \cos(2\vartheta) \right) w \right) - \frac{\partial}{\partial r} \left(\left(\alpha r - a r^3 + \frac{\sigma^2}{2r} \right) w \right) + \frac{\sigma^2}{2} \left(\frac{\partial^2 w}{\partial r^2} + \frac{1}{r^2} \frac{\partial^2}{\partial \vartheta^2} \right) = 0. \tag{1.21}$$

Progress using this computer-assisted strategy was achieved in [57] but didn't manage to compute w on the full domain $\mathbb{R}_+ \times \mathbb{T}$ but rather only an approximation of it on the bounded annular domain $[0.5, 1.5] \times \mathbb{T}$ (for $a = 1$, $b = 3.5$ $\alpha = 1$, $\beta = 1$ and $\sigma = 1.3$). First, observe that the singularity on $\{0\} \times \mathbb{T}$ is straightforwardly removable as an artifact of a polar coordinate change of variable. For instance, if we write

$$w(r, \vartheta) = (1 + u(r, \vartheta)) \nu(\mathrm{d}r, \mathrm{d}\vartheta), \qquad \nu(\mathrm{d}r, d\vartheta) = \frac{r}{Z} \exp\left(\frac{2}{\sigma^2} \left(-a \frac{r^4}{4} + \alpha \frac{r^2}{2} \right) \right) \mathrm{d}r \mathrm{d}\vartheta,$$

where ν is a probability measure, then

$$-r^2 \frac{\partial}{\partial \vartheta} \left(\left(b + \sqrt{a^2+b^2} \cos(2\vartheta) \right) u \right) + (-ar^3 + \alpha r) \frac{\partial u}{\partial r} + \frac{\sigma^2}{2} \Delta u = -2\sqrt{a^2+b^2} r^2 \sin(2\vartheta) \tag{1.22}$$

where

$$\Delta = \frac{1}{r}\frac{\partial}{\partial r}\left(r\frac{\partial}{\partial r}\right) + \frac{1}{r^2}\frac{\partial^2}{\partial \vartheta^2}$$

is the polar coordinate Laplacian on $\mathbb{R}^2 \simeq \mathbb{R}_+ \times \mathbb{T}$. However, approaching the full problem (1.21) on $\mathbb{R}^2 \simeq \mathbb{R}_+ \times \mathbb{T}$ is much more challenging.

This difficulty stems from the fact that the the overwhelming majority of computer-assisted resolutions of PDEs take advantage of the effortless construction of compact operators on bounded domains, making them approximable by finite rank operators (e.g. in [11, 215]). For instance, $(\Delta - \mathrm{id})^{-1}$ looses its compactness when considered on the full space $L^2(\mathbb{R}^2)$.

1.1.1 An approach on Freud-weighted Sobolev spaces

A natural functional analytic approach on unbounded spaces is to turn to an analysis on weighted Sobolev spaces and in particular to make use of the gradient diffusion operator

$$\mathfrak{L} = (ar^3 - \alpha r)\partial_r - \Delta \tag{1.23}$$

which is a positive semi-definite self-adjoint operator on $L^2(\nu)$ and should play the same role as the Laplacian Δ on $\mathbb{T}^d$ [20, 189]. We could therefore try to solve the equivalent zero-finding problem

$$F(u) = u - \mathfrak{L}^{-1}\left\{2\sqrt{a^2+b^2}r^2\sin(2\vartheta) - r^2\frac{\partial}{\partial\vartheta}\left(\left(b+\sqrt{a^2+b^2}\cos(2\vartheta)\right)u\right)\right\} = 0$$

by applying Theorem 1.1, for instance on the weighted Sobolev space

$$H^1_0(\nu) = \left\{v \in H^1(\nu) \mid \int_{\mathbb{R}^2} v \mathrm{d}\nu = 0\right\}.$$

However, a full numerical analysis of this space, e.g. the construction and use of an associated basis, is so far too difficult and out of the scope of the present work. As a first step, we considered one-dimensional differential equations involving the closely-related operator

$$\mathfrak{L} = (x^3 - \kappa x)\partial_x - \partial_{xx} \tag{1.24}$$

on the associated Sobolev space $H^1(\exp(-\frac{x^4}{4} + \kappa\frac{x^2}{2}))$. While this one-dimensional analysis is simpler, it already led to the first mathematically rigorous numerical analytic work on the use of so-called Freud-type (i.e. associated to a double-well potential) orthogonal polynomials [47, 108] and spaces to solve differential equations. We delve into this analysis in Chapter 3.

1.1.2 An approach on Hermite-weighted Sobolev spaces

Another approach to the problem (1.22) is to make the change of variable

$$r \longmapsto \sqrt{r}, \qquad \vartheta \longmapsto \vartheta/2$$

such that Eq. (1.22) becomes

$$-\frac{\partial}{\partial\vartheta}\left(\left(b+\sqrt{a^2+b^2}\cos\vartheta\right)u\right) + (-ar+\alpha)\frac{\partial u}{\partial r} + \sigma^2\Delta u = -\sqrt{a^2+b^2}\sin\vartheta. \tag{1.25}$$

Now, identifying the generator of the spherically symmetric Ornstein–Uhlenbeck process

$$\mathfrak{L} = ar\partial_r - \sigma^2\Delta, \tag{1.26}$$

one can attempt to solve the zero-finding problem

$$F(u) = u - \mathfrak{L}^{-1}\left\{\sqrt{a^2+b^2}r\sin\vartheta - \frac{\partial}{\partial\vartheta}\left(\left(b+\sqrt{a^2+b^2}\cos\vartheta\right)u + \alpha\frac{\partial u}{\partial r}\right)\right\} = 0 \tag{1.27}$$

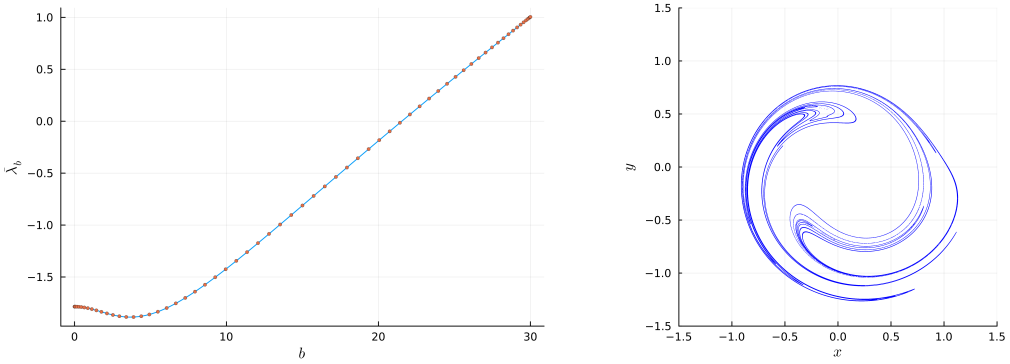
by using Theorem 1.1 on the weighted Sobolev space $H^1_0(\nu)$ where the probability measure ν is given by $\nu(\mathrm{d}r,\mathrm{d}\vartheta) = re^{-r^2/\sigma^2}\mathrm{d}r\mathrm{d}\vartheta$. Because much more is known about this Gaussian setting, e.g. the eigenfunctions of $\mathfrak{L}$ (made up of Hermite-like polynomials [75, 189]), one could hope to solve Eq. (1.21) via this approach. This approach is developed in Chapter 2 and we attempt to apply this strategy on problem (1.27) in Chapter 4.

1.1.3 Resolution via the adjoint method on the computer

While the aforementioned work led to the development of a rich theory of numerical analysis of weighted Sobolev spaces, we will see in Chapter 4 that this approach was unfortunately not quite good enough to enclose the solution of the stationary Fokker-Planck equation (1.21).

To bypass this issue, in Chapter 5, we develop a so-called computer-assisted *adjoint method* [18, 24] to directly enclose the ergodic average (1.19) without having to solve (1.21) but instead based on a non-rigorous resolution of the associated Poisson equation [46, 188]. This makes this approach very powerful and broadly applicable as not based on an application of the Theorem 1.1. Furthermore, we are able to combine this method with *continuation* techniques [51] to not only enclose λ_b for one single parameter value b but for a whole parameter range.

When applied in the case of the present problem of the enclosure of the Lyapunov exponent λ_b associated to the Hopf system (1.18), we obtained the following result.



(a) Graph of the function $b \mapsto \bar{\lambda}_b$; the orange points are sampled at Chebyshev nodes.

(b) Snapshot of a chaotic random attractor of (1.18) with $b = 21.5381$.

Figure 1.1: Quantitative and qualitative random dynamics induced by (1.18) with $a = \alpha = 4$ and $\sigma = \sqrt{2}$.

Theorem 1.4. Consider the stochastic flow $(\varphi_t)_{t\geq 0}$ on $\mathcal{M} = \mathbb{R}^2$ generated by the Hopf normal form with additive noise, i.e. by the stochastic differential equation (1.18). Let $\beta \in \mathbb{R}$ and fix $a = \alpha = 4$, $\sigma = \sqrt{2}$. Let λ_b denote the Lyapunov exponent of this system for a shear parameter

b, and $b \mapsto \bar{\lambda}_b$ be the function represented in Figure 1.1a (and whose precise description can be found at [78]). Then, for *all* $b \in [0, 30]$

$$|\lambda_b - \bar{\lambda}_b| \leq 3.41 \times 10^{-4}.$$

Proof. See Section 5.6 □

Corollary 1.5. Consider λ_b as in Theorem 1.4, then there exists $b^* \in (21.5323, 21.5381)$ such that $\lambda_{b^*} = 0$. Furthermore, $\lambda_b < 0$ for $b \in [0, 21.5322]$ and $\lambda_b > 0$ for $b \in [21.5381, 30]$.

The study of the Lyapunov exponent for system (1.18) was initiated in [94], where it was numerically conjectured that the Lyapunov exponent λ was positive for b large enough. After several attempts pointing to this result [57, 97, 100], the conjecture was recently proved in the asymptotic regime $b \to \infty$ in [24, 73]. Theorem 1.4 complements these results by covering the non-asymptotic regime. In particular, we obtain a precise estimate of the shear parameter value b^* at which the transition from negative to positive Lyapunov exponent occurs.

1.2 Resolution of differential equations on weighted Sobolev spaces

1.2.1 Functional Analysis on weighted Sobolev spaces

In the previous section, to play the role of the usual Laplacian on unbounded domains, we hinted at the study of an operator $\mathfrak{L}$ defined by (1.23), (1.24) or (1.26) to recover some compactness on $\mathbb{R}^d$. More generally, for a $\mathcal{C}^2$ potential $V : \mathbb{R}^d \to \mathbb{R}$, we can consider the operator

$$\mathfrak{L} = \nabla V \cdot \nabla - \Delta. \tag{1.28}$$

The operator $\mathfrak{L}$ is well-studied as $-\mathfrak{L}$ is the generator of the overdamped Langevin diffusion

$$\mathrm{d}x_t = -\nabla V(x_t)\mathrm{d}t + \sqrt{2}\mathrm{d}B_t. \tag{1.29}$$

If $e^{-V} \in L^1(\mathbb{R}^d)$, the potential V is said to be confining and the diffusion process (1.29) has the probability measure

$$\nu(\mathrm{d}x) = \frac{e^{-V}}{Z}\mathrm{d}x, \qquad Z = \int_{\mathbb{R}^d} e^{-V}\mathrm{d}x$$

as a stationary measure [189]. It is then natural to consider the study of $\mathfrak{L}$ on the weighted Sobolev space

$$H^n(\nu) = \left\{ f \in L^2(\nu) \mid \partial_\beta f \in L^2(\nu) \text{ for all } \beta \in \mathbb{N}^d, |\beta| \leq n \right\}.$$

For instance, $\mathfrak{L}$ is a self-adjoint positive semi-definite operator on $(L^2(\nu), \langle \cdot, \cdot \rangle)$ and $\mathfrak{L}$ can be seen as a Dirichlet form on $H^1(\nu)$. Indeed, observe that for all $u, v \in H^2(\nu)$,

$$\langle u, \mathfrak{L}v \rangle = \int_{\mathbb{R}^d} u(\mathfrak{L}v)\mathrm{d}\nu = -\int_{\mathbb{R}^d} (\nabla u \cdot \nabla v)\mathrm{d}\nu = \int_{\mathbb{R}^d} (\mathfrak{L}u)v\mathrm{d}\nu = \langle \mathfrak{L}u, v \rangle,$$

similarly to the Laplacian Δ on a bounded domain. Furthermore, under certain conditions [189, 224], a Poincaré inequality can be recovered on $H^1(\nu)$, i.e. there exists $C_P > 0$ such that for all

$u \in H^1(\nu)$

$$\mathrm{Var}_\nu(u) = \int_{\mathbb{R}^d} u^2 \mathrm{d}\nu - \left(\int_{\mathbb{R}^d} u \mathrm{d}\nu\right)^2 \leq C_P \int_{\mathbb{R}^d} |\nabla u|^2 \mathrm{d}\nu, \tag{1.30}$$

or equivalently

$$\int_{\mathbb{R}} u^2 \mathrm{d}\nu \leq C_P \int_{\mathbb{R}} |\nabla u|^2 \mathrm{d}\nu \qquad \text{for all } u \in H^1_0(\nu) = \left\{ u \in H^1(\nu) \mid \int_{\mathbb{R}^d} u \mathrm{d}\nu = 0 \right\}. \tag{1.31}$$

This means that the analysis of this setting is really similar to the one of a first course on elliptic PDEs. For instance, this directly implies that the Lax–Milgram theorem can be applied.

Proposition 1.6. Suppose there is a Poincaré inequality of the form (1.30) on $H^1(\nu)$. Let $H^{-1}(\nu)$ denote the dual with respect to $\langle \cdot, \cdot \rangle$ of

$$H^1_0(\nu) := \left\{ u \in H^1(\nu) \middle| \int_{\mathbb{R}} u \mathrm{d}\nu = 0 \right\}.$$

Then for all $g \in H^{-1}(\nu)$, there exists a unique $u \in H^1_0(\nu)$ such that for all $v \in H^1_0(\nu)$

$$\int_{\mathbb{R}} \nabla u \cdot \nabla v \mathrm{d}\nu = \int_{\mathbb{R}} g v \mathrm{d}\nu.$$

We denote $u = \mathfrak{L}^{-1} g$. Furthermore, $\mathfrak{L}^{-1} : H^{-1}(\nu) \to H^1_0(\nu)$ is a bounded linear operator.

Proof. Using the Poincaré inequality (1.31), this follows immediately from the Lax–Milgram Theorem [61, Corollary V.8]. □

In the case where we further have that the embedding $H^1(\nu) \hookrightarrow L^2(\nu)$ is compact (e.g. if $V(x) = x^2$), then we may hope to use CAPs to solve equations of the form

$$\mathfrak{L} u = f(x, u, \nabla u). \tag{1.32}$$

Such equations, in addition of being related to diffusion processes can appear in other contexts. For instance, since

$$e^{-V/2} \mathfrak{L}(e^{V/2} \cdot) = -\Delta + \frac{1}{4}(V'(x))^2 - \frac{1}{2} V''(x),$$

we may consider Schrödinger-type equations [150, 189]

$$-\Delta u + W(x) u = f(x, u), \qquad W(x) := \frac{1}{4}(V'(x))^2 - \frac{1}{2} V''(x).$$

Furthermore, in the Gaussian case $V(x) = x^2/4$, since

$$e^{-V} \mathfrak{L}(e^{V} \cdot) = -\frac{d}{2} - \frac{x}{2} \cdot \nabla - \Delta \tag{1.33}$$

an important example to consider will be equations of the type

$$L u = f(x, u, \nabla u), \qquad L := -\frac{x}{2} \cdot \nabla - \Delta. \tag{1.34}$$

This form of equation appears when considering *rapidly decaying* self-similar profiles of parabolic semilinear equations [2, 34, 84, 102]. We analyse equations of the type (1.34) in more detail in

Chapter 2.

1.2.2 Numerical Analysis on weighted Sobolev spaces

Since the Functional Analysis of the operator $\mathfrak{L}$ seems to suitable to use CAPs to solve equations of the type (1.32), what remains to be seen is how to approach such equation numerically. In particular, we need to choose a suitable basis to

1. solve the equation numerically,
2. obtain estimates of the type (1.15) necessary to the CAP.

If we restrict ourself to dimension $d = 1$, since we want to work with $L^2(\nu)$, a natural idea is to make use of orthonormal polynomials $\{p_n\}_{n\in\mathbb{N}}$ on $L^2(\nu)$, that is a sequence of polynomials of increasing degree with

$$\langle p_n, p_m\rangle = \int_{\mathbb{R}} p_n p_m \mathrm{d}\nu = \delta_{mn}, \qquad Z := \int_{\mathbb{R}} e^{-V(x)}\mathrm{d}x.$$

However, outside of classical families (Fourier, Jacobi, Hermite, Laguerre), because they can be tricky to work with, orthogonal polynomials are rarely used in the resolution of differential equations. Furthermore, when wanting to build a CAP based on Theorem 1.1 and especially when considering nonlinear problems, we may want to also work with an $H^1(\nu)$-basis to be able to make use of Sobolev embeddings [61, Chapter IX.3]. The construction of polynomial bases on $H^1(\nu)$, so-called *Sobolev orthogonal polynomials*, was introduced in the 1960s [5]. Despite being the subject of a large literature [5, 169, 170, 172, 213], they have however not been used outside of classical weights for what should be their main purpose: the resolution of differential equations [170]. One immediate issue is that when considering a standard inner product

$$\int_{\mathbb{R}} u'v'\mathrm{d}\nu + \Lambda \int_{\mathbb{R}} uv\mathrm{d}\nu, \qquad \Lambda > 0,$$

the induced polynomials depend non-trivially on the chosen constant Λ and are therefore not "canonical" [170]. Naturally, what we would like is to take $\Lambda = 0$ and use the inner product

$$\int_{\mathbb{R}} u'v'\mathrm{d}\nu.$$

However, such a bilinear form would not define an inner product on $H^1(\nu)$ as it would not dominate the $L^2(\nu)$-norm and not be definite (this is easily shown by taking $u = v = 1$). This is due to the fact that there does not hold a "classical" Poincaré inequality on $H^1(\nu)$. However, it does hold on $H^1_0(\nu)$ by (1.31). We thus define the inner product

$$(u, v) := \int_{\mathbb{R}} u'v'\mathrm{d}\nu + \int_{\mathbb{R}} u\mathrm{d}\nu \int_{\mathbb{R}} v\mathrm{d}\nu$$

on $H^1(\nu)$ which induces a norm Lipschitz equivalent to the standard $H^1(\nu)$ norm and thus induces a Hilbert structure on $H^1(\nu)$.

Therefore, in this thesis, we are able to construct a first natural Hilbert basis of $(\cdot,\cdot)$-orthonormal polynomials $\{q_n\}_{n\in\mathbb{N}}$ for $H^1(\nu)$. We will see that this basis is much simpler than previous constructions of Sobolev orthogonal polynomials. Moreover, we will be able to use them in the resolution

of some PDEs which are naturally posed on weighted Sobolev spaces.

In particular, we shall be able to extend explicit estimates of the type (1.15) to the setting of weighted Sobolev spaces $H^1(e^{-V}/Z)$, at least in the case where V is polynomial. For instance, in the case of the Freud weight $V(x) = x^4/4 - \kappa x^2/2$, we are able to prove:

Theorem 1.7. Consider $V(x) = x^4/4 - \kappa x^2/2$, then there exist $C > 0$ and $N \in \mathbb{N}$ such that for all $m \geq N$ and $u \in \overline{\mathrm{Span}\{q_j\}_{j>m}}^{H^1(\nu)}$

$$\|u\|_{L^2(\nu)} \leq \frac{C}{m^{3/4}} \|u\|_{H^1(\nu)}. \tag{1.35}$$

In particular, if $\kappa = 4$, the above holds for $C = 1.2233$ and $N = 2,187$.

Proof. See Section 3.3.3. □

Additionally to these advances in Numerical Analysis, we also introduce new techniques for computer-assisted proofs for differential equations on Hilbert spaces by developing rigorous quadrature rules and proposing new sharp ℓ^2-estimates for the application of Theorem 1.1.

1.2.3 Some results

With these techniques, we were able to rigorously enclose solutions of various classical differential equations on $\mathbb{R}^d$, using Theorem 1.1. For instance, consider the semilinear heat equation [102]

$$\partial_t v = \Delta v + v^3, \tag{1.36}$$

on $\mathbb{R}^2$. Under the similarity transformation $v(t,x) = t^{-1/(p-1)} u(x/\sqrt{t})$, u is a self-similar profile of Eq. (1.36) if it solves the elliptic partial differential equation

$$Lu = \frac{1}{2}u + u^3, \tag{1.37}$$

where $L = -\frac{x}{2} \cdot \nabla - \Delta u$. We obtain the following numerical solution $\bar{u}$ to (1.37).

Theorem 1.8. Let $\bar{u} : \mathbb{R}^2 \to \mathbb{R}$ be the function whose restriction to the disk $\{(x,y) \mid x^2 + y^2 \leq 4^2\}$ is represented on Fig 1.2 and whose description is available at [80]. There exists a solution $u^\star \in H^2(e^{|x|^2/4}, \mathbb{R}^2)$ to Eq. (1.37) such that

$$\|u^\star - \bar{u}\|_{H^2(e^{|x|^2/4})} \leq 1.6 \times 10^{-3},$$

where $\|f\|_{H^2(e^{|x|^2/4})} := \|Lf\|_{L^2(e^{|x|^2/4})}$ for all $f \in H^2(e^{|x|^2/4})$.

Proof. See Section 2.4.5. □

As hinted in Section 1.2.1, we are also able to solve Schrödinger-type equations. For instance, consider the Gross–Pitaevskii equation with sextic potential

$$i\partial_t v = -\partial_{xx} v + W(x)v + |v|^2 v, \tag{1.38}$$

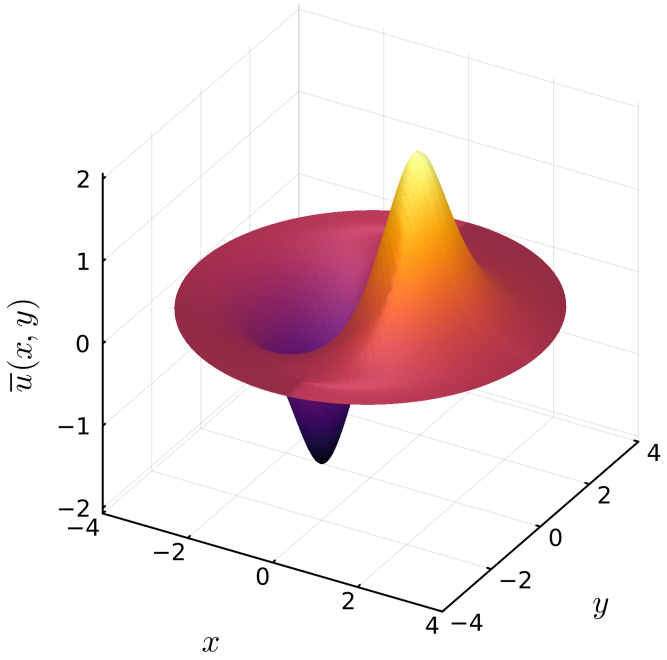


Figure 1.2: Non-radial numerical solution $\bar{u}$ to Eq. (1.37).

where $W(x) = x^6/4 - \kappa x^4/2 + cx^2 + d$. Looking for standing wave solutions of the form $v(t,x) = e^{i\omega t}\varphi(x)$ of Eq. (1.38), we obtain that φ satisfies the elliptic equation

$$-\partial_{xx}\varphi + W(x)\varphi + \varphi^3 = \omega\varphi. \tag{1.39}$$

Theorem 1.9. Let $c = 5/2$, $d = 2$, $\kappa = 4$, $\omega = 8$ and $\bar{\varphi} : \mathbb{R} \to \mathbb{R}$ be the function whose restriction to the interval $[-5, 5]$ is depicted in Figure 1.3, and whose precise description is available at [79] in the file `GP_eq/ubar1`. There exists an even *strictly positive* solution $\varphi_1^\star \in H^1(\mathbb{R})$ to Eq. (1.39) such that

$$\|\varphi_1^\star - \bar{\varphi}_1\|_{H^1(\mathbb{R})} \leq 3.89 \times 10^{-101},$$

where $\|\cdot\|_{H^1(\mathbb{R})}$ is the standard H^1-norm on $\mathbb{R}$ equipped with the Lebesgue measure $\mathrm{d}x$, i.e. $\|\varphi\|_{H^1(\mathbb{R})} = \left(\int_{\mathbb{R}} \varphi^2 \mathrm{d}x + \int_{\mathbb{R}} (\varphi')^2 \mathrm{d}x\right)^{1/2}$.

Proof. See Section 3.4 □

1.3 Rigorous enclosure of ergodic averages of stochastic flows

Let us come back to our original problem, the computation of Lyapunov exponents for stochastic flows $(\varphi_t)_{t\geq 0}$ satisfying stochastic differential equations with additive noise

$$\mathrm{d}\varphi_t(\omega, x) = X_0(\varphi_t(\omega, x))\mathrm{d}t + \sigma \mathrm{d}B_t(\omega), \qquad \varphi_0(\omega, x) = x \in \mathcal{M} \tag{1.40}$$

on a d-dimensional manifold $\mathcal{M} = \mathbb{T}^{d_1} \times \mathbb{R}^{d_2}$, where $(B_t)_{t\geq 0}$ denotes a d-dimensional Brownian motion on a probability space $(\Omega, \mathbb{P})$. Under the assumption that the Markov process $(\varphi_t)_{t\geq 0}$

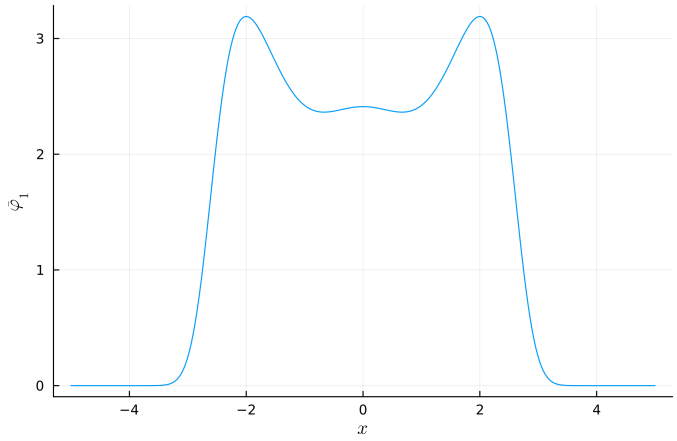


Figure 1.3: Plot of a numerical solution $\bar{\varphi}_1$ to Eq. (1.39) with $c = 5/2$, $d = 2$, $\kappa = 4$ and $\omega = 8$.

possesses a unique ergodic probability measure μ (and additional integrability conditions), $(\varphi_t)_{t\geq 0}$ has a constant Lyapunov exponent

$$\lambda := \lim_{t\to\infty} \frac{1}{t} \log \|D\varphi_t(\omega, x)v\|, \tag{1.41}$$

for $(\mathbb{P} \times \mu)$-almost every $(\omega, x) \in \Omega \times \mathcal{M}$, Lebesgue-almost every $v \in T_x\mathcal{M}$.

In the example of the Hopf normal form with additive noise of Section 1.1, λ could be obtained as the ergodic average (1.19) for the associated process (1.20). More generally, the Lyapunov exponent λ can be calculated via the so-called *Furstenberg–Kashminskii formula* [71, 112, 152]

$$\lambda = \int_{\mathbf{P}\mathcal{M}} Q(x, s)\tilde{\mu}(\mathrm{d}x, \mathrm{d}s), \qquad Q(x, s) = \langle s, DX_0(x)s\rangle, \tag{1.42}$$

if there exists a unique stationary measure $\tilde{\mu}(\mathrm{d}\xi) = \tilde{w}(\xi)\mathrm{d}\xi$ for the so-called *projective process* $(\xi_t)_{t\geq 0} = (\varphi_t, s_t)_{t\geq 0}$ on the projective bundle $\mathbf{P}\mathcal{M}$ where $(s_t)_{t\geq 0}$ solves the variational equation

$$\mathrm{d}s_t = h(\varphi_t, s_t)\mathrm{d}t := (DX_0(\varphi_t)s_t - Q(\varphi_t, s_t)s_t)\mathrm{d}t, \tag{1.43}$$

(see Section 5.3.1 for a proof). As illustrated by the example of Section 1.1, it is in general not simple to enclose $\tilde{\mu}(\mathrm{d}\xi) = \tilde{w}\mathrm{d}\xi$ by solving solving the stationary Fokker–Planck equation

$$\tilde{\mathcal{L}}^*\tilde{w} = 0$$

where

$$\tilde{\mathcal{L}}^* = -\nabla_x \cdot (X_0\cdot) - \nabla_s \cdot (h\cdot) + \frac{\sigma^2}{2}\Delta_x \tag{1.44}$$

which is the $L^2(\mathbf{P}\mathcal{M})$-adjoint of the generator of $(\xi_t)_{t\geq 0}$

$$\tilde{\mathcal{L}} = X_0 \cdot \nabla_x + h \cdot \nabla_s + \frac{\sigma^2}{2}\Delta_x. \tag{1.45}$$

In the case of the example of the Hopf normal form of Section 1.1, the Furstenberg–Khasminskii formula (1.42) and the projective process (φ_t, s_t) given by Eq. (1.40) & (1.43) can be further

simplified to formula (1.19) and system (1.20). In this case, solving for the elliptic Fokker–Planck equation (1.21) is difficult because posed on an unbounded domain. However, contrary to this example where the Fokker–Planck equation $\tilde{\mathcal{L}}^*\tilde{w} = 0$ reduces to the elliptic equation (1.21), in general, the Fokker–Planck operator $\tilde{\mathcal{L}}^*$ associated to the projective process $(\xi_t)_{t\geq 0} = (\varphi_t, s_t)_{t\geq 0}$ is not elliptic (in the s direction) as apparent in (1.44). Even on the bounded domain $\mathbb{T}^d$, where many techniques are available (Fourier series, Banach algebra,...), there is currently no general computer-assisted (or even numerical analytic) method to study hypoellitptic operators of the type (1.44). Therefore, it is not straightforward to apply Theorem 1.1 in this context.

To bypass this issue and avoid solving Eq. (1.44) rigorously, we adapt a well-known technique in the theory of stochastic dynamical systems, *the adjoint method* [18], to make it amenable to computer-assisted tools. This method relies on the observation that (under some regularity and integrability conditions [24]) for $u \in \mathcal{C}^2(\mathbf{P}\mathcal{M})$, the function

$$\tilde{\mathcal{L}}u$$

has $\tilde{\mu}$-mean zero. Indeed, for instance, assume that $\mathcal{M} = \mathbb{T}^d$ such that we avoid any technical consideration, then if $\tilde{w} \in \mathcal{C}^2(\mathbf{P}\mathcal{M})$, for any $u \in \mathcal{C}^2(\mathbf{P}\mathcal{M})$

$$\int_{\mathbf{P}\mathcal{M}} (\tilde{\mathcal{L}}u)(\xi)\tilde{\mu}(\mathrm{d}\xi) = \int_{\mathbf{P}\mathcal{M}} (\tilde{\mathcal{L}}u)(\xi)\tilde{w}(\xi)\mathrm{d}\xi = \int_{\mathbf{P}\mathcal{M}} u(\xi)(\tilde{\mathcal{L}}^*\tilde{w})(\xi)\mathrm{d}\xi = 0,$$

as $\tilde{\mathcal{L}}\tilde{w} = 0$. Therefore, we can "rewrite" formula (1.42) for the Lyapunov exponent λ as

$$\lambda = \int_{\mathbf{P}\mathcal{M}} (Q - \tilde{\mathcal{L}}u)\mathrm{d}\tilde{\mu}. \tag{1.46}$$

While we still do not know $\mathrm{d}\tilde{\mu} = \tilde{w}(\xi)\mathrm{d}\xi$, if u is well-chosen such that the integrand $Q - \tilde{\mathcal{L}}u$ is more manageable, we can hope to get a better bounds on λ. Ideally, we would like u to be the solution of the *Poisson problem* [46, 188]

$$\tilde{\mathcal{L}}u = Q - \lambda.$$

Clearly, it is not in general possible to solve exactly for u but, on the computer, one can hope to build a very good approximation $\bar{u}$ for u. Assume that we have found $\bar{\lambda} \approx \lambda$ for instance via a Monte-Carlo method [205], then we can attempt to find numerically $\bar{u} \in \mathcal{C}^2(\mathbf{P}\mathcal{M})$ such that

$$\tilde{\mathcal{L}}\bar{u} \approx Q - \bar{\lambda}.$$

Defining $\bar{Q} := \tilde{\mathcal{L}}\bar{u} + \bar{\lambda} \in \mathcal{C}^0(\mathbf{P}\mathcal{M})$, then by (1.46),

$$\lambda = \int_{\mathbf{P}\mathcal{M}} (Q - \tilde{\mathcal{L}}\bar{u})\mathrm{d}\tilde{\mu} = \int_{\mathbf{P}\mathcal{M}} (Q - \bar{Q} + \lambda)\mathrm{d}\tilde{\mu}.$$

and therefore, since $\mathrm{d}\tilde{\mu} = \tilde{w}\mathrm{d}\xi$

$$|\lambda - \bar{\lambda}| = \left| \int_{\mathbf{P}\mathcal{M}} (Q - \bar{Q})\mathrm{d}\tilde{\mu} \right| \tag{1.47}$$

where λ is the unknown to enclose but $Q, \bar{Q}$ and $\bar{\lambda}$ are known. For instance, if Q and $\bar{Q}$ are L^∞,

we can immediately apply Hölder's inequality to obtain the estimate

$$|\lambda - \bar{\lambda}| = \left| \int_{\mathbf{P}\mathcal{M}} (Q - \bar{Q}) \mathrm{d}\tilde{\mu} \right| \leq \|Q - \bar{Q}\|_\infty \int_{\mathbf{P}\mathcal{M}} \mathrm{d}\tilde{\mu} = \|Q - \bar{Q}\|_\infty. \tag{1.48}$$

as $\tilde{\mu}$ is a probability measure. Here is an example where this estimate (1.48) is used.

Theorem 1.10. Consider the cellular flow with sinks $(\varphi_t)_{t\geq 0}$ on $\mathcal{M} = \mathbb{T}^2$ generated by the stochastic differential equation

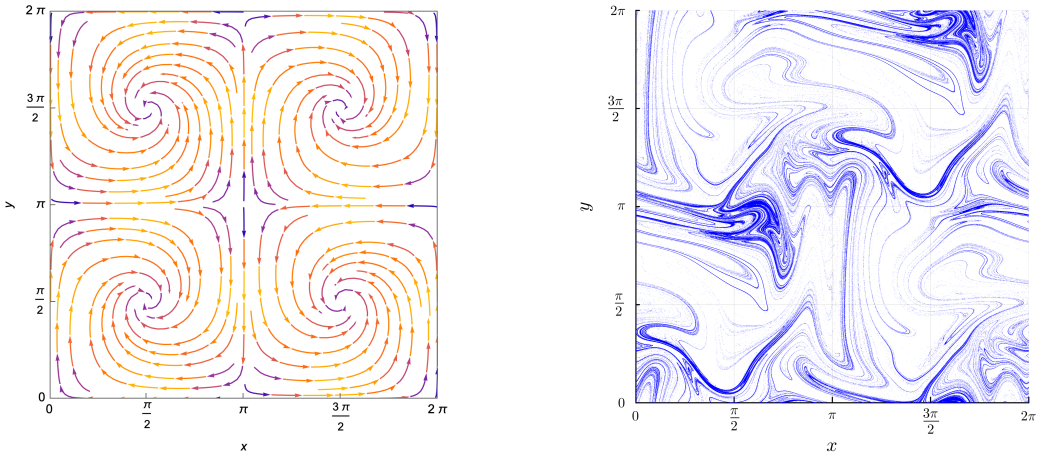
$$\begin{cases} \mathrm{d}x_t &= (\cos(x_t)/2 - \cos y_t) \sin x_t \mathrm{d}t + \sigma \mathrm{d}B_t^1, \\ \mathrm{d}y_t &= (\cos(y_t)/2 + \cos x_t) \sin y_t \mathrm{d}t + \sigma \mathrm{d}B_t^2. \end{cases} \tag{1.49}$$

Then, for $\sigma = \sqrt{2}$, the following bounds hold for the (top) Lyapunov exponent λ defined by (5.2):

$$\lambda = 0.0558453099857 \pm 10^{-13} > 0. \tag{1.50}$$

Here and everywhere else in this thesis, expressions like $\lambda = x \pm r$ mean that $\lambda \in [x - r, x + r]$.

Proof. See Section 5.4. □



(a) Phase portrait of the vector field (1.49) with $\sigma = 0$.

(b) Snapshot of a chaotic random attractor of (1.49) with $\sigma = \sqrt{2}$.

Figure 1.4: Deterministic and random dynamics of (1.49).

The positivity of the Lyapunov exponent has strong implications on the dynamics of $(\varphi_t)_{t\geq 0}$.

Corollary 1.11. For $\sigma = \sqrt{2}$, system (1.49) generates a random strange attractor and a random weak horseshoe.

Proof. Since the stochastic flow $(\varphi_t)_{t\geq 0}$ generated by (1.49) induces a family of independently composed random diffeomorphisms of the compact space $\mathcal{M} = \mathbb{T}^2$, the positivity of the Lyapunov exponent implies the existence of a random strange attractor [161]. Furthermore, applying the results of [138] also shows the existence of a random weak horseshoe. We refer to these two references for precise definitions of these objects. □

Corollary 1.11 is a typical example showcasing the complementarity of computer-assisted proofs with more traditional mathematical tools. Indeed, computer-assisted proofs enable the usage of powerful theoretical results whose assumptions (in that case, the assumption that the system has a positive Lyapunov exponent) are often very challenging to check in practice otherwise.

Let us say that this technique is naturally generalised in Chapter 5 to stochastic differential equations with multiplicative noise, on a more general manifold $\mathcal{M}$ and to general ergodic averages Q and can be combined with continuation methods as observed in Theorem 1.4.

Organisation of the thesis

Chapters 2 and 3 are concerned with the study of equations in weighted Sobolev spaces $H^n(\nu) = H^n(e^{-V}/Z)$ as outlined in Section 1.2.

- In Chapter 2, we first start with the more simple and classical Gaussian case, i.e. $V(x) = x^2/4$ and are more particularly concerned with equations of the type for self-similar profiles of semilinear parabolic equations solving elliptic problems of the type (1.34). We thus work directly under the change of unknown (1.33). This chapter is based on the paper [53].
- In Chapter 3, we develop a more general approach to the resolution of differential equations in weighted Sobolev spaces. We focus on the semiclassical case where V is a polynomial and in particular in the case of the double-well potential $V(x) = x^4/4 - \kappa x^2/2$. This chapter is based on the paper [54].

In Chapter 4, we come back to the problem of determining the sign of the Lyapunov exponent (1.19) for the Hopf normal form and describe one approach to attempt to solve the Fokker–Planck equation (1.21). While this approach was not quite successful, it contains potentially interesting ideas for the analysis of (1.21) or for other computer-assisted proofs. This chapter is partially based on the paper [55].

In Chapter 5, we give a full description of the computer-assisted adjoint method outlined in Section 1.3 and apply it rigorously to show the positivity of the Lyapunov exponent (1.41) for several stochastic flows. This chapter is based on the paper [55].

2

Constructive proofs for some semilinear PDEs on $H^2(e^{|x|^2/4})$

This chapter is based on the paper [53].

2.1 Introduction

Partial differential equations (PDEs) are fundamental in the modelling of many physical and biological systems, and the computation of their solutions is often well understood on bounded domains. However, certain PDEs can lose some key features such as particular solutions or conservation laws when restricted to a bounded domain. Furthermore, many problems, such as the ones studied in this chapter, are more natural to consider on an unbounded domain, either because their structure leads to simpler proofs or because they automatically give rise to localised solutions whose decay is intrinsically prescribed by the equation.

Among those, diffusion problems (both linear and nonlinear), many of which are natural to consider on $\mathbb{R}^d$, have a simple treatment on bounded domains based on standard Sobolev spaces but which fails to directly extend on unbounded domains. Many alternative techniques have been developed or applied to the study of diffusions on $\mathbb{R}^d$ such as variational formulations [102, 150, 228], Lyapunov (including energy/entropy) techniques and shooting methods for radial solutions [62, 190]. In particular, one popular approach is to recover some estimates which hold in the bounded case such as the Poincaré inequality by working on weighted Sobolev spaces instead.

Slightly more recently, a new family of tools has emerged, namely computer-assisted proofs (CAPs), which are complementary to the classical techniques. One of the benefits of CAPs is that the existence results they provide always come hand in hand with a quantitative description of the obtained solutions. Another advantage is that CAPs typically generalise in a straightforward way to systems, which is not necessarily the case for some of the aforementioned techniques. Given a PDE, abstractly written as $F(u) = 0$, and a numerically obtained approximate solution $\bar{u}$, a

common feature of many CAPs is to consider an associated Newton-like operator of the form

$$T(u) = u - AF(u), \tag{2.1}$$

where A is a well-chosen approximation of $DF(\bar{u})^{-1}$, and then to prove that T is a contraction on a small neighbourhood of $\bar{u}$, in a suitable norm [219].

Following the seminal chapters of Nakao [180] and Plum [191], many authors contributed to the further development and popularisation of computer-assisted proofs for elliptic PDEs (see e.g. [10, 90, 124, 185, 204, 221, 226, 232, 234]), but the vast majority of these works can only be applied to problems on bounded domains. Until recently, the main exception was the technique developed by Plum, which takes A equal to $DF(\bar{u})^{-1}$ and relies on eigenvalues bounds obtained via the so-called homotopy method in order to control $\|DF(\bar{u})^{-1}\|$. This approach can handle a variety of problems on unbounded domains, see [231] for a recent example and [181, Part II] for a more general presentation. Regarding other CAP techniques on unbounded domains, but for more specific problems, we also mention [177] which studies the spectrum of coupled harmonic oscillators, and [178] which deals with eigenvalue exclusion for localised perturbations of a one-dimensional periodic Schrödinger operator. Lately, other general CAP methodologies were developed for (systems of) PDEs on unbounded domains, first specifically for radial solutions [217, 218], and then for more general solutions in [66, 67]. In these recent approaches, one goes back to a problem on a bounded domain, either by compactifying the domain, or by dealing separately with the solutions at infinity, or by introducing a periodised problem whose solutions approximate those of the original problem. Such techniques are well-suited to study localised solutions of equations having only bounded coefficients.

In this chapter, we study elliptic PDEs of the form

$$Lu := -\Delta u - \frac{x}{2} \cdot \nabla u = f(x, u, \nabla u), \quad x \in \mathbb{R}^d, \tag{2.2}$$

and develop new computer-assisted tools for such equations. Equations of the form (2.2) have already been studied extensively, as they naturally appear in different contexts such as the ones we present below, or when studying self-similarity in various problems (see [2, 34, 84] or [143] in the case of the Navier–Stokes equations).

As a first example, consider the nonlinear heat equation

$$\partial_t v = \Delta v - \varepsilon |v|^{p-1} v, \qquad \varepsilon = \pm 1. \tag{2.3}$$

If u solves (2.2) with $f(x, u, \nabla u) = f(u) = u/(p-1) - \varepsilon |u|^{p-1} u$, i.e.

$$Lu = \frac{u}{p-1} - \varepsilon |u|^{p-1} u, \tag{2.4}$$

then $v(t, x) = t^{-1/(p-1)} u(x/\sqrt{t})$ is a self-similar solution of (2.3). One typically seeks "physical" solutions, having Gaussian decay or as critical points of some energy functional. In the radial case, a thorough description of solutions can then be achieved via shooting or ODE methods (see [62, 190, 233] and references therein). Alternatively, a variational approach [102, 228] identifies such solutions by working directly on weighted Sobolev spaces.

As a second example, notice that, if $u(x) = e^{-|x|^2/8}\varphi(x)$ for an arbitrary function φ, then

$$Lu = e^{-|x|^2/8}\left(-\Delta\varphi + \left(\frac{|x|^2}{16} + \frac{d}{4}\right)\varphi\right), \tag{2.5}$$

therefore equation (2.2) is also connected to Schrödinger equations. Indeed, consider for instance the critical nonlinear Schrödinger equation

$$i\partial_t v + \Delta v + \varepsilon|v|^{4/d}v = 0, \tag{2.6}$$

for $\varepsilon = \pm 1$. It is established (also via variational methods) in [150] that (2.6) has self-similar solutions of the form

$$v(t,x) = (1+t^2)^{-d/4}\exp\left(\frac{it|x|^2}{4(1+t^2)}\right)e^{i\omega\arctan t}\varphi\left(\frac{\sqrt{2}x}{(1+t^2)^{1/2}}\right),$$

where $\omega \in \mathbb{R}$ and $\varphi : \mathbb{R}^d \longrightarrow \mathbb{C}$ solves

$$-\Delta\varphi + \frac{|x|^2}{16}\varphi + \frac{\omega}{2}\varphi = \frac{\varepsilon}{2}|\varphi|^{4/d}\varphi. \tag{2.7}$$

Using the aforementioned change of unknown $\varphi(x) = e^{|x|^2/8}u(x)$, we get back to equation (2.2) for u, with

$$f(x,u,\nabla u) = f(x,u) = \left(\frac{d}{4} - \frac{\omega}{2}\right)u + \frac{\varepsilon}{2}e^{|x|^2/(2d)}|u|^{4/d}u.$$

In this chapter, we develop a computer-assisted approach based on (2.1) to study both radial and non-radial solutions of (2.2), which provides a precise and quantitative description of self-similar solutions of equations (2.3) and (2.6). Defining

$$H^n(\mu) = \left\{f \in L^2(\mu) \mid \partial_\beta f \in L^2(\mu) \text{ for all } \beta \in \mathbb{N}^d, |\beta| \le n\right\}, \qquad \mu(x) = \frac{\Gamma(d/2)}{(2\sqrt{\pi})^d}e^{|x|^2/4},$$

we will rigorously enclose solutions in $H^2(\mu)$ with respect to the norm $\|\cdot\|_{H^2(\mu)} := \|L\cdot\|_{L^2(\mu)}$, where $L^2(\mu)$ is equipped with the usual inner product

$$\langle u, v\rangle = \int_{\mathbb{R}^d} u(x)v(x)\mu(x)\mathrm{d}x,$$

and where L will be shown to be a positive $L^2(\mu)$ self-adjoint operator. Here are examples of results that can be obtained using this approach.

Theorem 2.1. Let $d = 2$, $p = 5/3$, $\varepsilon = 1$ and $\bar{u} : \mathbb{R}^2 \to \mathbb{R}$ be the radial function whose radial profile restricted to the interval $[0,4]$ is represented in Figure 2.1, and whose precise description is available at [80]. There exists a positive radial solution $u^\star \in H^2(\mu)$ to Eq. (2.4) such that

$$\|u^\star - \bar{u}\|_{H^2(\mu)} \le 1.6 \times 10^{-23}.$$

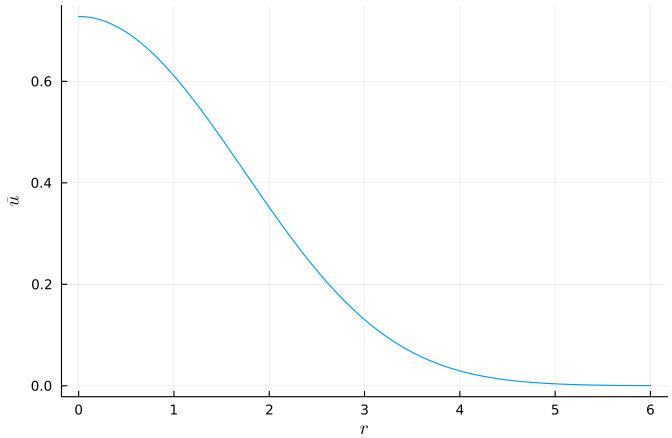


Figure 2.1: Plot of an approximate self-similar radial profile $\bar{u}$ to Eq. (2.3) with $\varepsilon = +1$, $d = 2$ and $p = 5/3$.

Theorem 2.2. Let $d = 2$, $\varepsilon = -1$, $\omega = -5/2$, and $\bar{\varphi} : \mathbb{R}^2 \to \mathbb{R}$ be the function whose restriction to the disk $\{(x, y) \mid x^2 + y^2 \leq 7^2\}$ is represented in Figure 2.2, and whose precise description is available at [80]. There exists a solution $\varphi^\star \in H^2(\mathbb{R}^2)$ to Eq. (2.7) such that

$$\|\varphi^\star - \bar{\varphi}\|_{H^2(\mathbb{R}^2)} \leq 3.8 \times 10^{-8}.$$

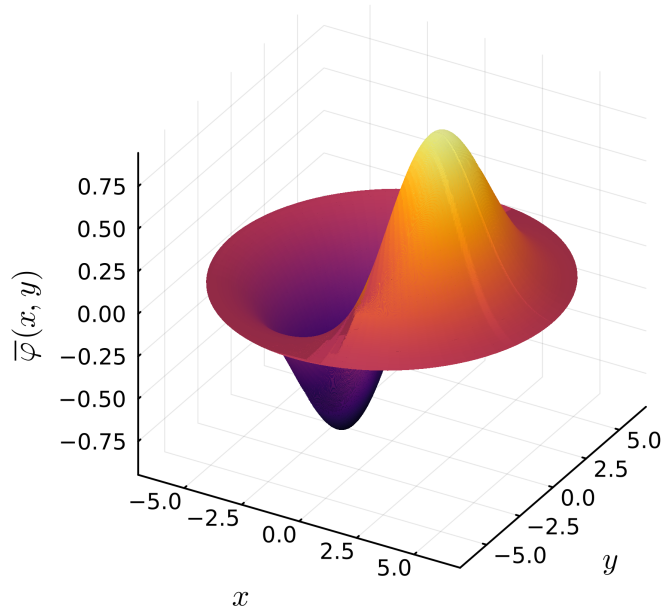


Figure 2.2: Plot of a non-radial numerical solution $\bar{\varphi} = e^{r^2/8}\bar{u}$ to Eq. (2.7) with $d = 2$, $\varepsilon = -1$ and $\omega = -5/2$.

More results with different self-similar profiles associated to the nonlinear heat and Schrödinger equations can be found in Section 2.4 and Section 2.5.

Remark 2.3. While the radial solutions we obtain were already known to exist thanks to previous works [62, 190, 228], our results also provide a precise description of these solutions. Furthermore,

our methods can also deal with non-radial solutions, without relying on a perturbation argument. The only other work we are aware of where non-radial solutions are found is [102, Remark 3.11], which relies on local bifurcation theory and therefore only holds for p close to specific values.

Remark 2.4. Beyond the results themselves, we believe part of the interest of this chapter lies in the computer-assisted tools that are developed in order to handle equations of the form (2.2), and in the underlying ideas which may prove useful for CAPs, and more largely for numerical analysis, in a broader context.

- Our CAPs are based on a spectral expansion of the solution, which is a common approach on bounded domains, but has proven challenging on unbounded domains. This is made possible by departing from the usual paradigm which consists in choosing the basis only in terms of the leading order differential operator (i.e. Δ in (2.2)), so that this operator becomes easy to invert by hand. Indeed, the basis we use makes $L := -\left(\Delta + \frac{x}{2} \cdot \nabla\right)$ diagonal (and therefore trivial to invert), but the operator Δ alone does not have a well-behaved inverse with respect to this basis.

- Extracting some compactness is usually key for CAPs based on (2.1), and can be especially challenging on unbounded domains. Here, compactness is retrieved by working with appropriately weighted Sobolev spaces (see Section 2.2.2).

- We use spherical coordinate basis functions of the Hilbert space $H^2(\mu)$ which are the counterparts of the spherical harmonics in the Hermite–Laguerre family and allow us to handle our problems globally and with a unified treatment. To the best of our knowledge, this is the first occurrence of the use of these bases to solve partial differential equations, even from a purely numerical perspective. Indeed, this differs from the previous literature (both theoretical [102] and computational [111]) on this family of problems which have exhibited (multivariate) Hermite functions as an eigenbasis for L. While at first glance, these bases might appear tricky to work with (especially in nonlinear problems), we demonstrate that they are well-suited to our problems. We show that they can be handled efficiently to both provide a spectral method to find numerical solutions to problems of the form (2.2) and then validate these solutions rigorously. On the one hand, these bases allow us to handle non-radial solutions to radially symmetric equations. On the other hand, in the case of radial solutions, these bases allow an approach based on the analysis of the operator L while exploiting the dimensionality reduction given by radial equations.

- As already mentioned, spectral expansions are common in CAPs for nonlinear equations, but only when they are associated to a Banach algebra structure which facilitates the control of nonlinearities. The basis used in this chapter does not enjoy this property, but we still manage to handle some nonlinear terms, thanks to a combination of rigorous quadrature and Sobolev embeddings, in a fashion which is more reminiscent of CAPs based on finite elements [181, Part I].

- Still regarding nonlinear terms, let us mention that we also handle non-polynomial nonlinearities, namely a fractional power p in (2.3). The existing CAP techniques based on spectral methods are more convenient to use when only polynomial nonlinearities occur, and therefore a common approach in the presence of non-polynomial terms is to first reformulate the equation in a polynomial one, typically adding several new unknowns and associated equations in the process [133, 151, 162]. For a different approach allowing to directly treat some

non-polynomial terms without adding extra equations and unknowns, but relying heavily on a Banach algebra structure, we refer to [59]. One can also approximate smooth non-polynomial terms using interpolation and computable error bounds [8, 105, 222], but once again, the Banach algebra structure is then typically used to control perturbations around a given approximate solution. In the current work, we directly deal with the fractional power in a somewhat ad-hoc manner that also does not necessitate the introduction of extra equations and unknowns, and works without a Banach algebra.

Our approach can also handle some equations featuring first-order derivatives, when f in (2.2) really does depend on ∇u. As an example, we also study self-similar solutions of a generalised viscous Burgers equation on $\mathbb{R}_+$ (see, e.g. [2, 201])

$$\partial_t v + v^2 \partial_x v = \partial_{xx} v, \tag{2.8}$$

of the form

$$v(t,x) = t^{-1/4} u\left(\frac{x}{\sqrt{t}}\right).$$

Then, one has to find a profile u which solves an equation akin to (2.2) with $f(x,u,\partial_x u) = u/4 - u^2\partial_x u$:

$$\partial_{xx} u + \frac{x}{2}\partial_x u + \frac{u}{4} - u^2 \partial_x u = 0, \quad x \in \mathbb{R}_+. \tag{2.9}$$

Finally, let us conclude the introduction by emphasising that there have been previous occurrences of CAPs of somewhat different nature for self-similar solutions, and that this topic has been attracting a lot of attention recently for fluid flows [64, 74].

The remainder of the chapter is organised as follows. We start by presenting the main important properties of the operator L, together with appropriate weighted Sobolev spaces and bases of eigenfunctions in Section 2.2.1. We show how this setting allows us to recover a crucial Poincaré inequality and projection error estimates in Section 2.2.2, and provide some explicit constants for the Sobolev embeddings between these weighted spaces in Section 2.2.3. The CAP methodology and the associated fixed point problem where all these ingredients will be brought together is then introduced in Section 2.2.4. Proving the existence of a fixed point requires us to explicitly evaluate (or at least upper-bound) several quantities associated to an approximate solution, and we present in Section 2.3 a quadrature scheme allowing us to compute these quantities rigorously. In Section 2.4, we then focus on self-similar profiles for the nonlinear heat equation. Explicit bounds allowing to use the CAP in the case of radial solutions and with an integer exponent p are derived in Section 2.4.1, and used in Section 2.4.2 to obtain our first set of results. In Section 2.4.3 we provide a sufficient condition which we use to prove the positivity of the obtained solutions. We then show how to deal with some fractional exponents p in Section 2.4.4, and with non-radial solutions in Section 2.4.5. Self-similar solutions of the nonlinear Schrödinger equations are treated in an analogous manner in Section 2.5, and we end in Section 2.6 with a generalised viscous Burgers equation. All the computations presented in this chapter have been implemented in `Julia`, using the `IntervalArithmetic.jl` library [198] for interval arithmetic. The computer-assisted parts of the proofs can be reproduced using the code available at [80].

2.2 Functional analytic preliminaries

2.2.1 Properties of the operator L

One of the main ideas of this chapter is to make use of the operator

$$L = -\frac{x}{2} \cdot \nabla - \Delta,$$

to play the role analogous to that of the Laplacian $-\Delta$ as it is usually employed for computer-assisted proofs on a bounded domain. Indeed, consider the weighted space $L^2(\mu)$, with scalar product

$$\langle u, v \rangle = \int_{\mathbb{R}^d} u(x)v(x)\mu(x)\mathrm{d}x,$$

where $\mu(x) = e^{|x|^2/4}/Z$, $Z = 2^{d-1}\omega_{d-1}$ where $\omega_{d-1} = 2\pi^{d/2}/\Gamma(d/2)$ denotes the surface area of the $(d-1)$-dimensional sphere $\mathbb{S}^{d-1}$ (this choice of normalisation is made in order to match the usual convention in numerical analysis). By integration by parts, we obtain the Dirichlet form

$$\langle \nabla u, \nabla v \rangle = \langle u, Lv \rangle, \qquad \text{for all } u \in H^1(\mu), v \in \mathcal{D}(L) = H^2(\mu), \tag{2.10}$$

which yields that L is a positive self-adjoint operator on $L^2(\mu)$, and can be analysed in the same "Hilbertian" fashion as $-\Delta$ is in a first course on elliptic PDEs, as will be seen below. We refer to [148] for more properties of L, and note that the above Dirichlet form structure is also often exploited in the analysis of the generators of reversible diffusions (see for instance [189]).

In the previous literature on the operator L [102, 111], its eigenbasis is usually given in cartesian coordinates in terms of Hermite functions

$$L\Psi_\beta = -\left(\frac{x}{2} \cdot \nabla + \Delta\right)\Psi_\beta = \frac{d+|\beta|}{2}\Psi_\beta, \qquad \text{where } \Psi_\beta(x) = e^{-|x|^2/4}\prod_{i=1}^{d-1} H_{\beta_i}(x_i/2), \qquad \beta \in \mathbb{N}^d, \tag{2.11}$$

where H_n denotes the Hermite polynomial of degree n. This basis might be suitable for some problems, but since the equations treated in this chapter are radially symmetric, we will instead use bases in spherical coordinates (except for $d = 1$).

Definition 2.5 (Spherical coordinate basis)**.** For $d \in \{2, 3\}$, define the following orthogonal basis of $L^2(\mu)$.

- For $d = 2$, $m \in \mathbb{N}$, $l \in \mathbb{Z}$, $x_1 = r\cos\vartheta$, $x_2 = r\sin\vartheta$,

$$\psi_{l,m}(r,\vartheta) = e^{-r^2/4}(r/2)^{|l|}L_m^{(|l|)}(r^2/4)\begin{cases}\cos l\vartheta & \text{if } l \geq 0\\ -\sin l\vartheta & \text{if } l < 0,\end{cases} \tag{2.12}$$

  where $L_m^{(\alpha)}$ denotes the generalised Laguerre polynomial of degree m and parameter α (see [1, p. 775]).

- For $d = 3$, $m \in \mathbb{N}$, $k \in \mathbb{Z}$, $l \in \mathbb{N}_{\geq |k|}$, $x_1 = r\sin\vartheta\cos\phi$, $x_2 = r\sin\vartheta\sin\phi$, $x_3 = r\cos\vartheta$

$$\psi_{k,l,m}(r,\vartheta,\phi) = e^{-r^2/4}(r/2)^l L_m^{(l+1/2)}(r^2/4)P_l^k(\cos\vartheta)\begin{cases}\cos k\phi & \text{if } k \geq 0\\ -\sin k\phi & \text{if } k < 0,\end{cases}$$

  where P_l^k denotes the associated Legendre polynomial of order k and degree l (see [1, Chapter 8]).

Remark 2.6. For $d = 2$, the $\psi_{l,m}$'s are weighted and reformulated versions of the so-called Hermite polynomials of complex variables [142]. See [75] for the derivations of some of these relations.

Lemma 2.7. The families $\{\psi_{l,m}\}$ and $\{\psi_{k,l,m}\}$ from Definition 2.5 are eigenfunctions of L for $d = 2$ and $d = 3$ respectively.

- For $d = 2$, $m \in \mathbb{N}$, $l \in \mathbb{Z}$,

$$L\psi_{l,m} = -\left(\frac{r}{2}\frac{\partial\psi_{l,m}}{\partial r} + \frac{1}{r}\frac{\partial}{\partial r}\left(r\frac{\partial\psi_{l,m}}{\partial r}\right) + \frac{1}{r^2}\frac{\partial^2\psi_{l,m}}{\partial\vartheta^2}\right) = \left(\frac{2+|l|}{2} + m\right)\psi_{l,m}.$$

- For $d = 3$, $m \in \mathbb{N}$, $k \in \mathbb{Z}$, $l \in \mathbb{N}_{\geq |k|}$,

$$\begin{aligned} &L\psi_{k,l,m}\\ &= -\left(\frac{r}{2}\frac{\partial\psi_{k,l,m}}{\partial r} + \frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial\psi_{k,l,m}}{\partial r}\right) + \frac{1}{r^2\sin\vartheta}\frac{\partial}{\partial\vartheta}\sin\vartheta\left(\frac{\partial\psi_{k,l,m}}{\partial\vartheta}\right) + \frac{1}{r^2\sin^2\vartheta}\frac{\partial^2\psi_{k,l,m}}{\partial\phi^2}\right)\\ &= \left(\frac{3+l}{2} + m\right)\psi_{k,l,m}.\end{aligned}$$

The construction of the bases given in Definition 2.5 hinges on the following lemma.

Lemma 2.8. Let f be a hyperspherical function on $\mathbb{S}^{d-1}$ of order $l \in \mathbb{N}$, i.e.

$$\Delta_{\mathbb{S}^{d-1}} f = -l(l+d-2)f,$$

where $\Delta_{\mathbb{S}^{d-1}}$ denotes the Laplace-Beltrami operator on $\mathbb{S}^{d-1}$. Then $e^{-r^2/4}(r/2)^l L_m^{(l+d/2-1)}(r^2/4)f$ is an eigenfunction of L with eigenvalue $(d+l)/2 + m$ on $\mathbb{R}^d$.

Proof. This follows from separation of the radial variable and the spherical variables and by identifying the Laguerre differential equation after the change of variable $z = r^2/4$. □

In order to obtain the bases of Definition 2.5, it then suffices to have orthogonal bases of the eigenspaces of $\Delta_{\mathbb{S}^{d-1}}$, and this construction can also be used in higher dimensions (e.g. by using [136] for the construction of an eigenbasis of $\Delta_{\mathbb{S}^{d-1}}$). Note that as a consequence, this directly generalises the known corresponding bases for the harmonic Schrödinger operator and for the generator of the radially symmetric Ornstein–Uhlenbeck process. Furthermore, the linear relationship between bivariate Hermite and Laguerre polynomials observed in [75] for $d = 2$ (and the one known for $d = 1$) can be generalised by the above pattern.

Corollary 2.9 (Radial eigenbasis)**.** For $d \in \mathbb{N}$, let $\alpha = d/2 - 1$ and let $\psi_n(r) := L_n^{(\alpha)}(r^2/4)e^{-r^2/4}$, then

$$L\psi_n = -\left(\frac{r}{2} + \frac{d-1}{r}\right)\frac{\partial\psi_n}{\partial r} - \frac{\partial^2\psi_n}{\partial r^2} = \left(\frac{d}{2} + n\right)\psi_n.$$

Note that with these bases, we can handle radial equations globally without treating either the behaviour at infinity or at the origin separately (see for instance [218] for an example of CAP where the behaviours at the origin and at infinity are handled separately).

2.2.2 Spaces, norms and Poincaré inequality

One of the main challenges of computer-assisted proofs on unbounded domains is that the embedding $H^1(\Omega) \hookrightarrow L^2(\Omega)$ is not compact anymore for $\Omega = \mathbb{R}^d$, as no Poincaré inequality even holds. Observe that in our setting with weighted spaces, the eigenbasis of L together with (2.10) immediately implies a genuine Poincaré inequality

$$\|u\|_{L^2(\mu)} \leq \sqrt{\frac{2}{d}\langle \nabla u, \nabla u\rangle} = \sqrt{\frac{2}{d}}\,\|\nabla u\|_{L^2(\mu)} \qquad \text{for all } u \in H^1(\mu), \tag{2.13}$$

since $d/2$ is the smallest eigenvalue of L. We can therefore consider on $H^1(\mu)$ the scalar product $\langle \cdot, \cdot \rangle_{H^1(\mu)} = \langle \nabla \cdot, \nabla \cdot \rangle$ and its associated norm, which is equivalent to the usual $H^1(\mu)$-norm. Similarly, on the space $H^2(\mu)$ we consider the scalar product $\langle \cdot, \cdot \rangle_{H^2(\mu)} = \langle L\cdot, L\cdot \rangle$ and associated norm, which is also equivalent to the usual $H^2(\mu)$-norm (see Lemma 2.16).

Notice that these choices of norms yield, in a similar fashion to (2.13),

$$\|u\|_{H^1(\mu)} \leq \sqrt{\frac{2}{d}}\|u\|_{H^2(\mu)} \qquad \text{for all } u \in H^2(\mu). \tag{2.14}$$

Notation 2.10. We denote by $\|u\|_\infty$ the essential supremum of $|u|$, i.e. for a measure ν on Ω,

$$\|u\|_\infty := \inf\{M \mid |u(x)| \leq M \text{ for } \nu\text{-a.e. } x \in \Omega\}.$$

Our notation does not depend on ν, as all the measures we will be using are equivalent (i.e. they have the same null sets). Finally, we adopt the usual convention that u is said to be continuous if it has a continuous representative.

Another important feature of our setup is that that $L^{-1} : L^2(\mu) \to H^1(\mu)$ is well-defined (say via the Lax–Milgram theorem [61, Corollary V.8], using (2.10) and (2.13)) and compact. More quantitatively, if Π_n denotes the orthogonal projection in $L^2(\mu)$ onto $\mathrm{Span}\{\psi \mid L\psi = \lambda\psi \text{ with } \lambda \leq d/2 + n\}$, (2.10) yields the following error estimates

$$\|L^{-1}(f - \Pi_n f)\|_{H^1(\mu)} \leq \sqrt{\frac{2}{d+2n+1}}\|f - \Pi_n f\|_{L^2(\mu)} \qquad \text{for all } f \in L^2(\mu), \tag{2.15}$$

and

$$\|f - \Pi_n f\|_{L^2(\mu)} \leq \frac{2}{d+2n+1}\,\|f - \Pi_n f\|_{H^2(\mu)} \qquad \text{for all } f \in H^2(\mu), \tag{2.16}$$

which are critical for our CAPs, and in particular for controlling the quality of the approximate inverse A that will be defined in Section 2.2.4.

Remark 2.11. Let us highlight two evident but useful properties of the orthogonal projector Π_n. First, Π_n commutes with L (and L^{-1}). Second Π_n is also an orthogonal projection with respect to the $H^1(\mu)$ and $H^2(\mu)$ scalar products. In particular, $\Pi_n(L^2(\mu)) = \Pi_n(H^1(\mu)) = \Pi_n(H^2(\mu))$.

2.2.3 Sobolev embeddings

To control the nonlinearities in our setting, Sobolev embeddings play a crucial role. We start by recalling some $H^1(\mu)$-embeddings proved in [102, 157, 228].

Theorem 2.12. We have the following Sobolev embeddings:

(i) If $d = 1$, $u \in H^1(\mu) \implies e^{x^2/8}u \in \mathcal{C}^0(\mathbb{R})$.

(ii) If $d = 2$, $H^1(\mu) \subset L^p(\mu)$ for all $p \in [2, \infty)$.

(iii) If $d \geq 3$, $H^1(\mu) \subset L^p(\mu)$ for all $p \in [2, 2d/(d-2)]$.

While in principle, this shows the feasibility of a computer-assisted proof using this functional framework, in practice we also require the corresponding embedding constants that we derive below.

Notation 2.13. In this section, we make use of classical embeddings between Sobolev spaces without weights in order to derive the needed results on weighted spaces. When we include $\mathbb{R}^d$ in the notation, e.g. $L^2(\mathbb{R}^d)$, this means we refer to the space without weight.

Lemma 2.14. Let $\theta(x) = |x|^2/4$ and denoting $\|u\|_{H^1(e^\theta)} := \|\nabla u\|_{L^2(e^\theta)}$, then for all $u \in H^1(e^\theta)$

$$\|u\|_{L^p(e^\theta)} \leq \|e^{(1/2-1/p)\theta}u\|_{L^p(e^\theta)} \leq C(d,p)\|u\|^a_{L^2(e^\theta)}\|u\|^{1-a}_{H^1(e^\theta)}, \tag{2.17}$$

where $a = 1 + d(1/p - 1/2)$ and:

- for $d = 1$, $p \in [2, \infty]$ and $C(1,p) = 2^{1/2-1/p}$;
- for $d = 2$, $p \in [2, \infty)$ and, writing $p = 2(k + r)$ with $k \in \mathbb{N}^* = \mathbb{N}\backslash\{0\}$ and $r \in [0, 1)$,

$$C(2, 2(k+r)) = (k!)^{1/(k+r)}\,(k+1)^{r/(k+r)};$$

- for $d \geq 3$, $p \in [2, 2d/(d-2)]$ and

$$C(d,p) = \left(\frac{1}{d(d-2)\pi}\right)^{(1-a)/2}\left\{\frac{(d-1)!}{\Gamma(d/2)}\right\}^{1/2-1/p}.$$

Proof. First, notice that $(1/2 - 1/p)\theta \geq 0$ since $p \geq 2$, which yields the first inequality in (2.17). Then, we note that for all $u \in H^1(e^\theta)$ and $\varphi = e^{|x|^2/8}u$,

$$-\frac{1}{2}\int_{\mathbb{R}^d}(x \cdot \nabla\varphi)\,\varphi \mathrm{d}x = \frac{d}{4}\int_{\mathbb{R}^d}\varphi^2 \mathrm{d}x, \tag{2.18}$$

as already shown in the proof of [102, Lemma 4.17]. Indeed, for any $\varphi \in \mathcal{C}^\infty_c(\mathbb{R})$, an integration by part yields

$$\int_{\mathbb{R}^d}(x \cdot \nabla\varphi)\,\varphi \mathrm{d}x = -\int_{\mathbb{R}^d}\varphi\nabla \cdot (x\varphi)\mathrm{d}x = -\int_{\mathbb{R}^d}\varphi(x \cdot \nabla\varphi)\mathrm{d}x - d\int_{\mathbb{R}^d}\varphi^2 \mathrm{d}x,$$

which gives (2.18), and this identity still holds for $\varphi = e^{|x|^2/8}u$ by a density argument. Therefore,

$$\begin{aligned}\|\nabla u\|^2_{L^2(e^\theta)} &= \int_{\mathbb{R}^d}\left|\nabla\varphi - \frac{x}{4}\varphi\right|^2 \mathrm{d}x \\ &= \int_{\mathbb{R}^d}\left(|\nabla\varphi|^2 - \frac{\varphi}{2}(x \cdot \nabla\varphi) + \frac{|x|^2}{16}\varphi^2\right)\mathrm{d}x\end{aligned}$$

$$= \int_{\mathbb{R}^d} \left[|\nabla \varphi|^2 + \varphi^2 \left(\frac{d}{4} + \frac{|x|^2}{16} \right) \right] \mathrm{d}x$$

which yields

$$\|\nabla \varphi\|_{L^2(\mathbb{R}^d)} \leq \|\nabla u\|_{L^2(e^\theta)}. \tag{2.19}$$

- For $d = 1$, from the proof of [61, Theorem VIII.7], we have that

$$\|\varphi\|_\infty \leq 2^{1/2} \|\varphi\|_{L^2(\mathbb{R})}^{1/2} \|\varphi'\|_{L^2(\mathbb{R})}^{1/2}.$$

  Therefore,

$$\|e^{\theta/2} u\|_\infty \leq 2^{1/2} \|u\|_{L^2(e^\theta)}^{1/2} \|u\|_{H^1(e^\theta)}^{1/2}, \tag{2.20}$$

  which is the announced inequality for $p = \infty$. For $2 \leq p < \infty$, Hölder's inequality yields

$$\begin{aligned} \|e^{\theta(1/2-1/p)} u\|_{L^p(e^\theta)} &\leq \left(\|e^{\theta/2} u\|_\infty^{p-2} \|u\|_{L^2(e^\theta)}^2 \right)^{1/p} \\ &= \|e^{\theta/2} u\|_\infty^{1-2/p} \|u\|_{L^2(e^\theta)}^{2/p} \\ &\leq 2^{1/2-1/p} \|u\|_{L^2(e^\theta)}^{1/2+1/p} \|u\|_{H^1(e^\theta)}^{1/2-1/p}. \end{aligned}$$

- Now, for $d = 2$, we are in the "limiting case", so from [61, Corollary IX.11], for $k \in \mathbb{N}^*$

$$\|\varphi\|_{L^{2k}(\mathbb{R}^2)} \leq k^{1/k} \|\varphi\|_{L^{2(k-1)}(\mathbb{R}^2)}^{(k-1)/k} \|\nabla \varphi\|_{L^2(\mathbb{R}^2)}^{1/k},$$

  and by induction on $k \in \mathbb{N}^*$

$$\|\varphi\|_{L^{2k}(\mathbb{R}^2)} \leq (k!)^{1/k} \|\varphi\|_{L^2(\mathbb{R}^2)}^{1/k} \|\nabla \varphi\|_{L^2(\mathbb{R}^2)}^{1-1/k}.$$

  Now, by interpolation, for $2k \leq 2(k+r) \leq 2(k+1)$, we get

$$\|\varphi\|_{L^{2(k+r)}(\mathbb{R}^2)} \leq (k!)^{1/(k+r)} (k+1)^{r/(k+r)} \|\varphi\|_{L^2(\mathbb{R}^2)}^{1/(k+r)} \|\nabla \varphi\|_{L^2(\mathbb{R}^2)}^{1-1/(k+r)},$$

  and thus

$$\begin{aligned} \|e^{\theta(k+r-1)/(2(k+r))} u\|_{L^{2(k+r)}(e^\theta)} &= \|\varphi\|_{L^{2(k+r)}(\mathbb{R}^2)} \\ &\leq (k!)^{1/(k+r)} \, (k+1)^{r/(k+r)} \|u\|_{L^2(e^\theta)}^{1/(k+r)} \|u\|_{H^1(e^\theta)}^{1-1/(k+r)}. \end{aligned}$$

- For $d \geq 3$, proceed similarly and use [206] (see also [102, Lemma 4.17]). □

Corollary 2.15. For all $u \in H^1(\mu)$,

$$\|u^p\|_{L^2(\mu)} \leq \|e^{(p-1)|x|^2/8} u^p\|_{L^2(\mu)} \leq c(d,p) \|u\|_{H^1(\mu)}^p,$$

where

- for $d = 1$, $p \in [1, \infty)$, $c(1,p) = 2^{(5p-3)/4}$;
- for $d = 2$, $p = k + r \in [1, \infty)$ with $k \in \mathbb{N}^*$ and $r \in [0,1)$, $c(2, k+r) = (2\sqrt{\pi})^{k+r-1} k! (k+1)^r$;

- for $d \geq 3$, $p \in [1, d/(d-2)]$ and

$$c(d,p) = \left(\frac{2}{d}\right)^{p/2} \left\{ \left(\frac{2}{d-2}\right)^{d/4} \frac{\Gamma(d)^{1/2}}{\Gamma(d/2)} \right\}^{p-1}.$$

Proof. Noting that $\mu = e^{\theta}/Z$ where $Z = 2^{d-1}\omega_{d-1}$ where $\omega_{d-1} = 2\pi^{d/2}/\Gamma(d/2)$ and applying Lemma 2.14 followed by the Poincaré inequality (2.13) yields

$$\begin{aligned}
\|u^p\|_{L^2(\mu)} &= \|e^{(p-1)\theta/2} u^p\|_{L^2(\mu)} \\
&= \frac{1}{\sqrt{Z}} \|e^{\theta(1/2-1/2p)} u\|^p_{L^{2p}(e^{\theta})} \\
&\leq \frac{\left(C(d,2p)\sqrt{Z}\right)^p}{\sqrt{Z}} \left(\sqrt{\frac{2}{d}}\right)^{p+d(1/2-p/2)} \|u\|^p_{H^1(\mu)} \\
&= (C(d,2p))^p \left(\frac{2^d \pi^{d/2}}{\Gamma(d/2)}\right)^{\frac{p-1}{2}} \left(\frac{2}{d}\right)^{p/2+d(1/4-p/4)} \|u\|^p_{H^1(\mu)}.
\end{aligned}$$

One then just has to check that

$$c(d,p) = (C(d,2p))^p \left(\frac{2^d \pi^{d/2}}{\Gamma(d/2)}\right)^{\frac{p-1}{2}} \left(\frac{2}{d}\right)^{p/2+d(1/4-p/4)}. \qquad \square$$

While the $H^1(\mu) \to L^2(\mu)$ embeddings will prove useful for some intermediate estimates, our CAP will mainly be conducted in $H^2(\mu)$. We derive the required embeddings with explicit constants below.

Lemma 2.16. For all $f \in L^2(\mu)$, there exists a unique $u \in H^2(\mu)$ such that $Lu = f$, and $L^{-1} : L^2(\mu) \to H^2(\mu)$ is bounded, so that $\|\cdot\|_{H^2(\mu)} := \|L \cdot\|_{L^2(\mu)}$ indeed induces the $H^2(\mu)$ topology. Furthermore, if $u \in H^2(\mu)$ and $\varphi = e^{|x|^2/8} u$, then $\varphi \in H^2(\mathbb{R}^d)$ and

$$\|D^2\varphi\|_{L^2(\mathbb{R}^d)} = \|\Delta\varphi\|_{L^2(\mathbb{R}^d)} \leq \sqrt{Z}\|u\|_{H^2(\mu)}, \tag{2.21}$$

where $\|D^2\varphi\|_{L^2(\mathbb{R}^d)} = \left(\sum_{i,j=1}^d \|\partial_{x_i x_j}\varphi\|^2_{L^2(\mathbb{R})}\right)^{1/2}$ denotes the Frobenius norm of the Hessian $D^2\varphi$ of φ.

Proof. The qualitative version of this lemma is the content of [148, Lemma 2.1.(vii)] (The additional fact that $\varphi \in H^2(\mathbb{R}^d)$ follows from [61, Theorem IX.25]). Given the bounds obtained in the proof of [148, Lemma 2.1.(vii)], for all $u \in H^2(\mu)$ the estimates below hold by density for $\varphi = e^{|x|^2/8}u$. Using (2.5), we have that

$$\int_{\mathbb{R}^d} (Lu)^2 \, e^{|x|^2/4} \mathrm{d}x = \int_{\mathbb{R}^d} \left[|\Delta\varphi|^2 + \left(\frac{d}{4} + \frac{|x|^2}{16}\right)\varphi^2 \right] \mathrm{d}x - \int_{\mathbb{R}^d} \varphi\Delta\varphi \left(\frac{d}{2} + \frac{|x|^2}{8}\right) \mathrm{d}x.$$

Now, by integration by parts, the last term simplifies to

$$\begin{aligned}
-\int_{\mathbb{R}^d} \varphi\Delta\varphi \left(\frac{d}{2} + \frac{|x|^2}{8}\right) \mathrm{d}x &= \int_{\mathbb{R}^d} |\nabla\varphi|^2 \left(\frac{d}{2} + \frac{|x|^2}{8}\right) \mathrm{d}x + \int_{\mathbb{R}^d} \varphi \left(\frac{x}{4} \cdot \nabla\varphi\right) \mathrm{d}x \\
&= \int_{\mathbb{R}^d} |\nabla\varphi|^2 \left(\frac{d}{2} + \frac{|x|^2}{8}\right) \mathrm{d}x - \frac{d}{8}\int_{\mathbb{R}^d} \varphi^2 \mathrm{d}x \qquad \text{using (2.18)}.
\end{aligned}$$

Adding back this term, we get

$$\int_{\mathbb{R}^d} (Lu)^2 \, e^{|x|^2/4} \mathrm{d}x \geq \int_{\mathbb{R}^d} |\Delta\varphi|^2 \, \mathrm{d}x + \frac{d}{2} \int_{\mathbb{R}^d} |\nabla\varphi|^2 \, \mathrm{d}x + \frac{d}{8} \int_{\mathbb{R}^d} \varphi^2 \mathrm{d}x, \tag{2.22}$$

and in particular

$$\|D^2\varphi\|_{L^2(\mathbb{R}^d)} = \|\Delta\varphi\|_{L^2(\mathbb{R}^d)} \leq \|Lu\|_{L^2(e^{|x|^2/4})} \leq \sqrt{Z}\|u\|_{H^2(\mu)},$$

where the first equality follows from [200, Lemma 2.5, Corollary 2.13], since $\varphi \in H^2(\mathbb{R}^d)$. □

Applying a similar argument as in Lemma 2.14, we then obtain the following embeddings.

Corollary 2.17. We have the following Sobolev embeddings:

(i) If $d \in \{1, 2, 3\}$, $u \in H^2(\mu) \implies e^{|x|^2/8} u \in L^\infty(\mathbb{R}^d)$.

(ii) If $d = 4$, $H^2(\mu) \subset L^p(\mu)$ for all $p \in [2, \infty)$.

(iii) If $d \geq 5$, $H^2(\mu) \subset L^p(\mu)$ for all $p \in [2, 2d/(d-4)]$.

Proof. The proof follows from the application of the Sobolev embeddings given by [61, Corollary IX.13] on $\varphi = e^{|x|^2/8} u \in H^2(\mathbb{R}^d)$. □

Remark 2.18. Note that these embeddings are sufficient to cover the range of exponent p for the semilinear heat equation for which rapidly decaying self-similar solutions are known to exist [102].

We now provide an explicit embedding constant for the case that we will need for our examples, namely (i) in Corollary 2.17, for $d \in \{2, 3\}$ (for $d = 1$, one can use the $H^1(\mu)$-embedding from Corollary 2.15 together with (2.14)).

Lemma 2.19. Let $d \in \{2, 3\}$, then there exists $C(d) > 0$ such that for all $u \in H^2(\mu)$

$$\|e^{|x|^2/8} u\|_\infty \leq C(d)\|u\|_{H^2(\mu)},$$

where $C(d)$ can be chosen as

$$C(d) = \sqrt{Z}\left(\frac{2}{d}C_0 + \sqrt{\frac{2}{d}}C_1 + C_2\right),$$

with

$$C_0 = 0.56419, \quad C_1 = 0.79789, \quad C_2 = 0.23033, \quad \text{if } d = 2;$$

$$C_0 = 0.52319, \quad C_1 = 1.0228, \quad C_2 = 0.37467, \quad \text{if } d = 3.$$

Proof. Letting once again $\varphi = e^{|x|^2/8} u$, we have that $\varphi \in H^2(\mathbb{R}^d)$ by Lemma 2.16. We can thus use the embedding from $H^2(\mathbb{R}^d)$ to $L^\infty(\mathbb{R}^d)$, with the explicit constants provided in [181, Example 6.12.(a)]:

$$\|\varphi\|_\infty \leq C_0\|\varphi\|_{L^2(\mathbb{R}^d)} + C_1\|\nabla\varphi\|_{L^2(\mathbb{R}^d)} + C_2\|D^2\varphi\|_{L^2(\mathbb{R}^d)}.$$

Then, noticing that $\|u\|_{L^2(\mu)} \leq \frac{2}{d}\|u\|_{H^2(\mu)}$ (by a direct computation or by combining (2.13) and (2.14)), we get

$$\|\varphi\|_{L^2(\mathbb{R}^d)} = \sqrt{Z}\|u\|_{L^2(\mu)} \leq \sqrt{Z}\frac{2}{d}\|u\|_{H^2(\mu)}.$$

Similarly, starting from (2.19) and using once more (2.14), we get

$$\|\nabla\varphi\|_{L^2(\mathbb{R}^d)} \leq \sqrt{Z}\|u\|_{H^1(\mu)} \leq \sqrt{Z}\sqrt{\frac{2}{d}}\|u\|_{H^2(\mu)},$$

and (2.21) provides the last missing inequality. □

2.2.4 The fixed-point theorem

As is common in the CAP literature, our approach will rely on a fixed-point theorem allowing for the *a posteriori validation* of an appropriate numerical solution $\bar{u}$, that is, a proof of the existence of a solution $u^\star$ to

$$Lu = f(x, u, \nabla u), \tag{2.23}$$

in an explicit neighbourhood of $\bar{u}$ in a Banach space $\mathcal{X}$. This is achieved by constructing a well-chosen map $T : \mathcal{X} \to \mathcal{X}$ with solutions of Eq. (2.23) as its fixed points and which is contracting in a neighbourhood of $\bar{u} \in \mathcal{X}$. In order to actually prove that T is a contraction, we will a corollary of Theorem 1.1 for polynomials polynomial nonlinearities (see [181, 215, 232] and the references therein for variants). Indeed, if T is polynomial in u of degree p, we reformulate conditions (1.4) and (1.5) into bounding $D^kT(\bar{u})$ for $k \in \{1, \dots, p\}$.

Corollary 2.20. Let $T : \mathcal{X} \to \mathcal{X}$ be a polynomial of degree p and let $\bar{u} \in \mathcal{X}$ be such that there exist $Y, Z_1, \dots, Z_p \geq 0$ such that

$$\|T(\bar{u}) - \bar{u}\|_{\mathcal{X}} \leq Y, \tag{2.24}$$

$$\|D^kT(\bar{u})h^k\|_{\mathcal{X}} \leq Z_k\|h\|_{\mathcal{X}}^k \qquad \text{for all } h \in \mathcal{X} \text{ and } k \in \{1, \dots, p\}. \tag{2.25}$$

Introducing the radii polynomials

$$P(\delta) = Y - \delta + \sum_{k=1}^{p} \frac{Z_k}{k!}\delta^k,$$

$$Q(\delta) = -1 + \sum_{k=1}^{p} \frac{Z_k}{(k-1)!}\delta^{k-1},$$

if there exists $\delta > 0$ such that $P(\delta) < 0$, then denoting $\underline{\delta}$ the smallest positive root of P and $\bar{\delta}$ the unique positive root of Q, for all $\delta \in (\underline{\delta}, \bar{\delta})$ T has a unique fixed point $u^\star \in \bar{B}(\bar{u}, \delta) \subset \mathcal{X}$.

Proof. See for instance [58, Corollary 4.4]. □

We now explain how to construct suitable operator T in order to study solutions of equation (2.23). Provided $g : u \mapsto f(\cdot, u, \nabla u)$ maps $H^2(\mu)$ to $L^2(\mu)$, our general problem

$$Lu = f(x, u, \nabla u)$$

can be reformulated as finding a zero of the map $F : H^2(\mu) \to H^2(\mu)$, where

$$F(u) = u - L^{-1} f(x, u, \nabla u).$$

Note that if $Dg(\bar{u})$ in fact maps $H^2(\mu)$ to $H^1(\mu)$, then $DF(\bar{u})$ is a compact perturbation of the identity. In particular, and this is a key aspect common to many such computer-assisted proofs, we can expect to find an accurate approximate inverse of $DF(\bar{u})$ which is also a compact perturbation of the identity. This motivates the introduction of the linear map $A : H^2(\mu) \to H^2(\mu)$ such that $\Pi_n A \Pi_n = A_n$ is an approximate inverse of $\Pi_n DF(\bar{u})\Pi_n$ computed numerically, and where $\Pi_n A(I - \Pi_n) = (I - \Pi_n)A\Pi_n = 0$ and $(I - \Pi_n)A(I - \Pi_n) = I - \Pi_n$. That is, using the block decomposition associated with the orthogonal projection Π_n, we have

$$A = \begin{pmatrix} A_n & 0 \\ 0 & I \end{pmatrix},$$

and we expect such an A to be accurate approximate inverse of $DF(\bar{u})$ if n is large enough. This statement will be made quantitative in Section 2.4.1, by leveraging the explicit compactness estimate (2.16), which allows us to obtain a computable upper bound for $\|I - ADF(\bar{u})\|_{H^2(\mu),H^2(\mu)}$.

We therefore consider the quasi-Newton operator $T : H^2(\mu) \longrightarrow H^2(\mu)$ with

$$T(u) = u - AF(u),$$

which we expect to be contracting near $\bar{u}$. Provided A is invertible (this will be an automatic consequence of verifying assumption (1.7)), zeros of F are indeed in one-to-one correspondence with fixed points of T. In Sections 2.4 to 2.6, we derive suitable estimates Y and Z_k's allowing us to apply Corollary 2.20 or Corollary 2.20 to this fixed-point operator T for the different equations mentioned in the introduction.

Remark 2.21. One could choose to perform a computer-assisted proof in $H^1(\mu)$ instead of $H^2(\mu)$, but the class of treatable problems would be more restricted and this would not directly yield L^∞-estimates on the solution in dimension $d \in \{2, 3\}$.

2.3 Handling nonlinearities via quadrature rules

To derive the bounds Y and Z_1 needed for our CAP (See Corollary 2.20), we will need to rigorously compute quantities like $\|\bar{u}^p\|_{L^2(\mu)}$. In the more classical case of Fourier series, $\bar{u}$ is typically a finite Fourier series (i.e. a trigonometric polynomial), and $\bar{u}^p$ is then still a finite Fourier series (provided p is an integer), whose integral or norm is therefore straightforward to compute exactly. In contrast, in our setting, whenever $u \neq 0$ and $v \neq 0$ belong to $\Pi_n(H^2(\mu))$, the product uv does not belong to $P_{n'}(H^2(\mu))$ for any $n' \in \mathbb{N}$. However, we can still compute exactly $\|uv\|_{L^2(\mu)}$ (or $\|\bar{u}^p\|_{L^2(\mu)}$), and we explain how this can be done in this section.

For clarity, we focus here on the case of the radial equation

$$Lu = u/(p-1) - \varepsilon u^p, \quad \varepsilon = \pm 1, \ p \in \mathbb{N},$$

giving rise to self-similar solutions of the semilinear heat equation, but all the constructions can be adapted to the other examples. We denote by $\{\hat{\psi}_m\}_{m=0}^{\infty}$ the normalisation of the orthogonal basis $\{\psi_m\}_{m=0}^{\infty}$ (see Corollary 2.9) with respect the $L^2(\mu)$-inner product $\langle\cdot,\cdot\rangle$, i.e.

$$\hat{\psi}_m(r) = \sqrt{\frac{m!}{\Gamma(m+\alpha+1)}} L_m^{(\alpha)}(r^2/4)e^{-r^2/4}, \qquad \alpha = \frac{d}{2} - 1.$$

We will solve our problem with respect to this basis and look for our numerical approximation $\bar{u}$ in $\mathrm{Span}\{\hat{\psi}_m\}_{m=0}^{n}$ (which is the set of radial functions in $\Pi_n(H^2(\mu))$). We can then write $\bar{u}$ in terms of its "Fourier" coefficients:

$$\bar{u} = \sum_{m=0}^{n} \bar{u}_m \hat{\psi}_m \qquad \bar{\mathbf{u}} = (\bar{u}_0, \dots, \bar{u}_n). \tag{2.26}$$

Since our computer-assisted proof will mostly rely on a Hilbertian approach, one of the main challenges is to be able to compute many projections and integrals (eventually rigorously) on unbounded domains. Such endeavour might appear naive given the lack of simple error control on Gauss–Laguerre quadrature and the notorious difficulties of working with this family of bases [110]. Furthermore, we would ideally like to solve (via gradient descent or Newton's method) the Galerkin problem

$$\left\langle L\bar{u} - \bar{u}/(p-1) + \varepsilon \bar{u}^p, \hat{\psi}_j \right\rangle = 0 \qquad \text{for all } j \in \{0, \dots, n\}, \tag{2.27}$$

without further approximating the problem. We show that this can in fact be achieved relatively efficiently for a nonlinearity of moderate degree by simply adapting the Gauss–Laguerre quadrature. Consider more generally the problem of evaluating (eventually rigorously) integrals of the form

$$\int_{\mathbb{R}^d} \prod_{k=1}^{m} f_k(x)\mu(x)\mathrm{d}x,$$

for $f_k \in \mathrm{Span}\{\hat{\psi}_m\}_{m=0}^{n}$. For instance, $\|\bar{u}^p\|_{L^2(\mu)}$ can be written in this form, but also the coefficients of $\Pi_n(\bar{u}^p)$ given by $\langle \bar{u}^p, \hat{\psi}_m\rangle$ for $m = 0, \dots, n$. Since we are in the radial setting, this boils down to evaluating integrals of the form

$$\int_0^{\infty} \prod_{k=1}^{m} f_k(r)(r/2)^{d-1} e^{r^2/4}\mathrm{d}r, \tag{2.28}$$

with $f_k(r) = p_k(r^2/4)e^{-r^2/4}$ for some polynomial p_k of degree at most n. Note that all calculations can be thought to be done with respect to the variable $z = r^2/4$.

Remark 2.22. When we have to deal with non-radial solutions, we also use spherical coordinates, and the projections and integrals with respect to the spherical variables only involve sines and cosines and thus do not require a quadrature. This is another advantage of using spherical coordinates instead of cartesian ones (i.e., of using the bases of Definition 2.5 instead of (2.11)), for which nontrivial quadratures would be required in every direction.

We now show how to exactly compute integrals of the form (2.28).

Lemma 2.23. Let $p_1, \dots, p_m$ be polynomials of degree at most n and let $N \in \mathbb{N}$ be such that

$2N-1 \geq mn$. Then, for $\alpha > -1$ and $\beta > 0$

$$\int_0^\infty z^\alpha e^{-\beta z} \prod_{k=1}^m p_k(z)\mathrm{d}z = \beta^{-\alpha-1} \sum_{i=1}^N W_i \prod_{k=1}^m p_k\left(\frac{z_i}{\beta}\right), \tag{2.29}$$

where z_i denotes the i^{th} root of $L_N^{(\alpha)}$ and

$$W_i = \frac{\Gamma(N+\alpha+1)z_i}{N!(N+1)^2[L_{N+1}^{(\alpha)}(z_i)]^2} \qquad i = 1, \ldots, N.$$

Proof. This follows from using the chain rule for the change of variables $z \mapsto z/\beta$ and the N^{th} Gauss–Laguerre quadrature (see [110, Formula 4.1]) which is exact for polynomials of degree $2N-1$ or less. □

In our implementation, p_k will usually be written as

$$p_k = \sum_{j=0}^n a_j^k L_j^{(\alpha)} / \|\psi_j\|_{L^2(\mu)}.$$

Thus, the above quadrature rule would be written as

$$\int_0^\infty z^\alpha e^{-\beta z} \prod_{k=1}^m p_k(z)\mathrm{d}z = \beta^{-\alpha-1} \sum_{i=1}^N W_i \prod_{k=1}^m \sum_{j=0}^n a_j^k L_j^{(\alpha)}\left(\frac{z_i}{\beta}\right) = \beta^{-\alpha-1} \sum_{i=1}^N W_i \prod_{k=1}^m (V\mathbf{a}^k)_i,$$

where $\mathbf{a}^k = (a_j^k)_{0\leq j\leq n}$ and $V = (V_{ij}) = (L_j^{(\alpha)}(z_i/\beta)/\|\psi_j\|_{L^2(\mu)})$ is a (pseudo)-Vandermonde matrix. However, this matrix has very large entries so that (2.29) as written needs to be computed in high precision arithmetic. When (2.29) needs to be evaluated fast and accurately, it proves better to use a regularised Vandermonde matrix $\bar{V} = \mathrm{Diag}(\beta^{-\alpha-1}W)^{1/m}V$ so that

$$\int_0^\infty z^\alpha e^{-\beta z} \prod_{k=1}^m p_k(z)\mathrm{d}z = \sum_{i=1}^N \prod_{k=1}^m (\bar{V}\mathbf{a}^k)_i.$$

In practice, $\bar{V}$ can be precomputed once (using high precision if needed but then possibly stored in lower precision) and after this is done both the rigorous and non-rigorous computations can be carried out in a manageable amount of time.

Remark 2.24. In practice, $\bar{V}$ proves much better behaved than V and easier to work with. It could be interesting to further investigate the properties of $\bar{V}$.

Example 2.25. In both the rigorous and non-rigorous parts, one needs to compute the matrix

$$G_{ij} = \langle \hat{\psi}_i, \bar{u}^{p-1}\hat{\psi}_j \rangle$$

which can be written as $G = \bar{V}^T \mathrm{Diag}(\bar{V}\bar{\mathbf{u}})^{p-1}\bar{V}$ for $m = p+1$ and $\beta = p$ (and $\bar{\mathbf{u}}$ as in (2.26)).

Note that here the nonlinearity in the Galerkin problem is not approximated by its so-called *pseudospectral* projection (usually obtained by collocation) found in the previous related literature [126, 111].

Like the validation procedure, the quadrature is implemented rigorously in `Julia` using the package `IntervalArithmetic.jl` [198]. Our implementation also relies on approximating the

roots of $L_N^{(\alpha)}$ with high precision, using initial guesses given by `FastGaussQuadrature.jl` [208] and refining them using Newton's method in `BigFloat` arithmetic. The roots are then enclosed rigorously by combining the Fundamental Theorem of Algebra and the Intermediate Value Theorem (recall that the roots of orthogonal polynomials are always simple and real). V is then computed by recursion. While this quadrature might appear expensive, in our experience for problems with $N \leq 2000$, the enclosure of the roots together with the computation of $\bar{V}$ only took a few minutes on a standard laptop.

Remark 2.26. Hermite and Laguerre bases are far less popular than Fourier and Chebyshev for computer-assisted proofs, or in numerical analysis for this matter. One reason is the lack of simple and global error control on interpolation and quadrature. However, polynomials are well-controlled in the bulk, and the tails of $\hat{\psi}_m$ can be controlled via the following estimate of Szegö [1, formula 22.14.13]

$$|\hat{\psi}_m(r)| \leq \hat{\psi}_m(0) e^{-r^2/8} = \frac{1}{\Gamma(\alpha+1)} \sqrt{\frac{\Gamma(m+\alpha+1)}{m!}} e^{-r^2/8}, \tag{2.30}$$

if $\alpha = d/2 - 1 \geq 0$, i.e. if $d \geq 2$.In particular, this estimate in theory allows for integration with rigorous error control, say by bluntly integrating in the bulk via interval arithmetic. Since our method will only rely on integration, it might handle more general nonlinearities. Note that this estimate immediately provides L^∞-bounds on finite linear combinations of the $\hat{\psi}_m$'s.

2.4 The semilinear heat equation

In this section, we are interested in the semilinear heat equation

$$\partial_t v = \Delta v - \varepsilon |v|^{p-1} v \qquad \text{on } \mathbb{R}^d, \tag{2.31}$$

with $p > 1$. It is well-known that if u solves the nonlinear elliptic problem

$$-\Delta u - \frac{x}{2} \cdot \nabla u - \frac{u}{p-1} + \varepsilon |u|^{p-1} u = 0, \tag{2.32}$$

then $v(t,x) = t^{-1/(p-1)} u(x/\sqrt{t})$ is a self-similar solution of (2.31). These solutions are relevant when studying the asymptotic behaviour of solutions to Eq. (2.31). Indeed, provided that $v(0,\cdot) \in H^1(\mu)$, they appear as (possibly unstable) "omega-limit points" [148] of $v(t,\cdot)$ in the sense that there exists a solution u to Eq. (2.32) and $t_n \to \infty$ such that

$$\lim_{n\to\infty} \left\| t_n^{1/(p-1)} v(t_n, \cdot) - u\left(\frac{\cdot}{\sqrt{t_n}}\right) \right\|_\infty = 0.$$

Let us first focus on positive radial solutions of Eq. (2.32) (we will later show in Section 2.4.3 that the solutions we obtain are indeed positive) which have been the subject of [62, 190], so that Eq. (2.32) becomes

$$Lu = -\partial_r^2 u - \left(\frac{d-1}{r} + \frac{r}{2}\right) \partial_r u = \frac{u}{p-1} - \varepsilon u^p. \tag{2.33}$$

Furthermore, let us assume first for simplicity that $p \in \mathbb{N}$. An example with a non-integer power p will be presented in Section 2.4.4, and non-radial solutions will be studied in Section 2.4.5.

2.4.1 Suitable bounds for the validation

In this section, we apply the general strategy outlined in Section 2.2.4 to Eq. (2.33), and derive computable estimates Y and Z_k satisfying the assumptions of Corollary 2.20. Since we are first looking for radial solutions, we restrict ourselves to the Hilbert space

$$\mathcal{H} = \overline{\mathrm{Span}\{\psi_m\}_{m=0}^{\infty}}^{H^2} \subset H^2(\mu).$$

Throughout this section, we then assume $\bar{u}$ is an element of $\mathcal{H}_n := \mathrm{Span}\{\psi_m\}_{m=0}^{n} \subset \mathcal{C}_0^\infty(\mathbb{R}_+)$. In particular, $\|\bar{u}\|_\infty$ is finite and can be computed rigorously (or at least upper-bounded rigorously, say via the estimate (2.30)). This quantity will appear in several of the estimates to come.

In order to study Eq. (2.33), we consider

$$\begin{aligned} F : \mathcal{H} &\longrightarrow \mathcal{H}, \\ u &\longmapsto u - L^{-1}\left(\frac{u}{p-1} - \varepsilon u^p\right), \end{aligned} \tag{2.34}$$

and T defined as in Section 2.2.4. Since we work in $\mathcal{H}$, the approximate inverse A involved in T is naturally taken to go from $\mathcal{H}$ to $\mathcal{H}$, so that $T : \mathcal{H} \to \mathcal{H}$. We obtain the following formulae for $DT^k(\bar{u})$

$$\begin{cases} DT(\bar{u})h &= h - ADF(\bar{u})h = h - A(h - L^{-1}(h/(p-1) - \varepsilon p\bar{u}^{p-1}h)) \\ D^kT(\bar{u})h^k &= -\varepsilon\dfrac{p!}{(p-k)!}AL^{-1}(\bar{u}^{p-k}h^k) \qquad 1 < k \leq p. \end{cases}$$

Notation 2.27. Recall Notation 2.10 and Remark 2.11. Our analysis will mostly be done in μ-weighted spaces, and we may shorten the notation by omitting the μ. Henceforth, $\|\cdot\|_{H^2}$ (resp. $\|\cdot\|_{H^1}$, $\|\cdot\|_{L^2}$) will always denote $\|\cdot\|_{H^2(\mu)}$ (resp. $\|\cdot\|_{H^1(\mu)}$, $\|\cdot\|_{L^2(\mu)}$). Furthermore, we denote by $\{\hat{\psi}_m\}_{m=0}^{\infty}$ the normalisation of the radial orthogonal basis $\{\psi_m\}_{m=0}^{\infty}$ (introduced in Corollary 2.9) with respect the $L^2(\mu)$-inner product $\langle\cdot,\cdot\rangle$, and let $\lambda_m = d/2 + m$ so that $L\hat{\psi}_m = \lambda_m\hat{\psi}_m$. We denote $\Pi_\infty = I - \Pi_n$ the complementary projection to Π_n (in $L^2(\mu)$ or $H^2(\mu)$). Note that Π_n, and therefore also Π_∞, leave $\mathcal{H}$ invariant, and we abuse notation and still denote by Π_n and Π_∞ their restriction to $\mathcal{H}$ so that $\Pi_n : \mathcal{H} \to \mathcal{H}$ is the orthogonal projection onto $\mathcal{H}_n$. We also denote by $\mathcal{H}_\infty = \Pi_\infty(\mathcal{H})$ the orthogonal complement of $\mathcal{H}_n$ in $\mathcal{H}$. Finally, since our implementation will be with respect to the $L^2(\mu)$-basis, in what follows, vectors in $\mathbb{R}^{n+1}$ are identified with the corresponding decomposition with respect to $\{\hat{\psi}_m\}_{m=0}^{n}$ and we aim at stating final estimates with respect to the $L^2(\mu)$-norm.

The bound Y

It suffices to estimate

$$\begin{aligned} \|T(\bar{u}) - \bar{u}\|_{H^2}^2 &= \|AF(\bar{u})\|_{H^2}^2 \\ &= \|\Pi_n(AF(\bar{u}))\|_{H^2}^2 + \|\Pi_\infty(AF(\bar{u}))\|_{H^2}^2 \\ &= \|A_n(\Pi_nF(\bar{u}))\|_{H^2}^2 + \|\Pi_\infty F(\bar{u})\|_{H^2}^2 \\ &= \|A_n(\Pi_nF(\bar{u}))\|_{H^2}^2 + \|\Pi_\infty L^{-1}(\bar{u}^p)\|_{H^2}^2 \\ &= \|A_n(\Pi_nF(\bar{u}))\|_{H^2}^2 + \left(\|L^{-1}\bar{u}^p\|_{H^2}^2 - \|\Pi_nL^{-1}(\bar{u}^p)\|_{H^2}^2\right). \end{aligned}$$

Thus, we may choose

$$Y^2 := \|LA_n(\Pi_n F(\bar{u}))\|_{L^2}^2 + \left(\|\bar{u}^p\|_{L^2}^2 - \|\Pi_n(\bar{u}^p)\|_{L^2}^2\right).$$

Note that all the terms in Y can be evaluated rigorously by means of a quadrature rule (see Lemma 2.23) and the output is expected to be small provided the truncation level n is large enough. In particular, the first term can practically be made arbitrarily small in the non-rigorous computation of $\bar{u}$.

Remark 2.28. Here and in many subsequent places, we slightly abuse notation, in the sense that the number Y that we will actually compute is only an upper bound of the quantity Y defined above. Indeed, we use interval arithmetic to control rounding errors, and in later estimates we also only upper-bounds quantities like $\|\bar{u}\|_\infty$ rather than trying to compute them *exactly*.

The bound Z_1

We choose to compute Z_1 by treating finite and infinite dimensional parts separately, and therefore take

$$Z_1 := \left\| \begin{pmatrix} Z^{11} & Z^{12} \\ Z^{21} & Z^{22} \end{pmatrix} \right\|_2$$

where the Z^{ij} are real numbers satisfying

$$\begin{cases} \|\Pi_n DT(\bar{u})\Pi_n\|_{H^2,H^2} & \leq Z^{11}, \\ \|\Pi_\infty DT(\bar{u})\Pi_n\|_{H^2,H^2} & \leq Z^{21}, \\ \|\Pi_n DT(\bar{u})\Pi_\infty\|_{H^2,H^2} & \leq Z^{12}, \\ \|\Pi_\infty DT(\bar{u})\Pi_\infty\|_{H^2,H^2} & \leq Z^{22}. \end{cases} \tag{2.35}$$

Indeed, for $h \in \mathcal{H}$ with $\|h\|_{H^2} = 1$, write $h = h_n + h_\infty$ such that $h_n \in \mathcal{H}_n$, $h_\infty \in \mathcal{H}_\infty$. Then,

$$\begin{aligned} \|DT(\bar{u})h\|_{H^2} &= \sqrt{\|\Pi_n DT(\bar{u})h\|_{H^2}^2 + \|\Pi_\infty DT(\bar{u})h\|_{H^2}^2} \\ &\leq \sqrt{\left(\|\Pi_n DT(\bar{u})h_n\|_{H^2} + \|\Pi_n DT(\bar{u})h_\infty\|_{H^2}\right)^2 + \left(\|\Pi_\infty DT(\bar{u})h_n\|_{H^2} + \|\Pi_\infty DT(\bar{u})h_\infty\|_{H^2}\right)^2} \\ &\leq \sqrt{\left(Z^{11}\|h_n\|_{H^2} + Z^{12}\|h_\infty\|_{H^2}\right)^2 + \left(Z^{21}\|h_n\|_{H^2} + Z^{22}\|h_\infty\|_{H^2}\right)^2} \\ &= \left\| \begin{pmatrix} Z^{11} & Z^{12} \\ Z^{21} & Z^{22} \end{pmatrix} \begin{pmatrix} \|h_n\|_{H^2} \\ \|h_\infty\|_{H^2} \end{pmatrix} \right\|_2 \\ &\leq Z_1 \qquad \text{since } \|h_n\|_{H^2}^2 + \|h_\infty\|_{H^2}^2 = 1. \end{aligned}$$

In the following subsections, we derive computable bounds Z^{ij} satisfying (2.35).

The bound Z^{11}

For $h_n \in \mathcal{H}_n$,

$$\Pi_n DT(\bar{u})h_n = \Pi_n(I - ADF(\bar{u}))h_n = (I_n - A_n\Pi_n DF(\bar{u})\Pi_n)h_n$$

by construction of A. Then, we get the estimate

$$\|\Pi_n DT(\bar{u})\Pi_n\|_{H^2,H^2} = \|I_n - A_n\Pi_n DF(\bar{u})\Pi_n\|_{H^2,H^2} = \|L(I_n - A_n\Pi_n DF(\bar{u})\Pi_n)L^{-1}\|_{L^2,L^2} =: Z^{11},$$

which is expected to be small because $A_n \approx (\Pi_n DF(\bar{u})\Pi_n)^{-1}$. Using the isometric isomorphism between $L^2(\mu)$ and ℓ^2, this quantity Z^{11} is in fact nothing but the 2-norm of an $(n+1)\times(n+1)$ matrix, whose entries can be evaluated rigorously. For $M \in \mathbb{R}^{(n+1)\times(n+1)}$, we may bound above its 2-norm with the estimate $\|M\|_2 \le \sqrt{\|M\|_1\|M\|_\infty}$. While this estimate is not sharp in general, it is good enough for our purpose, as we only need to compute $\|M\|_2$ either when M is very close to being zero (and we only need an estimate which is below 1), or where $\|M\|_2$ is not the crucial estimate.

The bound Z^{21}

For $h_n \in \mathcal{H}_n$, we get that

$$\begin{aligned}\Pi_\infty DT(\bar{u})h_n &= -\Pi_\infty DF(\bar{u})h_n \\ &= \Pi_\infty L^{-1}(h_n/(p-1) - \varepsilon p\bar{u}^{p-1}h_n) \\ &= -\varepsilon p\Pi_\infty L^{-1}(\bar{u}^{p-1}h_n),\end{aligned}$$

and thus,

$$\|\Pi_\infty DT(\bar{u})h_n\|_{H^2} = p\|\Pi_\infty(\bar{u}^{p-1}h_n)\|_{L^2}.$$

Then, writing $h_n \in \mathcal{H}_n$ as

$$h_n = \sum_{m=0}^{n} a_m\hat{\psi}_m,$$

we get

$$\Pi_\infty(\bar{u}^{p-1}h_n) = \sum_{m=0}^{n} a_m\Pi_\infty(\bar{u}^{p-1}\hat{\psi}_m).$$

Thus,

$$\begin{aligned}&\|\Pi_\infty(\bar{u}^{p-1}h_n)\|_{L^2} \\ &\le \sum_{m=0}^{n}\|a_m\Pi_\infty(\bar{u}^{p-1}\hat{\psi}_m)\|_{L^2} \qquad \text{by Minkowski inequality} \\ &\le \sum_{m=0}^{n}|a_m\lambda_m|\|\lambda_m^{-1}\Pi_\infty(\bar{u}^{p-1}\hat{\psi}_m)\|_{L^2} \\ &\le \left(\sum_{m=0}^{n}\lambda_m^{-2}\|\Pi_\infty(\bar{u}^{p-1}\hat{\psi}_m)\|_{L^2}^2\right)^{1/2}\left(\sum_{m=0}^{n}\lambda_m^2 a_m^2\right)^{1/2} \qquad \text{by Cauchy–Schwarz inequality} \\ &= \left(\sum_{m=0}^{n}\lambda_m^{-2}\|\Pi_\infty(\bar{u}^{p-1}\hat{\psi}_m)\|_{L^2}^2\right)^{1/2}\|h_n\|_{H^2}.\end{aligned}$$

Introducing the vector $w \in \mathbb{R}^{n+1}$ with

$$w_m := \|\Pi_\infty(\bar{u}^{p-1}\hat{\psi}_m)\|_{L^2} = \left(\|\bar{u}^{p-1}\hat{\psi}_m\|_{L^2}^2 - \|\Pi_n(\bar{u}^{p-1}\hat{\psi}_m)\|_{L^2}^2\right)^{1/2},$$

and identifying w with an element of $\Pi_n(L^2(\mu)) \subset L^2(\mu)$, we get

$$\|\Pi_\infty DT(\bar{u})\Pi_n\|_{H^2,H^2} \le p\|L^{-1}w\|_{L^2} =: Z^{21}.$$

Note that w_m is expected to be small, especially for small m, whereas for larger m the λ_m^{-2} factors also contribute to making $\|L^{-1}w\|_{L^2}^2 = \sum_{m=0}^n \lambda_m^{-2} w_m^2$ small.

The bound Z^{12}

Now, for $h_\infty \in \mathcal{H}_\infty$,

$$\begin{aligned}
\Pi_n DT(\bar{u})h_\infty &= -\Pi_n ADF(\bar{u})h_\infty \\
&= \Pi_n AL^{-1}h_\infty/(p-1) - \varepsilon p\Pi_n AL^{-1}(\bar{u}^{p-1}h_\infty) \\
&= L^{-1}\Pi_n h_\infty/(p-1) - \varepsilon p A_n \Pi_n L^{-1}(\bar{u}^{p-1}h_\infty) \\
&= -\varepsilon p A_n L^{-1}\Pi_n(\bar{u}^{p-1}h_\infty) \qquad \text{since } h_\infty \in \mathcal{H}_\infty.
\end{aligned}$$

Then, for $m \in \{0, \dots n\}$, we estimate

$$\begin{aligned}
|\langle \bar{u}^{p-1}h_\infty, \hat{\psi}_m\rangle| &= |\langle \bar{u}^{p-1}\hat{\psi}_m, h_\infty\rangle| \\
&= |\langle \Pi_\infty(\bar{u}^{p-1}\hat{\psi}_m), h_\infty\rangle| \qquad \text{since } h_\infty \in \mathcal{H}_\infty \\
&\le \|\Pi_\infty(\bar{u}^{p-1}\hat{\psi}_m)\|_{L^2}\|h_\infty\|_{L^2} \qquad \text{by Cauchy–Schwarz inequality} \\
&\le \frac{\|h_\infty\|_{H^2}}{\lambda_{n+1}}\|\Pi_\infty(\bar{u}^{p-1}\hat{\psi}_m)\|_{L^2} \qquad \text{by (2.16)}.
\end{aligned}$$

Thus, reusing the vector w introduced in the previous subsection,

$$\|\Pi_n DT(\bar{u})\Pi_\infty\|_{H^2,H^2} \le \frac{p}{\lambda_{n+1}}\left\| \left|A_n L^{-1}\right| w\right\|_{H^2} = \frac{p}{\lambda_{n+1}}\left\| \left|LA_n L^{-1}\right| w\right\|_{L^2} =: Z^{12},$$

where for $M \in \mathbb{R}^{(n+1)\times(n+1)}$, $|M| = (|M|_{ij}) = (|M_{ij}|)$.

The bound Z^{22}

For $h_\infty \in \mathcal{H}_\infty$,

$$\Pi_\infty DT(\bar{u})h_\infty = -\Pi_\infty DF(\bar{u})h_\infty = \Pi_\infty L^{-1}((1/(p-1) - \varepsilon p\bar{u}^{p-1})h_\infty.$$

Thus,

$$\begin{aligned}
\|\Pi_\infty DT(\bar{u})h_\infty\|_{H^2} &= \|(1/(p-1) - \varepsilon p\bar{u}^{p-1})h_\infty\|_{L^2} \\
&\le \|1/(p-1) - \varepsilon p\bar{u}^{p-1}\|_\infty \|h_\infty\|_{L^2} \qquad \text{by Hölder's inequality} \\
&\le \frac{(1/(p-1) + p\|\bar{u}\|_\infty^{p-1})}{\lambda_{n+1}}\|h_\infty\|_{H^2} \qquad \text{by (2.16)}.
\end{aligned}$$

Thus, we may choose

$$Z^{22} := \frac{1/(p-1) + p\|\bar{u}\|_\infty^{p-1}}{\lambda_{n+1}},$$

where $\|\bar{u}\|_\infty$ can be computed (or at least upper-bounded) using (2.30). Note that while $T : \mathcal{H} \to \mathcal{H}$ may not be compact, $DT(\bar{u}) : \mathcal{H} \to \mathcal{H}$ is, provided $\bar{u} \in L^\infty(\mathbb{R}^d)$.

The bounds Z_k for $1 < k \leq p$

If $d \leq 2$, or $p \leq d/(d-2)$ for $d \geq 3$, we can use the H^1-Sobolev embeddings given by Lemma 2.14, which yields, for $h \in \mathcal{H}$,

$$\begin{aligned}
\left\|D^k T(\bar{u})h^k\right\|_{H^2} &= \frac{p!}{(p-k)!}\left\|AL^{-1}(\bar{u}^{p-k}h^k)\right\|_{H^2} \\
&\leq \frac{p!}{(p-k)!}\|A\|_{H^2,H^2}\|L^{-1}(\bar{u}^{p-k}h^k)\|_{H^2} \\
&\leq \frac{p!}{(p-k)!}\|LAL^{-1}\|_{L^2,L^2}\|\bar{u}^{p-k}h^k\|_{L^2} \\
&\leq \frac{p!\|\bar{u}\|_\infty^{p-k}}{(p-k)!}\|LAL^{-1}\|_{L^2,L^2}\|h^k\|_{L^2} \qquad \text{by Hölder's inequality} \\
&\leq \frac{p!\|\bar{u}\|_\infty^{p-k}}{(p-k)!}\|LAL^{-1}\|_{L^2,L^2}c(d,k)\|h\|_{H^1}^k \\
&\leq \frac{p!\|\bar{u}\|_\infty^{p-k}}{(p-k)!}\|LAL^{-1}\|_{L^2,L^2}c(d,k)\lambda_0^{-k/2}\|h\|_{H^2}^k,
\end{aligned}$$

where $c(d,k)$ is given by Corollary 2.15 and we have used (2.14). Thus, we may choose

$$Z_k := \frac{p!\|\bar{u}\|_\infty^{p-k}}{(p-k)!}\lambda_0^{-k/2}c(d,k)\|LAL^{-1}\|_{L^2,L^2}, \tag{2.36}$$

where

$$\|LAL^{-1}\|_{L^2,L^2} \leq \max\left\{\|LA_nL^{-1}\|_{L^2,L^2}, 1\right\}.$$

Note that instead of using $\|\bar{u}\|_\infty$, for $k < p$, we may derive a bound only using the embedding $H^1(\mu) \hookrightarrow L^{2p}(\mu)$, but this is not expected to be as sharp.

For $d \in \{2,3\}$, we may instead use Lemma 2.19 relying on H^2-Sobolev embeddings

$$\begin{aligned}
\left\|D^k T(\bar{u})h^k\right\|_{H^2} &\leq \frac{p!\|\bar{u}\|_\infty^{p-k}}{(p-k)!}\|LAL^{-1}\|_{L^2,L^2}\|h^k\|_{L^2} \\
&\leq \frac{p!\|\bar{u}\|_\infty^{p-k}}{(p-k)!}\|LAL^{-1}\|_{L^2,L^2}\|h\|_\infty^{k-1}\|h\|_{L^2} \\
&\leq \frac{p!\|\bar{u}\|_\infty^{p-k}}{\lambda_0(p-k)!}\|LAL^{-1}\|_{L^2,L^2}C(d)^{k-1}\|h\|_{H^2}^k,
\end{aligned}$$

where $C(d)$ is given by Lemma 2.19. Thus, we may also choose

$$Z_k := \frac{p!\|\bar{u}\|_\infty^{p-k}}{\lambda_0(p-k)!}C(d)^{k-1}\|LAL^{-1}\|_{L^2,L^2}. \tag{2.37}$$

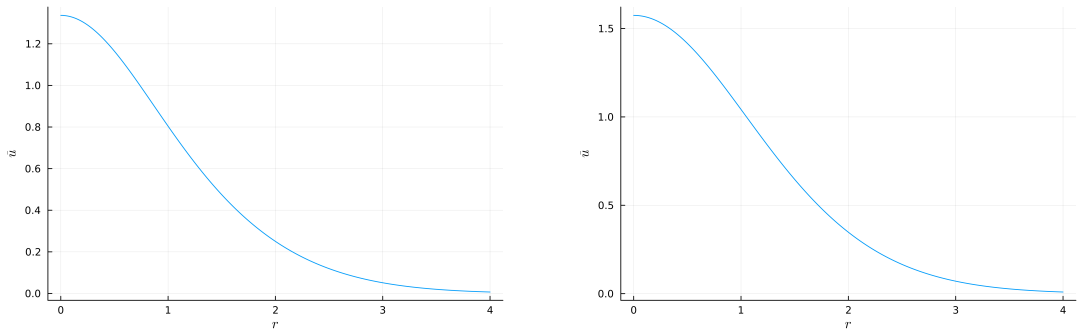
In practice, when $d \in \{2,3\}$, if both estimates are valid, we take for Z_k the minimum between (2.36) and (2.37).

2.4.2 Results

We first focus on the case $\varepsilon = -1$ in (2.33), such that the equation reads

$$Lu = -\partial_r^2 u - \left(\frac{d-1}{r} + \frac{r}{2}\right)\partial_r u = \frac{u}{p-1} + u^p. \tag{2.38}$$

In the cases $(d,p) = (2,3)$ and $(d,p) = (3,2)$, we find the numerical solutions plotted below with $n = 500$. One could of course use fewer coefficients (i.e., take n smaller), but the bound Y measuring the residual error and then the error bound $\underline{\delta}$ would then become larger.



(a) $d = 2$, $p = 3$ (b) $d = 3$, $p = 2$

Figure 2.3: Representation of the numerical approximate solutions $\bar{u}$ to Eq. (2.38) which are validated in Theorem 2.29. Note that the spatial domain of course has to be truncated for the plot, but these approximate solutions are actually defined and computed on $[0,\infty)$ thanks to our choice of basis (see Corollary 2.9).

	$\varepsilon = -1$, $d = 2$, $p = 3$	$\varepsilon = -1$, $d = 3$, $p = 2$
Y	$6.830397272197097 \times 10^{-13}$	$1.4114627225937143 \times 10^{-21}$
Z_1	0.009916643027658332	0.008621565176356588
Z_2	170.320283777825	17.04079355792355
Z_3	719.2983917297151	0
$\underline{\delta}$	$6.898810312173614 \times 10^{-13}$	$1.4237375688374744 \times 10^{-21}$
$\bar{\delta}$	0.0057434127215418	0.05817677630175133

Table 2.1: Results for the a posteriori validation with the bounds given in Section 2.4.1 and $\bar{u}$ represented in Figure 2.3.

Theorem 2.29. For $(d,p) = (2,3)$ (resp. $(d,p) = (3,2)$), let $\bar{u} : \mathbb{R}_+ \to \mathbb{R}$ be the radial function whose restriction to the interval is represented in Figure 2.3a (resp. Figure 2.3b) and whose precise description in terms of "Fourier" coefficients in the basis $\{\hat{\psi}_m\}_{m=0}^n$ is available at [80], then there exists a solution $u^\star \in \mathcal{H}$ to Eq. (2.38) such that

$$\|u^\star - \bar{u}\|_{H^2(\mu)} \leq \underline{\delta},$$

where $\underline{\delta}$ is as in Table 2.1. It is the only solution to Eq. (2.38) in $\mathcal{H}$ such that $\|u^\star - \bar{u}\|_{H^2(\mu)} \leq \bar{\delta}$.

Proof. We consider $F : \mathcal{H} \to \mathcal{H}$ defined in (2.34). In the file `Heat/d2_p3/proof.ipynb` (resp. `Heat/d3_p2/proof.ipynb`) at [80], we construct A_n (and thus indirectly A and T) as outlined in Section 2.2.4. Following the estimates of Section 2.4.1, we obtain the upper bounds in Table 2.1 for Y and the Z_k's to conclude with Corollary 2.20. □

2.4.3 Proving positivity a posteriori

Similarly to the previous literature on the semilinear heat equation, we also wish to verify the (strict) positivity of our radial solutions in this work. Note that even if $\bar{u}$ were proven to be strictly positive, for any $\delta > 0$, $B(\bar{u}, \delta)$ necessarily contains functions that are eventually negative at $+\infty$, e.g. $\bar{u} - (\delta/2)\hat{\psi}_m / \|\hat{\psi}_m\|_{H^2(\mu)}$ for large enough m. Thus, the positivity of $u^\star$ cannot be deduced directly. Since $\bar{u}$ decays faster than our L^∞-control, a direct comparison of $\bar{u}$ and $u^\star$ is only sufficient in a neighbourhood of zero. We thus resort to a maximum principle argument to show the (strict) positivity of $u^\star$ away from zero with the lemma below.

Lemma 2.30. Let $b : \mathbb{R}^d \to \mathbb{R}^d$, $c : \mathbb{R}^d \to \mathbb{R}$ two $\mathcal{C}^0$ functions and $\varphi : \mathbb{R}^d \to \mathbb{R}$ a $\mathcal{C}^2$ function such that

$$-\Delta\varphi + b \cdot \nabla\varphi + c\varphi = 0. \tag{2.39}$$

Assume there exists $r_0 > 0$ such that $c(x) > 0$ for all $|x| \geq r_0$. Assume further that $\varphi(x) > 0$ for all $|x| \leq r_0$, and that $\varphi(x) \underset{|x|\to\infty}{\longrightarrow} 0$. Then, $\varphi(x) > 0$ for all $x \in \mathbb{R}^d$.

This statement is essentially due to the maximum principle, which can be used even though we are on an unbounded domain because we already control the behaviour of the solution at infinity.

Proof. We argue by contradiction and assume that φ is nonpositive somewhere. Then, since $\varphi(x) \underset{|x|\to\infty}{\longrightarrow} 0$, there exists $x_0 \in \mathbb{R}^d$ such that $\varphi(x_0) = \min_{\mathbb{R}^d} \varphi \leq 0$, and we must have $|x_0| > r_0$. Let U be a connected open subset of $\mathbb{R}^d$ containing x_0, such that $|x| \geq r_0$ for all $x \in U$, and such that there exists x in ∂U with $|x| = r_0$. Since φ reaches its (nonpositive) minimum over $\bar{U}$ at the interior point x_0, while c is positive in U, the strong maximum principle yields that φ must be constant on $\bar{U}$. In particular, φ is nonpositive on ∂U, which contradicts the fact that the $\varphi(x)$ is positive for all $|x| \leq r_0$. □

Note that with $\varepsilon = -1$ in (2.33), we are in the "bad-sign" case of the semilinear heat equation, so that the strong maximum principle and the above lemma cannot be applied directly to equation (2.32). However, $\varphi = e^{|x|^2/8} u^\star$ satisfies an equation of the form (2.39), therefore its (strict) positivity can be verified via Lemma 2.30, which in turn is equivalent to the (strict) positivity of $u^\star$. For clarity, let us denote below a radial solution $u^\star$ as a function of $r = |x|$.

Corollary 2.31. Let $u^\star \in H^1(\mu)$ be a solution of Eq. (2.33) and $r_0 > 0$ be such that

$$\frac{d}{4} + \frac{r^2}{16} - \frac{1}{p-1} + \varepsilon u^\star(r)^{p-1} > 0 \qquad \text{for all } r \geq r_0. \tag{2.40}$$

If in addition, $u^\star(r) > 0$ for all $r \leq r_0$, then $u^\star(r) > 0$ for all $r \in \mathbb{R}_+$.

Proof. Define

$$\begin{aligned}\varphi : \mathbb{R}_+ &\longrightarrow \mathbb{R}\\ r &\longmapsto e^{r^2/8}u^\star(r).\end{aligned}$$

If $u^\star \in H^1(\mu)$ is a solution to Eq. (2.33), then by [102, Theorem 3.12, Proposition 3.15] it is also a classical solution in the sense that $u^\star \in \mathcal{C}^2(\mathbb{R}^d)$. Since $u^\star(|\cdot|) \in \mathcal{C}^2(\mathbb{R}^d)$, we observe that $u^\star \in H^1(\mathbb{R}_+, e^{r^2/4})$ and thus from the proof of Lemma 2.14 in the case $d = 1$, we have that $\varphi \in H^1(\mathbb{R}_+)$. Therefore, from [61, Corollary VIII.8], $\lim_{r\to+\infty} \varphi(r) = 0$. Now, letting $b = 0$ and

$$c(x) = \frac{d}{4} + \frac{|x|^2}{16} - \frac{1}{p-1} + \varepsilon u^\star(|x|)^{p-1},$$

we have that $\varphi(|\cdot|)$ solves the equation

$$-\Delta\varphi + c\varphi = 0.$$

Since $c, \varphi(|\cdot|) \in \mathcal{C}^2(\mathbb{R}^d)$ fulfil the assumptions of Lemma 2.30, under condition (2.40), we obtain that $\varphi(|x|) > 0$ for all $x \in \mathbb{R}^d$ and thus $u^\star(r) > 0$ for all $r \in \mathbb{R}_+$. □

In the case $d \in \{1, 2, 3\}$, it is straightforward to find some r_0 such that condition (2.40) holds by using the L^∞-bound obtained from Lemma 2.19 and using the estimate (2.30). Similarly, checking $u^\star$ is positive on $[0, r_0]$ can be achieved efficiently by using Lemma 2.19 and by using interval arithmetic to evaluate $P_m\bar{u}$ on $[0, r_0]$ for some small m and using the estimate (2.30) to bound $|(I - P_m)\bar{u}(r)|$. Let us remark that alternatively (in particular for $d \geq 4$), L^∞-estimates on $u^\star$ could be obtained by bootstrap arguments along the line of the proof of [102, Theorem 3.12]. By iteratively applying such arguments, one may also be able to obtain $\mathcal{C}^k$-bounds on $u^\star - \bar{u}$.

Corollary 2.32. Let $u^\star \in H^2(\mu)$ be as given by Theorem 2.29, $u^\star$ is strictly positive on $\mathbb{R}^d$.

Remark 2.33. In the event that the positivity of $u^\star$ is verified, in the case of $\varepsilon = -1$, since $u^\star \in C^2(\mathbb{R}_+)$, we immediately obtain that it is a classical solution (in the sense of [190]) of

$$\partial_r^2 u + \left(\frac{d-1}{r} + \frac{r}{2}\right)\partial_r u + \frac{u}{p-1} + |u|^{p-1}u = 0, \tag{2.41}$$

and since $u^\star$ is rapidly decaying, the results of [190] can be applied and yield $u^\star(r) = \mathcal{O}(r^{2/(p-1)-d}e^{-r^2/4})$. Furthermore, [233, Theorem 1] and [179] ensure that $u^\star$ is the unique rapidly decaying and strictly positive solution of Eq. (2.33) and of Eq. (2.32) respectively. The analogous result for the case $\varepsilon = +1$ is given by [62].

2.4.4 An example with a fractional exponent

In the case $\varepsilon = +1$, rapidly decaying self-similar solutions only exist for $p < 1 + 2/d$ [62, 102], and therefore integer exponents are excluded as soon as $d > 1$. We now explain how our method can be generalised to handle cases when the exponent p is a rational number. We focus on enclosing the positive self-similar profile of the nonlinear heat equation with $\varepsilon = +1$, $d = 2$ and $p = 5/3$. We thus aim to solve

$$Lu - \frac{3}{2}u + u^{5/3} = 0, \tag{2.42}$$

where we choose the real branch $x \in \mathbb{R} \mapsto x^{5/3} := (\sqrt[3]{x})^2 x$. We first look for an approximate solution $\bar{u} = \bar{U}^3$ such that

$$\bar{U}(r) = q(r)e^{-r^2/12},$$

where q is an even polynomial. The fractional exponent can then be *rigorously* handled via a quadrature as in Lemma 2.23. For instance, here, we first start by finding an approximate solution $\tilde{u}$ via a pseudospectral method [111], and compute for $n \in 3\mathbb{N}$

$$q(r) = \sum_{m=0}^{n/3} a_m L_m(r^2/12) \qquad \text{where } a_m \approx \frac{1}{6}\int_0^\infty L_m(r^2/12)\sqrt[3]{\tilde{u}(r)} r \mathrm{d}r,$$

so that $\bar{U} \approx \sqrt[3]{\tilde{u}}$. Finally, we define $\bar{u} := \bar{U}^3$ to apply Theorem 1.1. From here, $\bar{u}$ can be identified as a vector of $n+1$ intervals as in (2.26) and computations can be carried out in the same manner as in the other examples. Note that here, we cannot expect $\bar{u}$ to achieve the minimal error $\min_{u\in\Pi_n(\mathcal{H})} \|F(u)\|_{H^2(\mu)}$. Hence, we need to take more basis functions to achieve a comparable error as $\tilde{u}$, actually around s times more where the degree of the nonlinearity is $p = q/s$.

Remark 2.34. It is clear that this approach can work with any rational exponent with an odd denominator. In the case of an exponent with an even denominator, this approach can only work if $\bar{U}$ can be verified to be nonnegative. Beyond the fact that this verification most likely requires a lengthy computation, finding such nonnegative $\bar{U}$ in the first place probably needs some fine-tuning. A more sophisticated approach would be to bypass this issue by reformulating the problem as a differential-algebraic equation as in [52], but this would probably require additional bounds with an adapted functional analysis.

Now, analysing the function $x \mapsto x^{2/3} := (\sqrt[3]{x})^2$, one finds that for all $x, y \in \mathbb{R}$,

$$\left|\frac{\mathrm{d}y^{5/3}}{\mathrm{d}y} - \frac{\mathrm{d}x^{5/3}}{\mathrm{d}x}\right| = \frac{5}{3}\left|y^{2/3} - x^{2/3}\right| \le \frac{5}{3}|x-y|^{2/3}.$$

Thus, writing $\|DT(u)\|_{H^2,H^2} \le \|DT(\bar{u})\|_{H^2,H^2} + \|DT(u) - DT(\bar{u})\|_{H^2,H^2}$ and estimating that for $h \in H^2(\mu)$

$$\begin{aligned}
\|(DT(u) - DT(\bar{u}))h\|_{H^2} &\le \frac{5}{3}\|AL^{-1}(u^{2/3} - \bar{u}^{2/3})h\|_{H^2} \\
&\le \frac{5}{3}\|LAL^{-1}\|_{L^2,L^2}\|(u^{2/3} - \bar{u}^{2/3})h\|_{L^2} \\
&\le \frac{5}{3}\|LAL^{-1}\|_{L^2,L^2}\|(u^{2/3} - \bar{u}^{2/3})\|_\infty\|h\|_{L^2} \\
&\le \frac{5}{3}\|LAL^{-1}\|_{L^2,L^2}\|(u-\bar{u})\|_\infty^{2/3}\|h\|_{L^2} \qquad \text{by (2.4.4)} \\
&\le \frac{5}{3}C(2)^{2/3}\|LAL^{-1}\|_{L^2,L^2}\|u-\bar{u}\|_{H^2}^{2/3}\|h\|_{H^2} \qquad \text{by Lemma 2.19,}
\end{aligned}$$

we may choose

$$\mathcal{W}(\delta) := Z_{5/3}\delta^{2/3}$$

satisfying (1.5), where Z_1 is as in Section 2.4.1 and

$$Z_{5/3} = \frac{5}{3}C(2)^{2/3}\|LAL^{-1}\|_{L^2,L^2}.$$

For this example, we choose $n = 1200$ and find $\bar{u}$ depicted in Figure 2.1.

Proof of Theorem 2.1. We consider $F : \mathcal{H} \to \mathcal{H}$ defined in (2.34). In the file `Heat/fractional/proof.ipynb` at [80], we load a precomputed $\bar{U}$ and compute $\bar{u} = \bar{U}^3$, then we construct A_n (and thus indirectly A and T) as outlined in Section 2.2.4, and we find the following sufficient bounds:

$$\begin{aligned} Y &= 1.5917976375189734 \times 10^{-23}, \\ Z_1 &= 0.002929002447260958, \\ Z_{5/3} &= 19.560776011689786, \\ \underline{\delta} &= 1.5964737129311592 \times 10^{-23} \\ \bar{\delta} &= 0.011508269024627918. \end{aligned}$$

We conclude with Theorem 1.1. Finally, positivity is deduced from Corollary 2.31. □

2.4.5 An example of a non-radial solution

Let us now turn to the problem of finding (real-valued) non-radial solutions to problem (2.32). We limit ourselves to the case $\varepsilon = -1, d = 2, p = 3$ here (though, such construction can be generalised), so that the problem remains polynomial while allowing for solutions that are not necessarily positive. In polar coordinates, the equation for $u(r, \vartheta) = e^{-r^2/8}\varphi(r\cos\vartheta, r\sin\vartheta)$ reads

$$Lu = \frac{1}{2}u + u^3, \tag{2.43}$$

where

$$Lu = -\frac{r}{2}\frac{\partial u}{\partial r} - \Delta = -\frac{r}{2}\frac{\partial u}{\partial r} - \frac{1}{r}\frac{\partial}{\partial r}\left(r\frac{\partial u}{\partial r}\right) - \frac{1}{r^2}\frac{\partial^2 u}{\partial \vartheta^2}.$$

Observe that since the equation itself is radially symmetric, if $u : \mathbb{R}_+ \times \mathbb{T} \to \mathbb{R}$ is a solution to Eq. (2.43), then so is $u(\,\cdot\,, \cdot + \vartheta_0)$ for any phase $\vartheta_0 \in \mathbb{T}$. Thus, our approach which relies on a contraction principle, and hence requires local uniqueness, cannot possibly work directly on $H^2(\mu)$. By treating the problem in polar coordinates, instead of using cartesian coordinates with the Hermite basis (2.11), we get a natural way of dealing with the translation invariance in the angular variable.

We thus restrict the problem to an appropriate subspace, namely

$$\mathcal{H} = \overline{\mathrm{Span}\,\{\psi_{k,m} \mid k \in \mathbb{N}, m \in \mathbb{N}\}}^{H^2} \subset H^2(\mu),$$

where $\psi_{k,m}$ are as in Definition 2.5, and, as before, we denote by $\hat{\psi}_{k,m}$ the normalisation of $\psi_{k,m}$ with respect to the $L^2(\mu)$-inner product $\langle\cdot,\cdot\rangle$. Since we restricted ourselves to nonnegative k's, $\mathcal{H}$ is nothing but the space of $H^2(\mu)$-functions which are even with respect to ϑ. Solving for Eq. (2.43) in this space addresses the above symmetry "issue" and it is straightforward to check that

$$\begin{aligned} F : \mathcal{H} &\longrightarrow \mathcal{H} \\ u &\longmapsto u - L^{-1}\left(\frac{u}{2} + u^3\right) \end{aligned} \tag{2.44}$$

is well-defined and compact. In this respect, our strategy goes along the same line as the one employed in [11] to find non-radial solutions of analogous semilinear equations on the disc. In the most general setting, the above-defined space $\mathcal{H}$ shall be used, but one can simplify the proof

further if the solution has a zero projection onto certain frequencies. In our example, we will perform our computer-assisted proof in the subspace

$$\tilde{\mathcal{H}} = \overline{\mathrm{Span}\left\{\psi_{2k+1,m} \mid k \in \mathbb{N}, m \in \mathbb{N}\right\}}^{H^2} \subset \mathcal{H} \subset H^2(\mu).$$

Working on such subspaces can also automatically discard other non-zero solutions which are not of interest such as radial ones. Here, we have that

$$L\psi_{2k+1,m} = \lambda_{k+m}\psi_{2k+1,m}, \qquad \lambda_j := \frac{3}{2} + j,$$

and the $\psi_{2k+1,m}$ for $k, m \in \mathbb{N}$ form a Hilbert basis of $\tilde{\mathcal{H}}$. Note that the definition of λ_j in that context is slightly different from the one introduced in Notation 2.27. In particular, this change reflects the fact that the first eigenvalue of L restricted to $\tilde{\mathcal{H}}$ is strictly larger than $d/2 = 1$, which slightly improves the Poincaré inequalities (2.13) and (2.14) on $\tilde{\mathcal{H}}$.

The estimates for the radii polynomials coefficients are essentially the same as in Section 2.4.1, with Π_n now denoting the projection onto $\mathrm{Span}\left\{\psi_{2k+1,m} \mid k \in \mathbb{N}, m \in \mathbb{N} \text{ with } k+m \leq n\right\}$, and

$$w_{k,m} := \|\Pi_\infty(\bar{u}^2\hat{\psi}_{2k+1,m})\|_{L^2(\mu)} = \left(\|\bar{u}^2\hat{\psi}_{2k+1,m}\|^2_{L^2(\mu)} - \|\Pi_n(\bar{u}^2\hat{\psi}_{2k+1,m})\|^2_{L^2(\mu)}\right)^{1/2}.$$

The computation of integrals described in Section 2.3 is adapted as follows:

- the integral is first reformulated as a sum of integrals of product of functions, separable in r and ϑ components so as to apply Fubini's Theorem,
- the integrals with respect to ϑ are treated via the multiplication formula for cosines and orthogonality,
- the integrals with respect to r are of the form (2.29) after the change of variable $z = r^2/4$.

As for the L^∞-bounds on $\hat{\psi}_{2k+1,m}$, we have that $|\hat{\psi}_{2k+1,m}(r,\vartheta)| \leq |\hat{\psi}_{2k+1,m}(r,0)|$, and we compute the local extrema of $r \mapsto \partial_r\hat{\psi}_{2k+1,m}(r,0)$ by enclosing its zeros (which must all be real), this time using `PolynomialRoots.jl`, the Julia implementation of [199].

Remark 2.35. In practice, while we might do the computer-assisted proof with many basis functions, we set some of the entries of $\bar{u}$ to zero to eliminate unnecessary computational costs so that the validation can be performed within a manageable amount of time on a personal computer.

We choose $n = 150$ (i.e. 11,476 basis functions) and obtain the approximate solution $\bar{u}$ depicted in Figure 2.4.

Theorem 2.36. Let $\bar{u} : \mathbb{R}^2 \to \mathbb{R}$ be the function whose restriction to the disk $\{(x,y) \mid x^2 + y^2 \leq 4^2\}$ is represented on Fig 2.4 and whose description in terms of "Fourier" coefficients in $\{\hat{\psi}_{2k+1,m}\}_{k\geq 0, k+m\leq n}$ is available at [80]. There exists a solution $u^\star \in \tilde{\mathcal{H}}$ to Eq. (2.43) such that

$$\|u^\star - \bar{u}\|_{H^2(\mu)} \leq \underline{\delta} = 0.0016.$$

Proof. We consider $F : \tilde{\mathcal{H}} \to \tilde{\mathcal{H}}$ defined in (2.44). In the file `Heat/asymmetric/proof.ipynb` at [80], we construct A_n (and thus indirectly A and T) as outlined in Section 2.2.4, we find the

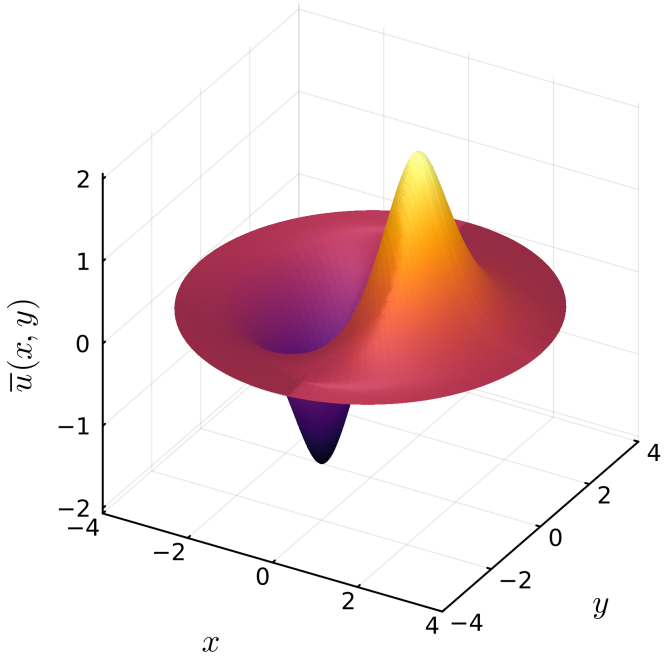


Figure 2.4: Plot of a non-radial numerical solution $\bar{u}$ to Eq. (2.43).

following sufficient bounds:

$$\begin{aligned} Y &= 0.0011482317939412424, \\ Z_1 &= 0.09887537542580953, \\ Z_2 &= 236.2041502678645, \\ Z_3 &= 456.22972624236917, \\ \bar{\delta} &= 0.003801071181766125, \end{aligned}$$

and we conclude with Corollary 2.20. □

2.5 Self-similar solutions of the nonlinear Schrödinger equation

Let us now turn to the critical nonlinear Schrödinger equation

$$i\partial_t v + \Delta v + \varepsilon |v|^{4/d} v = 0, \tag{2.45}$$

for $\varepsilon = \pm 1$. It is known [150] that this equation admits self-similar solutions of the form

$$v(t,x) = (1+t^2)^{-d/4} \exp\left(\frac{it|x|^2}{4(1+t^2)}\right) e^{i\omega \arctan t} \varphi\left(\frac{\sqrt{2}x}{(1+t^2)^{1/2}}\right), \tag{2.46}$$

for any $\omega \in \mathbb{R}$, as soon as $\varphi : \mathbb{R}^d \longrightarrow \mathbb{C}$ solves

$$-\Delta\varphi + \frac{|x|^2}{16}\varphi + \frac{\omega}{2}\varphi = \frac{\varepsilon}{2}|\varphi|^{4/d}\varphi. \tag{2.47}$$

Assuming $\varphi(x) = e^{|x|^2/8}u(x)$, we get the equation

$$Lu = \left(\frac{d}{4} - \frac{\omega}{2}\right) u + \frac{\varepsilon}{2} e^{(p-1)|x|^2/8} |u|^{4/d} u, \tag{2.48}$$

where $p = 4/d + 1$.

Remark 2.37. In [150], Eq. (2.47) is solved via variational methods for φ in the Hilbert space

$$\mathcal{X} = \left\{\varphi \in H^1(\mathbb{R}^d) : |x|\varphi \in L^2(\mathbb{R}^d)\right\},$$

but this is equivalent to solving Eq. (2.48) for $u \in H^1(e^{|x|^2/4})$. Furthermore, an enclosure of a solution $u^\star$ to (2.48) around $\bar{u}$ with respect to the $H^2(\mu)$-norm will automatically yield an enclosure for a solution $\varphi^\star := e^{|x|^2/8}u^\star$ to (2.47) around $\bar{\varphi} := e^{|x|^2/8}\bar{u}$ with respect to the $H^2(\mathbb{R}^d)$-norm by inequality (2.21).

In the radial case, we thus aim to find a non-trivial zero of

$$F(u) = u - L^{-1}\left(\left(\frac{d}{4} - \frac{\omega}{2}\right) u + \frac{\varepsilon}{2} e^{(p-1)r^2/8} u^p\right). \tag{2.49}$$

We get similar estimates for the radii polynomials coefficients as in Section 2.4.1 and take

$$\begin{aligned}
Y &= \left\{ \|LA_n(\Pi_n F(\bar{u}))\|^2_{L^2(\mu)} + \frac{1}{4}\left(\|e^{(p-1)r^2/8}\bar{u}^p\|^2_{L^2(\mu)} - \|\Pi_n(e^{(p-1)r^2/8}\bar{u}^p)\|^2_{L^2(\mu)} \right) \right\}^{1/2} \\
Z^{11} &= \|L(I_n - A_n\Pi_n DF(\bar{u})\Pi_n)L^{-1}\|_{L^2(\mu),L^2(\mu)} \\
Z^{21} &= \frac{p}{2}\|L^{-1}w\|_{L^2(\mu)} \\
Z^{12} &= \frac{p}{2\lambda_{n+1}} \left\| \left|LA_nL^{-1}\right| w \right\|_{L^2(\mu)} \\
Z^{22} &= \frac{\|d/4 - \omega/2 + \varepsilon p(e^{r^2/8}\bar{u})^{p-1}/2\|_\infty}{\lambda_{n+1}} \\
Z_k &= \frac{p!}{d(p-k)!} C(d)^{k-1} \|LAL^{-1}\|_{L^2(\mu),L^2(\mu)} \|e^{r^2/8}\bar{u}\|^{p-k}_\infty \\
\text{or } Z_k &= \frac{p!}{2(p-k)!}\left(\frac{2}{d}\right)^{k/2} c(d,k) \|LAL^{-1}\|_{L^2(\mu),L^2(\mu)} \|e^{r^2/8}\bar{u}\|^{p-k}_\infty,
\end{aligned}$$

where

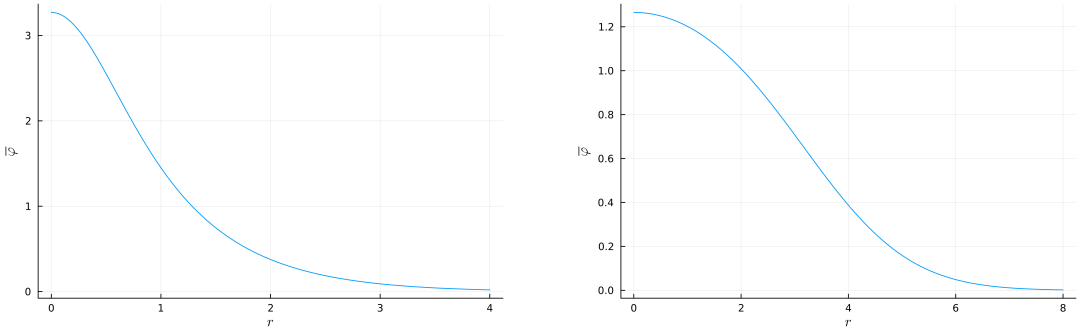
$$w_m := \|\Pi_\infty((e^{r^2/8}\bar{u})^{p-1}\hat{\psi}_m)\|_{L^2(\mu)} = \left(\|(e^{r^2/8}\bar{u})^{p-1}\hat{\psi}_m\|^2_{L^2(\mu)} - \|\Pi_n((e^{r^2/8}\bar{u})^{p-1}\hat{\psi}_m)\|^2_{L^2(\mu)} \right)^{1/2}.$$

Similarly, the quadrature rule of Section 2.3 can be adapted. For instance, the matrix

$$G_{ij} = \langle \hat{\psi}_i, e^{(p-1)r^2/8}\bar{u}^{p-1}\hat{\psi}_j \rangle$$

can be written as $G = \bar{V}^T \mathrm{Diag}(\bar{V}\bar{\mathbf{u}})^{p-1}\bar{V}$ for $\bar{V}$ as in Section 2.3, with $m = p+1$ and $\beta = (p+1)/2$. One could also study the positivity of our radial solutions by applying Lemma 2.30 to Eq. (2.47).

Furthermore, one can find non-radial solutions by adapting the setup and the above bounds analogously to Section 2.4.5.



(a) $\varepsilon = +1$, $d = 2$, $\omega = 2$ (b) $\varepsilon = -1$, $d = 2$, $\omega = -2$

Figure 2.5: Plots of the numerical approximations $\bar{\varphi} = e^{|x|^2/8}\bar{u}$ to Eq. (2.47).

	$\varepsilon = +1$, $d = 2$, $\omega = 2$	$\varepsilon = -1$, $d = 2$, $\omega = -2$	$\varepsilon = -1$, $d = 2$, $\omega = -5/2$
Y	$1.10976243687315 \times 10^{-7}$	$1.5107943983942 \times 10^{-33}$	$7.7098399586773 \times 10^{-9}$
Z_1	0.0159474482138791	0.0094441948748148	0.040651432114283
Z_2	77.796328353367	468.05753022221	109.713908018849
Z_3	134.269405908538	1264.7114345257	486.145035940895
$\underline{\delta}$	$1.1277557297873 \times 10^{-7}$	$1.52519871732857 \times 10^{-33}$	$8.0365405162453 \times 10^{-9}$
$\bar{\delta}$	0.00778742238332	0.00211029551244486	0.0085809580990918
η	$1.89177452668397 \times 10^{-6}$	$7.1523768316161 \times 10^{-33}$	$3.7687132530124 \times 10^{-8}$
$\dim(\Pi_n\mathcal{H})$	501	501	5151
Figure	2.5a	2.5b	2.2

Table 2.2: Results for the a posteriori validation of the solutions to Eq. (2.47) in Theorem 2.38.

Theorem 2.38. For $d = 2$ and $(\varepsilon, \omega) = (+1, 2)$, (resp. $(\varepsilon, \omega) = (-1, -2)$, resp. $(\varepsilon, \omega) = (-1, -5/2)$), let $\bar{\varphi}$ be the function depicted on a compact set in Figure 2.5a (resp. 2.5b, resp. 2.2) and whose description in terms of "Fourier" coefficients is available at [80]. There exists a solution $\varphi^\star \in H^2(\mathbb{R}^d)$ to Eq. (2.47) such that

$$\|\varphi^\star - \bar{\varphi}\|_{H^2(\mathbb{R}^2)} \leq \eta,$$

where η is as in Table 2.2.

Proof. We consider F defined in (2.49). In the file `Schrodinger/plus/proof.ipynb` (resp. `Schrodinger/minus/proof.ipynb`, resp. `Schrodinger/asymmetric/proof.ipynb`) at [80], we construct A_n (and thus indirectly A and T) as outlined in Section 2.2.4 and following the estimates above, we obtain the upper bounds in Table 2.2 for Y and the Z_k's to conclude with Corollary 2.20. Now, observe that from combining (2.22) with the Poincaré inequalities (2.13) and (2.14), for $d \geq 2$,

for all $u \in H^2(\mu)$ and $\varphi = e^{|x|^2/8}u$, we have that

$$\|\varphi\|^2_{H^2(\mathbb{R}^d)} := \|D^2\varphi\|^2_{L^2(\mathbb{R}^d)} + \|\nabla\varphi\|^2_{L^2(\mathbb{R}^d)} + \|\varphi\|^2_{L^2(\mathbb{R}^d)} \leq Z\left[1 + \max\left(0, 1 - \frac{d}{8}\right)\frac{4}{d^2}\right]\|u\|^2_{H^2(\mu)}.$$

And thus, for $d = 2$, we may choose $\eta = (\sqrt{7Z}/2)\underline{\delta}$. □

Note that the third case of Theorem 2.38 corresponds to Theorem 2.2.

2.6 An example with first order terms

In this final section, we consider a toy problem whose interest lies in the fact that it leads to an equation of the form (2.2) with a first-order term, i.e. a right-hand side of the form $f(x, u, \nabla u)$ with an actual dependence on ∇u. We focus on a generalised viscous Burgers equation on $\mathbb{R}_+$ with Neumann boundary condition

$$\begin{cases} \partial_t v + v^2\partial_x v = \partial_{xx} v, \\ \partial_x v(t, 0) = 0 \qquad\qquad \text{for all } t > 0. \end{cases} \tag{2.50}$$

Then, under the similarity transformation

$$v(t, x) = t^{-1/4}u\left(\frac{x}{\sqrt{t}}\right),$$

v solves Eq. (2.50) for $t > 0$ if u solves

$$Lu - \frac{u}{4} + u^2\frac{\partial u}{\partial x} = 0, \qquad x \geq 0. \tag{2.51}$$

Similar problems have been studied in [2, 201] and the references therein. This equation can be approached with our method, as $u \in H^2(\mu)$ implies that $u \in \mathcal{C}^1_0(\mathbb{R})$ and thus $u^2\partial_x u \in L^2(\mu)$.

Remark 2.39. We deal with a one-dimensional example here for simplicity, but terms like $(u\cdot\nabla)u$ could in principle also be handled in dimension $d \in \{2, 3\}$, as $u \in H^2(\mu)$ is then still enough to guarantee that $(u \cdot \nabla)u \in L^2(\mu)$ since $u \in L^\infty(\mathbb{R}^d)$.

In order to enforce the Neumann boundary condition, we symmetrise the problem and work on the Hilbert space

$$\mathcal{H} = \overline{\text{Span}\{\hat{\psi}_m\}_{m=0}^\infty}^{H^2} = \overline{\text{Span}\{e^{-x^2/4}\hat{H}_{2m}(x/2)\}_{m=0}^\infty}^{H^2},$$

i.e. we make use of "even half-Hermite series" where $\hat{H}_n = H_n/\sqrt{2^n n!\sqrt{\pi}}$ denotes a normalised Hermite polynomial. Note that working on $\mathcal{H}$ is equivalent to working on $H^2(\mathbb{R}_+, e^{x^2/4})$ with the additional Neumann boundary condition (see also [228, Section 3]). Furthermore, for clarity, in what follows, all elements of $L^2(\mu)$ that we will consider should be treated as functions on $\mathbb{R}_+$ having an even extension on $\mathbb{R}$. In particular, for such functions u and v, we have that

$$\langle u, v\rangle = \int_{-\infty}^{\infty} uv\mu(x)\mathrm{d}x = \frac{1}{2}\int_{-\infty}^{\infty} uve^{x^2/4}\mathrm{d}x = \int_0^\infty uve^{x^2/4}\mathrm{d}x.$$

We consider

$$\begin{aligned} F : \mathcal{H} &\longrightarrow \mathcal{H} \\ u &\longmapsto u + L^{-1}\left(-\frac{u}{4} + u^2\partial_x u\right), \end{aligned} \tag{2.52}$$

and construct our fixed point operator $T : \mathcal{H} \to \mathcal{H}$ as outlined in 2.2.4. Note that T is still polynomial with respect to u in this case and most bounds for the validation can be derived similarly as in Section 2.4.1:

$$\begin{aligned} Y &= \left\{\|LA_n(\Pi_n F(\bar{u}))\|^2_{L^2(\mu)} + \left(\|\bar{u}^2\partial_x\bar{u}\|^2_{L^2(\mu)} - \|\Pi_n(\bar{u}^2\partial_x\bar{u})\|^2_{L^2}\right)\right\}^{1/2}, \\ Z^{11} &= \|L(I_n - A_n\Pi_n DF(\bar{u})\Pi_n)L^{-1}\|_{L^2(\mu),L^2(\mu)}, \\ Z^{21} &= \|L^{-1}w\|_{L^2(\mu)}, \\ Z^{22} &= \frac{\|1/4 + 2\bar{u}\partial_x\bar{u}\|_\infty}{\lambda_{n+1}} + \frac{\|\bar{u}\|^2_\infty}{\sqrt{\lambda_{n+1}}}, \\ Z_2 &= 2^{15/4}\|LAL^{-1}\|_{L^2(\mu),L^2(\mu)}(\sqrt{2}\|\bar{u}\|_\infty + \|\partial_x\bar{u}\|_\infty), \\ Z_3 &= 96\|LAL^{-1}\|_{L^2(\mu),L^2(\mu)}, \end{aligned}$$

with

$$\begin{aligned} w_m :&= 2\|\Pi_\infty(\bar{u}\hat{\psi}_m\partial_x\bar{u})\|_{L^2} + \|\Pi_\infty(\bar{u}^2\partial_x\hat{\psi}_m)\|_{L^2} \\ &= 2\left(\|\bar{u}\hat{\psi}_m\partial_x\bar{u}\|^2_{L^2} - \|\Pi_n(\bar{u}\hat{\psi}_m\partial_x\bar{u})\|^2_{L^2}\right)^{1/2} + \left(\|\bar{u}^2\partial_x\hat{\psi}_m\|^2_{L^2} - \|\Pi_n(\bar{u}^2\partial_x\hat{\psi}_m)\|^2_{L^2}\right)^{1/2}. \end{aligned}$$

The only estimate which requires substantial adaptations is Z^{12}. For $h_\infty \in \mathcal{H}_\infty$, we get

$$\begin{aligned} \langle 2\bar{u}\partial_x\bar{u}h_\infty + \bar{u}^2\partial_x h_\infty, \hat{\psi}_m\rangle &= \langle \partial_x(\bar{u}^2 h_\infty), \hat{\psi}_m\rangle \\ &= \int_0^\infty \partial_x(\bar{u}^2 h_\infty)\hat{\psi}_m e^{x^2/4}\mathrm{d}x \\ &= \bar{u}(0)^2 h_\infty(0)\hat{\psi}_m(0) - \int_0^\infty \bar{u}^2 h_\infty \partial_x(\hat{\psi}_m e^{x^2/4})\mathrm{d}x \qquad \text{by parts.} \end{aligned} \tag{2.53}$$

We deal with both terms appearing in (2.53) separately. First, writing h_∞ as

$$h_\infty = \sum_{m=n+1}^\infty a_m\hat{\psi}_m,$$

we have that

$$\begin{aligned} h_\infty(0)^2 &= \left(\sum_{m=n+1}^\infty a_m\hat{\psi}_m(0)\right)^2 \\ &\le \left(\sum_{m=n+1}^\infty \lambda_m^2 a_m^2\right)\left(\sum_{m=n+1}^\infty \frac{\hat{\psi}_m(0)^2}{\lambda_m^2}\right) \qquad \text{by Cauchy–Schwarz inequality} \\ &= \frac{\|h_\infty\|^2_{H^2(\mu)}}{\Gamma(1/2)^2}\sum_{m=n+1}^\infty \frac{\Gamma(m+1/2)}{(m+1/2)^2 m!} \qquad \text{by (2.30)} \end{aligned}$$

$$
\begin{aligned}
&= \frac{\|h_\infty\|^2_{H^2(\mu)}}{\pi}\left(\sum_{m=0}^{\infty}\frac{\Gamma(m+1/2)}{(m+1/2)^2 m!} - \sum_{m=0}^{n}\frac{\Gamma(m+1/2)}{(m+1/2)^2 m!}\right)\\
&\leq \frac{\|h_\infty\|^2_{H^2(\mu)}}{\pi}\left(\pi^{3/2}\log 4 - \sum_{m=0}^{n}\frac{\Gamma(m+1/2)}{(m+1/2)^2 m!}\right)\\
&\leq \|h_\infty\|^2_{H^2(\mu)} S_n,
\end{aligned}
$$

where

$$
S_n = \frac{1}{\pi}\left(\pi^{3/2}\log 4 - \sum_{m=0}^{n}\frac{\Gamma(m+1/2)}{(m+1/2)^2 m!}\right).
$$

Now, for the integral term in (2.53),

$$
\begin{aligned}
&\left|\int_0^\infty \bar{u}^2 h_\infty \partial_x(\hat{\psi}_m e^{x^2/4})\mathrm{d}x\right|\\
=&\left|\int_0^\infty \bar{u}^2 h_\infty \left(\partial_x\hat{\psi}_m + \frac{x}{2}\hat{\psi}_m\right)e^{x^2/4}\mathrm{d}x\right|\\
\leq&\left|\left\langle h_\infty, \bar{u}^2\left(\partial_x\hat{\psi}_m + \frac{x}{2}\hat{\psi}_m\right)\right\rangle\right|\\
\leq&\left|\left\langle h_\infty, \Pi_\infty\left(\bar{u}^2\left(\partial_x\hat{\psi}_m + \frac{x}{2}\hat{\psi}_m\right)\right)\right\rangle\right| \qquad \text{as } h_\infty \in \mathcal{H}_\infty\\
\leq&\|h_\infty\|_{L^2(\mu)}\left\|\Pi_\infty\left(\bar{u}^2\left(\partial_x\hat{\psi}_m + \frac{x}{2}\hat{\psi}_m\right)\right)\right\|_{L^2(\mu)}\\
\leq&\frac{\|h_\infty\|_{H^2(\mu)}}{\lambda_{n+1}}\left(\left\|\bar{u}^2\left(\partial_x\hat{\psi}_m + \frac{x}{2}\hat{\psi}_m\right)\right\|^2_{L^2(\mu)} - \left\|P_n\left(\bar{u}^2\left(\partial_x\hat{\psi}_m + \frac{x}{2}\hat{\psi}_m\right)\right)\right\|^2_{L^2(\mu)}\right)^{1/2}.
\end{aligned}
$$

Thus, with

$$
\tilde{w}_m = \bar{u}(0)^2\hat{\psi}_m(0)\sqrt{S_n} + \frac{1}{\lambda_{n+1}}\left(\left\|\bar{u}^2\left(\partial_x\hat{\psi}_m + \frac{x}{2}\hat{\psi}_m\right)\right\|^2_{L^2(\mu)} - \left\|P_n\left(\bar{u}^2\left(\partial_x\hat{\psi}_m + \frac{x}{2}\hat{\psi}_m\right)\right)\right\|^2_{L^2(\mu)}\right)^{1/2},
$$

we can choose

$$
Z^{12} = \left\| \left|LA_nL^{-1}\right| \tilde{w}\right\|_{L^2(\mu)}.
$$

An estimate based on Parseval's identity on $H^1(\mu)$ is also possible, but gives similar results.

Remark 2.40. Note that if $u(x) = q(x)e^{-x^2/4}$ for a polynomial q, then $\partial_x u(x) = (\partial_x q(x) - x/2q(x))e^{-x^2/4}$ and thus the integrals necessary to compute our bounds can also be evaluated with quadrature rules as in Section 2.3. Concerning L^∞-bounds, from [96, (18.14.9)], we have that for all $m \in \mathbb{N}$

$$
\|\hat{\psi}_m\|_\infty \leq \|\hat{\psi}_m e^{x^2/8}\|_\infty = \|e^{-x^2/8}\hat{H}_{2m}(x/2)\|_\infty \leq \pi^{-1/4},
$$

and for all $m \in \mathbb{N}^*$

$$
\|\partial_x\hat{\psi}_m\|_\infty \leq \left\|\sqrt{m}e^{-x^2/4}\hat{H}_{2m-1}(x/2) - \frac{x}{2}\hat{\psi}_m\right\|_\infty \leq \pi^{-1/4}\left(\sqrt{m} + \frac{1}{\sqrt{e}}\right) \qquad \text{as } \left\|\frac{x}{2}e^{-x^2/8}\right\|_\infty = \frac{1}{\sqrt{e}}.
$$

With $n = 1500$, we find the approximate solution $\bar{u}$ represented in Figure 2.6.

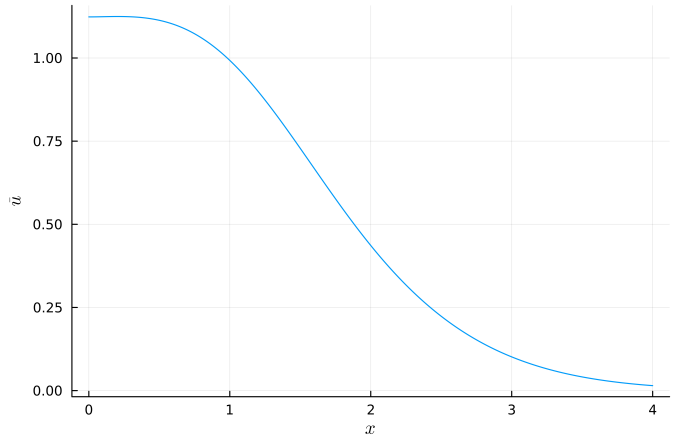


Figure 2.6: Plot of the numerical solution $\bar{u}$ to Eq. (2.51).

Theorem 2.41. Let $\bar{u} : \mathbb{R}_+ \to \mathbb{R}$ be the function represented on the interval $[0, 4]$ in Fig 2.6 and whose description in terms of "Fourier" coefficients in $\{\hat{\psi}_m\}_{m=0}^n$ is available at [80], then there exists a positive solution $u^\star \in \mathcal{H}$ to Eq. (2.51) such that

$$\|u^\star - \bar{u}\|_{H^2(\mu)} \leq 10^{-3}.$$

Proof. We consider $F : \mathcal{H} \to \mathcal{H}$ defined in (2.52). In the file `Burger/proof.ipynb` at [80], we construct A_n (and thus indirectly A and T) as outlined in Section 2.2.4 and following the estimates above, we find the following sufficient bounds:

$$\begin{aligned} Y &= 0.00075636391, \\ Z_1 &= 0.065135932, \\ Z_2 &= 343.3917, \\ Z_3 &= 556.478, \\ \bar{\delta} &= 0.00271646316, \end{aligned}$$

and we conclude with Corollary 2.20 to the existence of a solution $u^\star \in \mathcal{H}$ to Eq. (2.51). As Eq. (2.51) can be seen as an ordinary differential equation with a smooth vector field, we immediately get that $u^\star \in \mathcal{C}^\infty(\mathbb{R}_+)$ and thus we can apply Lemma 2.30 (again to $\varphi = e^{|x|^2/8}u^\star$) with $b(x) = u^{\star 2}(x)$ and $c(x) = x^2/16 - xu^{\star 2}(x)/4$, to get that $u^\star$ is positive. □

2.7 Relationship with the Ornstein-Uhlenbeck process

In this chapter, we studied equations of the form

$$Lu = f(x, u, \nabla u), \qquad L := -\frac{x}{2} \cdot \nabla - \Delta. \tag{2.54}$$

L can actually be seen as analogous to the operator

$$\mathfrak{L} = \frac{x}{2} \cdot \nabla - \Delta = e^{|x|^2/4} L(e^{-|x|^2/4} \cdot) - \frac{d}{2}\mathrm{id}$$

where $-\mathfrak{L}$ is the generator of the Ornstein-Uhlenbeck process

$$\mathrm{d}X_t = -\frac{X_t}{2}\mathrm{d}t + \sqrt{2}\mathrm{d}B_t.$$

The equation (2.54) can actually be seen as a nonlinear Fokker–Planck equation as $L = \mathfrak{L}^* + (d/2)\mathrm{id}$ (where $\mathfrak{L}^*$ denotes the $L^2(\mathbb{R}^d)$-adjoint of $\mathfrak{L}$).

The functional analysis of such operator $\mathfrak{L}$ is well established [20, 189] and can straightforwardly be generalised to

$$\mathfrak{L} = \nabla V \cdot \nabla - \Delta$$

where $-\mathfrak{L}$ generates the Markov semi-group associated to a Brownian particle $(X_t)_{t\geq 0}$ evolving under a confining potential $V : \mathbb{R}^d \to \mathbb{R}$

$$\mathrm{d}X_t = -\frac{X_t}{2}\mathrm{d}t + \sqrt{2}\mathrm{d}B_t.$$

Therefore, a natural question is whether our numerical analysis can be expanded to study equations of the form

$$\mathfrak{L}u = \nabla V \cdot \nabla u - \Delta u = f(x, u)$$

for a less classical potential V. We study this problem in dimension $d = 1$ in the next chapter, with a particular focus on the potential

$$V(x) = \frac{x^4}{4} - \kappa\frac{x^2}{2}$$

3

Solutions of differential equations in Freud-weighted Sobolev spaces

This chapter is based on the paper [54].

3.1 Introduction

Given a potential $V \in \mathcal{C}^2(\mathbb{R})$, it is well-known that if the Gibbs probability measure $\nu(\mathrm{d}x) := e^{-V}\mathrm{d}x/Z$ has finite moments of all orders, then one may construct a Hilbert basis of orthonormal polynomials $\mathcal{P} = \{p_n\}_{n\in\mathbb{N}}$ on $(L^2(\nu), \langle\cdot,\cdot\rangle)$, that is

$$\langle p_n, p_m\rangle = \int_{\mathbb{R}} p_n p_m \mathrm{d}\nu = \delta_{mn}, \qquad Z := \int_{\mathbb{R}} e^{-V(x)}\mathrm{d}x.$$

Orthogonal polynomials [1, 92, 120, 182, 203] have been a topic of interest since the birth of Numerical Analysis and much is known about their construction, asymptotic behaviour, relation with special functions and random matrices, zeroes etc. However, disappointingly, almost all the resolutions of differential equations with orthogonal polynomials are achieved using the classical families (Fourier, Hermite, Jacobi and Laguerre) [98]. One of the reasons is that these classical families have the property that the derivative of a classical orthogonal polynomial is a polynomial in the same family. Therefore, these bases allow for simple representations of the differentiation operator ∂_x (typically diagonal, maybe up to a shift), which makes them very convenient for the study of differential equations.

However, some (non-quantitative) results in Functional Analysis [19, 20] (most notably in Probability Theory) show that the Sobolev embedding $H^1(\nu) \hookrightarrow L^2(\nu)$ is often compact, even beyond the classical weights. In principle, this allows for the approximation of compact operators on these spaces with finite-dimensional matrices on the computer, in order to solve equations of the form

$$\mathfrak{L}u = f(u), \qquad \mathfrak{L} := V'(x)\partial_x - \partial_{xx}, \tag{3.1}$$

which are naturally posed in $H^1(\nu)$, where $\mathfrak{L}$ is a well-studied operator in Probability Theory. Note that this type of equations are equivalent to (possibly nonlinear) Fokker–Planck equations and Schrödinger type equations [189, §4.9]. Ideally, for both theoretical and practical purposes, we would like to have $\mathfrak{L}$ diagonal with respect to the associated orthogonal polynominal basis $\{p_n\}$. Unfortunately, it is established [20, 21, 22, 174] that this only occurs if the p_n's belong to a classical family, suggesting that working with respect to non-classical weights is much more intricate.

Taking inspiration from this functional analytic theory, in this work, we overcome the apparent hurdles of working with non-classical orthogonal polynomials, and show that it is in fact possible to effectively solve some differential equations with respect to non-classical weights [171], numerically but also rigorously.

3.1.1 A natural Sobolev Hilbert structure

A first problem arising in the numerical treatment of differential equations on weighted Sobolev spaces is that it is not so immediate that there exists a natural complete inner product, i.e. a natural Hilbert structure on such spaces. For instance, on bounded domains with appropriate boundary conditions (say Dirichlet), the simple norm induced by $\langle \nabla \cdot, \nabla \cdot \rangle$ defines a natural Hilbert structure. This simplifies the tackling of problems with Finite Elements, Chebyshev or Fourier bases. However, on weighted Sobolev spaces on unbounded domains, this inner product does not define a complete topology, essentially because there does not hold a classical Poincaré inequality, i.e. there does not exist $C_P > 0$ such that

$$\int_{\mathbb{R}} u^2 \mathrm{d}\nu \leq C_P \int_{\mathbb{R}} (u')^2 \mathrm{d}\nu \qquad \text{for all } u \in H^1(\nu).$$

However, a fundamental tool in the analysis of weighted Sobolev spaces [48] is that there often holds a modified Poincaré inequality on $H^1(\nu)$: there exists $C_P > 0$ such that

$$\int_{\mathbb{R}} u^2 \mathrm{d}\nu - \left(\int_{\mathbb{R}} u \mathrm{d}\nu \right)^2 \leq C_P \int_{\mathbb{R}} (u')^2 \mathrm{d}\nu \qquad \text{for all } u \in H^1(\nu). \tag{3.2}$$

From now on, we will simply refer to (3.2) as the Poincaré inequality on $H^1(\nu)$. It allows us to immediately give a natural inner product on $H^1(\nu)$

$$(u, v) := \int_{\mathbb{R}} u'v' \mathrm{d}\nu + \int_{\mathbb{R}} u \mathrm{d}\nu \int_{\mathbb{R}} v \mathrm{d}\nu, \tag{3.3}$$

whose induced norm (henceforth denoted $\| \cdot \|_{H^1(\nu)}$) can be shown to be Lipschitz equivalent to the standard norm on $H^1(\nu)$; demonstrating that $(H^1(\nu), (\cdot, \cdot))$ is indeed a Hilbert space.

While this new inner product may appear "unusual" at first sight, it is actually very natural; for instance, it reduces to the inner product $\langle \partial_x \cdot, \partial_x \cdot \rangle$ on the subspace of ν-mean zero functions of $H^1(\nu)$. Furthermore, it allows us to propose a natural solution to the problem of the construction of orthogonal polynomials $\mathcal{Q} = \{q_n\}_{n \in \mathbb{N}}$ on a non-classical Sobolev space $H^1(\nu)$.

Proposition 3.1. For all $n \geq 1$, the polynomials $\mathcal{Q} = \{q_n\}_{n\in\mathbb{N}}$ orthonormal with respect to $(\cdot,\cdot)$ are uniquely defined by the properties

$$q_n' = p_{n-1} \qquad \text{and} \qquad \int_{\mathbb{R}} q_n \mathrm{d}\nu = 0.$$

Proof. It suffices to check that these are orthonormal with respect to $(\cdot,\cdot)$, the uniqueness (up to sign) follows from the Gram–Schmidt algorithm. □

Note that the q_n's do not *scricto sensu* fall under the usual construction of orthogonal polynomials on a Sobolev space [5, 169, 170, 172, 213] which should be induced by an inner product of the type

$$\int_{\mathbb{R}} uv\mathrm{d}\nu_0 + \int_{\mathbb{R}} u'v'\mathrm{d}\nu_1 \qquad \text{for some Borel measures } \nu_0, \nu_1. \tag{3.4}$$

However, from now on, we will refer to the basis $\mathcal{Q} = \{q_n\}_{n\in\mathbb{N}}$ associated to the scalar product (3.3) as *Sobolev orthogonal polynomials*. There is a vast literature on polynomials orthogonal with respect to an inner product of the form (3.4) (See [169, 170, 172, 213] and references therein). Particularly when considering non-classical weights, the construction from (3.4) encounters several difficulties:

- A serious issue is that many of the particular cases of (3.4) studied in the literature (e.g. taking ν_1 to be some discrete measure) do not necessarily induce a meaningful Sobolev topology.
- Barring some special cases, the construction of such orthogonal basis is typically very involved [170, 213].
- They are often not practical in the Numerical Analysis of differential equations, which should be their main purpose (See [170, §12] for a discussion).

In some sense, our approach is more topological and directly inspired from the Functional Analysis of weighted Sobolev spaces. Proposition 3.1 shows that the q_n's can be indeed simply obtained by integrating the p_n's which is a natural (maybe naive) first approach when considering this problem. For instance, in the semi-classical setting [171] of V being a even polynomial, we will see that the q_n's can be inexpensively evaluated from the p_n's via the resolution of a banded triangular linear system.

More than that, we will show that they are quite useful in the Numerical Analysis of differential equations on weighted Sobolev spaces.

Example 3.2. Consider the case of the Gaussian measure, i.e. $V(x) = x^2/2$ such that $\nu(\mathrm{d}x) = e^{-x^2/2}\mathrm{d}x/\sqrt{2\pi}$. Then ∂_x acts very simply on the basis $\{p_n\}$, namely $p_n' = \sqrt{n}\, p_{n-1}$ for all $n \geq 1$ and therefore $q_n = p_n/\sqrt{n}$ for $n \geq 1$: in that case, the Sobolev orthonormal polynomials are simply renormalized classical orthogonal polynomials. However, we emphasize that, in general, q_n need not be proportional to p_n, and indeed this will not be the case in the main example considered in this chapter, as we have to work with non-classical weights.

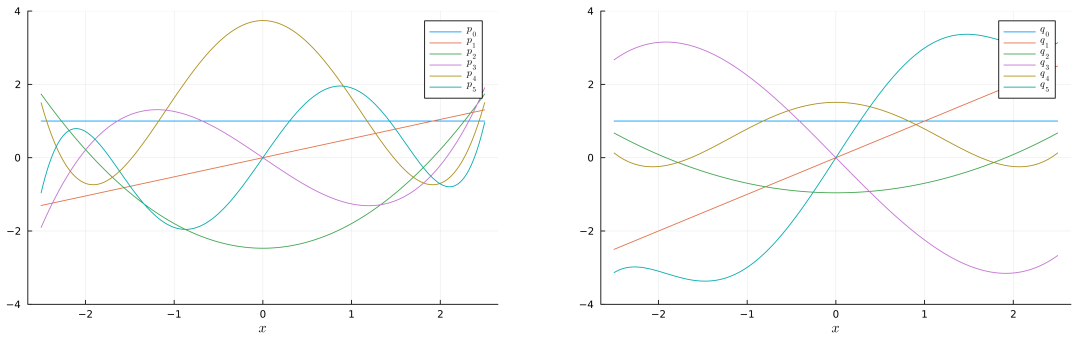
3.1.2 A Numerical-Functional Analysis of Freud-weighted Sobolev spaces

While our approach may agree on classical settings, as previously mentioned, we are mainly interested in problems outside of these families. A natural example to consider is the case of *Freud-*

weighted spaces associated with a quartic (or double-well) potential

$$V(x) = \frac{x^4}{4} - \kappa\frac{x^2}{2}, \qquad \kappa \in \mathbb{R},$$

as the first step departing from the classical paradigm. We will show that this already leads to a rich theory bringing together several ideas in Numerical and Functional Analysis.



(a) $p_1, \dots p_5$ orthonormal with respect to $\langle \cdot, \cdot \rangle$ (b) $q_1, \dots q_5$ orthonormal with respect to $(\cdot, \cdot)$

Figure 3.1: Plots of orthonormal polynomials with respect to $\nu(\mathrm{d}x) = e^{-V(x)}\mathrm{d}x/Z$ with $V(x) = x^4/4 - \kappa x^2/2$ with $\kappa = 4$.

In this context, the operator $\mathfrak{L} = -\partial_{xx} + V'\partial_x$ of Eq. (3.1) becomes

$$\mathfrak{L} = (x^3 - \kappa x)\partial_x - \partial_{xx}.$$

Note that this operator or very closely related operators are of importance as they appear in the probabilistic treatment of several models of *noise-induced phenomena* in Random Dynamics such as:

- the stochastic resonance phenomenon for the noisy Duffing oscillator [76, 104, 189] or Benzi–Parisi–Sutera–Vulpiani model [35] (which we will soon be able to quantify rigorously),
- the Hopf bifurcation with additive noise [24, 55, 94, 73],
- the Desai–Zwantig model [93],
- the (non)-destruction of the pitchfork bifurcation by additive noise [68, 87]. See also [38] for a recent example where our methods could be applied.

Our approach relies on exploiting the structure of the bidiagonal differentiation operator with respect to the bases $\{p_n\}$ and $\{q_n\}$ to give a thorough and precise Numerical and Functional Analysis of the Sobolev space $H^1(\nu)$. Our techniques are to be put in perspective with the related work [56].

For instance, our method allows us to compute the optimal Poincaré inequality constant C_P on $H^1(\nu)$ [48]. Note that, in general, even giving a non-sharp upper bound on C_P is not trivial [20, 43, 48, 50, 146, 223] especially when V is not convex (which can be the case here depending on the value of κ). In contrast, in this particular case, we can give a very tight enclosure for C_P.

Theorem 3.3. Consider $V(x) = x^4/4 - \kappa x^2/2$ with $\kappa = 4$, the best Poincaré inequality constant

C_P in (3.2) is given by

$$C_P = 33.58004242 \pm 2.3 \times 10^{-7}. \tag{3.5}$$

In fact, we can do much better by rigorously proving and quantifying the compactness of the embedding $H^1(\nu) \hookrightarrow L^2(\nu)$, a rare occurrence in Numerical Analysis.

Theorem 3.4. Consider $V(x) = x^4/4 - \kappa x^2/2$, then there exist constructible $C > 0$ and $N \in \mathbb{N}$ such that for all $m \geq N$ and $u \in \overline{\text{Span}\{q_j\}_{j>m}}^{H^1(\nu)}$

$$\|u\|_{L^2(\nu)} \leq \frac{C}{m^{3/4}} \|u\|_{H^1(\nu)}. \tag{3.6}$$

In particular, if $\kappa = 4$, the above holds for $C = 1.2233$ and $N = 2,187$.

It is well-established [3, 60, 70, 81, 111, 180] that such kind of estimates are useful in the numerical resolution of partial differential equations (PDEs), as they constitute a key ingredient to show the convergence of spectral methods. To the best of our knowledge, this is the first derivation of such compactness estimate in a non-classical setting. Indeed, while in classical polynomial settings, these estimates can be obtained trivially from a diagonal differentiation operator (e.g. see Example 3.13) or a well-structured integration operator (e.g. in Chebyshev [163]), much work is needed to obtain Theorem 3.4.

Remark 3.5. Note that this embedding is "more compact" than the known Hermite/Gaussian embedding $H^1(e^{-x^2/2}/\sqrt{2\pi}) \hookrightarrow L^2(e^{-x^2/2}/\sqrt{2\pi})$ which only decays like $1/\sqrt{n}$ (See Example 3.13). This agrees with our expectation that the compactness of the embedding $H^1(\nu) \hookrightarrow L^2(\nu)$ should get better as the potential V is more confining (i.e. as V grows faster, see also Conjecture 3.10).

Brought together, these insights allow for the resolution of new differential equations in a natural and mathematically rigorous framework, using the topology of Freud-weighted spaces and using Sobolev orthogonal polynomials. To showcase that our approach does indeed provide an excellent numerical framework beyond numerical experiments, we incorporate our estimates into computer-assisted proofs (CAPs) to provide some *rigorous* bounds on our numerical approximations, proving the *existence* of a nearby solution.

We first consider the Gross–Pitaevskii equation with sextic potential

$$i\partial_t v = -\partial_{xx} v + W(x)v + |v|^2 v, \tag{3.7}$$

where $W(x) = x^6/4 - \kappa x^4/2 + cx^2 + d$. We look for standing wave solutions $v(t,x) = e^{i\omega t}\varphi(x)$ of Eq. (3.7) where φ satisfies the elliptic semilinear equation

$$-\partial_{xx}\varphi + W(x)\varphi + \varphi^3 = \omega\varphi \tag{3.8}$$

which can be reformulated as an equation of the form 3.1. Within our framework which makes use of Sobolev orthgonal polynomials and estimates such as (3.6), we not only obtain accurate approximate solutions to this equation plotted in Figures 1.3 and 3.2, but also prove the existence of *true* solutions of Eq. (3.8) nearby. The very small error bounds obtained below showcase that using Sobolev orthogonal polynomials to numerically solve such equations leads to very efficient numerical methods.

In addition to Theorem 1.9, we have the following.

Theorem 3.6. Let $c = 5/2$, $d = 2$, $\kappa = 4$, $\omega = 8$ and $\bar{\varphi}_2 : \mathbb{R} \to \mathbb{R}$ be the function whose restriction to the interval $[-5, 5]$ is depicted in Figure 3.2, and whose precise description is available at [79] in the file `GP_eq/ubar2`. There exists an even solution $\varphi_2^\star \in H^1(\mathbb{R})$ to Eq. (3.8) such that

$$\|\varphi_2^\star - \bar{\varphi}_2\|_{H^1(\mathbb{R})} \leq 8.64 \times 10^{-141},$$

where $\|\cdot\|_{H^1(\mathbb{R})}$ is the standard H^1-norm on $\mathbb{R}$ equipped with the Lebesgue measure $\mathrm{d}x$, i.e. $\|\varphi\|_{H^1(\mathbb{R})} = \left(\int_{\mathbb{R}} \varphi^2 \mathrm{d}x + \int_{\mathbb{R}} (\varphi')^2 \mathrm{d}x\right)^{1/2}$.

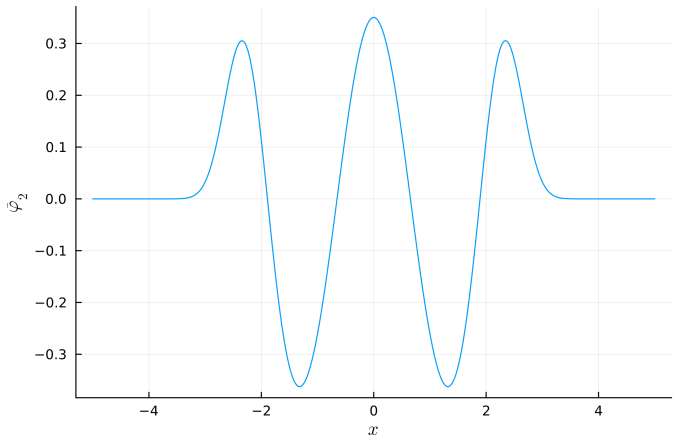


Figure 3.2: Plot of a numerical solution $\bar{\varphi}_2$ to Eq. (1.39) with $c = 5/2$, $d = 2$, $\kappa = 4$ and $\omega = 8$.

Computer-assisted proofs have become more and more common in the study of differential equations, and we refer to the expository article [219], the surveys [124, 147] the books [181, 212] and the references therein for an overview of the field. A the notable feature of the computer-assisted proofs performed in this work is that they deal with problems on unbounded domains, for which fewer techniques are available (See [181, Part II], and the more recent [218, 53, 66]). Our proofs belong to the family of CAPs based on spectral methods, but with the unusual twist that we work between two different bases $\{p_n\}$ and $\{q_n\}$. Moreover, the dominant operator $\mathfrak{L}$ is not going to be diagonal but merely bidiagonal or tridiagonal in these bases, which means we have to resort to some of the tools developed in [56] in order to control its inverse. Furthermore, contrary to usual computer-assisted proofs, the formulae for the representations of our differential operators are not known explicitly in closed form and their coefficients are actually challenging to control.

3.1.3 A differential counterpart to Freud's conjecture

We recall that any family of orthogonal polynomials associated to a positive weight function satisfies a three-term recurrence relation. When the weight function is even, this recurrence relation simplifies to

$$x p_n = a_{n+1} p_{n+1} + a_n p_{n-1}, \qquad n \geq 1, \tag{3.9}$$

where the coefficients a_n are positive and $a_0 = 0$. To any even potential V, we can therefore associate a unique (positive) sequence $(a_n)_{n\geq 0}$ satisfying (3.9), with $a_0 = 0$. Under the hood, the proofs of Theorems 3.3 and 3.4 (and ultimately Theorems 1.9 and 3.6) rely crucially on quantifying *explicitly* the asymptotic growth of the positive sequence $(a_n)_{n\geq 0}$ satisfying (3.9). This can be accomplished by first deriving a recurrence relation satisfied by the coefficients a_n themselves. For

instance, in the case, where V is polynomial, we have the following.

Lemma 3.7. There exists a *computable* set of homogeneous polynomials $\left\{R_j : \mathbb{R}^{2j-1} \to \mathbb{R}\right\}_{j=1}^{\infty}$ having positive integer coefficients and with $\deg R_j = j-1$ such that, for every $k \in \mathbb{N}^*$ and every even polynomial potential $V(x) = \sum_{j=1}^{k} c_j \frac{x^{2j}}{2j}$, the positive sequence $(b_n)_{n\in\mathbb{N}} = (a_n^2)_{n\in\mathbb{N}}$ satisfies the recurrence relation

$$\frac{n}{b_n} = \sum_{j=1}^{k} c_j R_j(b_{n-j}, \dots, b_n, \dots, b_{n+j}), \tag{3.10}$$

where $(a_n)_{n\in\mathbb{N}}$ is the sequence associated to V via (3.23).

Proof. See Remark 3.30. □

In our case of the quartic potential $V(x) = x^4/4 - \kappa x^2/2$, we have that $R_1 = 1$ and $R_2(x_{-1}, x_0, x_1) = x_{-1} + x_0 + x_1$ such that $(b_n)_{n\in\mathbb{N}} = (a_n^2)_{n\in\mathbb{N}}$ is the (unique) positive solution to the recurrence relation

$$\frac{n}{b_n} = b_{n-1} + b_n + b_{n+1} - \kappa, \qquad n \geq 1, \tag{3.11}$$

which is known as the *discrete Painlevé I equation* (See also [47]). From (3.11), one expects that $b_n \sim \sqrt{n}/\sqrt{3}$. However, (3.11) has high sensitivity on initial conditions and we furthermore require a tight quantitative control on the b_n's. We achieve this control via computer assistance which gives a substantial improvement on previous non-constructive approaches [4, 82, 108, 130, 164, 183] which could not in general produce rigorous estimates such as the one below. Our work establishes an important connection between the said Freud's conjecture and the compact embedding of weighted Sobolev spaces previously established (in a non-quantitative manner) by probability theorists [19, 20].

Proposition 3.8. Let $(b_n)_{n\in\mathbb{N}}$ be the unique positive solution to the recurrence relation (3.11). For all $c^- < 1$ and $c^+ > 1$, there exists $N \in \mathbb{N}$ such that for all $n \geq N$

$$c^- \frac{\sqrt{n}}{\sqrt{3}} \leq b_n \leq c^+ \frac{\sqrt{n}}{\sqrt{3}}. \tag{3.12}$$

In particular, if $\kappa = 4$, $c^- = 0.987$ and $c^+ = 1.025$, the above holds for $N = 2,187$.

Proposition 3.9 (A particular case of Freud's conjecture)**.** Let $V(x) = x^{2k}/(2k) + O(x^{2k})$ be an even polynomial potential of degree $2k$, then we have the following growth for the positive sequence $(b_n)_{n\in\mathbb{N}} = (a_n^2)_{n\in\mathbb{N}}$ defined by (3.9)

$$b_n \sim n^{\frac{1}{k}} \begin{pmatrix} 2k-1 \\ k \end{pmatrix}^{-\frac{1}{k}}. \tag{3.13}$$

Proof. See [91]. □

For instance, this conjecture is proved in the case $V(x) = x^{2k}/(2k)$ [166]. This allows us in turn to speculate the following on the compactness of the embedding $H^1(\nu) \hookrightarrow L^2(\nu)$.

Conjecture 3.10. Let $V(x) = x^{2k}/(2k) + O(x^{2k})$ be an even polynomial potential of degree $2k$ and denote by $\{q_n\}_{n\in\mathbb{N}}$ the Sobolev orthogonal polynomials with respect to $\mathrm{d}\nu = e^{-V}\mathrm{d}x/Z$. Then

there exist constructible $C > 0$ and $N \in \mathbb{N}$ such that for all $m \geq N$ and $u \in \overline{\mathrm{Span}\{q_j\}_{j>m}}^{H^1(\nu)}$

$$\|u\|_{L^2(\nu)} \leq \frac{C}{m^{\frac{2k-1}{2k}}} \|u\|_{H^1(\nu)}. \tag{3.14}$$

Heuristics. On $H^1(\nu)$, taking a derivative is essentially equivalent to multiplying by V' in the sense that they induce the same loss of regularity (they both send $H^1(\nu)$ to $L^2(\nu)$). This will be discussed further and more precisely in the subsequent sections, see in particular Remark 3.28. Since V' is of degree $(2k-1)$ and equivalent to x^{2k-1} at infinity, multiplying by V' essentially amounts to multiplying by x $(2k-1)$ times, i.e. applying $(2k-1)$ times the recurrence relation (3.9). Therefore, using (3.13) and ignoring multiplicative constants, we expect to have

$$\|p_n\|_{H^1(\nu)} = \|p_n'\|_{L^2(\nu)} \gtrsim \|V' p_n\|_{L^2(\nu)} \gtrsim \|x^{2k-1} p_n\|_{L^2(\nu)} \gtrsim \|a_n^{2k-1} p_n\|_{L^2(\nu)} \gtrsim n^{\frac{2k-1}{2k}} \|p_n\|_{L^2(\nu)}$$

This yields the proposed compactness estimate (3.14). □

Remark 3.11. Note that (3.14) is known to hold for $k = 1$ (See example 3.13), and that we prove the case $k = 2$ with Theorem 3.4. On the other hand, as $k \to \infty$ then $\exp(-x^{2k}/(2k)) \to \mathbb{1}_{[-1,1]}$, such that the asymptotic of (3.14) as $k \to \infty$ agrees with the compactness on the embedding $H^1([-1,1]) \hookrightarrow L^2([-1,1])$ which decays like $1/m$.

Organisation of the chapter

The remainder of the chapter is organised as follows. In Section 3.2, we first recall some results about weighted Sobolev spaces and Poincaré inequalities, and then discuss our construction of Sobolev orthogonal polynomials and the structure of operators with respect to orthogonal polynomial bases. Building on these insights, we focus in Section 3.3 on the case of the quartic potential $V(x) = x^4/4 - \kappa x^2/2$, and prove embedding estimates for $H^1(\nu) \hookrightarrow L^2(\nu)$, i.e. Theorems 3.3 and 3.4, as well as Proposition 3.8 on which they rely crucially. In Section 3.4, we apply these estimates to solve the Gross–Pitaevskii equation with sextic potential and prove Theorems 1.9 and 3.6.

3.2 Weighted Sobolev spaces

3.2.1 The Functional Analytic point of view

The present work is motivated by the study of the overdamped Langevin (or Smoluchowski) dynamics

$$\mathrm{d}X_t = -V'(X_t)\mathrm{d}t + \sqrt{2}\mathrm{d}B_t, \tag{3.15}$$

for a potential $V \in \mathcal{C}^2(\mathbb{R})$ which induce a reversible diffusion process $(X_t)_{t\geq 0}$ with stationary probability (Gibbs) measure

$$\nu(\mathrm{d}x) = \frac{e^{-V(x)}}{Z}\mathrm{d}x \qquad Z = \int_{\mathbb{R}} e^{-V}\mathrm{d}x,$$

where V and ν will always be of this form unless stated otherwise. The Markov semi-group $(T_t)_{t\geq 0}$ of $(X_t)_{t\geq 0}$ is generated by $-\mathfrak{L}$, where

$$\mathfrak{L} = V'(x)\partial_x - \partial_{xx}$$

is a positive self-adjoint operator with respect to the L^2-inner product $\langle\cdot,\cdot\rangle$. Indeed, by parts, one has that

$$\langle u, \mathfrak{L}v\rangle = \int_{\mathbb{R}} u(\mathfrak{L}v)\mathrm{d}\nu = \int_{\mathbb{R}} u'v'\mathrm{d}\nu = \int_{\mathbb{R}} (\mathfrak{L}u)v\mathrm{d}\nu = \langle \mathfrak{L}u, v\rangle, \qquad \text{for all } u, v \in H^1(\nu), \tag{3.16}$$

which can thus also be written as a Dirichlet form. An accessible introduction to this theory can be found in [189, §4] (See also [48] for a nice introduction to Poincaré inequalities) but we emphasize that various aspects of this theory can be generalised [19, 20], to higher dimensions and to various geometries.

Much of this theory relies on the following Poincaré inequality on $H^1(\nu)$, i.e. on the existence of a constant $C_P > 0$ such that for all $u \in H^1(\nu)$,

$$\int_{\mathbb{R}} u^2\mathrm{d}\nu - \left(\int_{\mathbb{R}} u\mathrm{d}\nu\right)^2 \leq C_P \int_{\mathbb{R}} (u')^2\mathrm{d}\nu. \tag{3.17}$$

For instance [189, Theorem 4.4], such Poincaré inequality immediately implies the exponential ergodicity of the process $(X_t)_{t\geq 0}$ evolving under (3.15). A criterion for the Poincaré inequality (3.17) to hold and which will be sufficient for our purposes is given by the following proposition. See [48] for various functional analytic aspects related to this Poincaré inequality.

Proposition 3.12. Suppose that the potential V is such that

$$\lim_{x\to\pm\infty} \frac{(V'(x))^2}{2} - V''(x) = +\infty,$$

then there holds a Poincaré inequality of the form (3.17) on $H^1(\nu) = H^1(e^{-V}/Z)$.

Proof. See [224, Theorem A.1]. □

This criterion essentially amounts to V having to grow faster than linearly at infinity. Note that a more sophisticated way to verify the Poincaré inequality is via the Muckenhoupt criterion [20, Theorem 4.5.1] which is actually an equivalent statement and gives (large) bounds on the optimal Poincaré constant C_P (See also [224, §A.19]).

Example 3.13. Consider the case of the Gaussian measure, i.e. $V(x) = x^2/2$ such that $\nu(\mathrm{d}x) = e^{-x^2/2}\mathrm{d}x/\sqrt{\pi}$. Then, we have the following Poincaré inequality, for all $u \in H^1(\nu)$,

$$\int_{\mathbb{R}} u^2\mathrm{d}\nu - \left(\int_{\mathbb{R}} u\mathrm{d}\nu\right)^2 \leq \int_{\mathbb{R}} (u')^2\mathrm{d}\nu.$$

This is easily shown by decomposing u in terms of the orthonormal Hermite polynomials $\mathcal{P} = \{p_n\}_{n\in\mathbb{N}}$ [1, §22]. One can actually improve this further and obtain the compactness estimates

$$\|u\|_{L^2(\nu)} \leq \frac{1}{\sqrt{n}}\|u\|_{H^1(\nu)},$$

for all $u \in \overline{\mathrm{Span}\{p_m\}_{m\geq n}}^{H^1(\nu)}$.

The Hermite case is actually one of the few settings for which such constructive compactness estimates have so far been able to be proved. This stems from the diagonal nature of the operator ∂_x when represented with respect to $\mathcal{P}$ (See [21, 22, 174]). This is a shame, as from the probability theoretic point of view, the Hermite case (associated to the so-called Ornstein–Uhlenbeck process) is a limiting in the classification of diffusion semi-groups generated by $-\mathfrak{L}$ and associated to ν (See [20, §7.7] for a discussion, see also [19, 149]).

However, the embedding $H^1(\nu) \hookrightarrow L^2(\nu)$ is known to be compact (without quantitative estimates) in a much broader setting.

Theorem 3.14. Let $V(x) = x^{2k}/(2k) + O(x^{2k})$ be a polynomial potential such that $k \geq 1$, then $H^1(\nu) = H^1(e^{-V}/Z)$ is compactly embedded in $L^2(\nu)$.

Proof. The case $k = 1$ follows from Example 3.13. The case $k > 1$, it suffices to check that V satisfies the assumptions of [149, Theorem 1.4] which implies the compactness of the embedding $H^1(\nu) \hookrightarrow L^2(\nu)$ by [20, Theorem 6.4.2]. This last theorem (which is non constructive) relies on the fact that if $k > 1$, the semi-group $(T_t)_{t\geq 0}$ is "ultracontractive" (the property that T_t sends a function $u \in L^1(\nu)$ to $T_t u \in L^\infty(\mathbb{R})$ for all $t > 0$ and in particular is associated to a L^∞-kernel representation for $t > 0$). □

As stated in Conjecture 3.10, we expect that if $V(x) \sim |x|^p$ as $x \to \infty$ for $p \in (1, \infty)$, then the embeddings should get quantitatively better as p increases. We note that in the limiting case $p = 1$, while the Poincaré inequality (3.17) holds, the embedding $H^1(\nu) \hookrightarrow L^2(\nu)$ does not (See [20, §4.4.1]).

Finally, we emphasize that, once the Poincaré inequality (3.17) is available, all the Functional Analysis on $H^1(\nu)$ is reduced to textbook analysis of elliptic PDEs on Hilbert spaces [61, 103]. For instance, concerning the well-posedness of

$$\mathfrak{L}u = g, \qquad \int_{\mathbb{R}} g \mathrm{d}\nu = 0,$$

we have the following the weak formulation given by Proposition 1.6. Similarly, $\mathfrak{L}$ has positive unbounded discrete spectrum, etc.

3.2.2 Sobolev orthogonal polynomials

A problem naturally arising in Numerical Analysis is the construction of *Sobolev orthonormal polynomials* on the Sobolev space $H^1(\nu)$ and their use in the resolution of partial differential equations [170]. A first approach could consist in using the standard inner product on $H^1(\nu)$:

$$\int_{\mathbb{R}} u'v' \mathrm{d}\nu + \Lambda \int_{\mathbb{R}} uv \mathrm{d}\nu \qquad u, v \in H^1(\nu),\ \Lambda > 0,$$

which is a specific instance of (3.4). However, orthogonal polynomials generated with such inner product have not been very successul in the Numerical Analysis of PDEs. In particular, these polynomials have not achieved the quantification of compactness between weighted Sobolev spaces, in non-classical settings. Furthermore, even the construction of such basis is not necessarily simple;

showing that in some sense the above inner product is not the "correct" choice. In particular, it is unclear what value of Λ should be chosen, as each one gives rise to a different basis of orthonormal polynomials (even up to rescaling).

To construct a natural basis of Sobolev orthonormal polynomials, we propose to instead use the Poincaré inequality on $H^1(\nu)$.

Theorem 3.15. Suppose that ν is a probability measure such that on $H^1(\nu)$, there holds a Poincaré inequality, i.e. there exists a constant $C_P > 0$ such that for all $u \in H^1(\nu)$

$$\mathrm{Var}_\nu(u) = \int_{\mathbb{R}} u^2 \mathrm{d}\nu - \left(\int_{\mathbb{R}} u \mathrm{d}\nu \right)^2 \leq C_P \int_{\mathbb{R}} (u')^2 \mathrm{d}\nu. \tag{3.18}$$

Then the inner product $(\cdot, \cdot)$ defined by

$$(u, v) = \int_{\mathbb{R}} u'v' \mathrm{d}\nu + \int_{\mathbb{R}} u \mathrm{d}\nu \int_{\mathbb{R}} v \mathrm{d}\nu \qquad u, v \in H^1(\nu)$$

defines a Hilbert structure on $H^1(\nu)$ inducing its topology. In particular, $H^1(\nu)$ is complete under the induced norm $\| \cdot \|_{H^1(\nu)} := \sqrt{(\cdot, \cdot)}$.

Proof. Verifying that $(\cdot, \cdot)$ is indeed an inner product is straightforward. In particular, if $(u, u) = 0$, then

$$\int_{\mathbb{R}} (u')^2 \mathrm{d}\nu = 0 \qquad \text{and} \qquad \left(\int_{\mathbb{R}} u \mathrm{d}\nu \right)^2 = 0.$$

The first inequality implies that u' is identically zero such that u is constant. Then, the second equality in turn implies that u is identically zero, proving the positive-definiteness. Now, let us show that the induced norm $\| \cdot \|_{H^1(\nu)} := \sqrt{(\cdot, \cdot)}$ is Lipschitz-equivalent to the standard Sobolev $H^1(\nu)$-norm defined by

$$\left(\int_{\mathbb{R}} (u')^2 \mathrm{d}\nu + \int_{\mathbb{R}} u^2 \mathrm{d}\nu \right)^{1/2} \qquad u \in H^1(\nu).$$

The fact that $\| \cdot \|_{H^1(\nu)}$ is dominated by the standard Sobolev $H^1(\nu)$-norm is a direct consequence of the Cauchy–Schwarz inequality (or Jensen's inequality or that the variance is positive). Now for the other direction, the Poincaré inequality (3.18) shows that

$$\|u\|^2_{L^2(\nu)} = \langle u, u \rangle = \int u^2 \mathrm{d}\nu \leq \max(1, C_P) \left\{ \int_R (u')^2 \mathrm{d}\nu + \left(\int_{\mathbb{R}} u \mathrm{d}\nu \right)^2 \right\} = \max(1, C_P) \|u\|^2_{H^1(\nu)}.$$

Since, it is clear that for $u \in H^1(\nu)$, $\langle u', u' \rangle \leq \|u\|^2_{H^1(\nu)}$, this finishes the proof. □

Remark 3.16. On the space of mean-zero functions

$$H^1_0(\nu) := \left\{ u \in H^1(\nu) \middle| \int_{\mathbb{R}} u \mathrm{d}\nu = 0 \right\},$$

the standard Poincaré inequality

$$\int_{\mathbb{R}} u^2 \mathrm{d}\nu \leq C_P \int_{\mathbb{R}} (u')^2 \mathrm{d}\nu. \tag{3.19}$$

holds, it is actually equivalent to (3.18).

After identifying that $q_0 = p_0 = 1$, one can thus think of the construction of the mean-zero Sobolev orthonormal polynomials $\{q_n\}_{n=1}^{\infty}$ as the orthogonalisation of the basis $\{p_n\}_{n=1}^{\infty}$ of $H_0^1(\nu)$ with respect to the inner product

$$\int_{\mathbb{R}} u'v' \mathrm{d}\nu, \qquad \text{for } u, v \in H_0^1(\nu),$$

which is another way to show Proposition 3.1, i.e.

$$q_n' = p_{n-1} \qquad \text{and} \qquad \int_{\mathbb{R}} q_n \mathrm{d}\nu = 0.$$

Remark 3.17. Note that, up to normalisation, the q_n's do not depend on any possible additional weighting coefficients Λ_1 and Λ_2 that could be appended to form an inner product of the form

$$\Lambda_1 \int_{\mathbb{R}} u'v' \mathrm{d}\nu + \Lambda_2 \int_{\mathbb{R}} u \mathrm{d}\nu \int_{\mathbb{R}} v \mathrm{d}\nu \qquad u, v \in H^1(\nu).$$

Remark 3.18. Note that in the case $V(x) = x^4/4$, our Freud–Sobolev orthogonal polynomials are different to the ones obtained in [119], which do not actually correspond to the $H^1(e^{-V}/Z)$-topology.

Some examples outside of our setting

The main focus of this chapter is on measures of the form $\nu(\mathrm{d}x) = e^{-V}\mathrm{d}x/Z$ supported on the whole real line. However, even for different measures, our construction of Sobolev orthogonal polynomials can be used as soon as a form of Poincaré inequality is at hand, and in some specific cases it produces back classical orthogonal polynomials.

Example 3.19 (The Legendre case)**.** Consider $\mathrm{d}\nu = \mathrm{d}x/2$ on $[-1, 1]$, where the orthonormal polynomials are the Legendre polynomials [1, §22]. While this example does not sit within the general setting of this chapter, it satisfies the assumptions of Theorem 3.15. Indeed on $H^1(\nu)$, we have the Poincaré–Wirtinger inequality [103, §5.8.1] (See also [20, §4.5.2])

$$\int_{-1}^{1} u^2 \mathrm{d}\nu - \left(\int_{-1}^{1} u \mathrm{d}\nu\right)^2 \leq C_P \int_{-1}^{1} (u')^2 \mathrm{d}\nu, \qquad C_P = \frac{4}{\pi^2}.$$

The Sobolev orthogonal polynomials q_n associated to the scalar product (3.3) are then given by

$$q_0 = 1, \qquad q_1 = \frac{p_1}{\sqrt{3}}, \qquad q_2 = \frac{p_2}{\sqrt{15}}, \qquad q_n = \frac{1}{\sqrt{2n-1}}\left(\frac{p_n}{\sqrt{2n+1}} - \frac{p_{n-2}}{\sqrt{2n-3}}\right) \quad \text{for } n \geq 3.$$

Note that $q_n(-1) = q_n(1) = 0$ for all $n \geq 3$, which furthermore shows that the q_n's cannot simply be some (even rescaled) Jacobi polynomials, as those have interlacing zeros in (-1,1). For for $n \geq 3$, the q_n's in fact coincide with some so-called Legendre associated polynomials [1, §8], which are the natural extension of the Jacobi polynomials at the parameters $\alpha = \beta = -1$.

Note that it might sometimes be more natural to construct H^1-Sobolev orthogonal polynomials

$\{q_n\}_{n\in\mathbb{N}}$ with respect to an inner product with two different measures ν and $\tilde{\nu}$

$$\int_{\mathbb{R}} u'v'\mathrm{d}\nu + \int_{\mathbb{R}} u\mathrm{d}\tilde{\nu}\int_{\mathbb{R}} v\mathrm{d}\tilde{\nu}, \tag{3.20}$$

which extends our construction of Sobolev orthogonal polynomials naturally. For instance, in the case of beta distributions we have the following.

Example 3.20 (The Jacobi family)**.** Let $\alpha,\beta>0$ and denote $\nu_{\alpha,\beta}(\mathrm{d}x)=(1-x)^{\alpha}(1+x)^{\beta}\mathrm{d}x/Z_{\alpha,\beta}$ on $[-1,1]$, for which the p_n's are Jacobi polynomials of parameter (α,β) [1, §22]. Then, on $H^1(\nu_{\alpha,\beta})\cap L^2(\nu_{\alpha-1,\beta-1})$, there holds a Poincaré inequality

$$\int_{-1}^{1} u^2\mathrm{d}\nu_{\alpha-1,\beta-1} - \left(\int_{-1}^{1} u\mathrm{d}\nu_{\alpha-1,\beta-1}\right)^2 \leq C_P\int_{-1}^{1}(u')^2\mathrm{d}\nu_{\alpha,\beta}, \qquad C_P=\alpha+\beta.$$

See [20, §2.7.4] for more details about the associated semi-group. Then the q_n's associated to the inner product (3.20) (with $\nu=\nu_{\alpha,\beta}$ and $\tilde{\nu}=\nu_{\alpha-1,\beta-1}$) are nothing but the (rescaled) Jacobi polynomials associated to $\nu_{\alpha-1,\beta-1}$. Observe that the Legendre-Sobolev polynomials on $H^1(\nu_{0,0})$ (Example 3.19), cannot be constructed via this inner product as we require $\alpha,\beta>0$.

Similarly, concerning the gamma distributions, we have the following.

Example 3.21 (The Laguerre family)**.** For $\alpha>-1$, denote $\nu_\alpha=x^\alpha e^{-x}\mathrm{d}x/Z_\alpha$ on $\mathbb{R}_+=[0,\infty)$ such that the p_n's are orthonormal Laguerre polynomials of parameter α [1, §22].

- If $\alpha>0$, on $H^1(\nu_\alpha)\cap L^2(\nu_{\alpha-1})$, we have the Poincaré inequality [20, §4.4.1]

  $$\int_0^{\infty} u^2\mathrm{d}\nu_{\alpha-1} - \left(\int_0^{\infty} u\mathrm{d}\nu_{\alpha-1}\right)^2 \leq \int_0^{\infty}(u')^2\mathrm{d}\nu_\alpha,$$

  such that the q_n's associated to the inner product (3.20) (with $\nu=\nu_\alpha$ and $\tilde{\nu}=\nu_{\alpha-1}$) are (rescaled) Laguerre polynomials of parameter $(\alpha-1)$.

- In the case $\alpha=0$, we have the Poincaré inequality [20, §4.4.1]

  $$\int_0^{\infty} u^2\mathrm{d}\nu_0 - \left(\int_0^{\infty} u\mathrm{d}\nu_0\right)^2 \leq 4\int_0^{\infty}(u')^2\mathrm{d}\nu_0.$$

  In a similar way as in the Legendre case, for $n\geq 2$, the q_n's correspond to a natural extension of the Laguerre polynomials at the parameter $\alpha=-1$ (which are not orthogonal with respect to a probability measure). They are for instance obtained by generalising the closed form of the Laguerre polynomials.

3.2.3 The differentiation operator

Notation 3.22. In the rest of this chapter, so that all our statements are precise, we denote the ℓ^2- representation of an element u of a weighted Sobolev space

- by $[u]_{L^2}$ if we consider its representation with respect to the orthonormal basis $\mathcal{P}=\{p_n\}_{n=0}^{\infty}$ of $L^2(\nu)$,
- by $[u]_{H^1}$ if we consider its representation with respect to the orthonormal basis $\mathcal{Q}=\{q_n\}_{n=0}^{\infty}$ of $H^1(\nu)$.

That is, $[u]_{L^2} \in \ell^2$ is the infinite vector of coefficients $\langle p_n, u\rangle$, and $[u]_{H^1} \in \ell^2$ is the infinite vector of coefficients (q_n, u). Furthermore, for the sake of clarity, we may shorten some notations by omitting the ν. Henceforth, $\|\cdot\|_{H^1}$ (resp. $\|\cdot\|_{L^2}$) will always denote $\|\cdot\|_{H^1(\nu)}$ (resp. $\|\cdot\|_{L^2(\nu)}$).

Given an operator $\mathcal{A}$ acting between two weighted Sobolev spaces, for instance $\mathcal{A} : H^1 \to L^2$, we denote by $[\mathcal{A}]_{H^1\to L^2} : \ell^2 \to \ell^2$ the operator such that $[\mathcal{A}u]_{L^2} = [\mathcal{A}]_{H^1\to L^2}\,[u]_{H^1}$. In other words, $[\mathcal{A}]_{H^1\to L^2}$ is the infinite matrix representing the operator $\mathcal{A}$ with basis $\mathcal{Q}$ for the domain and basis $\mathcal{P}$ for the range. We use similar arrow notations for operator norms, i.e.,

$$\|\mathcal{A}\|_{H^1\to L^2} = \sup_{\substack{u\in H^1\\ u\neq 0}} \frac{\|\mathcal{A}u\|_{L^2(\nu)}}{\|u\|_{H^1(\nu)}},$$

and note that

$$\|\mathcal{A}\|_{H^1\to L^2} = \|[\mathcal{A}]_{H^1\to L^2}\|_{\ell^2\to\ell^2}\,.$$

When the two spaces are the same, we sometimes write $[\mathcal{A}]_{L^2}$ instead of $[\mathcal{A}]_{L^2\to L^2}$.

In order to eventually deal with $\mathfrak{L}$, we first consider the (unbounded) differentiation operator ∂_x, which we write with respect to $\mathcal{P}$, i.e.,

$$[\partial_x]_{L^2\to L^2} = D = \begin{pmatrix} 0 & \cdots \\ \vdots & D_{>0} \end{pmatrix}.$$

As a differentiation operator acting on a polynomial basis, D is strictly upper triangular. The submatrix $D_{>0}$, which corresponds to ∂_x from the subspace of mean zero functions of $L^2(\nu)$ to $L^2(\nu)$, will play a central role in the analysis to come.

As made clear by Proposition 3.29, the operator ∂_x (or equivalently D) is closely related to the change of basis matrix $P = [\mathrm{id}]_{L^2\to H^1}$ from $\mathcal{P}$ to $\mathcal{Q}$, i.e. the matrix such that $[u]_{H^1} = P\,[u]_{L^2}$.

Proposition 3.23. The change of basis matrix P from $\mathcal{P}$ to $\mathcal{Q}$ is given by

$$P = [\mathrm{id}]_{L^2\to H^1} = \begin{pmatrix} 1 & 0 & \cdots \\ 0 & & \\ \vdots & & D_{>0} \end{pmatrix}. \tag{3.21}$$

Proof. We normalized the p_n and q_m so that $p_0 = q_0 = 1$, which explains the first column of P. The first row of zeros is an immediate consequence of the fact that the p_n all have mean 0 for $n \geq 1$. Finally, using that the q_m also all have mean 0 for $m \geq 1$, we get

$$\begin{aligned}(q_m, p_n) &= \langle q_m', p_n' \rangle + \langle q_m, 1\rangle\langle p_n, 1\rangle \\ &= \langle p_{m-1}, p_n' \rangle \\ &= D_{m-1,n}.\end{aligned}$$ □

These observations are useful for the resolution of differential equations involving the operator $\mathfrak{L}$ such as (3.8).

Proposition 3.24. We have that

$$[\mathfrak{L}]_{L^2} = D^T D \qquad \text{and} \qquad [\mathfrak{L}]_{H_0^1} = D_{>0} D_{>0}^T.$$

Proof. This follows from (3.16) such that for all $u, v \in H^1$

$$\langle u, \mathfrak{L} v\rangle = \langle u', v'\rangle = [\partial_x u]_{L^2}^T [\partial_x v]_{L^2} = (D[u]_{L^2})^T (D[v]_{L^2}) = [u]_{L^2}^T D^T D [v]_{L^2}.$$ □

Since D is upper triangular, $[\mathfrak{L}]_{L^2} = D^T D$ gives a Cholesky factorisation (LU) of $[\mathfrak{L}]_{L^2}$, whereas $[\mathfrak{L}]_{H_0^1} = D_{>0} D_{>0}^T$ gives a *reverse Cholesky* factorisation (UL) of $[\mathfrak{L}]_{H_0^1}$. UL decompositions are rather uncommon as they are typically non-unique in infinite dimensions but it seems to be canonical in this case.

This allows for a simple inversion of the operator $\mathfrak{L}$. This is particularly the case if the potential V is polynomial. Indeed, we have

Lemma 3.25. Let $V(x) = x^{2k}/(2k) + O(x^{2k})$ be a polynomial of degree $2k$, and $\nu(\mathrm{d}x) = e^{-V}\mathrm{d}x/Z$. Then, for all $m \leq n - 2k$

$$D_{m,n} = \langle p_m, p_n' \rangle = 0$$

such that D (and P) are upper triangular operators on ℓ^2 of upper bandwidth $(2k-1)$.

Proof. Let $m < n$, then

$$\begin{aligned}\langle p_m, p_n' \rangle &= \frac{1}{Z}\int_{-\infty}^{+\infty} p_m(x) p_n'(x) e^{-V(x)}\mathrm{d}x \\ &= -\frac{1}{Z}\int_{-\infty}^{+\infty} p_n(x)\left(p_m(x)e^{-V(x)}\right)'\mathrm{d}x \qquad \text{By parts} \\ &= \frac{1}{Z}\int_{-\infty}^{+\infty} p_n(x)p_m(x)V'(x)e^{-V(x)}\mathrm{d}x - \frac{1}{Z}\int_{-\infty}^{+\infty} p_n(x)p_m'(x)e^{-V(x)}\mathrm{d}x \\ &= \int_{-\infty}^{+\infty} p_n(x)p_m(x)V'(x)\nu(\mathrm{d}x) \qquad \text{By orthogonality since } \deg(p_m') = m-1 < n.\end{aligned}$$

Since $V'p_m$ is a polynomial of degree $m + 2k - 1$, the above term is zero by orthogonality if $m + 2k - 1 < n$, i.e. $m \leq n - 2k$. □

Remark 3.26. In the case of a polynomial potential V, one can think of the basis $\{p_n\}_{n\in\mathbb{N}}$ as semi-classical in the sense that $[\partial_x]_{L^2}$ is banded with upper bandwidth $(2k-1)$, in contrast with the classical case of Hermite polynomial ($\nu(\mathrm{d}x) = e^{-x^2}\mathrm{d}x/Z$) where $[\partial_x]_{L^2}$ is diagonal. This, in turn, implies that $[\mathfrak{L}]_{L^2}$ is banded with bandwidth $(4k-3)$, extending the result of [174].

Remark 3.27. Of course, if V is an even polynomial then for all $m = n \mod 2$, $D_{m,n} = \langle p_m, p_n' \rangle = 0$.

Remark 3.28. Observe that

$$\mathfrak{L} = -\mathcal{J} \circ \partial_x \qquad \text{where } \mathcal{J}\cdot = -V' \cdot + \partial_x \cdot$$

is the so-called probability flux (or current) operator [189]. Now, for $u, v \in H^1(\nu)$,

$$\begin{aligned} \langle u, \partial_x v \rangle &= \frac{1}{Z} \int_{\mathbb{R}} u(\partial_x v) e^{-V} \mathrm{d}x \\ &= -\frac{1}{Z} \int_{\mathbb{R}} v \partial_x (u e^{-V}) \mathrm{d}x \\ &= -\frac{1}{Z} \int_{\mathbb{R}} v(-V'u + \partial_x u) e^{-V} \mathrm{d}x \\ &= \langle -\mathcal{J} u, v \rangle, \end{aligned}$$

which shows that $-\mathcal{J}$ is the $L^2(\nu)$-adjoint of ∂_x, and provides another proof of the first identity of Proposition 3.24. Another consequence of this observation is that

$$D^T = [-\mathcal{J}]_{L^2} = [V'\cdot]_{L^2} - D, \qquad \text{and thus} \qquad [V'\cdot]_{L^2} = D + D^T,$$

where $[V'\cdot]_{L^2}$ is the multiplication operator by V'. This means that the coefficients of $[V'\cdot]_{L^2}$ grow at the same speed as the ones of D, which is consistent with the expectation that multiplying by V' loses as much regularity as differentiating once on a ν-weighted Sobolev space. Furthermore, when V is a polynomial, note that one can therefore deduce the differentiation matrix D, directly from the multiplication by V' operator, and thus from the multiplication by x (Jacobi) operator.

3.3 Functional and Numerical Analysis on Freud-weighted Sobolev spaces

We consider the double-well potential

$$V(x) = \frac{x^4}{4} - \kappa \frac{x^2}{2}, \tag{3.22}$$

so that

$$\mathrm{d}\nu = \frac{e^{-V(x)}}{Z} \mathrm{d}x, \qquad \text{with } Z = \int_{-\infty}^{+\infty} \exp\left(-\frac{x^4}{4} + \kappa \frac{x^2}{2}\right) \mathrm{d}x,$$

where Z can be expressed and computed via the use of Bessel functions.

3.3.1 Freud-type orthogonal polynomials

The orthonormal polynomials with respect to ν are the so-called *Freud-type* orthonormal polynomials $\{p_n\}_{n\in\mathbb{N}}$ and constitute a family of *semi-classical* orthonormal polynomials. These p_n's can be constructed recursively via a three-term recurrence formula of the form

$$\begin{cases} p_0 &= 1 \\ x p_n &= a_{n+1} p_{n+1} + a_n p_{n-1}, \qquad \text{where } a_n > 0, \end{cases} \tag{3.23}$$

without any p_n term in the right hand side. since V is even.

Furthermore, in the case of Freud-type polynomials, one can give an "explicit" recurrence formula for the positive sequence $(a_n)_{n\in\mathbb{N}}$. Indeed, the sequence $(b_n)_{n\in\mathbb{N}} := (a_n^2)_{n\in\mathbb{N}}$ satisfies the so-called discrete Painlevé I equation

$$\frac{n}{b_n} = b_{n-1} + b_n + b_{n+1} - \kappa, \quad n \geq 1, \tag{3.24}$$

with $b_0 = 0$ and

$$b_1 = \int_{\mathbb{R}} x^2 \nu(\mathrm{d}x) = \frac{\displaystyle\int_{-\infty}^{+\infty} x^2 \exp\left(-\frac{x^4}{4} + \kappa\frac{x^2}{2}\right)\mathrm{d}x}{\displaystyle\int_{-\infty}^{+\infty} \exp\left(-\frac{x^4}{4} + \kappa\frac{x^2}{2}\right)\mathrm{d}x}, \tag{3.25}$$

which can also be computed via Bessel functions.

In view of Lemma 3.25 and Remark 3.27, p_n' should be a linear combination of p_{n-1} and p_{n-3} and we furthermore have the following:

Proposition 3.29. Let $\{p_n\}_{n\in\mathbb{N}}$ be the basis of orthonormal polynomials of $L^2(\nu) = L^2(e^{-V}/Z)$ generated by (3.23) and (3.24), then

$$p_n' = \frac{n}{a_n} p_{n-1} + a_n a_{n-1} a_{n-2} p_{n-3}. \tag{3.26}$$

Proof. This can be obtained rather easily from Remark 3.28. Indeed, applying (3.23) three times to express $x^3 p_n$ yields

$$\begin{aligned} V'(x)p_n &= (x^3 - \kappa x)p_n \\ &= a_{n+1}a_{n+2}a_{n+3}p_{n+3} + a_{n+1}\left(a_{n+2}^2 + a_{n+1}^2 + a_n^2 - \kappa\right)p_{n+1} \\ &\quad + a_n a_{n-1}a_{n-2}p_{n-3} + a_n\left(a_{n+1}^2 + a_n^2 + a_{n-1}^2 - \kappa\right)p_{n-1}. \end{aligned}$$

Using that $[V']_{L^2} = D + D^T$ and that D is upper triangular allows us to extract the formula for p_n', namely

$$p_n' = a_n a_{n-1} a_{n-2} p_{n-3} + a_n\left(a_{n+1}^2 + a_n^2 + a_{n-1}^2 - \kappa\right)p_{n-1},$$

and using (3.24) (with $a_n = b_n^2$) gives (3.26). □

Remark 3.30. Proposition 3.29 is exactly the implication $(iv) \implies (ii)$ of the main Theorem of [47], but they instead directly observe that by looking at the leading coefficient of p_n (and thus of p_n') in terms of monomials

$$\langle p_{n-1}, p_n\rangle = \int_{\mathbb{R}} p_n p_{n-1}\mathrm{d}\nu = \frac{n}{a_n}.$$

This calculation does not actually depend on the chosen polynomial $V(x) = x^{2k}/(2k) + O(x^{2k})$, and thus by computing

$$\langle p_{n-1}, V'p_n\rangle = \langle p_{n-1}, p_n\rangle$$

by applying $2k-1$ times the recurrence formula (3.23), one can automatically deduce recurrence

the relation on the a_n's. Identifying the polynomial R_j such that

$$\langle x^{2j+1} p_n, p_{n-1} \rangle = a_n R_j(a_{n-j+1}^2, \dots, a_n^2, \dots, a_{n+j-1}^2)$$

shows Lemma 3.7. Similar formulations of these recurrence relations are for instance found in [83, 166].

Proposition 3.29 means that the differential operator D and change of basis operator P are bidiagonal and can be written as

$$D = \begin{pmatrix} 0 & \alpha_1 & 0 & \beta_1 & & \\ & 0 & \alpha_2 & 0 & \beta_2 & \\ & & \ddots & \ddots & \ddots & \ddots \\ & & & & & \end{pmatrix} \quad \text{and} \quad P = \begin{pmatrix} 1 & 0 & 0 & & & \\ & \alpha_1 & 0 & \beta_1 & & \\ & & \alpha_2 & 0 & \beta_2 & \\ & & & \ddots & \ddots & \ddots \\ & & & & & \end{pmatrix},$$

where

$$\alpha_n = \frac{n}{a_n}, \qquad \beta_n = a_n a_{n+1} a_{n+2}. \tag{3.27}$$

Remark 3.31. Bonan and Nevai [47] actually prove that $[\partial_x]_{L^2}$ is bidiagonal if and only if V is of the form (3.22), up to a translation and scaling (in x).

In order to justify the invertibility of P and to get explicit compactness estimates for its inverse, we need a precise control on the growths of the α_n's and the β_n's, and thus on the growth of the b_n's. Indeed, using the triangular structure of P one can easily derive a formal inverse P^{-1}, but to prove that this yields a well defined and bounded operator, and to then get quantitative compactness estimates, we will need an estimate of the form

$$\frac{\beta_n}{\alpha_n} \leq \theta < 1 \qquad \text{for all } n \geq N, \tag{3.28}$$

with an explicit threshold N and constant θ. This condition, which naturally appears in our proof of Theorem 3.4 in Section 3.3.3, was also already used in [56] in the slightly more general context of tridiagonal operators.

Looking at (3.24), a formal calculation suggests that $b_n \sim \sqrt{n}/\sqrt{3}$ as $n \to \infty$, and this can in fact be established rigorously [4, §6]. From the formulas (3.27) and the fact that $a_n = \sqrt{b_n}$, we get $\beta_n/\alpha_n \to 1/3$, which shows the existence of a $\theta < 1$ and of an N large enough such that (3.28) holds. However, since we require explicit N and θ, we need more quantitative estimates on the a_n's (or equivalently on the b_n's), like the ones stated in Proposition 3.8, with explicit constants c^- and c^+. In order to establish these bounds, we have to overcome the following difficulties. While the recurrence relation (3.24) might seem in appearance very innocent, it turns out that it is extremely unstable and sensitive to initial conditions. More is in fact true [4, 47]: the initial condition given by (3.25) is the unique one such that $b_n \geq 0$ for all $n \in \mathbb{N}$. In particular, this suggests that one cannot get estimates solely from (3.24), the positivity condition being crucial. This furthermore constitutes a computational challenge as even calculating a finite number of terms in double precision quickly diverges from the positive solution.

We point out the analysis of the recurrence relation (3.24) has been the topic of a vast literature [4, 37, 82, 107, 130, 164, 166, 167, 168, 183] including the celebrated Freud's conjecture and its proof in the case $\kappa = 0$ [108] (See [4, §2] for a nice historical review of the problem). However, quantitative bounds like (3.29) with explicit constants do not seem to be already available, and we obtain those via a computer-assisted proof, which, although based on a fixed point argument, has some unorthodox features.

Finally, let us emphasize we do not have access to an explicit form of the p_n's and q_n's, and nor of the a_n's, but we show in this work that these explicit descriptions are in fact not necessary (contrarily to what was suggested in [141]) in order to successfully use these bases in practice. This is demonstrated in an unequivocal manner via the establishment of Theorems 1.9 and 3.6, which use these bases both for the obtention of the approximate solutions, and for deriving the compactness estimates required for the proof.

3.3.2 A precise analysis of the discrete Painlevé I equation

Proof of Proposition 3.8. The qualitative statement, namely that for all $0 < c^- < 1 < c^+$, there exists N such that (3.12) holds for all $n \geq N$, follows directly from the fact that $b_n \sim \sqrt{n}/\sqrt{3}$, which is for instance proved nicely in [4, §6]. However, such asymptotic analysis does not provide quantitative bounds on the b_n's. The quantitative statement follows from a computer-assisted proof and adapts a construction first proposed in [164] (which gives quantitative bounds in the case $\kappa = 0$) and greatly simplified in [130] in the case of this particular recurrence. We describe below a procedure where, for a given κ and fixed c^- and c^+ close enough to 1, we find the smallest possible N such that, for $(b_n)_{n\in\mathbb{N}}$ satisfying (3.24) and (3.25), we get

$$c^- \frac{\sqrt{n}}{\sqrt{3}} \leq b_n \leq c^+ \frac{\sqrt{n}}{\sqrt{3}}, \tag{3.29}$$

for all $n \geq N$.

Step 1 (Set-up of a fixed-point problem)**.** Adapting the strategy in [130], we introduce

$$f(x) = -x + \sqrt{1 + x^2} \qquad \text{and} \qquad g_n(x, y) = \frac{x + y - \kappa}{2\sqrt{n}}, \ n \geq 1,$$

and the map $S : \mathbb{R}^{\mathbb{N}^*} \to \mathbb{R}^{\mathbb{N}^*}$ such that, for $b \in \mathbb{R}^{\mathbb{N}^*}$,

$$\begin{aligned} (Sb)_n &= \sqrt{n} f(g(b_{n-1}, b_{n+1})), \qquad \text{for } n > 1, \\ (Sb)_1 &= f(g(0, b_2)), \end{aligned}$$

where $\mathbb{R}^{\mathbb{N}^*}$ is endowed with the product topology. It is then straightforward to check that, if $Sb = b$, then, defining $b_0 = 0$, b satisfies the recurrence relation (3.24), and we thus seek a fixed point of S in $\mathbb{R}_+^{\mathbb{N}^*}$. Note that, by the aforementioned uniqueness of a positive solution of (3.24) (see [4, 47]), the solution to (3.24)-(3.25) is the unique fixed point of S in $\mathbb{R}_+^{\mathbb{N}^*}$.

Step 2 (Upper and lower bounds of a fixed point)**.** We keep following the ideas from [130, Theorem 2.1.(a)], which relies on a Banach lattice theory argument, and state the following lemma.

Lemma 3.32. If there are sequences $b^-, b^+ \in \mathbb{R}_+^{\mathbb{N}^*}$ such that for all $n \in \mathbb{N}^*$

$$0 \le b_n^- \le (Sb^+)_n \le (Sb^-)_n \le b_n^+, \tag{3.30}$$

then the unique positive solution b of (3.24) satisfies $b_n^- \le b_n \le b_n^+$ for all $n \in \mathbb{N}^*$.

Proof. The inequality $(Sb^+)_n \le (Sb^-)_n$ is implied by $b_n^- \le b_n^+$, as from its definition S is monotone decreasing with respect to the canonical partial order $\le$ on $\mathbb{R}_+^{\mathbb{N}^*}$. Now, for the same reason, we have that for all $n \in \mathbb{N}^*$,

$$(S(K))_n \subset [b_n^-, b_n^+], \quad \text{where} \quad K = \prod_{n=1}^{\infty} [b_n^-, b_n^+] \subset \mathbb{R}^{\mathbb{N}^*}.$$

Thus $S(K) \subset K$, which is convex and compact in $\mathbb{R}^{\mathbb{N}^*}$ by Tychonoff's theorem. Since $S : \mathbb{R}^{\mathbb{N}^*} \to \mathbb{R}^{\mathbb{N}^*}$ is continuous and $\mathbb{R}^{\mathbb{N}^*}$ is locally convex, by Schauder–Tychonoff theorem, we have that there exists $b \in K$ such that $Sb = b$. Since $K \subset \mathbb{R}^{\mathbb{N}^*}$, this fixed point is the positive solution of (3.24), and the fact that b belongs to K finishes the proof. □

We are now going to get explicit enclosures of b by constructing explicit sequences b^- and b^+ satisfying the assumptions of Lemma 3.32.

Step 3 (Criterion for very large n)**.** We henceforth assume that $\kappa > 0$ (the same procedure, with slightly different conditions, can be used if $\kappa < 0$ or $\kappa = 0$). Let $c^+ > 1$ and $c^- < 1$ such that there exists $N_1 > 1$ satisfying

$$\sqrt{12 + \left(c^+ \sqrt{1 - \frac{1}{N_1}} + c^+ \sqrt{1 + \frac{1}{N_1}} - \frac{\sqrt{3}\kappa}{\sqrt{N_1}} \right)^2} - 2c^+ - 2c^- \ge 0, \tag{3.31}$$

and

$$\sqrt{12 + (2c^-)^2} + \frac{\sqrt{3}\kappa}{\sqrt{N_1}} - c^- \left(\sqrt{1 - \frac{1}{N_1}} + \sqrt{1 + \frac{1}{N_1}} \right) - 2c^+ \le 0. \tag{3.32}$$

Note that, if c^- and c^+ are both close enough to 1, such an N_1 always exists. For all $n \ge N_1$, let

$$b_n^+ = c^+ \frac{\sqrt{n}}{\sqrt{3}}, \qquad b_n^- = c^- \frac{\sqrt{n}}{\sqrt{3}}. \tag{3.33}$$

Then, for $n > N_1$,

$$\begin{aligned}
(Sb^+)_n &= \sqrt{n} \left(\sqrt{\frac{\left(\frac{c^+\sqrt{n-1}}{\sqrt{3}} + \frac{c^+\sqrt{n+1}}{\sqrt{3}} - \kappa \right)^2}{4n}} + 1 - \frac{\frac{c^+\sqrt{n-1}}{\sqrt{3}} + \frac{c^+\sqrt{n+1}}{\sqrt{3}} - \kappa}{2\sqrt{n}} \right) \\
&= \frac{\sqrt{n}}{2\sqrt{3}} \left(\sqrt{12 \left(c^+ \sqrt{1 - \frac{1}{n}} + c^+ \sqrt{1 + \frac{1}{n}} - \frac{\sqrt{3}\kappa}{\sqrt{n}} \right)^2} + \frac{\sqrt{3}\kappa}{\sqrt{n}} - c^+ \left(\sqrt{1 - \frac{1}{n}} + \sqrt{1 + \frac{1}{n}} \right) \right) \\
&\ge \frac{n}{2\sqrt{3}} \left(\sqrt{12 + \left(c^+ \sqrt{1 - \frac{1}{N_1}} + c^+ \sqrt{1 + \frac{1}{N_1}} - \frac{\sqrt{3}\kappa}{\sqrt{N_1}} \right)^2} - 2c^+ \right),
\end{aligned}$$

and similarly, we get that

$$(Sb^-)_n = \frac{\sqrt{n}}{2\sqrt{3}}\left(\sqrt{12+\left(c^-\sqrt{1-\frac{1}{n}}+c^-\sqrt{1+\frac{1}{n}}-\frac{\sqrt{3}\kappa}{\sqrt{n}}\right)^2}+\frac{\sqrt{3}\kappa}{\sqrt{n}}-c^-\left(\sqrt{1-\frac{1}{n}}+\sqrt{1+\frac{1}{n}}\right)\right)$$
$$\leq \frac{\sqrt{n}}{2\sqrt{3}}\left(\sqrt{12+(2c^-)^2}+\frac{\sqrt{3}\kappa}{\sqrt{N_1}}-c^-\left(\sqrt{1-\frac{1}{N_1}}+\sqrt{1+\frac{1}{N_1}}\right)\right).$$

Thanks to (3.31)-(3.32), we do get that

$$0 \leq b_n^- \leq (Sb^+)_n \leq (Sb^-)_n \leq b_n^+,$$

for all $n > N_1$.

Step 4 (Construction of K)**.** We start by defining b^+ and b^- as in as in (3.33), for all $n \geq 1$.

- Picking N_1 as in Step 3, i.e. satisfying (3.31)–(3.32), we already have proven that (3.30) holds for all $n > N_1$.
- However, we do not expect the threshold given by (3.31)–(3.32) to be sharp. We therefore look for the smallest $N_2 \leq N_1$ such that (3.30) holds for all $n > N_2$. In principle it could be that $N_2 = N_1$, but in practice we typically get $N_2 \ll N_1$.
- For $n \leq N_2$, we gradually decrease b_n^- and increase b_n^+ by ε-inflation [173], until (3.30) holds for all $n \geq 1$.

All the calculations are guaranteed via interval arithmetic. If this step succeeds, We have constructed $b^- = (b_n^-)_{n\geq 1}$ and $b^+ = (b_n^+)_{n\geq 1}$ such that (3.30) holds for all $n \in \mathbb{N}^*$. Thus, we can apply Lemma 3.32, which yields that $b_n^- \leq b_n \leq b_n^+$ for all $n \in \mathbb{N}^*$. In particular the estimate (3.29) holds for all $n > N_2$.

Step 5 (Estimates for small n)**.** Finally, we compute b_1 with extended precision using the formula

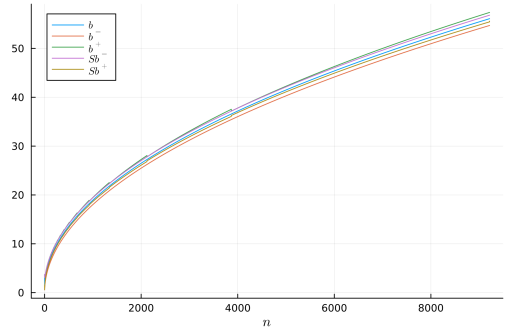
$$b_1 = \int_{\mathbb{R}} x^2 \nu(\mathrm{d}x) = \frac{\kappa^2 I_{-\frac{1}{4}}\left(\frac{\kappa^2}{8}\right) + \kappa^2\left(I_{\frac{3}{4}}\left(\frac{\kappa^2}{8}\right) + I_{\frac{5}{4}}\left(\frac{\kappa^2}{8}\right)\right) + \left(\kappa^2+4\right) I_{\frac{1}{4}}\left(\frac{\kappa^2}{8}\right)}{2\kappa\left(I_{-\frac{1}{4}}\left(\frac{\kappa^2}{8}\right) + I_{\frac{1}{4}}\left(\frac{\kappa^2}{8}\right)\right)},$$

where I_γ denotes the modified Bessel function of the first kind with parameter γ (and can be evaluated rigorously with `Arb` [144]). Recall that we assumed $\kappa > 0$, otherwise a slightly different expression in terms of Bessel functions is obtained for b_1. We can then compute the b_n's by recursion, to find the smallest $N \in \mathbb{N}^*$ such that the estimate (3.29) also holds for all $n \in \{N, \dots, N_2\}$.

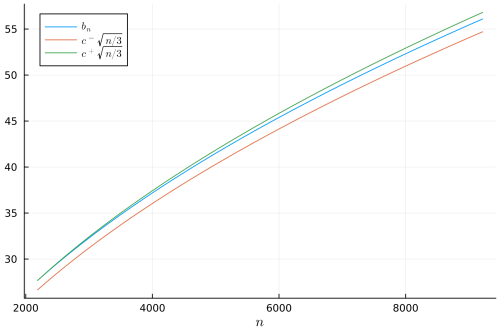
With $\kappa = 4$, $c^- = 0.987$ and $c^+ = 1.025$, the entire procedure is successful with $N_1 = 9,000,000$, $N_2 = 9,215$ and $N = 2,187$; the proof is performed at [79] in the file `GP_eq/Painleve_bounds.ipynb`. □

3.3.3 Compactness estimates

We now show how estimates on the growth of the positive solution of the discrete Painlevé I equation can be leveraged to quantify the compactness of the Sobolev embedding $H^1(\nu) \hookrightarrow L^2(\nu)$ and the Poincaré inequality on $H^1(\nu)$, i.e. we give quantitative versions of Proposition 3.12 and



(a) Construction of $(b_n^-)_{n\geq 1}$ and $(b_n^+)_{n\geq 1}$ by ε-inflation for $n \leq N_2$



(b) Verification of the bounds (3.29) for $n \in \{N, \dots, N_2\}$

Figure 3.3: Bounds on b_n for $k = 4$, $c^- = 0.987$ and $c^+ = 1.025$.

Theorem 3.14 via Theorems 3.3 and 3.4 respectively.First, using the upper bound on $b_n = a_n^2$ from Proposition 3.8, we now obtain explicit bounds on the coefficients

$$\alpha_n = \frac{n}{a_n} \quad \text{and} \quad \beta_m = a_n a_{n+1} a_{n+2}$$

of the (unbounded) ℓ^2-operator P introduced in Section 3.2.3, which in particular allow us to satisfy (3.28).

Corollary 3.33. For all $c^+ > 1$, there exists $N \in \mathbb{N}$ such that

$$b_n \leq c^+ \frac{\sqrt{n}}{\sqrt{3}}, \tag{3.34}$$

for all $n \geq N$. Defining

$$C_\alpha = \frac{\sqrt[4]{3}}{\sqrt{c^+}}, \qquad \theta = \frac{(c^+)^2}{3}\left(\left(1+\frac{1}{N}\right)\left(1+\frac{2}{N}\right)\right)^{1/4},$$

we get, for all $n \geq N$,

$$\alpha_n \geq C_\alpha n^{3/4} \qquad \text{and} \qquad \frac{\beta_n}{\alpha_n} \leq \theta. \tag{3.35}$$

In the case $\kappa = 4$, one can take $c^+ = 1.025$ and $N = 2,187$, which yields

$$C_\alpha \approx 1.299925254 \qquad \text{and} \qquad \theta \approx 0.350328462$$

Remark 3.34. Recall that $b_n \sim \sqrt{n/3}$ yields $\alpha_n \sim \sqrt[4]{3} n^{3/4}$ and $\beta_n \sim (n/3)^{3/4}$, and therefore $\beta_n/\alpha_n \sim 1/3$. In particular, up to taking N large enough, one can always get $\theta < 1$. Moreover, if c^+ is arbitrarily close to 1, then θ can be brought arbitrarily close to $1/3$. The above explicit values show that, in practice, we can indeed rather close to the optimal value of θ.

Note that we only needed the upper-bounds on b_n from Proposition 3.8 here, but the lower-bounds will also be used, in the Appendix A.1.

Remark 3.35. Of course, these estimates become worse and harder to obtain as κ gets larger. Furthermore, if c^- and c^+ were chosen to be further from 1, then N would be smaller, though the quality of C_α and θ would be worse. However, the crucial feature is for θ be strictly less than 1.

Notation 3.36. Note that the unbounded operator $\mathrm{id} : H^1(\nu) \subset L^2(\nu) \to H^1(\nu)$ obviously maps

even functions to even functions and odd functions to odd functions, which is reflected in the fact that the action of P on even and odd modes is decoupled. In the sequel, we only consider the subspace of even functions (the case of odd functions is analogous), which amounts to considering

$$P = \begin{pmatrix} 1 & 0 & & \\ & \alpha_2 & \beta_2 & \\ & & \alpha_4 & \ddots \\ & & & \ddots \\ & & & \end{pmatrix}.$$

Furthermore, for a matrix or operator A, we use the computational notations for selection of indices, e.g. $A_{1:n,-1}$ denotes the vector made up of the first n indices (i.e. the first index is 1 and notations are inclusive) of the last column of A.

The computational parts of the subsequent subsections are given at [79] in the file `GP_eq/Poincare.ipynb`.

Proof of Theorem 3.4

Observe that P^{-1} is the ℓ^2-representation of the embedding $\iota : H^1(\nu) \hookrightarrow L^2(\nu)$, that is

$$P^{-1} = [\iota]_{H^1 \to L^2}.$$

We thus aim to obtain compactness estimates via the analysis of the ℓ^2-operator P^{-1}. We first pick an even integer n, $n \geq N$, with respect to which we carve up our problem. Let us carve P as follows

$$P := \left(\begin{array}{c|c} P_{\leq n} & \\ \hline & \beta_n \\ & \\ & D_{>n} \end{array}\right) := \left(\begin{array}{c|cc} 1 & & \\ \hline & D_{\leq n} & \\ & & \beta_n \\ \hline & & D_{>n} \end{array}\right),$$

where

$$P_{\leq n} = \left(\begin{array}{c|c} 1 & 0 \quad \cdots \\ \hline 0 & \\ \vdots & \quad D_{\leq n} \\ & \end{array}\right) = \begin{pmatrix} 1 & 0 & & & & \\ & \alpha_2 & \beta_2 & & & \\ & & \alpha_4 & \ddots & & \\ & & & \ddots & \ddots & \\ & & & & \ddots & \beta_{n-2} \\ & & & & & \alpha_n \end{pmatrix},$$

and

$$D_{>n} = \begin{pmatrix} \alpha_{n+2} & \beta_{n+2} & & \\ & \alpha_{n+4} & \beta_{n+4} & \\ & & \alpha_{n+6} & \ddots \\ & & & \ddots \end{pmatrix}. \tag{3.36}$$

Computing the inverse of P seen as a two-by-two block matrix and using the Schur complement, one thus infer that

$$P^{-1} = \left(\begin{array}{c|c} P_{\leq n}^{-1} & -\beta_n (P_{\leq n}^{-1})_{:,-1} (D_{>n}^{-1})_{1,:} \\ \hline & \\ & D_{>n}^{-1} \\ & \end{array}\right) = \left(\begin{array}{c|c} 1 & \\ \hline & \begin{array}{c|c} D_{\leq n}^{-1} & -\beta_n (D_{\leq n}^{-1})_{:,-1} (D_{>n}^{-1})_{1,:} \\ \hline & \\ & D_{>n}^{-1} \\ & \end{array} \end{array}\right), \tag{3.37}$$

where we will show that $P^{-1} : \ell^2(\mathbb{N}^*) \to \ell^2(\mathbb{N}^*)$ is a bounded operator. Since

$$\|u\|_{L^2} = \|\iota u\|_{L^2} = \left\|P^{-1}[u]_{H^1}\right\|_{\ell^2},$$

and

$$\|u\|_{H^1} = \|[u]_{H^1}\|_{\ell^2},$$

in order to prove Theorem 3.4, we need to find a constant C such that, for all $u \in \overline{\mathrm{Span}\{q_j\}_{j>m}}^{H^1(\nu)}$,

$m \geq N$,

$$\left\| P^{-1}[u]_{H^1} \right\|_{\ell^2} \leq \frac{C}{m^{3/4}} \left\| [u]_{H^1} \right\|_{\ell^2}.$$

In the remainder of this proof, we take $n = N$, but some of the calculations will be reused in the proof of Theorem 3.3 with a different (larger) n.

Denoting $m = n + 2k$, $k \geq 0$, and recalling that we only work on even subspaces here, we therefore need to find C such that

$$\left\| \begin{pmatrix} -\beta_n (P_{\leq n}^{-1})_{:,-1} (D_{>n}^{-1})_{1,k+1:} \\ \hline (D_{>n}^{-1})_{:,k+1:} \end{pmatrix} \right\|_{\ell^2} \leq \frac{C}{(n+2k)^{3/4}}.$$

We are going to obtain two separate constants C_{12} and C_{22} such that

$$\|\beta_n (P_{\leq n}^{-1})_{:,-1} (D_{>n}^{-1})_{1,k+1:}\|_{\ell^2} \leq C_{12}(n+2k)^{-3/4} \qquad \text{and} \qquad \|(D_{>n}^{-1})_{:,k+1:}\|_{\ell^2} \leq C_{22}(n+2k)^{-3/4}, \tag{3.38}$$

and then take C defined by

$$C := \sqrt{C_{12}^2 + C_{22}^2} = \left\| \begin{pmatrix} C_{12} \\ C_{22} \end{pmatrix} \right\|_{\ell^2}.$$

Starting with C_{12}, note that by backward substitution, we get from (3.36) that

$$(D_{>n}^{-1})_{ij} = \begin{cases} \dfrac{(-1)^{i-j}}{\alpha_{n+2j}} \displaystyle\prod_{l=i}^{j-1} \frac{\beta_{n+2l}}{\alpha_{n+2l}}, & \text{for } i \leq j, \\ 0 & \text{otherwise.} \end{cases} \tag{3.39}$$

Using Corollary (3.33), assuming N is taken largen enough so that $\theta < 1$ (see Remark 3.34), we can therefore estimate

$$\begin{aligned} \|(D_{>n}^{-1})_{1,k+1:}\|_{\ell^2} &= \left(\sum_{j=k+1}^{\infty} \frac{1}{\alpha_{n+2j}^2} \prod_{l=1}^{j-1} \frac{\beta_{n+2l}^2}{\alpha_{n+2l}^2} \right)^{1/2} \\ &\leq \frac{1}{C_\alpha (n+2k)^{3/4}} \left(\sum_{j=1}^{\infty} \theta^{2(j-1)} \right)^{1/2}, \end{aligned}$$

and thus,

$$\|(D_{>n}^{-1})_{1,k+1:}\|_{\ell^2} \leq \frac{1}{C_\alpha\sqrt{1-\theta^2}(n+2k)^{3/4}}. \tag{3.40}$$

Since, by the extremal case of the Cauchy–Schwarz inequality,

$$\|\beta_n(P_{\leq n}^{-1})_{:,-1}(D_{>n}^{-1})_{1,k+1:}\|_{\ell^2} = \beta_n\|(P_{\leq n}^{-1})_{:,-1}\|_{\ell^2}\|(D_{>n}^{-1})_{1,k+1:}\|_{\ell^2},$$

we choose

$$C_{12} = \frac{\beta_n\|(P_{\leq n}^{-1})_{:,-1}\|_{\ell^2}}{C_\alpha\sqrt{1-\theta^2}}. \tag{3.41}$$

Turning our attention to C_{22}, let us first recall that for an operator $A : \ell^2(\mathbb{N}^*) \to \ell^2(\mathbb{N}^*)$,

$$\|A\|_{\ell^2} \leq \|A\|_{\ell^1}^{1/2}\|A\|_{\ell^\infty}^{1/2},$$

where $\|\cdot\|_{\ell^1}, \|\cdot\|_{\ell^\infty}$ can be evaluated easily via the formulae

$$\|A\|_{\ell^1} = \sup_{j\in\mathbb{N}^*}\|A_{:,j}\|_{\ell^1} \qquad \text{and} \qquad \|A\|_{\ell^\infty} = \sup_{i\in\mathbb{N}^*}\|A_{i,:}\|_{\ell^1}.$$

Using again (3.39) together with (3.35), we estimate, for all $i \geq 1$,

$$\|(D_{>n}^{-1})_{i,k+1:}\|_{\ell^1} = \sum_{j=i\vee(k+1)}^{\infty}\left|\frac{(-1)^{i-j}}{\alpha_{n+2j}}\prod_{l=i}^{j-1}\frac{\beta_{n+2l}}{\alpha_{n+2l}}\right| \leq \frac{1}{C_\alpha(n+2k)^{3/4}}\sum_{j=i}^{\infty}\theta^{j-i} \leq \frac{1}{C_\alpha(1-\theta)(n+2k)^{3/4}},$$

which yields

$$\|(D_{>n}^{-1})_{:,k+1:}\|_{\ell^\infty} \leq \frac{1}{C_\alpha(1-\theta)(n+2k)^{3/4}}.$$

Similarly, we estimate, for all $j \geq k+1$,

$$\|(D_{>n}^{-1})_{:,j}\|_{\ell^1} = \sum_{i=1}^{j}\left|\frac{(-1)^{i-j}}{\alpha_{n+2j}}\prod_{l=i}^{j-1}\frac{\beta_{n+2l}}{\alpha_{n+2l}}\right| \leq \frac{1}{C_\alpha(n+2k)^{3/4}}\sum_{i=1}^{j}\theta^{j-i} \leq \frac{1}{C_\alpha(1-\theta)(n+2k)^{3/4}},$$

which yields

$$\|(D_{>n}^{-1})_{:,k+1:}\|_{\ell^1} \leq \frac{1}{C_\alpha(1-\theta)(n+2k)^{3/4}}.$$

Combining the two above estimates, we get

$$\|(D_{>n}^{-1})_{:,k+1:}\|_{\ell^2} \leq \frac{1}{C_\alpha(1-\theta)}\frac{1}{(n+2k)^{3/4}},$$

such that we can choose

$$C_{22} = \frac{1}{C_\alpha(1-\theta)}. \tag{3.42}$$

When $\kappa = 4$, according to Proposition 3.8 we can pick $c^+ = 1.025$ and $N = 2,187$ in Corollary 3.33. Repeating the same analysis on the odd subspaces and taking the maximum of the two constants yields the announced value of the constant C, and finishes the proof of Theorem 3.4.

□

Proof of Theorem 3.3

Recalling Remark 3.16, the Poincaré constant is the smallest number C_P such that for all $u \in H_0^1(\nu)$,

$$\int_{\mathbb{R}} u^2 \mathrm{d}\nu \leq C_P \int_{\mathbb{R}} (u')^2 \mathrm{d}\nu,$$

i.e. such that

$$\|u\|_{L^2}^2 \leq C_P \|u'\|_{L^2}^2 = C_P \|u\|_{H^1}^2,$$

which means

$$C_p = \sup_{\substack{u \in H_0^1 \\ u \neq 0}} \frac{\|u\|_{L^2}^2}{\|u\|_{H^1}^2}.$$

Rephrasing this in terms of our operators P and $D_{>0}$, we have that the Poincaré constant is the smallest number C_P such that for all $u \in H_0^1(\nu)$,

$$\|[u]_{L^2}\|_{\ell^2}^2 = \|P^{-1}[u]_{H^1}\|_{\ell^2}^2 \leq C_P \|[u]_{H^1}\|_{\ell^2}^2.$$

Since $u \in H_0^1(\nu)$, i.e. $(q_0, u) = \langle p_0, u \rangle = 0$, and recalling (3.21), we get

$$C_P = \|D_{>0}^{-1}\|_{\ell^2}^2 = \sup_{\substack{v \in \ell^2(\mathbb{N}^*) \\ v \neq 0}} \frac{\|D_{>0}^{-1} v\|_{\ell^2}^2}{\|v\|_{\ell^2}^2}$$

and we therefore prove Theorem 3.3 by rigorously enclosing the norm of $D_{>0}^{-1}$.

First, since $D_{>0}^{-1}$ is upper triangular, using the carving and notations from Section 3.3.3 we have that $\|D_{\leq n}^{-1}\|_{\ell^2} \leq \|D_{>0}^{-1}\|_{\ell^2}$. A lower bound for the Poincaré constant is therefore given by

$$\bar{C}_P := \|D_{\leq n}^{-1}\|_{\ell^2}^2.$$

Since $D_{\leq n}$ is a finite matrix, $\bar{C}_P$ can be enclosed, sharply and rigorously, via the Gershgorin circle theorem:

- First, compute rigorously $M = D_{\leq n}^{-1}(D_{\leq n}^{-1})^T$, so that $\|D_{\leq n}^{-1}\|_{\ell^2} = \|M\|_{\ell^2}^{1/2}$. Since M is symmetric, $\|M\|_{\ell^2}$ is simply the maximum of $|\lambda(M)|$ over all the eigenvalues $\lambda(M)$ of M.
- Secondly, diagonalise M numerically, i.e. find Q such that $Q^{-1}MQ$ is approximately diagonal.
- Then, rigorously (i.e. in interval arithmetic) compute Q^{-1}; this can be achieved via the function `inv` in the Julia library `IntervalArithmetic.jl` [198].
- Rigorously compute $\bar{\Lambda} := Q^{-1}MQ$. Note that $\bar{\Lambda}$ and M have same spectrum.
- Enclose the spectrum of $\bar{\Lambda}$ (and thus M, which is a subset of $\mathbb{R}_+$) via the Gershgorin circle theorem. This gives an upper bound on $\|D_{\leq n}^{-1}\|_{\ell^2} = \|M\|_{\ell^2}^{1/2}$.
- Finally, take v the column of Q corresponding to the largest numerical eigenvalue of M in modulus, and rigorously compute $\|D_{\leq n}^{-1} v\|_{\ell^2} / \|v\|_{\ell^2}$, which gives a lower bound on $\|D_{\leq n}^{-1}\|_{\ell^2}$.

It thus remains to find an upper bound for C_P. We pick some $n \geq N$, extract $D_{>0}^{-1}$ from (3.37),

and proceeding as in the proof of Theorem 3.4, to get

$$C_P = \|D_{>0}^{-1}\|_{\ell^2} \leq \left\| \begin{pmatrix} \|D_{\leq n}^{-1}\|_{\ell^2} & \beta_n \|(D_{\leq n}^{-1})_{:,-1}(D_{>n}^{-1})_{1,:}\|_{\ell^2} \\ 0 & \|D_{>n}^{-1}\|_{\ell^2} \end{pmatrix} \right\|_{\ell^2}^2 \leq \left\| \begin{pmatrix} \bar{C}_P^{1/2} & C_{12} n^{-3/4} \\ 0 & C_{22} n^{-3/4} \end{pmatrix} \right\|_{\ell^2}^2,$$

where C_{12} and C_{22} are as in (3.41) and (3.42). We again pick $c^+ = 1.025$, this time with $n = 3,500$, which yields the announced enclosure for C_p. □

Remark 3.37. Note that

$$\bar{C}_P \leq C_P \leq \left\| \begin{pmatrix} \bar{C}_P^{1/2} & C_{12} n^{-3/4} \\ 0 & C_{22} n^{-3/4} \end{pmatrix} \right\|_{\ell^2}^2 = \bar{C}_P + \frac{C_{12}^2}{n^{3/2}} + O\left(\frac{1}{n^3}\right),$$

which explains the sharpness of the estimate (3.5) in Theorem 3.3.

Other embedding estimates

In the context of (nonlinear) PDEs, it is often useful to make use of Sobolev inequalities [61, Corollary IX.13] to deal with nonlinearities. In one dimension, this can be achieved via the derivation of L^∞-bounds which are also useful in the proof of the positivity of solutions to elliptic equations in the fashion of Section 2.4.3. Such bounds can be obtained via the standard inequality [61, Theorem VIII.7]

$$\|\varphi\|_\infty \leq \sqrt{2} \|\varphi\|_{L^2(\mathbb{R})}^{1/2} \|\varphi'\|_{L^2(\mathbb{R})}^{1/2}, \qquad \text{for all } \varphi \in H^1(\mathbb{R}).$$

By setting $\varphi = e^{-V/2} u$, we then obtain

$$\|e^{-V/2} u\|_\infty \leq \sqrt{2} \|e^{-V/2} u\|_{L^2(\mathbb{R})}^{1/2} \|(e^{-V/2} u)'\|_{L^2(\mathbb{R})}^{1/2}.$$

Now, observe that

$$e^{V/2}(u e^{-V/2})' = -\frac{1}{2} V' u + u' = \frac{1}{2}(-V' u + u') + \frac{1}{2} u' = \frac{1}{2} \left(\mathcal{J} u + \partial_x u \right),$$

where $\mathcal{J} = -V'(x) + \partial_x$, such that

$$\|(e^{-V/2} u)'\|_{L^2(\mathbb{R})} = \sqrt{Z} \|e^{V/2}(e^{-V/2} u)'\|_{L^2(\nu)} \leq \frac{\sqrt{Z}}{2} \left(\|\mathcal{J} u\|_{L^2} + \|\partial_x u\|_{L^2} \right).$$

Note that this calculation does not depend on the choice of V. Since $-\mathcal{J}$ is the $L^2(\nu)$-adjoint of ∂_x (cf. proof of Proposition 3.24, also Remark 3.28), it is expected that $\|\mathcal{J}\|_{H^1 \to L^2}$ is finite as

$$\|\mathcal{J}\|_{H^1(\nu) \to L^2(\nu)} = \|[\mathcal{J}]_{H^1 \to L^2}\|_{\ell^2} = \|[\mathcal{J}]_{L^2 \to L^2} P^{-1}\|_{\ell^2} = \| - D^T P^{-1}\|_{\ell^2} = \|D^T P^{-1}\|_{\ell^2}.$$

We furthermore need to quantify this bound and have the following lemma.

Lemma 3.38. For $V = x^4/4 - \kappa x^2/2$, if $\mathcal{J} = -V'(x) + \partial_x$, then there exist $c > 0$ such that for all $u \in H^1(\nu)$,

$$\|\mathcal{J} u\|_{L^2(\nu)} \leq c \|u\|_{H^1(\nu)}.$$

Furthermore, for all $u \in H^1(\nu)$,

$$\|e^{-V/2}u\|_\infty \leq \sqrt{Z(c+1)}\|u\|_{L^2(\nu)}^{1/2}\|u\|_{H^1(\nu)}^{1/2} \leq \sqrt{Z(c+1)}\max(1, C_P)^{1/4}\|u\|_{H^1(\nu)}, \tag{3.43}$$

and

$$\|e^{-V/2}u\|_{H^1(\mathbb{R})} \leq \sqrt{Z}\left(\max(1, C_P) + \frac{(c+1)^2}{4}\right)^{1/2}\|u\|_{H^1(\nu)}. \tag{3.44}$$

Finally, if $\kappa = 4$, we can choose $c = 24.6332$.

Proof. See Appendix A.1. □

3.4 The Gross–Pitaevskii equation with sextic potential

Notation 3.39. From the rest of this section, we fix some $n \in \mathbb{N}$ greater than N in Theorem 3.4 and for some $u \in L^2(\nu)$ (resp. H^1) we denote by $\Pi_n^{L^2}$ (resp. $\Pi_n^{H^1}$) the projection onto $\mathrm{Span}\{p_m\}_{m=0}^n$ (resp. $\mathrm{Span}\{q_m\}_{m=0}^n$) and by $\Pi_\infty^{L^2}$ (resp. $\Pi_\infty^{H^1}$) the projection onto $\overline{\mathrm{Span}\{p_m\}_{m>n}}^{L^2}$ (resp. $\overline{\mathrm{Span}\{q_m\}_{m>n}}^{H^1}$). Furthermore, we treat the problem of this section only with respect to even subspaces and polynomials of $L^2(\nu)$ and $H^1(\nu)$, and all operators are restricted to these subspaces.

We look for solutions of the Gross–Pitaevskii equation

$$-\partial_{xx}\varphi + W(x)\varphi + \varphi^3 = \omega\varphi,$$

where $W(x) = x^6/4 - \kappa x^4/2 + cx^2 + d$ is a sextic polynomial potential. We look for real even solutions φ of the above equation such that

$$\int_{\mathbb{R}} \varphi^2 W \mathrm{d}x < \infty. \tag{3.45}$$

Then, still with $V(x) = x^4/4 - \kappa x^2/2$, writing $u = e^{-V/2}\varphi$ gives

$$\mathfrak{L}u + e^{-V}u^3 - \omega u + r(x)u = 0$$

where $r(x) = (6 + 4c - \kappa^2)x^2/4 + (2d - \kappa)/2$. For simplicity, we choose parameters c and d such that $r(x) = 0$, though this term does not contain any additional difficulty. We are thus left with the equation

$$\mathfrak{L}u + e^{-V}u^3 - \omega u = 0, \tag{3.46}$$

which is equivalent to the zero-finding problem

$$F(u) := u - \tilde{\mathfrak{L}}^{-1}f(u) = u - \tilde{\mathfrak{L}}^{-1}(\omega u + u_0 - e^{-V}u^3) = 0, \qquad u_0 := \int_{\mathbb{R}} u \mathrm{d}\nu, \tag{3.47}$$

where we introduced $\tilde{\mathfrak{L}} := \mathfrak{L} + \Pi_0^{L^2} = \mathfrak{L} + \Pi_0^{H^1}$ in order to get rid of the one-dimensional kernel of $\mathfrak{L}$ and get an invertible operator.

Corollary 3.40. We have the following representations of $\tilde{\mathfrak{L}}$ on $L^2(\nu)$ and $H^1(\nu)$:

$$[\tilde{\mathfrak{L}}]_{L^2} = P^T P, \qquad [\tilde{\mathfrak{L}}]_{H^1} = PP^T \qquad \text{and} \qquad [\tilde{\mathfrak{L}}]_{H^1 \to L^2} = P^T. \tag{3.48}$$

Furthermore,

$$\|\Pi_\infty^{H^1}\tilde{\mathfrak{L}}^{-1}\Pi_\infty^{L^2}\|_{L^2\to H^1} \leq \frac{C_{22}}{n^{3/4}}, \qquad \|\Pi_\infty^{H^1}\tilde{\mathfrak{L}}^{-1}\|_{L^2\to H^1} \leq \frac{C}{n^{3/4}}, \tag{3.49}$$

where C_{22} and C are as in Section 3.3.3 and

$$\Pi_n^{H^1}\tilde{\mathfrak{L}}^{-1}\Pi_\infty^{L^2} = 0 \qquad \text{such that} \qquad \Pi_n^{H^1}\tilde{\mathfrak{L}}^{-1} = \Pi_n^{H^1}\tilde{\mathfrak{L}}^{-1}\Pi_n^{L^2}. \tag{3.50}$$

Proof. The identities in (3.48) follow from Proposition (3.24) by adding the action of $\tilde{\mathfrak{L}}$ on constants. Combining (3.48) with the estimates of Section 3.3.3, gives (3.49). The identities in (3.50) follow from the fact that P^T and thus $(P^{-1})^T$ is lower triangular. Note that we also have that for $u, v \in H^1(\nu)$,

$$\langle u, \tilde{\mathfrak{L}}v\rangle = \int_{\mathbb{R}} u'v' \mathrm{d}\nu + \int_{\mathbb{R}} u \mathrm{d}\nu \int_{\mathbb{R}} v \mathrm{d}\nu = (u, v). \qquad \square$$

Since $[\tilde{\mathfrak{L}}^{-1}]_{L^2\to H^1} = (P^{-1})^T$ which is a bounded (actually compact from Theorem 3.4) ℓ^2-operator, $\tilde{\mathfrak{L}}^{-1}$ is bounded and compact as an operator from $L^2(\nu)$ to $H^1(\nu)$. Moreover, by the Sobolev embeddings (see Section 3.3.3), $u \in H^1(\nu)$ implies $e^{-V/2}u \in L^\infty(\mathbb{R})$ and thus $e^{-V}u^3 \in L^2(\nu)$. Therefore, $F : H^1(\nu) \to H^1(\nu)$ is bounded and a compact perturbation of the identity. Given an approximate solution $\bar{u}$ to Eq. (3.47), this motivates the introduction of an operator $A : H^1(\nu) \to H^1(\nu)$ defined as

$$A = A_n + \Pi_\infty^{H^1},$$

where $A_n \approx (\Pi_n^{H^1} DF(\bar{u})\Pi_n^{H^1})^{-1}$ (note that $\Pi_n^{H^1} DF(\bar{u})\Pi_n^{H^1}$ is finite-dimensional, hence this approximate inverse can be computed numerically), so that $\approx DF(\bar{u})^{-1}$. This approximate inverse A can then be used to introduce a quasi-Newton (fixed-point) operator

$$\begin{array}{rccc} T: & \mathcal{H} & \longrightarrow & \mathcal{H} \\ & u & \longmapsto & u - AF(u), \end{array} \tag{3.51}$$

where

$$\mathcal{H} = \left\{u \in H^1(\nu) \mid u \text{ is even}\right\}.$$

This is a common reformulation for computer-assisted proofs, and we will show that $T : \mathcal{H} \to \mathcal{H}$ is a contraction around $\bar{u}$, such that there exists a true solution u to Eq. (3.46) in a tight and explicit neighbourhood around $\bar{u}$. Note that by Lemma 3.38, if we find a solution $u \in \mathcal{H} \subset H^1(\nu)$ to Eq. (3.46), then $\varphi = e^{-V}u$ satisfies the integrability condition (3.45).

Remark 3.41. Any Schrödinger operator with sextic potential

$$-\Delta + \frac{1}{4}x^6 - \frac{\kappa^2}{2}x^4 + ax^2 + b,$$

is tridiagonal symmetric (i.e. Jacobi) with respect to the weighted basis $\{e^{-V/2}p_n\}_{n=0}^\infty$, where $V(x) = x^4/4 - \kappa x^2/2$.

3.4.1 The Newton–Kantorovitch theorem

In order to show that T is actually a contraction on a neighbourhood of $\bar{u}$, we make use of the following statement (which is nothing but Corollary 2.20 with p $p = 3$) and can be interpreted as

a kind of Newton-Kantorovich theorem when its assumptions are expressed in terms of F rather than T.

Theorem 3.42. Let T be as in (3.51) and suppose that for some Y, Z_1, Z_2, Z_3

$$\begin{aligned} &\|T(\bar{u}) - \bar{u}\|_{H^1} \leq Y, \\ &\|D^k T(\bar{u}) h^k\|_{H^1} \leq Z_k \|h\|^k, \qquad \text{for all } h \in H^1(\nu), \text{ with } k = 1, 2, 3. \end{aligned}$$

Then assume that for the radii polynomials

$$\begin{aligned} Q(\delta) &= Y - \delta + \sum_{k=1}^{3} \frac{Z_k}{k!} \delta^k, \\ R(\delta) &= -1 + \sum_{k=1}^{3} \frac{Z_k}{(k-1)!} \delta^{k-1}, \end{aligned}$$

there exists $\delta > 0$ such that $Q(\delta) < 0$ Then, denoting $\underline{\delta}$ the smallest positive root of Q and $\bar{\delta}$ the unique positive root of R, for all $\delta \in (\underline{\delta}, \bar{\delta})$, T has a unique fixed point $u^\star \in \bar{B}(\bar{u}, \delta) \subset \mathcal{H}$.

3.4.2 The bounds

We first compute an approximate solution $\bar{u} \in \Pi_n^{H^1}(\mathcal{H}) \subset \mathcal{C}^\infty(\mathbb{R})$, for $n = 2500$ (such that $n > N = 2,187$ in the case $\kappa = 4$ of Theorem 3.4). Note that this implies that $\Pi_n^{L^2} \bar{u} = \Pi_n^{H^1} \bar{u} = \bar{u}$ and $\Pi_\infty^{L^2} \bar{u} = \Pi_\infty^{H^1} \bar{u} = 0$. We then derive below appropriate bounds Y, Z_1, Z_2, Z_3 to prove the existence of an actual solution u to Eq. (3.47) (and thus to Eq. (3.46)) close to $\bar{u}$ via Theorem 3.42. Our estimates rely on a carving of the problem in the fashion of Section 3.3.3.

Finally, much of our proofs will rely on rigorously computing integrals of polynomials against Freud-weights. This is done using a quadrature rule given in Appendix A.2 and implemented in the file `GP_eq/quadrature.jl` at [79].

The computation of the bounds Y, Z_1, Z_2, Z_3 and application of Theorem 3.42 can be found at [79] in the files `GP_eq/proof1.ipynb` and `GP_eq/proof2.ipynb` for Theroem 1.9 and 3.6 respectively.

The Y bound

We estimate the difference $T(\bar{u}) - \bar{u}$ as follows

$$\begin{aligned} \|T(\bar{u}) - \bar{u}\|_{H^1}^2 &= \|AF(\bar{u})\|_{H^1}^2 \\ &= \|A(\bar{u} - \tilde{\mathfrak{L}}^{-1} f(\bar{u}))\|_{H^1}^2 \\ &= \|\Pi_n^{H^1} A(\bar{u} - \tilde{\mathfrak{L}}^{-1} f(\bar{u}))\|_{H^1}^2 + \|\Pi_\infty^{H^1} A(\bar{u} - \tilde{\mathfrak{L}}^{-1} f(\bar{u}))\|_{H^1}^2 \qquad \text{By Parseval's identity} \\ &= \|A_n(\bar{u} - \Pi_n^{H^1} \tilde{\mathfrak{L}}^{-1} f(\bar{u}))\|_{H^1}^2 + \|\Pi_\infty^{H^1}(\bar{u} - \tilde{\mathfrak{L}}^{-1} f(\bar{u}))\|_{H^1}^2 \\ &= \|A_n(\bar{u} - \Pi_n^{H^1} \tilde{\mathfrak{L}}^{-1} \Pi_n^{L^2} f(\bar{u}))\|_{H^1}^2 + \|\Pi_\infty^{H^1} \tilde{\mathfrak{L}}^{-1} f(\bar{u})\|_{H^1}^2 \qquad \text{using (3.50).} \end{aligned}$$

The first term requires a finite computation and can therefore evaluated exactly, while the second term has to be decomposed as follows

$$\|\Pi_\infty^{H^1} \tilde{\mathfrak{L}}^{-1} f(\bar{u})\|_{H^1} \leq \|\Pi_\infty^{H^1} \tilde{\mathfrak{L}}^{-1} \Pi_n^{L^2} f(\bar{u})\|_{H^1} + \|\Pi_\infty^{H^1} \tilde{\mathfrak{L}}^{-1} \Pi_\infty^{L^2} f(\bar{u})\|_{H^1}.$$

Now, we have

$$\left[\Pi_\infty^{H^1}\tilde{\mathfrak{L}}^{-1}\Pi_n^{L^2}f(\bar{u})\right]_{H^1} = \left[\Pi_\infty^{H^1}\tilde{\mathfrak{L}}^{-1}\Pi_n^{L^2}\right]_{L^2\to H^1}\left[\Pi_n^{L^2}f(\bar{u})\right]_{L^2} = -\beta_n(D_n^{-1})_{1,:}(P_{\leq n}^{-1})_{:,-1}^T\left[\Pi_n^{L^2}f(\bar{u})\right]_{L^2},$$

so that

$$\|\Pi_\infty^{H^1}\tilde{\mathfrak{L}}^{-1}\Pi_n^{L^2}f(\bar{u})\|_{H^1} = \beta_n\|(D_n^{-1})_{1,:}\|_{\ell^2}\left|(P_{\leq n}^{-1})_{:,-1}^T\left[\Pi_n^{L^2}f(\bar{u})\right]_{L^2}\right|,$$

where we recall (3.40)

$$\|(D_n^{-1})_{1,:}\|_{\ell^2} \leq \frac{1}{C_\alpha\sqrt{1-\theta^2}}\frac{1}{n^{3/4}}. \tag{3.52}$$

We also have that

$$\begin{aligned}
\|\Pi_\infty^{H^1}\tilde{\mathfrak{L}}^{-1}\Pi_\infty^{L^2}f(\bar{u})\|_{H^1} &\leq \|\Pi_\infty^{H^1}\tilde{\mathfrak{L}}^{-1}\Pi_\infty^{L^2}\|_{L^2\to H^1}\|\Pi_\infty^{L^2}f(\bar{u})\|_{L^2}\\
&\leq \|\Pi_\infty^{H^1}\tilde{\mathfrak{L}}^{-1}\Pi_\infty^{L^2}\|_{L^2\to H^1}\|\Pi_\infty^{L^2}(\omega\bar{u}+\bar{u}_0-e^{-V}\bar{u}^3)\|_{L^2}\\
&\leq \|\Pi_\infty^{H^1}\tilde{\mathfrak{L}}^{-1}\Pi_\infty^{L^2}\|_{L^2\to H^1}\|\Pi_\infty^{L^2}(e^{-V}\bar{u}^3)\|_{L^2}\\
&\leq \|\Pi_\infty^{H^1}\tilde{\mathfrak{L}}^{-1}\Pi_\infty^{L^2}\|_{L^2\to H^1}\left(\|e^{-V}\bar{u}^3\|_{L^2}^2-\|\Pi_n^{L^2}(e^{-V}\bar{u}^3)\|_{L^2}^2\right)^{1/2}\\
&\leq \frac{C_{22}}{n^{3/4}}\left(\|e^{-V}\bar{u}^3\|_{L^2}^2-\|\Pi_n^{L^2}(e^{-V}\bar{u}^3)\|_{L^2}^2\right)^{1/2} \qquad \text{by (3.49)}.
\end{aligned}$$

We can thus take

$$\begin{aligned}
Y^2 :=& \|A_n(\bar{u}-\Pi_n^{H^1}\tilde{\mathfrak{L}}^{-1}\Pi_n^{L^2}f(\bar{u}))\|_{H^1}^2\\
&+\frac{1}{n^{3/2}}\left\{\frac{\beta_n}{C_\alpha\sqrt{1-\theta^2}}\left|(P_{\leq n}^{-1})_{:,-1}^T\left[\Pi_n^{L^2}f(\bar{u})\right]_{L^2}\right|+C_{22}\left(\|e^{-V}\bar{u}^3\|_{L^2}^2-\|\Pi_n^{L^2}(e^{-V}\bar{u}^3)\|_{L^2}^2\right)^{1/2}\right\}^2.
\end{aligned}$$

The Z_1 bound

We choose to compute Z_1 by treating finite and infinite dimensional parts separately, and therefore take

$$Z_1 := \left\|\begin{pmatrix} Z^{11} & Z^{12}\\ Z^{21} & Z^{22}\end{pmatrix}\right\|_2$$

where the Z^{ij} are real numbers satisfying

$$\begin{cases}
\|\Pi_n^{H^1}DT(\bar{u})\Pi_n^{H^1}\|_{H^1} & \leq Z^{11},\\
\|\Pi_\infty^{H^1}DT(\bar{u})\Pi_n^{H^1}\|_{H^1} & \leq Z^{21},\\
\|\Pi_n^{H^1}DT(\bar{u})\Pi_\infty^{H^1}\|_{H^1} & \leq Z^{12},\\
\|\Pi_\infty^{H^1}DT(\bar{u})\Pi_\infty^{H^1}\|_{H^1} & \leq Z^{22}.
\end{cases} \tag{3.53}$$

Indeed, for $h\in\mathcal{H}$ with $\|h\|_{H^1}=1$, write $h=h_n+h_\infty$ such that $h_n\in\Pi_n^{H^1}(\mathcal{H})$, $h_\infty\in\Pi_\infty^{H^1}(\mathcal{H})$. Then,

$$\begin{aligned}
\|DT(\bar{u})h\|_{H^1} &= \sqrt{\|\Pi_n^{H^1}DT(\bar{u})h\|_{H^1}^2+\|\Pi_\infty^{H^1}DT(\bar{u})h\|_{H^1}^2}\\
&\leq \sqrt{\left(\|\Pi_n^{H^1}DT(\bar{u})h_n\|_{H^1}+\|\Pi_n^{H^1}DT(\bar{u})h_\infty\|_{H^1}\right)^2+\left(\|\Pi_\infty^{H^1}DT(\bar{u})h_n\|_{H^1}+\|\Pi_\infty^{H^1}DT(\bar{u})h_\infty\|_{H^1}\right)^2}
\end{aligned}$$

$$
\begin{aligned}
&\leq \sqrt{\left(Z^{11}\|h_n\|_{H^1} + Z^{12}\|h_\infty\|_{H^1}\right)^2 + \left(Z^{21}\|h_n\|_{H^1} + Z^{22}\|h_\infty\|_{H^1}\right)^2} \\
&= \left\| \begin{pmatrix} Z^{11} & Z^{12} \\ Z^{21} & Z^{22} \end{pmatrix} \begin{pmatrix} \|h_n\|_{H^1} \\ \|h_\infty\|_{H^1} \end{pmatrix} \right\|_2 \\
&\leq Z_1 \qquad \text{since } \|h_n\|_{H^1}^2 + \|h_\infty\|_{H^1}^2 = 1.
\end{aligned}
$$

In the following subsections, we derive computable bounds Z^{ij} satisfying (3.53).

The bound Z^{11}

For $h_n \in \Pi_n^{H^1}(\mathcal{H})$,

$$
\Pi_n^{H^1} DT(\bar{u})h_n = \Pi_n^{H^1}(\mathrm{id} - ADF(\bar{u}))h_n = (\Pi_n^{H^1} - A_n \Pi_n^{H^1} DF(\bar{u})\Pi_n^{H^1})h_n,
$$

by construction of A. Then, we get the estimate

$$
\begin{aligned}
\|\Pi_n^{H^1} DT(\bar{u})\Pi_n^{H^1}\|_{H^1,H^1} &= \|\Pi_n^{H^1} - A_n \Pi_n^{H^1} DF(\bar{u})\Pi_n^{H^1}\|_{H^1,H^1} \\
&= \|[\Pi_n^{H^1}]_{H^1} - [A_n]_{H^1}[\Pi_n^{H^1} DF(\bar{u})\Pi_n^{H^1}]_{H^1}\|_{\ell^2} =: Z^{11}.
\end{aligned}
$$

This quantity is expected to be very small as A_n is constructed as a numerical inverse of $[\Pi_n^{H^1} DF(\bar{u})\Pi_n^{H^1}]_{H^1}$. This estimate is only the two-norm of a finite-dimensional matrix and we bound this quantity via the inequality $\|A\|_{\ell^2} \leq \|A\|_{\ell^1}^{1/2}\|A\|_{\ell^\infty}^{1/2}$.

The bound Z^{21}

For $h_n \in \Pi_n^{H^1}(\mathcal{H})$, we have

$$
\begin{aligned}
\|\Pi_\infty^{H^1} DT(\bar{u})h_n\|_{H^1} &= \|\Pi_\infty^{H^1}(h_n - ADF(\bar{u})h_n\|_{H^1} \\
&= \|\Pi_\infty^{H^1} DF(\bar{u})h_n\|_{H^1} \\
&= \|\Pi_\infty^{H^1}(h_n - \tilde{\mathfrak{L}}^{-1} Df(\bar{u})h_n\|_{H^1} \\
&= \|\Pi_\infty^{H^1} \tilde{\mathfrak{L}}^{-1} Df(\bar{u})h_n\|_{H^1} \\
&\leq \|\Pi_\infty^{H^1} \tilde{\mathfrak{L}}^{-1} \Pi_n^{L^2} Df(\bar{u})h_n\|_{H^1} + \|\Pi_\infty^{H^1} \tilde{\mathfrak{L}}^{-1} \Pi_\infty^{L^2} Df(\bar{u})h_n\|_{H^1}.
\end{aligned}
$$

On the one hand, we have

$$
\begin{aligned}
\left[\Pi_\infty^{H^1} \tilde{\mathfrak{L}}^{-1} \Pi_n^{L^2} Df(\bar{u})h_n\right]_{H^1} &= \left[\Pi_\infty^{H^1} \tilde{\mathfrak{L}}^{-1} \Pi_n^{L^2}\right]_{L^2 \to H^1} \left[\Pi_n^{L^2} Df(\bar{u})\Pi_n^{H^1}\right]_{H^1 \to L^2} [h_n]_{H^1} \\
&= -\beta_n (D_{>n}^{-1})_{1,:} ((P_{\leq n}^{-1})_{:,n})^T \left[\Pi_n^{L^2} Df(\bar{u})\Pi_n^{H^1}\right]_{H^1 \to L^2} [h_n]_{H^1},
\end{aligned}
$$

such that

$$
\begin{aligned}
\|\Pi_\infty^{H^1} \tilde{\mathfrak{L}}^{-1} \Pi_n^{L^2} Df(\bar{u})h_n\|_{H^1} &\leq \beta_n \|(D_{>n}^{-1})_{1,:}\|_{\ell^2} \left\|((P_{\leq n}^{-1})_{:,n})^T \left[\Pi_n^{L^2} Df(\bar{u})\Pi_n^{H^1}\right]_{H^1 \to L^2}\right\|_{\ell^2} \|h_n\|_{H^1} \\
&\leq \frac{\beta_n}{C_\alpha \sqrt{1-\theta^2}} \frac{1}{n^{3/4}} \left\|((P_{\leq n}^{-1})_{:,n})^T \left[\Pi_n^{L^2} Df(\bar{u})\Pi_n^{H^1}\right]_{H^1 \to L^2}\right\|_{\ell^2} \|h_n\|_{H^1},
\end{aligned}
$$

using (3.52). On the other hand, we have

$$\Pi_\infty^{H^1}\tilde{\mathfrak{L}}^{-1}\Pi_\infty^{L^2}Df(\bar{u})h_n = \Pi_\infty^{H^1}\tilde{\mathfrak{L}}^{-1}\Pi_\infty^{L^2}(\omega h_n + h_0 - 3e^{-V}\bar{u}^2h_n) = -3\Pi_\infty^{H^1}\tilde{\mathfrak{L}}^{-1}\Pi_\infty^{L^2}(e^{-V}\bar{u}^2h_n).$$

Now, writing h_n as

$$h_n = \sum_{m=0}^{n} a_m q_m,$$

we get by linearity

$$\begin{aligned}
\|\Pi_\infty^{L^2}(e^{-V}\bar{u}^2h_n)\|_{L^2}^2 &= \left\|\sum_{m=0}^{n} a_m\Pi_\infty^{L^2}(e^{-V}\bar{u}^2q_m)\right\|_{L^2}^2 \\
&\le \left(\sum_{m=0}^{n}|a_m|\|\Pi_\infty^{L^2}(e^{-V}\bar{u}^2q_m)\|_{L^2}\right)^2 \\
&\le \left(\sum_{m=0}^{n}a_m^2\right)\left(\sum_{m=0}^{n}\|\Pi_\infty^{L^2}(e^{-V}\bar{u}^2q_m)\|_{L^2}^2\right) \qquad \text{By Cauchy–Schwarz inequality} \\
&\le \sum_{m=0}^{n}\|\Pi_\infty^{L^2}(e^{-V}\bar{u}^2q_m)\|_{L^2}^2 \qquad \text{Since } \|h_n\|_{H^1}=1 \\
&\le \sum_{m=0}^{n}\|e^{-V}\bar{u}^2q_m\|_{L^2}^2 - \|\Pi_n^{L^2}(e^{-V}\bar{u}^2q_m)\|_{L^2}^2 \qquad \text{By Parseval's identity.}
\end{aligned}$$

This implies that

$$\begin{aligned}
\|\Pi_\infty^{H^1}\tilde{\mathfrak{L}}^{-1}\Pi_\infty^{L^2}Df(\bar{u})h_n\|L^2 &\le \|\Pi_\infty^{H^1}\tilde{\mathfrak{L}}^{-1}\Pi_\infty^{L^2}\|_{L^2\to H^1}\|\Pi_\infty^{L^2}Df(\bar{u})h_n\|L^2 \\
&\le \frac{3C_{22}}{n^{3/4}}\left(\sum_{m=0}^{n}\|e^{-V}\bar{u}^2q_m\|_{L^2}^2 - \|\Pi_n^{L^2}(e^{-V}\bar{u}^2q_m)\|_{L^2}^2\right)^{1/2}\|h_n\|_{H^1},
\end{aligned}$$

using (3.49). Thus, we can choose

$$\begin{aligned}
Z^{21} :=& \frac{1}{n^{3/4}}\left\{\frac{\beta_n}{C_\alpha\sqrt{1-\theta^2}}\left\|((P_{\le n}^{-1})_{:,n})^T\left[\Pi_n^{L^2}Df(\bar{u})\Pi_n^{H^1}\right]_{H^1\to L^2}\right\|_{\ell^2}\right. \\
&\left. + 3C_{22}\left(\sum_{m=0}^{n}\|e^{-V}\bar{u}^2q_m\|_{L^2}^2 - \|\Pi_n^{L^2}(e^{-V}\bar{u}^2q_m)\|_{L^2}^2\right)^{1/2}\right\}.
\end{aligned}$$

The bound Z^{12}

For $h_\infty \in \Pi_\infty^{H^1}(\mathcal{H})$, we have

$$\begin{aligned}
\|\Pi_n^{H^1}DT(\bar{u})h_\infty\|_{H^1} &= \|\Pi_n^{H^1}(h_\infty - ADF(\bar{u})h_\infty)\|_{H^1} \\
&= \|A_n\Pi_n^{H^1}DF(\bar{u})h_\infty\|_{H^1} \\
&= \|A_n\Pi_n^{H^1}(h_\infty - \tilde{\mathfrak{L}}^{-1}Df(\bar{u})h_\infty)\|_{H^1} \\
&= \|A_n\Pi_n^{H^1}\tilde{\mathfrak{L}}^{-1}Df(\bar{u})h_\infty\|_{H^1} \\
&= \|A_n\Pi_n^{H^1}\tilde{\mathfrak{L}}^{-1}\Pi_n^{L^2}Df(\bar{u})h_\infty\|_{H^1}
\end{aligned}$$

$$\leq \|A_n \Pi_n^{H^1} \tilde{\mathfrak{L}}^{-1} \Pi_n^{L^2} (Df(\bar{u}) \Pi_n^{L^2} h_\infty)\|_{H^1} + \|A_n \Pi_n^{H^1} \tilde{\mathfrak{L}}^{-1} \Pi_n^{L^2} (Df(\bar{u}) \Pi_\infty^{L^2} h_\infty)\|_{H^1}.$$

Note that $h_\infty = \Pi_\infty^{H^1} h$, where the projection is the H^1 one, therefore $\Pi_n^{L^2} h_\infty$ is not equal to 0. We start with the first term, for which we have

$$\begin{aligned}
&\left[A_n \Pi_n^{H^1} \tilde{\mathfrak{L}}^{-1} \Pi_n^{L^2} (Df(\bar{u}) \Pi_n^{L^2} h_\infty)\right]_{H^1} \\
&= [A_n]_{H^1} \left[\Pi_n^{H^1} \tilde{\mathfrak{L}}^{-1} \Pi_n^{L^2}\right]_{L^2 \to H^1} \left[\Pi_n^{L^2} Df(\bar{u}) \Pi_n^{L^2}\right]_{L^2} \left[\Pi_n^{L^2} \iota \Pi_\infty^{H^1}\right]_{H^1 \to L^2} [h_\infty]_{H^1} \\
&= -\,[A_n]_{H^1} (P_{\leq n}^{-1})^T \left[\Pi_n^{L^2} Df(\bar{u}) \Pi_n^{L^2}\right]_{L^2} \beta_n (P_{\leq n}^{-1})_{:,-1} (D_{>n}^{-1})_{1,:} [h_\infty]_{H^1}.
\end{aligned}$$

where we used that $[\iota]_{L^2 \to H^1} = P^{-1}$ and its carving given by (3.37). We thus get

$$\begin{aligned}
&\|A_n \Pi_n^{H^1} \tilde{\mathfrak{L}}^{-1} \Pi_n^{L^2} (Df(\bar{u}) \Pi_n^{L^2} h_\infty)\|_{H^1} \\
\leq &\beta_n \left\| [A_n]_{H^1} (P_{\leq n}^{-1})^T \left[\Pi_n^{L^2} Df(\bar{u}) \Pi_n^{L^2}\right]_{L^2} (P_{\leq n}^{-1})_{:,-1} \right\|_{\ell^2} \left\|(D_n^{-1})_{1,:}\right\|_{\ell^2} \|h_\infty\|_{H^1} \\
= &\frac{\beta_n}{C_\alpha \sqrt{1-\theta^2}} \frac{1}{n^{3/4}} \left\| [A_n]_{H^1} (P_{\leq n}^{-1})^T \left[\Pi_n^{L^2} Df(\bar{u}) \Pi_n^{L^2}\right]_{L^2} (P_{\leq n}^{-1})_{:,-1} \right\|_{\ell^2} \|h_\infty\|_{H^1},
\end{aligned}$$

where we have used (3.52). For the second term, we have

$$\Pi_n^{L^2} Df(\bar{u}) \Pi_\infty^{L^2} h_\infty = \Pi_n^{L^2} ((\omega - 3e^{-V}\bar{u}^2) \Pi_\infty^{L^2} h_\infty) = -3\Pi_n^{L^2} (e^{-V}\bar{u}^2 \Pi_\infty^{L^2} h_\infty),$$

and we now estimate each coefficient of the above term

$$\begin{aligned}
|\langle p_m, e^{-V}\bar{u}^2 \Pi_\infty^{L^2} h_\infty\rangle| &= |\langle p_m e^{-V}\bar{u}^2, \Pi_\infty^{L^2} h_\infty\rangle| \\
&= |\langle \Pi_\infty^{L^2} (p_m e^{-V}\bar{u}^2), \Pi_\infty^{L^2} h_\infty\rangle| \\
&\leq \|\Pi_\infty^{L^2} (p_m e^{-V}\bar{u}^2)\|_{L^2} \|\Pi_\infty^{L^2} h_\infty\|_{L^2} \\
&\leq \left(\|p_m e^{-V}\bar{u}^2\|_{L^2}^2 - \|\Pi_n^{L^2} (p_m e^{-V}\bar{u}^2)\|_{L^2}^2\right)^{1/2} \|D_{>n}^{-1}\|_{\ell^2} \|h_\infty\|_{H^1} \\
&\leq \frac{C_{22}}{n^{3/4}} \left(\|p_m e^{-V}\bar{u}^2\|_{L^2}^2 - \|\Pi_n^{L^2} (p_m e^{-V}\bar{u}^2)\|_{L^2}^2\right)^{1/2} \|h_\infty\|_{H^1} \qquad \text{using (3.38).}
\end{aligned}$$

Finally, writing $w_m = [-1,1] \left(\|p_m e^{-V}\bar{u}^2\|_{L^2}^2 - \|\Pi_n^{L^2} (p_m e^{-V}\bar{u}^2)\|_{L^2}^2\right)^{1/2}$, we obtain

$$\begin{aligned}
\|A_n \Pi_n^{H^1} \tilde{\mathfrak{L}}^{-1} \Pi_n^{L^2} (Df(\bar{u}) \Pi_\infty^{L^2} h_\infty)\|_{H^1} &\leq \frac{3C_{22}}{n^{3/4}} \left\| [A_n]_{H^1} \left[\Pi_n^{H^1} \tilde{\mathfrak{L}}^{-1} \Pi_n^{L^2}\right]_{L^2 \to H^1} w \right\|_{\ell^2} \\
&\leq \frac{3C_{22}}{n^{3/4}} \left\| [A_n]_{H^1} (P_{\leq n}^{-1})^T w \right\|_{\ell^2}.
\end{aligned}$$

We can therefore choose

$$Z^{12} := \frac{1}{n^{3/4}} \left\{ \frac{\beta_n}{C_\alpha \sqrt{1-\theta^2}} \left\| [A_n]_{H^1} (P_{\leq n}^{-1})^T \left[\Pi_n^{L^2} Df(\bar{u}) \Pi_n^{L^2}\right]_{L^2} (P_{\leq n}^{-1})_{:,-1} \right\|_{\ell^2} + 3C_{22} \left\| [A_n]_{H^1} (P_{\leq n}^{-1})^T w \right\|_{\ell^2} \right\}.$$

The bound Z^{22}

For $h_\infty \in \Pi_\infty^{H^1}(\mathcal{H})$,

$$\|\Pi_\infty^{H^1} DT(\bar{u}) h_\infty\|_{H^1} = \|h_\infty - \Pi_\infty^{H^1} ADF(\bar{u}) h_\infty\|_{H^1}$$

$$
\begin{aligned}
&= \|h_\infty - \Pi_\infty^{H^1} DF(\bar{u})h_\infty\|_{H^1} \\
&= \|h_\infty - \Pi_\infty^{H^1}(h_\infty - \tilde{\mathfrak{L}}^{-1} Df(\bar{u})h_\infty)\|_{H^1} \\
&= \|\Pi_\infty^{H^1} \tilde{\mathfrak{L}}^{-1} Df(\bar{u})h_\infty\|_{H^1} \\
&= \|\Pi_\infty^{H^1} \tilde{\mathfrak{L}}^{-1}(\omega - 3e^{-V}\bar{u}^2)h_\infty\|_{H^1} \\
&\leq \|\Pi_\infty^{H^1} \tilde{\mathfrak{L}}^{-1}\|_{L^2\to H^1} \|(\omega - 3e^{-V}\bar{u}^2)h_\infty\|_{L^2} \\
&\leq \frac{C}{n^{3/4}} \|(\omega - 3e^{-V}\bar{u}^2)\|_\infty \|h_\infty\|_{L^2} \qquad \text{by Hölder's inequality and (3.49)} \\
&\leq \frac{C^2}{n^{3/2}} \left\{ 3\|e^{-V/2}\bar{u}\|_\infty^2 + |\omega| \right\} \|h_\infty\|_{H^1} \qquad \text{by Theorem 3.4.}
\end{aligned}
$$

We thus choose

$$
Z^{22} := \frac{C^2}{n^{3/2}} \left\{ 3\|e^{-V/2}\bar{u}\|_\infty^2 + |\omega| \right\}.
$$

While other methods are possible, in practice, we simply use the estimate (3.43) to bound $\|e^{-V/2}\bar{u}\|_\infty$.

Note that our estimates are sharp in the sense that they agree with the estimates of the diagonal case (See Section 2.4.1) and that we observe in practice that Z^{22} is the largest of the Z^{ij}'s.

The bound Z_2

We have that for $h \in \mathcal{H}$,

$$
\begin{aligned}
\|D^2T(\bar{u})h^2\|_{H^1} &= \|AD^2F(\bar{u})h^2\|_{H^1} \\
&\leq \|A\|_{H^1} \|D^2F(\bar{u})h^2\|_{H^1} \\
&\leq \|A\|_{H^1} \|\tilde{\mathfrak{L}}^{-1}(D^2(\bar{u})h^2)\|_{H^1} \\
&\leq \|A\|_{H^1} \|\tilde{\mathfrak{L}}^{-1}\|_{L^2\to H^1} \|(D^2(\bar{u})h^2)\|_{L^2} \\
&\leq 6\|A\|_{H^1} \|(P^{-1})^T\|_{\ell^2} \|e^{-V}\bar{u}h^2\|_{L^2} \\
&\leq 6\|A\|_{H^1} \|P^{-1}\|_{\ell^2} \|\bar{u}\|_{L^2} \|e^{-V/2}h\|_\infty^2 \qquad \text{By Hölder's inequality} \\
&\leq 6\max(1, C_P)\|A\|_{H^1} \|\bar{u}\|_{L^2} (\sqrt{Z(c+1)}\max(1, C_P)^{1/4}\|h\|_{H^1})^2 \qquad \text{by (3.43)} \\
&\leq 6Z(c+1)\max(1, C_P)^{3/2} \|A\|_{H^1} \|\bar{u}\|_{L^2} \|h\|_{H^1}^2.
\end{aligned}
$$

We can thus choose

$$
Z_2 := 6Z(c+1)\max(1, C_P)^{3/2} \|A\|_{H^1} \|\bar{u}\|_{L^2}
$$

where $\|A\|_{H^1} = \max\{\|A_n\|_{H^1}, 1\}$.

The bound Z_3

Directly from the above bound we obtain that $h \in \mathcal{H}$,

$$
\begin{aligned}
\|D^3T(\bar{u})h^3\|_{H^1} &\leq 6\|A\|_{H^1} \|(P^{-1})^T\|_{\ell^2} \|e^{-V}h^3\|_{L^2} \qquad \text{by (3.43)} \\
&\leq 6Z(c+1)\max(1, C_P)^{3/2} \|A\|_{H^1} \|h\|_{L^2} \|h\|_{H^1}^2 \\
&\leq 6Z(c+1)\max(1, C_P)^{5/2} \|A\|_{H^1} \|h\|_{H^1}^3.
\end{aligned}
$$

and thus choose

$$Z_3 := 6Z(c+1)\max(1, C_P)^{5/2}\|A\|_{H^1}.$$

3.4.3 Proof of positivity in Theorem 1.9

To prove the positivity of φ_1^* in Theorem 1.9, we again rely on Lemma 2.30. By a usual bootstrap argument, if $\varphi = e^{-V/2}u \in H^1(\mathbb{R})$ is a solution to

$$-\partial_{xx}\varphi + W\varphi + \varphi^3 - \omega\varphi = 0,$$

then $\varphi \in \mathcal{C}^\infty(\mathbb{R}_+)$. Furthermore, since $\varphi \in H^1(\mathbb{R})$, by [61, Corollary VIII.8], $\lim_{r\to+\infty}\varphi(x) = 0$ as $|x| \to \infty$. We choose $c = W + \varphi^2 - \omega \in \mathcal{C}^\infty$. Denoting $\bar{\varphi} = e^{-V/2}\bar{u}$, by Lemma 3.38, we have that

$$\|\varphi - \bar{\varphi}\|_\infty \leq \sqrt{Z(c+1)}\max(1, C_P)^{1/4}\delta, \qquad \text{where } \|u - \bar{u}\|_{H^1(\nu)} \leq \delta \tag{3.54}$$

and

$$\|\varphi\|_\infty \leq \sqrt{Z(c+1)}\max(1, C_P)^{1/4}\|u\|_{H^1(\nu)} \leq \sqrt{Z(c+1)}\max(1, C_P)^{1/4}(\|\bar{u}\|_{H^1(\nu)} + \delta).$$

That allows us to find a positive real r_0 such that $c(x) = W(x) + \varphi^2(x) - \omega \geq W(x) - \omega > 0$ for all $|x| \geq r_0$. Then using the estimate (3.54) and rigorously evaluating $\bar{\varphi}$ on $[-r_0, r_0]$ finishes verifying the assumptions of Lemma 2.30.

4

Going back to the dynamics of the Hopf normal form

We now come back to the *fil rouge* of this thesis introduced in Section 1.1, namely the computation of the Lyapunov exponent λ_b of the stochastic flow $(\varphi_t)_{t\geq 0}$ induced by the Hopf normal form with additive noise

$$\mathrm{d}\begin{pmatrix} x_t \\ y_t \end{pmatrix} = \left[\begin{pmatrix} \alpha & -\beta \\ \beta & \alpha \end{pmatrix} \begin{pmatrix} x_t \\ y_t \end{pmatrix} - \begin{pmatrix} a & b \\ -b & a \end{pmatrix} \begin{pmatrix} x_t \\ y_t \end{pmatrix} (x_t^2 + y_t^2) \right] \mathrm{d}t + \sigma \mathrm{d} \begin{pmatrix} B_t^1 \\ B_t^2 \end{pmatrix}. \tag{4.1}$$

This system was first introduced in [94] in the context of random dynamical systems as a simple perturbation of the deterministic Hopf normal form. See also [95, 207, 229] for applications to ocean and laser dynamics. This system has been conjectured (see also [97]) to exhibit the *shear-induced chaos* scenario proposed in [165], for which the perturbation of a limit cycle induces a stretch-and-fold mechanism leading to chaos. This conjecture can be quantitatively translated into proving a transition from a negative to positive Lyapunov exponent λ_b as b increases. This problem was already attacked with computer-assisted techniques in [57], but this work only managed to establish such a transition for the *conditioned* Lyapunov exponent [72, 101], which in particular meant restricting the problem to a bounded domain. In this chapter, we first derive again the simplified Furstenberg–Khasminskii formula (1.19) for the Hopf normal form in Section 4.1 (based on [55, §6]). In the rest of this chapter, we present an attempt to enclose this Lyapunov exponent via the usual strategy of enclosing the solution of the Fokker–Planck equation (1.21). While this attempt was not quite successful, some ideas may remain useful in the theory of computer-assisted proofs for PDEs or in the analysis of the the Fokker–Planck equation (1.21).

4.1 Derivation of the Furstenberg–Khasminskii formula

As in [24, 57, 73, 94], we prepare the problem by reducing the formula for λ_b to an integral over the ergodic measure μ of a two-dimensional and uniformly elliptic diffusion.

In polar coordinates $x_t = r_t \cos\phi_t, y_t = r_t \sin\phi_t$, we have

$$\begin{cases} \mathrm{d}r_t &= \left(\alpha r_t - a r_t^3 + \dfrac{\sigma^2}{2r_t}\right)\mathrm{d}t + \sigma \mathrm{d}B_t^r \\ \mathrm{d}\phi_t &= (\beta + b r_t^2)\mathrm{d}t + \dfrac{\sigma}{r_t}\mathrm{d}B_t^\phi \end{cases} \tag{4.2}$$

where B_t^r, B_t^ϕ are independent Brownian motions

$$\mathrm{d}\begin{pmatrix} B_t^r \\ B_t^\phi \end{pmatrix} = \begin{pmatrix} \cos\phi_t & \sin\phi_t \\ -\sin\phi_t & \cos\phi_t \end{pmatrix} \mathrm{d}\begin{pmatrix} B_t^1 \\ B_t^2 \end{pmatrix}.$$

Now recall that we have the almost-sure limit

$$\lambda_b = \lim_{t\to\infty} \frac{1}{t} \log \|D\varphi_t v\|,$$

for $v \in \mathbb{S}^1$. We thus introduce

$$\varrho_t(\omega, x, v) = \|D\varphi_t(\omega, x)v\| \qquad \text{and} \qquad s_t(\omega, x, v) = \frac{D\varphi_t(\omega, x)v}{\|D\varphi_t(\omega, x)v\|} \in T_{\varphi_t(\omega,x)}\mathcal{M}. \tag{4.3}$$

and further writing $(s_t)_{t\geq 0} = (\cos\theta_t, \sin\theta_t)_{t\geq 0}$, we obtain

$$\begin{cases} \mathrm{d}\varrho_t &= \left(\alpha - 2ar_t^2 + \sqrt{a^2+b^2}\, r_t^2 \sin(2\theta_t - \chi_0 - 2\phi_t)\right)\varrho_t \mathrm{d}t \\ \mathrm{d}\theta_t &= \left(\beta + 2br_t^2 + \sqrt{a^2+b^2}\, r_t^2 \cos(2\theta_t - \chi_0 - 2\phi_t)\right)\mathrm{d}t \end{cases} \tag{4.4}$$

where $\chi_0 = \arccos(b/\sqrt{a^2+b^2})$. Now, letting $\vartheta_t = \theta_t - \chi_0/2 - \phi_t$ and subtracting (4.4) by (4.2), we obtain

$$\begin{cases} \mathrm{d}r_t &= \left(\alpha r_t - a r_t^3 + \dfrac{\sigma^2}{2r_t}\right)\mathrm{d}t + \sigma \mathrm{d}B_t^r & (4.5) \\ \mathrm{d}\vartheta_t &= \left(b r_t^2 + \sqrt{a^2+b^2}\, r_t^2 \cos(2\vartheta_t)\right)\mathrm{d}t - \dfrac{\sigma}{r_t}\mathrm{d}B_t^\phi & (4.6) \\ \mathrm{d}\varrho_t &= Q(r_t, \vartheta_t)\varrho_t \mathrm{d}t & (4.7) \end{cases}$$

where

$$Q(r, \vartheta) = \alpha - 2ar^2 + \sqrt{a^2+b^2}\, r^2 \sin 2\vartheta.$$

Since

$$\varrho_t = \exp\left(\int_0^t Q(\varphi_t, \vartheta_\tau)\mathrm{d}\tau\right),$$

by Birkhoff's ergodic theorem, we have almost-surely

$$\lambda_b = \lim_{t\to\infty} \frac{1}{t} \log \|D\varphi_t v\|$$

$$
\begin{aligned}
&= \lim_{t\to\infty} \frac{1}{t} \log \varrho_t \\
&= \lim_{t\to\infty} \frac{1}{t} \int_0^t Q(\varphi_t, \vartheta_\tau) \mathrm{d}\tau \\
&= \int_{\mathbb{R}_+ \times \mathbb{T}} Q(r, \vartheta) \mu(\mathrm{d}r, \mathrm{d}\vartheta),
\end{aligned}
$$

where μ is the unique stationary distribution of $(r_t, \vartheta_t)_{t\geq 0}$ given by Eq. (4.5)–(4.6). Note that this is a slightly different formulation than in [24, 57, 73, 94, 97] which factors in an additional symmetry. Our formulation turns out to be more practical for numerical purposes as it allows us to recover the polar coordinate Laplacian while still exploiting this symmetry. Indeed, we get that the generator of $(\xi_t)_{t\geq 0} = (r_t, \vartheta_t)_{t\geq 0}$ is

$$
\mathcal{L} = (\alpha r - a r^3) \frac{\partial}{\partial r} + \left(b r^2 + \sqrt{a^2 + b^2} r^2 \cos 2\vartheta \right) \frac{\partial}{\partial \vartheta} + \frac{\sigma^2}{2} \Delta
$$

where Δ is the polar coordinate Laplacian

$$
\Delta = \frac{1}{r} \frac{\partial}{\partial r} \left(r \frac{\partial}{\partial r} \right) + \frac{1}{r^2} \frac{\partial^2}{\partial \vartheta^2}.
$$

Moreover, note that since the generator $\mathcal{L}$ of $(r_t, \vartheta_t)_{t\geq 0}$ is uniformly elliptic and e.g. has $e^{ar^4/(4\sigma^2)}$ as a Lyapunov function, the process $(r_t, \vartheta_t)_{t\geq 0}$ indeed has a unique stationary measure μ on $\mathbb{R}^2 \simeq \mathbb{R}_+ \times \mathbb{T}$ [175]. We can thus write the Lyapunov exponent λ_b as

$$
\lambda_b = \int_{\mathbb{R}_+ \times \mathbb{T}} Q(r, \vartheta) w(r, \vartheta) \mathrm{d}r \mathrm{d}\vartheta, \tag{4.8}
$$

where $\mu(\mathrm{d}r, \mathrm{d}\vartheta) = w(r, \vartheta) \mathrm{d}r \mathrm{d}\vartheta$ and w is the mass one solution of the stationary Fokker-Planck equation

$$
-r^2 \frac{\partial}{\partial \vartheta} \left(\left(b + \sqrt{a^2 + b^2} \cos(2\vartheta) \right) w \right) - \frac{\partial}{\partial r} \left(\left(\alpha r - a r^3 + \frac{\sigma^2}{2r} \right) w \right) + \frac{\sigma^2}{2} \left(\frac{\partial^2 w}{\partial r^2} + \frac{1}{r^2} \frac{\partial^2}{\partial \vartheta^2} \right) = 0. \tag{4.9}
$$

4.2 Reformulation of the Fokker–Planck equation

In the rest of this chapter *only*, we make a further changes of variables and unknown and restrict ourselves to the case $\alpha = 0$. First, we write

$$
w(r, \vartheta) = (1 + u(r, \vartheta)) \frac{p(r)}{2\pi}, \tag{4.10}
$$

where $p(r) = \dfrac{2}{\sigma} \sqrt{\dfrac{2a}{\pi}} r \exp\left(\dfrac{a}{2\sigma^2} r^4 \right)$ is the stationary probability density of the radial process $(r_t)_{t\geq 0}$, and thus marginal of w onto r. Then making the change of variables

$$
r \mapsto \sqrt{\sigma r \sqrt{\frac{2}{a}}}, \qquad \vartheta \mapsto \frac{\vartheta}{2}, \qquad b \mapsto ab,
$$

we obtain the equation

$$2\partial_\vartheta\left(\left(\sqrt{1+b^2}\cos\vartheta+b\right)u\right)+2r\partial_r u-\Delta u=2\sqrt{1+b^2}\sin\vartheta \tag{4.11}$$

where $\Delta\cdot=\frac{1}{r}\partial_r(r\partial_r\cdot)+\frac{1}{r^2}\partial_{\vartheta\vartheta}\cdot$ is the polar-coordinate Laplacian on $\mathbb{R}^2\simeq\mathbb{R}_+\times\mathbb{T}$. Additionally, the Furstenberg–Khasminskii formula (4.8) becomes

$$\lambda_b=\sqrt{\frac{2a}{\pi}}\sigma\int_0^{2\pi}\int_0^\infty\left(\sqrt{1+b^2}\sin\vartheta-2\right)(1+u(r,\vartheta))\nu(\mathrm{d}r,\mathrm{d}\vartheta),\qquad \nu(\mathrm{d}r,\mathrm{d}\vartheta):=\frac{re^{-r^2}}{\pi}\mathrm{d}r\mathrm{d}\vartheta. \tag{4.12}$$

In order to apply the Newton–Kantorovich Theorem 1.1, as in Chapters 2 and 3, we need to identify a splitting

$$\mathfrak{L}u+\mathfrak{B}u=2\partial_\vartheta\left(\left(\sqrt{1+b^2}\cos\vartheta+b\right)u\right)+2r\partial_r u-\Delta u=2\sqrt{1+b^2}\sin\vartheta=f \tag{4.13}$$

of Eq. (4.11) such that $\mathfrak{L}$ is an easily invertible operator, ideally dominating the other term $\mathfrak{B}$ of the equation, in order to obtain an equivalent zero-finding problem

$$F(u)=u-\mathfrak{L}^{-1}(\mathfrak{B}u-f),\qquad f=2\sqrt{1+b^2}\sin\vartheta,$$

where F is a Banach self-mapping (and hopefully DF a compact perturbation of the identity).

We could for instance split the partial differential equation (4.11) as $\mathfrak{L}u+\mathfrak{B}u=f$ with

$$\mathfrak{L}u=2r\partial_r u-\Delta u,\qquad \mathfrak{B}u=2\partial_\vartheta\left(\left(\sqrt{1+b^2}\cos\vartheta+b\right)u\right), \tag{4.14}$$

where $\mathfrak{L}$ is the well-known and well-invertible part of the equation. Indeed, as in Chapter 3, $\mathfrak{L}$ is a nonnegative self-adjoint operator on $L^2(\nu)$ where $\nu(\mathrm{d}r,\mathrm{d}\vartheta)=(re^{-r^2}/\pi)\mathrm{d}r\mathrm{d}\vartheta$ on $\mathbb{R}_+\times\mathbb{T}\simeq\mathbb{R}^2$ (with a shift by $d/2$, it is actually equivalent to the operator L of Chapter 2). Note that $-\mathfrak{L}$ is the infinitesimal generator of a radially symmetric Ornstein–Uhlenbeck process. Furthermore, the spectrum of $\mathfrak{L}$ is well-known:

$$\mathfrak{L}H_n^m=2(|m|+2n)H_n^m,\qquad H_n^m(r,\vartheta)=r^{|m|}e^{im\vartheta}L_n^{(|m|)}(r^2), \tag{4.15}$$

where $L_n^{(\alpha)}$ denotes the generalised Laguerre polynomial of degree n and parameter α (see [1, p. 775]). The H_n^m's are sometimes known as Hermite polynomials of complex variables [142] or Hermite–Laguerre–Itô polynomials [75] and are unweighted and rescaled polynomial versions of the basis (2.12). By the spectral theorem, they form an orthogonal basis of $L^2(\nu)$.

However, we can choose a slightly better splitting than (4.14) with

$$\mathfrak{L}u=2b\partial_\vartheta u+2r\partial_r u-\Delta u,\qquad \mathfrak{B}u=2\partial_\vartheta\left(\left(\sqrt{1+b^2}\cos\vartheta\right)u\right),\qquad f=2\sqrt{1+b^2}\sin\vartheta, \tag{4.16}$$

where $\mathfrak{L}$ is now the generator of an Ornstein–Uhlenbeck process with radius-independent rotational speed b and is now "more dominant" than previously. While the eigenfunctions remain the same, the spectrum is now shifted away from the real line. That is, we now have

$$\mathfrak{L}H_n^m=2(ibm+|m|+2n)H_n^m \tag{4.17}$$

Concerning the choice of functional space for the resolution of Eq. (4.11), since we only need to compute the integral (4.12) where $\left(\sqrt{1+b^2}\sin\vartheta - 2\right) \in L^2(\nu)$, it is sufficient to enclose u in $L^2(\nu)$. We could choose u to have ν-mean zero, but by definition (4.10) of u, since the marginal of w onto r is p, it is clear that we can even take u to have angular-mean zero. Thus, we could attempt to enclose u in the space

$$L^2_\vartheta(\nu) = \left\{ v \in L^2(\nu) \mid \int_0^{2\pi} v(r,\vartheta)\mathrm{d}\vartheta = 0 \right\} = \overline{\mathrm{Span}\{H_n^m\}_{m\in\mathbb{Z}^*, n\in\mathbb{N}}}^{L^2(\nu)}$$

Therefore, since $\mathfrak{L}$ is invertible on $L^2_\vartheta(\nu)$ by (4.17), we can choose to solve the zero-finding problem

$$F(u) = u + \mathfrak{L}^{-1}(\mathfrak{B}u - f) = 0, \tag{4.18}$$

where $\mathfrak{L}$, $\mathfrak{B}$ and f are as in (4.16) and $L^2_\vartheta(\nu)$ is invariant under F. With $u \in L^2_\vartheta(\nu)$, we can actually simplify our formula (4.12) further to

$$\lambda_b = \sqrt{\frac{2a}{\pi}}\sigma\left(-\frac{1}{\pi} + \sqrt{1+b^2}\int_0^{2\pi}\int_0^\infty \sin\vartheta u(r,\vartheta)\nu(\mathrm{d}r,\mathrm{d}\vartheta)\right) \tag{4.19}$$

Remark 4.1. Note that the equation (4.11) does not have real analytic/polynomial coefficients when considered on $\mathbb{R}^2 \simeq \mathbb{R}_+ \times \mathbb{T}$. Indeed, under the change of variable $\tilde{x} = r\cos\vartheta, \tilde{y} = r\sin\vartheta$, $\cos\vartheta\partial_\vartheta = (\tilde{x}/\sqrt{\tilde{x}^2+\tilde{y}^2})(-\tilde{y}\partial_{\tilde{x}} + \tilde{x}\partial_{\tilde{y}})$.

Note that $u \mapsto \partial_\vartheta u$ (and thus $u \mapsto \partial_\vartheta(u\cos\vartheta)$ and $\mathfrak{B}$) is not relatively compact with respect to $\mathfrak{L}$. This can actually be seen directly from the difference between (4.15) and (4.17). More heuristically, it is well-known that, if $u \in H^1(\nu) = H^1(re^{-r^2}/\pi)$ is multiplied by r, one can in general only say that $ru \in L^2(\nu)$, that is $u \mapsto ru$ loses one order of regularity. Clearly, ∂_ϑ/r (as the second component of $\nabla = (\partial_r, \partial_\vartheta/r)$) is also equivalent to taking a derivative such that if $u \in H^2(\nu)$, one cannot hope for $u \mapsto \partial_\vartheta(\cos\vartheta u) : H^2(\nu) \to L^2(\nu)$ to be compact. Therefore, $\mathfrak{L}^{-1}\mathfrak{B}$ is not compact on $L^2_\vartheta(\nu)$ and this fact will be shown more precisely in the following section. This means that we will not be able to apply the method laid out in Chapter 1 and used in Chapters 2 and 3.

4.3 A nearly working strategy

Let us first observe that in the definition (4.18) of F, the only term that can map an angular frequency to another is $\mathfrak{L}^{-1}\mathfrak{B}$; and more precisely the map $u \mapsto \cos\vartheta u$ which maps the angular frequency m to the angular frequencies $m\pm 1$. Since we are seeking a solution $L^2_\vartheta(\nu)$, i.e. of angular mean zero, we can further decouple the problem as

$$F_\pm(u) = u + \mathfrak{L}^{-1}(\mathfrak{B}u - f_\pm) = 0, \qquad f_\pm = \pm\frac{e^{\pm i\vartheta}}{2i}. \tag{4.20}$$

where $\mathfrak{L}$ and $\mathfrak{B}$ remain as in (4.16). That is we can work on positive and negative frequencies separately; without loss of generality, by symmetry, we can only consider the positive frequencies, i.e. work on the space

$$\mathcal{H}_+ = \overline{\bigoplus_{m\in\mathbb{N}^*} \mathcal{H}_m}^{L^2(\nu)}, \qquad \mathcal{H}_m = \overline{\mathrm{Span}\{H_n^m\}_{n\in\mathbb{N}}}^{L^2(\nu)} \simeq L^2(2re^{-r^2}\mathrm{d}r).$$

Therefore, the operator $\mathfrak{L}^{-1}\mathfrak{B}$ on $\mathcal{H}_+$ can be decomposed as

$$\mathfrak{L}^{-1}\mathfrak{B} = \begin{pmatrix} & \boxed{\mathfrak{L}_1^{-1}\mathfrak{B}_{12}} & & \\ \boxed{\mathfrak{L}_2^{-1}\mathfrak{B}_{21}} & & \boxed{\mathfrak{L}_2^{-1}\mathfrak{B}_{23}} & \\ & \boxed{\mathfrak{L}_3^{-1}\mathfrak{B}_{32}} & & \ddots \\ & & \ddots & \end{pmatrix}$$

where $\mathfrak{B}_{m,m\pm1}$ is the action of $\mathfrak{B}$ on $\mathcal{H}_{m\pm1}$ projected on $\mathcal{H}_m$ and similarly for $\mathfrak{L}_m$. While the operator $\mathfrak{B}$ seems straightforward, as only involving simple operations in the variable ϑ; if we then want to apply $\mathfrak{L}_m^{-1}$, we actually need to make a change of basis which can be rather intricate. For instance, it is clear that the action of $\mathfrak{B}$ on $\mathcal{H}_{m\pm1}$ projected on $\mathcal{H}_m$, i.e. $\mathfrak{B}_{m,m\pm1}$, necessitates a change of basis from $\{r^{m\pm1}L_n^{(m\pm1)}(r^2)\}_{n\in\mathbb{N}}$ (odd polynomials in r if m is even) to $\{r^m L_n^{(m)}(r^2)\}_{n\in\mathbb{N}}$ (even polynomials in r if m is even). It thus appears impossible to invert $DF_+ = \mathrm{id} + \mathfrak{L}^{-1}\mathfrak{B}$ (or at least part of it) by hand.

Furthermore, to have some chance of inverting DF via a computer-assisted techniques used in Chapters 2 and 3 via Theorem 1.1, we would need for $\|\mathfrak{L}_m^{-1}\mathfrak{B}_{m,m\pm1}\|_{L^2(\nu)} \to 0$ as $m \to +\infty$. We are actually able to show the following:

Lemma 4.2. For all $m \in \mathbb{N}^*$, $\|\mathfrak{L}_m^{-1}\mathfrak{B}_{m,\pm1}\|_{L^2(\nu)} = 1/2$.

Proof. We first show that $\|\mathfrak{L}_m^{-1}\mathfrak{B}_{m,m\pm1}\|_{L^2(\nu)} \le 1/2$. Let $e^{i(m\pm1)\vartheta}v(r) \in \mathcal{H}_{m\pm1}$, then $\mathfrak{B}_{m,m\pm1}(e^{i(m\pm1)\vartheta}v) = i\sqrt{1+b^2}me^{im\vartheta}v$. Therefore, since $\|e^{i(m\pm1)\vartheta}v\|_{L^2(\nu)} = \|e^{im\vartheta}v\|_{L^2(\nu)}$, we have that $\|\mathfrak{B}_{m,m\pm1}\|_{L^2(\nu)} = |i\sqrt{1+b^2}m| = \sqrt{1+b^2}m$. By looking at the spectrum of $\mathfrak{L}$ (4.17), it is clear that

$$\|\mathfrak{L}_m^{-1}\|_{L^2(\nu)} = \min_{n\in\mathbb{N}} |2(ibm + |m| + 2n)| = 2\min\sqrt{b^2m^2 + (m+2n)^2} = 2\sqrt{1+b^2}.$$

Therefore, by submultiplicativity $\|\mathfrak{L}_m^{-1}\mathfrak{B}_{m,m\pm1}\|_{L^2(\nu)} \le 1/2$

We now prove that $\|\mathfrak{L}_m^{-1}\mathfrak{B}_{m,m\pm1}\|_{L^2(\nu)} \ge 1/2$. Take $v(r) = r^m L_0^{(m)}(r^2)$ such that $e^{i(m\pm1)}v \in L^2(\nu)$. Then, by (4.17), since $\mathfrak{L}_m(e^{im\vartheta}v) = \mathfrak{L}H_0^m = 2m(1+ib)H_0^m = 2m(1+ib)e^{im\vartheta}v$, as previously

$$\mathfrak{L}_m^{-1}\mathfrak{B}_{m,m\pm1}(e^{i(m\pm1)\vartheta}v) = i\sqrt{1+b^2}m\mathfrak{L}_m^{-1}(e^{im\vartheta}v) = \frac{i\sqrt{1+b^2}m}{2m(1+ib)}e^{im\vartheta}v = \frac{i\sqrt{1+b^2}}{2(1+ib)}e^{im\vartheta}v.$$

Therefore, since $\|e^{i(m\pm1)\vartheta}v\|_{L^2(\nu)} = \|e^{im\vartheta}v\|_{L^2(\nu)}$,

$$\|\mathfrak{L}_m^{-1}\mathfrak{B}_{m,m\pm1}\|_{L^2(\nu)} \ge \frac{\|\mathfrak{L}_m^{-1}\mathfrak{B}_{m,m\pm1}(e^{i(m\pm1)\vartheta}v)\|_{L^2(\nu)}}{\|e^{i(m\pm1)\vartheta}v\|_{L^2(\nu)}} = \left|\frac{i\sqrt{1+b^2}}{2(1+ib)}\right| \frac{\|e^{im\vartheta}v\|_{L^2(\nu)}}{\|e^{i(m\pm1)\vartheta}v\|_{L^2(\nu)}} = \frac{1}{2},$$

which finishes the proof. □

Therefore, $DF_+ = \mathrm{id} + \mathfrak{L}^{-1}\mathfrak{B}$ is not a compact perturbation of the identity on $\mathcal{H}_+$ and we cannot hope to apply the same method as in Chapter 2. Worse, if only we had $\|\mathfrak{L}_m^{-1}\mathfrak{B}_{m,m\pm1}\|_{L^2(\nu)} < 1/2 - \varepsilon < 1/2$ for m large enough, we could hope to apply the same theory as in Chapter 3 for inverting tridiagonal operators (see also [56]), but we are clearly here in a limiting case.

Trying to look instead at the fixed-point map

$$T(u) = u - F_\pm(u) = -\mathfrak{L}^{-1}(\mathfrak{B}u - f_\pm), \tag{4.21}$$

to apply Theorem 1.1, does not help much more. To show that T is contracting via Theorem 1.1, we would need to find $Y, Z_1 > 0$ such that

$$\|DT\|_{L^2(\nu)} = \|\mathfrak{L}^{-1}\mathfrak{B}\|_{L^2(\nu)} \leq Z_1 < 1.$$

Then, given an approximate solution $\bar{u}$, there would exist a fixed point $u^\star$ of T and thus a zero of F_+ such that

$$\|u^\star - \bar{u}\|_{L^2(\nu)} \leq \frac{Y}{1 - Z_1}, \qquad \|T(\bar{u}) - \bar{u}\|_{L^2(\nu)} = \|\bar{u} + \mathfrak{L}^{-1}(\mathfrak{B}\bar{u} - f_\pm)\|_{L^2(\nu)} \leq Y.$$

Note that in this case $\bar{u}$ would not necessarily have to be expressed (and thus solved for) with respect to the basis $\{H_n^m\}$ to give a good bound Y.

However, by straightforwardly generalising the calculation of Section 2.4.1, we are only able to show that

$$\begin{aligned}
\|DT\|_{L^2(\nu)} &= \|\mathfrak{L}^{-1}\mathfrak{B}\|_{L^2(\nu)} \\
&\leq \left\| \begin{pmatrix} & \boxed{\|\mathfrak{L}_1^{-1}\mathfrak{B}_{12}\|_{L^2(\nu)}} & & \\ \boxed{\|\mathfrak{L}_2^{-1}\mathfrak{B}_{21}\|_{L^2(\nu)}} & & \boxed{\|\mathfrak{L}_2^{-1}\mathfrak{B}_{23}\|_{L^2(\nu)}} & \\ & \boxed{\|\mathfrak{L}_3^{-1}\mathfrak{B}_{32}\|_{L^2(\nu)}} & & \ddots \\ & & \ddots & \end{pmatrix} \right\|_{\ell^2} \\
&= \left\| \begin{pmatrix} 0 & 1/2 & & \\ 1/2 & 0 & 1/2 & \\ & 1/2 & 0 & \ddots \\ & & \ddots & \ddots \end{pmatrix} \right\|_{\ell^2} \\
&= 1,
\end{aligned} \tag{4.22}$$

since the operator (4.22) has spectrum $[-1, 1]$ (it is actually the Jacobi matrix associated with the Chebyshev polynomials of the second kind and thus has spectral measure $(2/\pi)\sqrt{1-x^2}\mathrm{d}x$ on

$[-1,1]$ [227]). This is only on the verge of proving that T is contracting and therefore is not quite enough to apply Theorem 1.1.

4.4 Some ideas to bridge the gap

In this short section, we give the sketch for a few ideas to use the fact that T is nearly contracting to enclose a solution $u^\star$ to our equation. These ideas are based on the following observation:

1. If we perturb the problem (4.11) to

$$2\partial_\vartheta\left(\left((1-\varepsilon)\sqrt{1+b^2}\cos\vartheta+b\right)u_\varepsilon\right)+2r\partial_r u_\varepsilon-\Delta u_\varepsilon=2(1-\varepsilon)\sqrt{1+b^2}\sin\vartheta, \tag{4.23}$$

then, we can build a corresponding fixed-point operator T_ε as in (4.21) with fixed points corresponding to solutions of Eq. (4.23), that is

$$T_\varepsilon(u)=(1-\varepsilon)T(u)=-(1-\varepsilon)\mathfrak{L}^{-1}(\mathfrak{B}\mathfrak{u}-f_\pm)$$

where $\mathfrak{L}$, $\mathfrak{B}$ and $f_\pm$ are as before. Then if $\varepsilon>0$, $\|DT_\varepsilon\|_{L^2(\nu)}\leq 1-\varepsilon$, such that if we find a numerical solution $\bar{u}_\varepsilon$ to (4.23), there exists an "actual" solution $u_\varepsilon^\star$ to (4.23) such that

$$\|u_\varepsilon^\star-\bar{u}_\varepsilon\|_{L^2(\nu)}\leq\frac{\|T_\varepsilon(\bar{u}_\varepsilon)-\bar{u}_\varepsilon\|_{L^2(\nu)}}{\varepsilon}.$$

Writing, from (4.19)

$$\lambda_b^\varepsilon=\sqrt{\frac{2a}{\pi}}\sigma\left(-\frac{1}{\pi}+\sqrt{1+b^2}\int_0^\infty\sin\vartheta u_\varepsilon^\star(r,\vartheta)\nu(\mathrm{d}r,\mathrm{d}\vartheta)\right), \tag{4.24}$$

(where $\lambda_b^0=\lambda_b$) we could therefore have a bound on λ_b^ε given by

$$\begin{aligned}\left|\lambda_b^\varepsilon-\sqrt{\frac{2a}{\pi}}\sigma\left(-\frac{1}{\pi}+\sqrt{1+b^2}\int_{\mathbb{R}_+\times\mathbb{T}}\sin\vartheta\bar{u}_\varepsilon\mathrm{d}\nu\right)\right|&\leq\sqrt{\frac{2a(1+b^2)}{\pi}}\sigma\int_{\mathbb{R}_+\times\mathbb{T}}\sin\vartheta|u_\varepsilon^\star-\bar{u}_\varepsilon|\mathrm{d}\nu,\\&\leq\sqrt{\frac{2a(1+b^2)}{\pi}}\sigma\|\sin\vartheta\|_{L^2(\nu)}\|u_\varepsilon^\star-\bar{u}_\varepsilon\|_{L^2(\nu)}\\&\leq\sqrt{\frac{a(1+b^2)}{\pi}}\frac{\sigma}{\varepsilon}\|T_\varepsilon(\bar{u}_\varepsilon)-\bar{u}_\varepsilon\|_{L^2(\nu)}.\end{aligned}$$

For the right-hand side to be small, we would require $\|T_\varepsilon(\bar{u}_\varepsilon)-\bar{u}_\varepsilon\|_{L^2(\nu)}\ll\varepsilon$ (which is in principle not a problem if the numerical scheme for the resolution of $\bar{u}_\varepsilon$ is chosen appropriately but is clearly difficult if ε is too small).

2. Now observe that for all $\varepsilon\geq 0$, if u_ε is a solution to (4.23), then $w_\varepsilon=(1+u_\varepsilon)\nu(\mathrm{d}r,\mathrm{d}\psi)=(1+u_\varepsilon)re^{-r^2}/\pi$ solves the stationary Fokker-Planck equation

$$-2\frac{\partial}{\partial\vartheta}\left((\sqrt{1+b^2}(1-\varepsilon)\cos\vartheta+b)w_\varepsilon\right)-\frac{\partial}{\partial r}\left(-2\rho w_\varepsilon\right)+\Delta w_\varepsilon=0.$$

whose solutions are stationary densities for the diffusion process

$$\begin{cases} \mathrm{d}r_t &= (-2r_t + 1/r_t)\mathrm{d}t + \sqrt{2}\mathrm{d}W_t^1, \\ \mathrm{d}\vartheta_t &= 2(b + \sqrt{1+b^2}(1-\varepsilon)\cos\vartheta_t)\mathrm{d}t + \sqrt{2}/r_t\mathrm{d}W_t^2, \end{cases} \tag{4.25}$$

on $\mathbb{R}^2 \simeq \mathbb{R}_+ \times \mathbb{T}$. We could thus turn to the literature on ergodic diffusion processes to attempt to bound $(w_0 - w_\varepsilon)$ in a suitable topology and thus bridge the gap to conclude on the sign of the Lyapunov exponent λ_b. For instance, suppose that we are able to show that there exists a constant $C > 0$ such that for all $\varepsilon \in (0,1)$, $\|w_0 - w_\varepsilon\|_{L^1(\mathbb{R}^2)} \leq C\epsilon$. Then by Hölder, from (4.24), we would directly have the bound

$$|\lambda_b^\varepsilon - \lambda_b| \leq \sqrt{\frac{2a(1+b^2)}{\pi}} C\sigma\varepsilon.$$

3. Of the few approaches available to potentially achieve a bound of the type $\|w_0 - w_\varepsilon\|_{L^1(\mathbb{R}^2)} \leq C\epsilon$, we mention the following ones:

   - One first approach [45, p. 179] essentially relies on

     (a) quantifying the (sub)-exponential rate of convergence of the semi-group $(\mathcal{P}_t)_{t\geq 0}$ associated to (4.25) in a suitable topology, typically via a Lyapunov-type criterion,

     (b) and on bounding the growth of the gradient semigroup $(\nabla\mathcal{P}_t)_{t\geq 0}$, e.g. using [194].

     If these are possible, [45] gives a simple formula for a bound on $(w_0 - w_\varepsilon)$. However, the difficulty lies in obtaining the constants involved in the formula in the first place. While (b) is straightforward in this case (because the drift of (4.25) is Lipschitz in cartesian coordinates), (a) is in general difficult.

     – If we try to make use of one of the rare papers having a constructive approach to proving exponential ergodicity under a Lyapunov condition (e.g. [69]), the difficulty is now hidden in quantifying the so-called local *coupling condition* [69]. In the context of a diffusion processes on a state space $\mathcal{X}$ whose density evolve according to the semi-group $(\mathcal{P}_t^*)_{t\geq 0}$, this essentially reduces to proving that for any $x, y \in \mathcal{X}$, $\|\mathcal{P}_t^*(\delta_x - \delta_y)\|_{TV} < 2$ for $t > 0$, i.e. the densities $\mathcal{P}_t^*\delta_x$ and $\mathcal{P}_t^*\delta_y$ "overlap". While this would not be difficult to show in our case (because our diffusion process is uniformly elliptic), this cannot be shown in a constructive/quantitative manner in general.

     – Alternatively, we could try to make use of the pioneering work [99] which applies to diffusions with Lipschitz drift (which is the case here). However, it still leads to bounds which are far from usable in practice.

   - The most realistic approach is likely to use the work [46] which relies on bounds on the solution to the so-called *Poisson equation*: while the bound it provides on $(w_0 - w_\varepsilon)$ is very intricate, all the involved constants seem to be fully explicit. In particular, this bound ultimately rely on the Harnack inequality [44, §3.7(ii)], i.e. a bound on the ratio $\sup_C w_\varepsilon / \inf_C w_\varepsilon$ on a compact set. While this bound is explicit, it remained too large for our purpose.

The limitations of the above-mentioned approaches essentially lie in the fact that the needed bounds depend exponentially or super-exponentially on the growth of the drift (for instance in the case of the Harnack inequality). That is in our case, essentially $|b|$. Since we would like to work in the regime b large to confirm the positivity of the Lyapunov exponent λ_b, these approaches were not suitable to our problem.

Remark 4.3. While taking $\alpha \neq 0$ only adds a relatively compact perturbation with respect to $\mathfrak{L}$, it would make this approach much more difficult, especially computationally, even if the magnitude of α is taken to be very small ($\alpha \ll \varepsilon$).

These ideas to bridge the gap between w_ε and w_0, while some of them in principle applicable, were too difficult or unrealistic to implement in practice. We thus turned to developing a perpendicular (actually dual) approach to the traditional idea of solving for the Fokker–Planck equation (4.9). Indeed, solving for the stationary density of a diffusion process may be too much to ask for in general: it is in the theory equivalent to be able to enclose all moments of this probability density. However, to compute the Lyapunov exponent, we only need to enclose *one unique* average over this density.

We achieve this by making use of the above-mentioned Poisson equation. This leads to the method presented in the next chapter, which is much more broadly applicable beyond the particular example of the Hopf normal form.

5

Rigorous enclosure of Lyapunov exponents of stochastic flows

This chapter is based on the paper [55].

5.1 Introduction

We consider stochastic flows $(\varphi_t)_{t\geq 0}$ generated by nonlinear stochastic differential equations of the form

$$\mathrm{d}\varphi_t(\omega,x) = X_0(\varphi_t(\omega,x))\mathrm{d}t + \sum_{i=1}^{\ell} X_i(\varphi_t(\omega,x)) \circ \mathrm{d}B_t^i(\omega), \qquad \varphi_0(\omega,x) = x, \tag{5.1}$$

where $X_0, X_1, \ldots, X_\ell$ denote analytic and complete vector fields on an analytic Riemannian manifold $(\mathcal{M}, \langle\cdot,\cdot\rangle)$, the B^i's are independent standard Brownian motions over a filtered probability space $(\Omega, \mathcal{F}, (\mathcal{F}_t)_{t\geq 0}, \mathbb{P})$ and $\circ$ denotes Stratonovich integration. A central object in the study of the dynamics of the stochastic flow $(\varphi_t)_{t\geq 0}$ is the (top) Lyapunov exponent

$$\lambda(\omega,x,v) := \lim_{t\to\infty} \frac{1}{t} \log \|D\varphi_t(\omega,x)v\|. \tag{5.2}$$

Throughout this chapter, we assume the ergodicity of the Markov process $(\varphi_t)_{t\geq 0}$, in the sense that $(\varphi_t)_{t\geq 0}$ possesses a unique stationary probability measure μ on $\mathcal{M}$. Under the existence and uniqueness of such an ergodic measure (and mild integrability conditions), it is well-established by the celebrated Osdelets multiplicative ergodic theorem [113, 186] (see also [14, Chapters 3 & 4]) that the Lyapunov exponent λ is well-defined and constant for $(\mathbb{P}\times\mu)$-almost every $(\omega,x)\in\Omega\times\mathcal{M}$, Lebesgue-almost every $v\in\mathbf{P}(T_x\mathcal{M})$, the projective space of the tangent space $T_x\mathcal{M}$.

The Lyapunov exponent λ is an essential tool to characterise stochastic dynamics. It is an important ingredient in the proof of *synchronisation when λ is negative* [26, 106] and in the characterisation of various forms of *chaotic dynamics when λ is positive* [158, 161]. In particular, from (5.2),

it can be seen that it is linked to sensitivity to initial conditions, which is a quintessential feature of chaos. Thus, obtaining rigorous bounds on the Lyapunov exponent is crucial to understanding the dynamics of $(\varphi_t)_{t\geq 0}$. This has been a long-standing fundamental problem, highlighted for instance by Kingman [153]: "Pride of place among the unsolved problems of subadditive ergodic theory must go to [its] calculation". This question has already been studied extensively in [14, 39, 40, 41, 42] and in particular for stochastic flows [24, 29, 32, 73]. However, most existing results are restricted to the small noise limit $X_i \to 0$ (for $i \neq 0$) and to systems enjoying a particular structure, such as volume-preserving/incompressible/Hamiltonian stochastic flows [15, 29], for which establishing the positivity of the (top) Lyapunov exponent often follows from non-degeneracy conditions such as the Furstenberg criterion [112] (see [86] for a recent example), especially when the noise is small.

In this chapter, we propose a computer-assisted method for *rigorously enclosing* λ under mild conditions, which substantially reduces the problem of rigorously computing Lyapunov exponents for stochastic flows, and is in principle applicable to a wide range of low-dimensional Markovian random dynamical systems.

While computer-assisted methods have played an increasingly important role in the theory of dynamical systems [116, 147, 160, 176, 211, 219, 225], the problem of rigorously enclosing Lyapunov exponents has thus far remained very challenging: in the more manageable discrete-time setting, a substantial body of work resolves this problem, including [192] for random products of matrices and [77, 109, 114] for iterated function systems (see also [115, 193, 230] in the deterministic setting). In the case of stochastic flows induced by stochastic differential equations of the type (5.1), the tackling of this problem with computer-assisted methods is more recent, with a first attempt in [57] that only applied to specific SDEs conditioned to a bounded domain, and the successful treatment of a class of chaotic systems in the small noise limit in [33].

The approach proposed in this chapter is much more general, but has the same starting point as several other studies, namely, the formulation of the top Lyapunov exponent λ as an ergodic average via the limit (5.2), the so-called Furstenberg–Khasminskii formula [71, 112, 152]

$$\lambda = \int_{\mathbf{P}\mathcal{M}} Q \mathrm{d}\tilde{\mu}, \tag{5.3}$$

where the integrand Q has an explicit formula in terms of the vector fields $X_0, X_1, \ldots, X_\ell$ and is the mean infinitesimal growth rate of the linear flow along the so-called *projective process* $(\xi_t)_{t\geq 0} = (\varphi_t, s_t)_{t\geq 0}$ on $\mathbf{P}\mathcal{M} = \bigcup_{x\in\mathcal{M}} \mathbf{P}_x\mathcal{M}$, where

$$s_t(\omega, x, v) = \frac{D\varphi_t(\omega, x)v}{\|D\varphi_t(\omega, x)v\|} \in \mathbf{P}_{\varphi_t(\omega,x)}\mathcal{M};$$

and $\tilde{\mu}(\mathrm{d}\xi) = \tilde{w}(\xi)\mathrm{d}\xi$ is the ergodic probability measure of the Markov process $(\xi_t)_{t\geq 0}$ on $\mathbf{P}\mathcal{M}$, where $\mathrm{d}\xi$ denotes the (Riemannian) volume measure on $\mathbf{P}\mathcal{M}$ by abuse of notation.

Note that in general, the existence and uniqueness of such an invariant probability measure $\tilde{\mu}$ is non-trivial, but sufficient conditions for this to hold can be found in the literature, e.g. in [197]. It is a control-theoretic problem associated to the stochastic differential equation solved by $(\xi_t)_{t\geq 0}$

$$\mathrm{d}\xi_t = \tilde{X}_0(\xi_t)\mathrm{d}t + \sum_{i=1}^{\ell} \tilde{X}_i(\xi_t) \circ \mathrm{d}B_t^i, \qquad \xi_0 = (x, v), \tag{5.4}$$

with vector fields $\tilde{X}_0, \tilde{X}_1, \ldots, \tilde{X}_\ell$ on $\mathbf{P}\mathcal{M}$.

In all but a few cases (e.g. [23, 100]), obtaining bounds or even only the sign for λ via the Furstenberg–Khashminskii formula (5.3) has so far proven extremely difficult. A common strategy (in both the deterministic and random settings [57, 109, 114, 115, 230]) is to try to enclose $\tilde{w}$ rigorously and then integrate Q against $\tilde{w}$ to obtain bounds on λ via (5.3). In the context of stochastic flows, we could try to make use of computer-assisted proof methods [124, 181, 195, 219] to solve the stationary Fokker–Planck equation

$$\tilde{\mathcal{L}}^* \tilde{w} = 0, \tag{5.5}$$

where $\tilde{\mathcal{L}}^*$ denotes the adjoint in $L^2(\mathbf{P}\mathcal{M})$ of

$$\tilde{\mathcal{L}} = \tilde{X}_0 + \frac{1}{2} \sum_{i=1}^{\ell} \tilde{X}_i^2,$$

which is the infinitesimal generator of the process $(\xi_t)_{t \geq 0}$ written in Hörmander form. Such computer-assisted proof, if successful, would yield a precise and quantitative description of $\tilde{w}$, which would then allow to accurately enclose the integral (5.3) (see, e.g., [57]). However, the rigorous general treatment of general partial differential equations (PDEs) of the form (5.5) by computer-assisted means is for now far out of reach due to the typically *non-elliptic* nature of $\tilde{\mathcal{L}}^*$ (and $\tilde{\mathcal{L}}$). The gap to bridge is even greater when considering problems on an unbounded state space $\mathcal{M}$ [57]. This difficulty stems from the fact that both these aspects usually prevent the derivation of explicit a priori bounds to quantify errors on the computation of $\tilde{w}$. While there exist techniques [13, 122, 188] to prove the existence of a spectral gap for $\tilde{\mathcal{L}}^*$ (or $\tilde{\mathcal{L}}$), these are typically non-constructive, and thus do not provide an explicit bound on this spectral gap. Even when explicit bounds are available, for instance in some elliptic cases, they can be very intricate and lead to unusable values in practice, typically depending exponentially on $\|\tilde{X}_0\|$ [44, 46]. We will therefore depart from the usual strategy of estimating $\tilde{w}$ and develop a more flexible approach.

Nonetheless, in certain special cases, some estimates for (5.3) can be achieved analytically in an asymptotic parameter regime e.g. as $X_i \to 0$, $i \neq 0$ [32, 33, 73]. In such a regime, one can, for instance, make use of the so-called *adjoint method* proposed by Arnold, Papanicolaou and Wihstutz [18] (see [24, 30] for some recent examples).

In this chapter, we combine the adjoint method with computer-assisted techniques to obtain rigorous and tight bounds on Lyapunov exponents for general systems: we do not assume any asymptotic or perturbative regime, assuming only mild hypoellipticity conditions. Our method, which we now introduce in Section 5.1.1, is applicable to unbounded domains and does not necessitate any specific structure on (5.1). We showcase this in Section 5.1.2, which contains four examples of stochastic flows without specific structure or asymptotically small parameters, for which we establish the positivity of the (top) Lyapunov exponent. The first three examples feature the phenomenon of noise-induced chaos, i.e. a transition from negative to positive Lyapunov exponent with increasing noise level (although the Lyapunov exponent may become negative again if the noise is too large), and the last two address open conjectures.

5.1.1 Our method to rigorously enclose Lyapunov exponents

As already mentioned, working directly with the Furstenberg–Khashminskii formula (5.3) is often very difficult. The idea of the adjoint method introduced in [18] is to instead consider, for a well chosen u,

$$\int_{\mathbf{P}\mathcal{M}} \left(Q - \tilde{\mathcal{L}}u\right) \mathrm{d}\tilde{\mu}. \tag{5.6}$$

Indeed, since $\tilde{\mathcal{L}}^*\tilde{w} = 0$, we formally get

$$\int_{\mathbf{P}\mathcal{M}} \tilde{\mathcal{L}}u \mathrm{d}\tilde{\mu} = \int_{\mathbf{P}\mathcal{M}} \tilde{\mathcal{L}}u(\xi)\tilde{w}(\xi)\mathrm{d}\xi = \int_{\mathbf{P}\mathcal{M}} u(\xi)(\tilde{\mathcal{L}}^*\tilde{w}(\xi))\mathrm{d}\xi = 0, \tag{5.7}$$

and this calculation can be made rigorous under suitable integrability and growth assumptions on u, see for instance Lemma 5.5, which is based on [24, Proposition B.1]. Therefore, the (top) Lyapunov exponent λ is also given by (5.6), that is

$$\lambda = \int_{\mathbf{P}\mathcal{M}} \left(Q - \tilde{\mathcal{L}}u\right) \mathrm{d}\tilde{\mu}, \tag{5.8}$$

and one can try to pick a function u for which the integrand $(Q - \tilde{\mathcal{L}}u)$ is more approachable so that the right-hand side of (5.8) is easier to work with than the original Furstenberg–Khashminskii formula (5.3). Ideally, one would like to find a function u and a constant Λ such that $Q - \tilde{\mathcal{L}}u = \Lambda$, i.e., such that u and Λ solve the *Poisson equation*

$$\tilde{\mathcal{L}}u = Q - \Lambda, \tag{5.9}$$

because then we simply get $\lambda = \Lambda$ from (5.8). However, solving the Poisson equation (5.9) is not necessarily easier than solving the stationary Fokker–Planck equation (5.5), and finding an explicit solution is in general not possible.

For some specific problems, in an asymptotic regime, ad hoc choices of u that make (5.8) more manageable than (5.3) can sometimes be found, and we again refer to [24] for a recent example where this idea is used several times. In contrast, in this work we propose a generic and robust way of using the adjoint method on a broad class of systems, which leads to quantitative and accurate estimates on the Lyapunov exponent.

The main idea is that, even if the "optimal" u (the one solving (5.9)) cannot be found explicitly, for many problems we can still find *numerically* an approximate solution $\bar{u}$, and then use this approximate solution in (5.8) in order to derive estimates on λ, which are going to be sharp if $\bar{u}$ is an accurate approximate solution. Suppose for the moment that we have an approximation $\bar{\lambda}$ of λ (e.g., via a Monte-Carlo method [125, 154, 205]), and that we have obtained an approximate solution $\bar{u}$ to the Poisson problem (5.9), by solving numerically the equation

$$\tilde{\mathcal{L}}\bar{u} \approx Q - \bar{\lambda}.$$

How to find suitable $\bar{\lambda}$ and $\bar{u}$ in practice will be discussed in Section 5.2. Setting

$$\bar{Q} \overset{\text{def}}{=} \tilde{\mathcal{L}}\bar{u} + \bar{\lambda},$$

we expect to have $\bar{Q} \approx Q$. Furthermore, using $\bar{u}$ in (5.8) we get

$$\lambda = \int_{\mathbf{P}\mathcal{M}} \left(Q - \tilde{\mathcal{L}}\bar{u}\right) \mathrm{d}\tilde{\mu} = \int_{\mathbf{P}\mathcal{M}} \left(Q - \bar{Q}\right) \mathrm{d}\tilde{\mu} + \bar{\lambda},$$

hence

$$|\lambda - \bar{\lambda}| = \left| \int_{\mathbf{P}\mathcal{M}} (Q - \bar{Q}) \mathrm{d}\tilde{\mu} \right|. \tag{5.10}$$

That is, we control the difference between the approximate Lyapunov exponent $\bar{\lambda}$ (which we know explicitly) and the exact one λ (unknown), via the difference $Q - \bar{Q}$ (where both terms are known). Thus, the problem of enclosing λ has been reduced to the easier problem of bounding the integral in (5.10): while $\tilde{\mu}$ is still unknown, various inequalities can be applied to show that this integral is small. The derivation of such a bound mostly depends on the nature of Q (and $\bar{Q}$) and $\mathcal{M}$ and on a priori estimates on $\tilde{\mu}$. In this chapter, our strategy is mainly based on directly applying L^∞ and L^1 bounds globally. For instance, on a compact state space $\mathcal{M}$, the functions Q and $\bar{Q}$ are typically L^∞ and

$$|\lambda - \bar{\lambda}| = \left| \int_{\mathbf{P}\mathcal{M}} (Q - \bar{Q}) \mathrm{d}\tilde{\mu} \right| \leq \|Q - \bar{Q}\|_\infty \int_{\mathbf{P}\mathcal{M}} \mathrm{d}\tilde{\mu} = \|Q - \bar{Q}\|_\infty. \tag{5.11}$$

Note that $\bar{Q}$ is known explicitly in terms of $\bar{u}$ and $\bar{\lambda}$, therefore there is in principle no difficulty in getting an explicit upper bound for $\|Q - \bar{Q}\|_\infty$. In practice, this can be done efficiently using rigorous numerics and interval arithmetic [212], see Proposition 5.7 for more details. We emphasize that $\bar{u}$ and $\bar{\lambda}$ can and should be obtained using traditional numerics with floating-point arithmetic. The only steps that have to be carried out rigorously are the calculation of $\bar{Q}$, i.e., the application of $\tilde{\mathcal{L}}$ to $\bar{u}$, and then the estimation of $\|Q - \bar{Q}\|_\infty$. In contrast, even in specific situations in which one could have rigorously solved the stationary Fokker–Planck equation (5.5) or the Poisson equation (5.9) using a computer-assisted proof, this would be a computer-assisted proof for solving a PDE, for which the amount of rigorous numerics required would be much higher compared to the computer-assisted approach proposed here (see Remark 5.8 for more details). We also point out that our method does not only apply to the computation of top Lyapunov exponents but to any ergodic average of the form (5.3) where Q is given and explicit.

Estimate (5.11) is in some sense rather crude, as it does not seem to use any information on $\tilde{\mu}$, but this is in fact a strength of our approach. Indeed, obtaining quantitative information on $\tilde{\mu}$ can often be very hard, and being able to rigorously enclose λ without knowing anything about $\tilde{\mu}$ is part of what makes our method broadly applicable. Of course, if some information on $\tilde{\mu}$ is available then it may be leveraged to obtain sharper estimates (see for instance Section 5.6 and 5.7), but directly using the simple estimate (5.11) can already lead to very precise results such as the one in Theorem 1.10 below.

The above estimate (5.11) can be generalised to treat systems on a non-compact state space $\mathcal{M}$, where Q or $\bar{Q}$ may not be in L^∞, and one instead makes use of Foster–Lyapunov inequalities [69, 127, 175] to recover the necessary estimates (see Section 5.2.1). Examples with both bounded and unbounded state spaces are provided below.

5.1.2 Examples of results obtained with our method

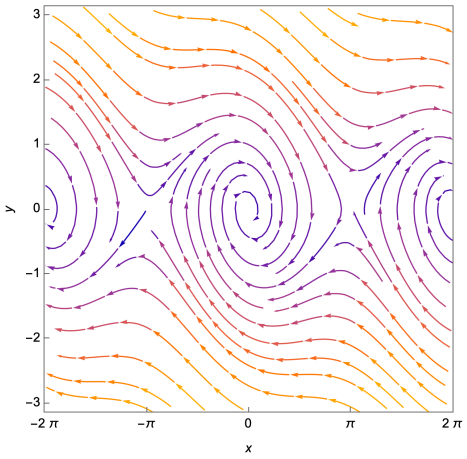
We illustrate the power of our method by providing sharp quantitative bounds on the Lyapunov exponent λ for several SDE examples, including the ones of Theorems 1.4 and 1.10, well beyond the previous state-of-the-art. More details on each of these systems, together with the proofs of the theorems, are given in Sections 5.4 to 5.7.

Theorem 5.1. Consider the stochastic flow $(\varphi_t)_{t\geq 0}$ on $\mathcal{M} = \mathbb{T} \times \mathbb{R}$ generated by the randomly forced pendulum equation

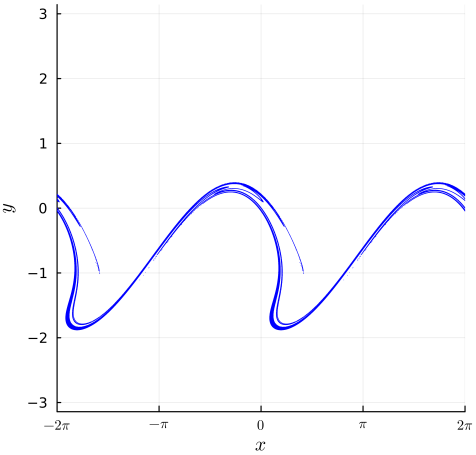
$$\begin{cases} \mathrm{d}x_t &= y_t \mathrm{d}t, \\ \mathrm{d}y_t &= -(\kappa \sin x_t + \gamma y_t)\mathrm{d}t + \sigma \mathrm{d}B_t. \end{cases} \tag{5.12}$$

Then, with gravitational constant $\kappa = 2/3$, friction coefficient $\gamma = 1/4$ and noise strength $\sigma = 4$, the Lyapunov exponent λ is positive with bounds

$$\lambda \in [0.0228, 0.0315].$$



(a) Phase portrait of the vector field (5.12) with $\sigma = 0$.



(b) Snapshot of a chaotic random attractor of (5.12) with $\sigma = 4$.

Figure 5.1: Deterministic and random dynamics of (5.12) for $\kappa = 2/3$ and $\gamma = 1/4$.

For system (5.12), proving that there is a positive Lyapunov exponent seems far out of reach without the use of our method. In particular, there are no clear mechanisms explaining the chaotic dynamics shown in Figure 5.1b. Moreover, the operators $\tilde{\mathcal{L}}$ and $\tilde{\mathcal{L}}^*$ are very much non-elliptic, since there is no noise acting on the x variable, and also on the projective variable s at all points of $\mathbf{P}\mathcal{M}$ (see Section 5.5 for the explicit formula). Due to this lack of ellipticity, one cannot use usual computer-assisted proofs to rigorously solve the Fokker–Planck equation (5.5) or the Poisson equation (5.9). The strategy based on the adjoint method proposed in this chapter bypasses these obstructions, since it only relies on an approximate solution of the Poisson equation. Nonetheless, the lack of ellipticity still impacts the output of our method, as it makes it more challenging in practice to find an accurate approximate solution $\bar{u}$, which partially explains why the enclosure of λ in Theorem 5.1 is not as sharp as the one in Theorem 1.10.

Next, we show that our method is robust and can be combined with continuation methods

recently introduced in [51] (see also [9]) to enclose Lyapunov exponents for a large parameter range.

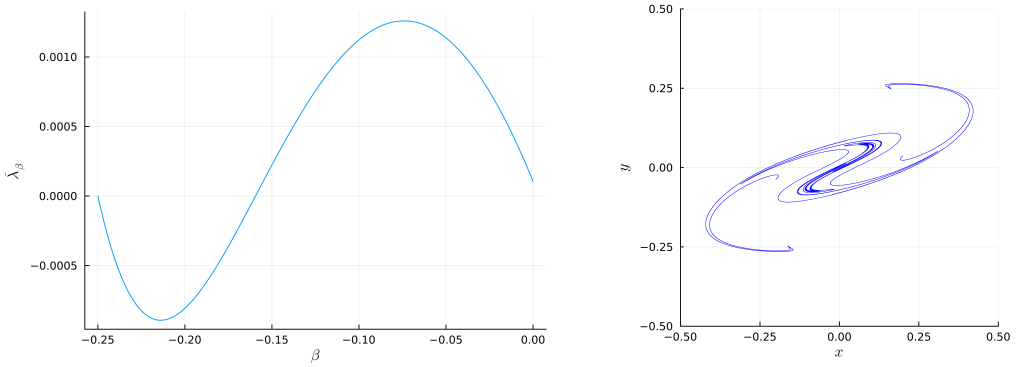
As an example, we consider the stochastic differential equation (5.1) on $\mathcal{M} = \mathbb{R}^2\backslash\{0\}$ with the vector fields

$$\begin{aligned} X_0(x,y) &= \left(\frac{\beta}{2} - \frac{b}{8}(x^2+y^2)\right)\begin{pmatrix} x \\ y \end{pmatrix} - \frac{3a}{8\nu}(x^2+y^2)\begin{pmatrix} y \\ -x \end{pmatrix}, \\ X_1(x,y) &= \frac{\sigma}{2\sqrt{2}\nu}\begin{pmatrix} x \\ -y \end{pmatrix}, \qquad X_2(x,y) = \frac{\sigma}{2\sqrt{2}\nu}\begin{pmatrix} y \\ x \end{pmatrix}, \qquad X_3(x,y) = \frac{\sigma}{2\nu}\begin{pmatrix} y \\ -x \end{pmatrix}, \end{aligned} \tag{5.13}$$

with $-\sigma^2/4\nu^2 < \beta \leq 0$, $a \geq 0$ and $b, \nu, \sigma > 0$. This system appears as a result of a stochastic averaging procedure for the stochastic Duffing–van der Pol equation on $\mathcal{M} = \mathbb{R}^2\backslash\{0\}$

$$\begin{cases} \mathrm{d}x_t &= -\nu y_t \mathrm{d}t \\ \mathrm{d}y_t &= \left(\nu x_t + \varepsilon^2\beta y_t + \frac{a}{\nu}x_t^3 - b x_t^2 y_t\right)\mathrm{d}t - \frac{\varepsilon\sigma}{\nu}x_t \mathrm{d}B_t \end{cases} \tag{5.14}$$

as $\varepsilon \to 0$. Baxendale [27] conjectures the following for the Lyapunov exponent λ_β associated to the stochastic differential equation (5.1) with vector fields (5.13): if $\sigma/\nu = 1$ and $b\nu/a = 1.24$, there exists $\beta^* \approx -0.17$ such that $\lambda_\beta < 0$ for $-\sigma^2/4\nu^2 = -1/4 < \beta < \beta^*$ and $\lambda_\beta > 0$ for $\beta^* < \beta < 0$. We provide an answer to this conjecture by proving that a transition from negative to positive Lyapunov exponent indeed occurs as β increases.



(a) Graph of the function $\beta \mapsto \bar{\lambda}_\beta$ from Theorem 5.2.

(b) Snapshot of a chaotic random attractor of (5.13) for $\beta = -0.1$.

Figure 5.2: Quantitative and qualitative random dynamics induced by (5.13), for $\sigma/\nu = a/\nu = 1$ and $b = 1.24$.

Theorem 5.2. Consider the stochastic differential equation (5.1) with vector fields (5.13). Assume that $\sigma/\nu = 1$ and $b\nu/a = 1.24$, and let $\beta \mapsto \bar{\lambda}_\beta$ be the function represented in Figure 5.2a (and whose precise description can be found at [78]). Then, for *all* $\beta \in (-1/4, 0]$,

$$|\lambda_\beta - \bar{\lambda}_\beta| \leq 2.2 \times 10^{-6}.$$

In Theorem 5.2, we give a uniform error bound in β for simplicity, but we in fact get tighter

bounds for some values of β (see Table 5.1). In particular, by refining the estimates close to the values of β for which λ_β vanishes, we obtain the following result.

Theorem 5.3. Assume that $\sigma/\nu = 1$ and $b\nu/a = 1.24$, then there exists $\beta^* \in (-0.159449, -0.159437)$ such that $\lambda_{\beta^*} = 0$. Furthermore, $\lambda_\beta < 0$ for $\beta \in (-0.249997, -0.159449]$ and $\lambda_\beta > 0$ for $\beta \in [-0.159437, 0]$.

Beyond the fact that Theorems 5.2 and 5.3 answer the conjecture from [27], this example is interesting because it features a singularity which needs to be handled at the origin. Another aspect of note is that, when $\beta = -1/4 = -\sigma^2/4\nu^2$, the system loses its ergodicity. Nonetheless, our method allows to treat the system for all $\beta \in (-1/4, 0]$, without any kind of singularity issue as β approaches $-1/4$. These two points will be addressed in more detail in Section 5.7.

Note that the above conjecture from [27], which was obtained using simulations [205], turned out to be slightly imprecise regarding the value β^* at which the transition from negative to positive Lyapunov exponent occurs. This illustrates the fact that one cannot reliably determine the sign of the Lyapunov exponent λ_β using purely numerical simulations when the magnitude of λ_β is small. In contrast, our method is very precise numerically and also provides guaranteed error bounds, which allows us to rigorously conclude regarding the sign of λ_β, even for β relatively close to the transition value β^*.

Finally, using the averaging results obtained in [27], we can say the following about the Duffing–van der Pol system (5.14).

Corollary 5.4. Consider the stochastic Duffing–van der Pol system (5.14), with $\sigma/\nu = 1$ and $b\nu/a = 1.24$. Then for ε small enough, the associated Lyapunov exponent $\hat{\lambda}_{\beta,\varepsilon}$ is well-defined and $\hat{\lambda}_{\beta,\varepsilon} \sim \varepsilon^2 \lambda_\beta$. Moreover,

- if $\beta \in [-0.159437, 0]$, there exists $\varepsilon_0 > 0$ such that for all $\varepsilon < \varepsilon_0$, $\hat{\lambda}_{\beta,\varepsilon}$ is positive;
- if $\beta \in (-0.249997, -0.159449]$, there exists $\varepsilon_0 > 0$ such that for all $\varepsilon < \varepsilon_0$, $\hat{\lambda}_{\beta,\varepsilon}$ is negative.

Proof. The facts that $\hat{\lambda}_{\beta,\varepsilon}$ is well-defined and that $\hat{\lambda}_{\beta,\varepsilon} \sim \varepsilon^2 \lambda_\beta$ as $\varepsilon \to 0$ follow from [27, Theorem 1.1.(iii)]. Corollary 5.4 is then a direct consequence of Theorem 5.3. □

The remainder of the chapter is organised as follows. The principle of the adjoint method is recalled in Section 5.2, where we also introduce a general framework allowing us to turn this idea into a computer-assisted proof, together with a first simple example. We then recall how the Furstenberg–Khasminskii formula can be derived and how the ergodicity of the projective process can be shown in Section 5.3. In Sections 5.4, 5.5, 5.6 and 5.7, we provide more background on each of the systems studied in Theorems 1.10, 5.1, 1.4 and 5.2 respectively, together with the proofs of each Theorem. Finally, Section 5.8 discusses potential further applications of our computer-assisted adjoint method. The computer-assisted parts of the proofs can be reproduced using the code deposited in [78].

5.2 The adjoint method using an approximate solution

5.2.1 General framework

In this section, we lay out the main method used in this chapter to enclose ergodic averages. Given a diffusion process $(x_t)_{t\geq 0}$ on a σ-compact manifold $\mathcal{X}$ (i.e. the countable union of compact submanifolds) induced by a stochastic differential equation (SDE) with complete vector fields

$$\mathrm{d}x_t = V_0(x_t)\mathrm{d}t + \sum_{i=1}^{\ell} V_i(x_t) \circ \mathrm{d}B_t^i, \tag{5.15}$$

assumed to have a unique stationary measure $\mu(\mathrm{d}x) = w(x)\mathrm{d}x$, and a $\mathcal{C}^2$ μ-integrable function $q : \mathcal{X} \to \mathbb{R}$, our aim is to rigorously enclose the integral

$$\mathcal{I} = \int_{\mathcal{X}} q\mathrm{d}\mu. \tag{5.16}$$

This includes the problem of enclosing Lyapunov exponents discussed in the introduction, for which the diffusion process to be considered is the projective process given by (5.4) (see also Section 5.3.1), but the method presented here applies to any ergodic average.

In order to study $\mathcal{I}$, we consider the operator

$$\mathcal{L} = V_0 + \frac{1}{2}\sum_{i=1}^{\ell} V_i^2 : \mathcal{C}^2(\mathcal{X}) \to \mathcal{C}^0(\mathcal{X}),$$

which is the (infinitesimal) generator of the solution process $(x_t)_{t\geq 0}$ satisfying Eq. (5.15). We aim to find $\bar{u} \in \mathcal{C}^2(\mathcal{X})$ and a constant $\bar{\mathcal{I}}$ such that

$$\mathcal{L}\bar{u} \approx q - \bar{\mathcal{I}}. \tag{5.17}$$

One may approach this problem by first approximating $\mathcal{I}$ with a numerical scheme such as a Monte-Carlo method to produce a candidate $\bar{\mathcal{I}} \approx \mathcal{I}$, and then solve for $\bar{u}$. However, we show below that such a step is not necessary. Indeed, because $\int \mathcal{L}\bar{u}\mathrm{d}\mu = 0$, for any $(\bar{u}, \bar{\mathcal{I}})$ satisfying (5.17) we automatically get $\bar{\mathcal{I}} \approx \mathcal{I}$. This allows us to first solve for $\bar{u}$ only, and then recover $\bar{\mathcal{I}}$, which often leads to a much more precise approximation of $\mathcal{I}$. In this chapter, we work under the following setting:

(S1) We have a Hilbert (orthonormal) basis $\{f_n\}_{n\in\mathbb{N}} \subset \mathcal{C}^2(\mathcal{X})$ for a judicious Hilbert space $(\mathcal{H}, (\cdot,\cdot))$ such that $f_0 = 1$.

(S2) For all $N \in \mathbb{N}$, there exists $M \geq N$ such that $\mathcal{L}$ maps $\Pi_N(\mathcal{H}) = \mathrm{Span}\{f_n\}_{n=0}^N$ to $\Pi_M(\mathcal{H}) = \mathrm{Span}\{f_m\}_{m=0}^M$, where Π_n denotes the projection in $\mathcal{H}$ onto $\mathrm{Span}\{f_i\}_{i=0}^n$.

(S3) There is a $\mathcal{C}^2$ positive function $W : \mathcal{X} \to \mathbb{R}_+^* := (0,\infty)$ such that

$$\sup_{m\in\mathbb{N}} \left\| \frac{f_m}{W} \right\|_\infty < \infty,$$

and $\mu(W) < \infty$. Furthermore, $\mu(W)$ and these suprema can be bounded explicitly.

(S4) There exists a $\mathcal{C}^2$ function $\tilde{W} : \mathcal{X} \to \mathbb{R}_+^*$ such that $\mathcal{L}\tilde{W} \leq c\tilde{W}$ for some $c < \infty$ and that for all $n \in \mathbb{N}$

$$\frac{|f_n(x)|}{\tilde{W}(x)} \longrightarrow 0 \qquad \text{as } |f_n(x)| \to \infty.$$

(S5) There is $n_0 \in \mathbb{N}$ such that $q \in \mathrm{Span}\{f_n\}_{n=0}^{n_0}$.

In practice, we take $W = \tilde{W}$, except for the Duffing–van der Pol example in Section 5.7; and if $\mathcal{X}$ is compact, we will simply take $W = \tilde{W} = 1$.

In the heuristic description of our approach in Section 5.1.1, we heavily used the fact that elements in the range of $\mathcal{L}$ have μ-mean equal to zero. The following lemma, which is a direct rewriting of [24, Proposition B.1] adapted to our framework, gives sufficient conditions allowing the use of this fact rigorously.

Lemma 5.5. Under assumptions (S1)–(S4), for all $n \in \mathbb{N}$,

$$\int_{\mathcal{X}} (\mathcal{L}f_n) \mathrm{d}\mu = 0. \tag{5.18}$$

Thus, by linearity, for any $u \in \Pi_N(\mathcal{H})$,

$$\int_{\mathcal{X}} (\mathcal{L}u) \mathrm{d}\mu = 0.$$

Proof. Fix $n \in \mathbb{N}$, it is clear that under assumptions (S2) and (S3), f_n and $\mathcal{L}f_n$ are μ-integrable. These two integrability conditions together with assumption (S4) and the fact that f_n is $\mathcal{C}^2$ imply (5.18) by [24, Proposition B.1]. □

The problem (5.17) is then expressed and solved numerically with respect to the Hilbert basis $\{f_n\}_{n\in\mathbb{N}}$, i.e. we represent the action of $\mathcal{L} : \Pi_N(\mathcal{H}) \to \Pi_M(\mathcal{H})$ by its Galerkin representation, the finite-dimensional matrix

$$(f_m, \mathcal{L}f_n)_{m\leq M, n\leq N},$$

and all the subsequent operations are equivalent to finite-dimensional linear algebra: we find $\bar{u}$, a *numerical* solution of the least-square problem

$$\operatorname*{argmin}_{u\in\Pi_N(\mathcal{H})} \|\Pi_0^\perp(\mathcal{L}u - q)\|_{\mathcal{H}}^2, \tag{5.19}$$

or of the linear problem

$$(\Pi_N \Pi_0^\perp \mathcal{L} \Pi_N \Pi_0^\perp) u = \Pi_0^\perp q.$$

In our experience, the first approach gives slightly better results. Note that this is a purely numerical guess; there is in general no theoretical guarantee or indication for this procedure to converge quickly as $N \to \infty$. For the main problems considered in this chapter, the usual compactness estimates do not hold and convergence is typically not of spectral nature [209]. The argument presented below will only provide a tight enclosure of λ if the approximate solution $\bar{u}$ is accurate enough, but we stress that we do not need any a priori estimate regarding the quality of $\bar{u}$.

Remark 5.6. For very high-dimensional sparse systems, it will in general prove better (for instance in terms of memory requirements) to make use of iterative methods to solve truncated or least-square versions of this problem [187, 210].

We now assume that an approximate solution $\bar{u} \in \Pi_N(\mathcal{H})$ of (5.17) has been computed for some N. In practice, we do so via (5.19), but we again emphasize that the way such a $\bar{u}$ is actually obtained is irrelevant for the estimates to come. In particular, none of the above computations need to have been performed rigorously. We are now ready give a fully justified and more detailed version of method presented in Section 5.1.1.

Proposition 5.7. Assume that the SDE (5.15) having complete vector fields and posed on a σ-compact manifold $\mathcal{X}$ has a unique stationary measure μ. Let $q : \mathcal{X} \to \mathbb{R}$ a $\mathcal{C}^2$ μ-integrable function, and $\mathcal{I}$ be the integral (5.16). Assume (S1)–(S5), and let $\bar{u} \in \Pi_N(\mathcal{H})$ for some $N \in \mathbb{N}$. Let

$$\bar{\mathcal{I}} \overset{\text{def}}{=} P_0(q - \mathcal{L}\bar{u}), \tag{5.20}$$

and

$$\bar{q} \overset{\text{def}}{=} \mathcal{L}\bar{u} + \bar{\mathcal{I}}. \tag{5.21}$$

Then

$$\mathcal{I} - \bar{\mathcal{I}} = \int_{\mathcal{X}} (q - \bar{q}) \mathrm{d}\mu. \tag{5.22}$$

Moreover, denoting by $\{\epsilon_m\}_{m=1}^M$ the coefficients of $q - \bar{q}$ with respect to the basis $\{f_m\}_{m\geq 0}$, i.e.

$$q - \bar{q} = \sum_{m=1}^{M} \epsilon_m f_m, \tag{5.23}$$

we have the estimate

$$|\mathcal{I} - \bar{\mathcal{I}}| \leq \mu(W) \sum_{m=1}^{M} |\epsilon_m| \left\| \frac{f_m}{W} \right\|_\infty. \tag{5.24}$$

Proof. By Lemma 5.5 we have $\int_{\mathcal{X}} (\mathcal{L}\bar{u}) \mathrm{d}\mu = 0$, and integrating (5.21) immediately yields (5.22). Then, thanks to assumptions (S2) and (S5), $q - \bar{q}$ belongs to $\Pi_M(\mathcal{H})$ for some $M \in \mathbb{N}$, hence $q - \bar{q}$ can be written as $\sum_{m=0}^{M} \epsilon_m f_m$. We note that, as claimed in (5.23), the first coefficient ϵ_0 is in fact 0, because (5.20) and (5.21) imply $q - \bar{q} = \Pi_0^\perp (q - \mathcal{L}\bar{u})$. We then simply estimate

$$|\mathcal{I} - \bar{\mathcal{I}}| = \left| \int_{\mathcal{X}} (q - \bar{q}) \mathrm{d}\mu \right| \leq \mu(W) \left\| \frac{(q - \bar{q})}{W} \right\|_\infty \leq \mu(W) \sum_{m=1}^{M} |\epsilon_m| \left\| \frac{f_m}{W} \right\|_\infty. \qquad \square$$

Estimate (5.24) gives us an enclosure of $\mathcal{I}$, which is expected to be tight if $\bar{u}$ is an accurate approximation of the solution u of the Poisson equation $\mathcal{L}u = q - \mathcal{I}$. Moreover, the right hand side of (5.24) can be explicitly and rigorously bounded. This only requires

- Rigorously applying $\mathcal{L}$ to the approximate solution $\bar{u}$ in order to obtain $\bar{\mathcal{I}}$ and $\bar{q}$ in (5.20)-(5.21), which then yields the coefficients ϵ_m,
- Getting computable upper-bounds for $\mu(W)$ and for $\left\| \frac{f_m}{W} \right\|_\infty$, for finitely many m's.

For instance, if we use Fourier series and $W = 1$ (as will be the case in some examples), we simply have $\left\| \frac{f_m}{W} \right\|_\infty = 1$ for all m. When using more involved bases, we get explicit bounds on $\left\| \frac{f_m}{W} \right\|_\infty$ using interval arithmetic together with some elementary estimates. In this work, we use the Julia package `IntervalArithmetic.jl` [198] to perform our rigorous calculations, and the required estimates are discussed case by case in the example sections.

Remark 5.8. The evaluation of $\bar{q}$ (5.21) which is the most expensive calculation in interval arithmetic is only a matrix-vector multiplication. This is in contrast with most computer-assisted proofs for ODEs or PDEs, which usually at least require a matrix-matrix multiplication, the inversion of a matrix, the resolution of a linear system or many matrix-vector multiplications in rigorous arithmetic. That allows for the treatment of problems with a much higher truncation dimension N which are especially necessary for non-elliptic problems on an unbounded multi-dimensional domain $\mathcal{X}$. Furthermore (at least for the rigorous part of the proof), provided $\mathcal{L}$ has a sparse representation with respect to $\{f_n\}_{n\in\mathbb{N}}$, this approach is not so limited by memory resources (which typically restrict computer-assisted proofs), as we can take full advantage of the sparsity of $\mathcal{L}$.

Remark 5.9. The main reason for the need for a weight function W, is that for our class of problems which are analytic, the Hilbert basis $\{f_n\}_{n\in\mathbb{N}}$ and q are typically of polynomial type and thus unbounded on an unbounded domain. In this case, $W(x)$ needs to grow exponentially or superexponentially as $|x| \to \infty$. Note that the existence of such weight or Lyapunov function is a standard ingredient for the proof of ergodicity of $(x_t)_{t\geq 0}$. When choosing W, there is of course a trade-off between the values of $\|f_m/W\|_\infty$ and $\mu(W)$.

Remark 5.10. Some of the assumptions of our setting can be loosened. For instance, instead of (S5), it is sufficient for q to be analytic and thus have geometrically decaying coefficients with respect to our Hilbert basis, but this would require an additional bound for the tail of this series. We could also choose to express the problem with respect to two different bases for arguments and images of $\mathcal{L}$. Moreover, working with a Hilbert basis for the domain of $\mathcal{L}$ is not strictly necessary, as will be showcased in Section 5.7.2. More generally, we stress that the setting presented in this section is only one approach among others that one could take for the rigorous enclosure of ergodic averages via the adjoint method. The present approach is most likely the simplest one but may not be suitable in every situation (e.g. if w is not exponentially decaying on an unbounded domain $\mathcal{M}$).

Note that other computational approaches [156, 184] based on polynomial optimisation and relying on the fact that $\mathcal{L}\bar{u}$ has μ-mean zero have previously been proposed. However, they instead rely on proving upper and lower bounds separately (or equivalently positivity/negativity conditions) which are less brutal than (5.24) but also much harder to verify computationally. It is unclear if this approach can be made rigorous or even computationally viable on nontrivial examples where $\mathcal{X}$ is multidimensional and $\mathcal{L}$ is not elliptic.

5.2.2 Example: The average Lyapunov exponent for the cellular flow with sinks

Consider the cellular flow with sinks $(\varphi_t)_{t\geq 0}$ on the two-torus $\mathcal{M} = \mathbb{T}^2$ generated by the differential equation

$$\begin{cases} \mathrm{d}x_t &= (\cos(x_t)/2 - \cos y_t)\sin x_t \mathrm{d}t + \sigma \mathrm{d}B_t^1 \\ \mathrm{d}y_t &= (\cos(y_t)/2 + \cos x_t)\sin y_t \mathrm{d}t + \sigma \mathrm{d}B_t^2 \end{cases}$$

where $\mathbb{T}^2 = (\mathbb{R}/\mathbb{Z})^2 \simeq [0, 2\pi)^2$ is endowed with the Riemannian structure inherited from $\mathbb{R}^2$ (throughout this chapter, the Riemannian structure on $\mathbb{T} = \mathbb{R}/\mathbb{Z}$ will always be inherited from $\mathbb{R}$). Since the noise is additive and the state space $\mathcal{M} = \mathbb{T}^2$ is compact, the Markov process $(\varphi_t)_{t\geq 0}$ is clearly ergodic with unique stationary measure μ on $\mathbb{T}^2$. This system is a modification of the

classical Hamiltonian cellular flow [63], and thus the incompressibility of the flow is lost. For this variant, one actually expects volume contraction along trajectories (see Figure 1.4a). This volume growth rate is given by the so-called *average Lyapunov exponent*

$$\lambda_\Sigma(\omega, x) = \lim_{t\to\infty} \frac{1}{2t} \log\det D\varphi_t(\omega, x).$$

Before turning our attention to the actual Lyapunov exponent λ for this system in Section 5.4, we first study here the simpler case of the average Lyapunov exponent, which provides an easy example to illustrate our method. By Liouville's formula [14, Theorem 2.3.32],

$$\det(D\varphi_t(\omega, x)) = \exp\int_0^t \mathrm{tr} D(X_0(\varphi_\tau))\mathrm{d}\tau = \exp\int_0^t \frac{\cos 2x_\tau + \cos 2y_\tau}{2}\mathrm{d}\tau.$$

Then, by Birkhoff's ergodic theorem, λ_Σ is constant $(\mathbb{P}\times\mu)$-almost surely and

$$\lambda_\Sigma = \lim_{t\to\infty} \frac{1}{2t}\int_0^t \frac{\cos 2x_\tau + \cos 2y_\tau}{2}\mathrm{d}\tau = \int_{\mathbb{T}^2} \frac{\cos 2x + \cos 2y}{4}\mu(\mathrm{d}x, \mathrm{d}y).$$

We thus aim to find numerical solutions $\bar{u}$ and $\bar{\lambda}_\Sigma$ to the Poisson problem

$$\mathcal{L}u = \left(\frac{\cos x}{2} - \cos y\right)\partial_x u + \left(\frac{\cos y}{2} + \cos x\right)\partial_y u + \frac{\sigma^2}{2}\left(\partial_x^2 + \partial_y^2\right)u = \frac{\cos 2x + \cos 2y}{4} - \lambda_\Sigma = q(x,y) - \lambda_\Sigma. \tag{5.25}$$

We choose the basis $\{f_i\}_{i\in\mathbb{N}} = \{\cos mx, \sin mx\}_{m\in\mathbb{N}} \otimes \{\cos ny, \sin ny\}_{n\in\mathbb{N}}$, fix $\sigma = \sqrt{2}$ (with $W = \tilde{W} = 1$), and in the file `cellular/proof_volume` at [78] we construct

$$\bar{u}(x,y) = \sum_{m=0}^{50}\sum_{n=0}^{50} a_{mn}\cos mx\cos ny + b_{mn}\cos mx\sin ny + c_{mn}\sin mx\cos ny + d_{mn}\sin mx\sin ny,$$

represented in Figure 5.3.

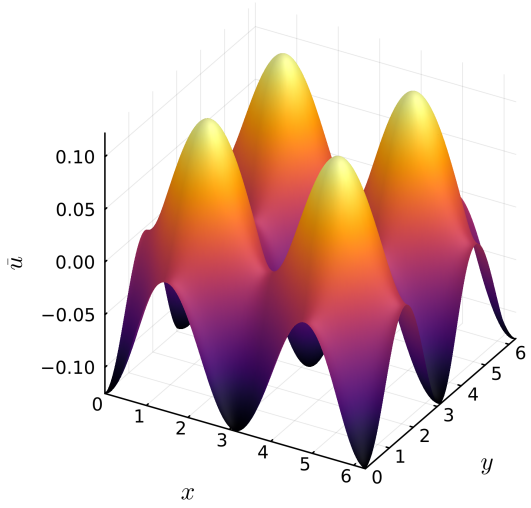


Figure 5.3: Plot of the numerical solution $\bar{u}$ to Eq. (5.25) with $\sigma = \sqrt{2}$.

Remark 5.11. Of course, one should normally try to reduce the dimension of the numerical problem by exploiting the symmetries of the system. For instance, in this case, one can observe in

Figure 5.3 that

$$\bar{u}(x,y) = \sum_{m=1}^{25}\sum_{n=1}^{25} a_{2m,2n}\cos 2mx \cos 2ny.$$

This is of importance when solving large linear systems.

We then choose

$$\bar{\lambda}_\Sigma := \frac{1}{(2\pi)^2}\int_{\mathbb{T}^2}(q-\mathcal{L}\bar{u})\,\mathrm{d}x\mathrm{d}y = -\frac{1}{(2\pi)^2}\int_{\mathbb{T}^2}(\mathcal{L}\bar{u})\,\mathrm{d}x\mathrm{d}y,$$

i.e., as in Eq. (5.21), $\bar{\lambda}_\Sigma$ is the projection of $q-\mathcal{L}\bar{u}$ on constants and

$$\bar{q} := \mathcal{L}\bar{u} + \bar{\lambda}_\Sigma.$$

Since

$$\bar{\lambda}_\Sigma = \int_{\mathbb{T}^2}\bar{q}\mathrm{d}\mu,$$

we thus have that

$$|\bar{\lambda}_\Sigma - \lambda_\Sigma| = \left|\int_{\mathbb{T}^2}(q-\bar{q})\mathrm{d}\mu\right| \leq \|q-\bar{q}\|_\infty.$$

Thus, by bounding the right-hand side, we find that

$$\lambda_\Sigma = -0.0308582892201142 \pm 5\times 10^{-16} < 0, \tag{5.26}$$

confirming that the stochastic flow $(\varphi_t)_{t\geq 0}$ is volume contracting. Note that q is a trigonometric polynomial, and that we constructed $\bar{u}$ as a trigonometric polynomial. Therefore, $\bar{q} = \mathcal{L}\bar{u} + \bar{\lambda}_\Sigma$ is also a trigonometric polynomial, and explicitly bounding $\|q-\bar{q}\|_\infty$ is straightforward (for instance using the ℓ^1-norm of the Fourier coefficients).

Of course, this particular problem could instead also be treated with more traditional computer-assisted methods by computing the stationary density w via the stationary Fokker–Planck equation $\mathcal{L}^* w = 0$ which is a uniformly elliptic equation on the torus $\mathbb{T}^2$ [12, 139, 181]. However, as already mentioned, our method requires significantly fewer computations than what would be needed for rigorously solving the stationary Fokker–Planck equation. But most importantly, our method does not make any assumption on the ellipticity of the operator $\mathcal{L}$ or on the compactness of the domain and can thus treat a much wider class of examples. This is for instance the case of the main problem of this chapter: the computations of Lyapunov exponents.

5.3 Lyapunov exponents via the projective process

In this section, we first recall how the Furstenberg–Khasminskii formula can be derived, and then give sufficient conditions for proving the ergodicity of the projective process.

5.3.1 The Furstenberg–Khasminskii formula

For the sake of presentation, let us consider first the additive noise case, i.e. $X_i = \sigma_i e_i$ for all $i \in \{1, \dots, d\}$ for some $\sigma_i \geq 0$ where $\mathcal{M} = \mathbb{T}^{d_1} \times \mathbb{R}^{d_2}$ (with $d = d_1 + d_2$). We then have that

$$\mathrm{d}\varphi_t = X_0(\varphi_t)\mathrm{d}t + \sum_{i=1}^{d} \sigma_i e_i \mathrm{d}B_t^i.$$

Then the Furstenberg–Khasminskii formula can be derived as follows. For $v \in \mathbf{P}_x\mathcal{M}$, we define

$$\varrho_t(\omega, x, v) = \|D\varphi_t(\omega, x)v\|, \qquad s_t(\omega, x, v) = \frac{D\varphi_t(\omega, x)v}{\|D\varphi_t(\omega, x)v\|} \in T_{\varphi_t(\omega,x)}\mathcal{M}. \tag{5.27}$$

Then $(s_t)_{t\geq 0}$ solves the random differential equation (a nonautonomous ordinary differential equation)

$$\frac{\mathrm{d}s_t}{\mathrm{d}t} = DX_0(\varphi_t)s_t - Q(\varphi_t, s_t)s_t, \tag{5.28}$$

where $Q(x, s) = \langle DX_0(x)s, s\rangle$ and similarly

$$\frac{\mathrm{d}\log \varrho_t}{\mathrm{d}t} = Q(\varphi_t, s_t) \quad \text{and} \quad \varrho_t = \exp \int_0^t Q(\varphi_\tau, s_\tau)\mathrm{d}\tau.$$

Therefore, if $(\xi_t)_{t\geq 0} = (\varphi_t, s_t)_{t\geq 0}$ has a unique invariant probability measure $\tilde{\mu}$ and $Q \in L^1(\tilde{\mu})$, by Birkhoff's ergodic theorem, we obtain the Furstenberg–Khasminskii formula

$$\lambda = \lim_{t\to\infty} \frac{1}{t} \log \varrho_t = \lim_{t\to\infty} \frac{1}{t} \int_0^t Q(\xi_\tau)\mathrm{d}\tau = \int_{\mathbf{P}\mathcal{M}} Q\mathrm{d}\tilde{\mu}.$$

In the multiplicative noise case,

$$\mathrm{d}\varphi_t = X_0(\varphi_t)\mathrm{d}t + \sum_{i=1}^{\ell} X_i(\varphi_t) \circ \mathrm{d}B_t^i, \qquad \varphi_0 = x,$$

the evolution equation of $(\xi_t)_{t\geq 0}$ has the form

$$\mathrm{d}\xi_t = \tilde{X}_0(\xi_t)\mathrm{d}t + \sum_{i=1}^{\ell} \tilde{X}_i(\xi_t) \circ \mathrm{d}B_t^i \qquad \xi_0 = (x, v),$$

where the vector fields $\tilde{X}_0, \tilde{X}_1, \dots, \tilde{X}_\ell$ on $\mathbf{P}\mathcal{M}$ are given by [71], which also gives a formula for the function Q in the multiplicative noise case, such that

$$\mathrm{d}\log \varrho_t = Q(\varphi_t, s_t)\mathrm{d}t + \sum_{i=1}^{\ell} \langle DX_i(\varphi_t)s_t, s_t\rangle \mathrm{d}B_t^i;$$

where the above equation is now written in Itô form. Provided

$$\frac{1}{t} \int_0^t \langle DX_i(\varphi_\tau)s_\tau, s_\tau\rangle \mathrm{d}B_\tau^i \xrightarrow{t\to\infty} 0, \qquad i = 1, \dots, \ell, \tag{5.29}$$

almost surely or in expectation with respect to $\mathbb{P} \times \tilde{\mu}$, then as before, by Birkhoff's ergodic theorem

$$\lambda = \int_{\mathbf{P}\mathcal{M}} Q \mathrm{d}\tilde{\mu}.$$

The limit (5.29) holds in expectation for instance if

$$\int_{\mathcal{M}} \|DX_i\|^2 \mathrm{d}\mu < \infty, \qquad i = 1, \dots, \ell, \tag{5.30}$$

which is a standard integrability condition for the multiplicative ergodic theorem [14, Theorem 4.2.13]. Indeed, under such integrability condition, a simple application of the Cauchy–Schwarz inequality and the Itô isometry yields that

$$\frac{1}{t} \int_{\mathbf{P}\mathcal{M}} \mathbb{E}\left[\left|\int_0^t \langle DX_i(\varphi_\tau)s_\tau, s_\tau\rangle \mathrm{d}B_\tau^i\right|\right] \mathrm{d}\tilde{\mu} \leq \frac{1}{\sqrt{t}} \left(\int_{\mathcal{M}} \|DX_i\|^2 \,\mathrm{d}\mu\right)^{1/2} \xrightarrow{t\to\infty} 0.$$

This implies that the limit (5.29) holds in expectation.

Remark 5.12. Lower Lyapunov exponents (see [17, Chapter 3] for a definition) can be obtained similarly [28] by generalising the projective process to a Grassmannian process. There is in principle no obstruction for our method to be applied to compute these additional Lyapunov exponents but, in this chapter, we mostly restrict ourselves to the top Lyapunov exponent for the sake of clarity. In particular, the bottom Lyapunov exponents can be obtained with a system similar and of the same dimension as the one studied in this work for the (top) Lyapunov exponent.

5.3.2 On the ergodicity of the projective process

Let us now address the question of the existence and uniqueness of a measure $\tilde{\mu}$ for the projective process $(\xi_t)_{t\geq 0}$. To this end, let us recall that the Lie bracket $[U, V]$ between two vector fields U and V is the vector field given by

$$[U, V](x) = DV(x)U(x) - DU(x)V(x).$$

We can now state the following nondegeneracy conditions.

Definition 5.13. Consider a stochastic differential equation written in Stratonovich form

$$\mathrm{d}x_t = V_0(x_t)\mathrm{d}t + \sum_{i=1}^{\ell} V_i(x_t) \circ \mathrm{d}B_t^i \tag{5.31}$$

with vector fields $V_0, V_1, \dots, V_\ell$ on a manifold $\mathcal{X}$. Then (5.31) is said to satisfy

(WH) the *weak* (or elliptic) Hörmander condition if $L(x)$ spans $T_x\mathcal{X}$ for all $x \in \mathcal{X}$ where $L = LA(V_0, V_1, \dots, V_\ell)$ denotes the Lie algebra generated by $V_0, V_1, \dots, V_\ell$.

(PH) the *parabolic* Hörmander condition if $L_0(x)$ spans $T_x\mathcal{X}$ for all $x \in \mathcal{X}$ where L_0 denotes the ideal generated by $V_1, \dots, V_\ell$ in L.

(SH) the *strong* Hörmander if $LA(V_1, \dots, V_\ell)$ spans $T_x\mathcal{X}$ for all $x \in \mathcal{X}$.

These conditions are typically checked by iterating the Lie Brackets

$$[\,[\ldots[V_{i_1}, V_{i_2}]\,,\ldots]\,, V_{i_n}]\,(x)$$

until they span $T_x\mathcal{X}$ for all $x \in \mathcal{X}$, where the allowed indices $i_1, \ldots, i_n$ depend on the condition to be checked. These conditions may be verified by hand e.g. in Section 5.5 or by computer assistance e.g. in Section 5.4.

Note that clearly $(SH) \implies (PH) \implies (WH)$, however only in some rare cases, does (WH) hold without (PH) (see [140] and its supplements and corrections). While the parabolic Hörmander (PH) condition implies that the Markov process $(x_t)_{t\geq 0}$ has smooth transition probabilities and is strong Feller [129, Theorem 1.3], the weak Hörmander condition (WH) implies the smoothness of stationary densities.

If a diffusion satisfies the strong Hörmander condition (SH), it is usually more straightforward to prove the existence and uniqueness of a stationary density [16]. If a diffusion does not satisfy the strong Hörmander condition (SH), it is said to be degenerate. If it only satisfies the parabolic Hörmander condition (PH) (i.e. is strong Feller) coupled with a recurrence/Lyapunov condition, then in general, one can only conclude the existence of a stationary measure [69, Section 6]. In order to obtain uniqueness, one typically has to prove the controllability or topological irreducibility of the Markov process $(x_t)_{t\geq 0}$ via the Stroock–Varadhan theorem [128, 202]. This last step is not needed when the diffusion satisfies the strong Hörmander condition (SH), as the controllability is automatic in that case.

Unfortunately, in the case of the projective process $(\xi_t)_{t\geq 0} = (\varphi_t, s_t)_{t\geq 0}$, the strong Hörmander condition (SH) is typically not satisfied. This is for instance clear in the additive noise case (see Eq. (5.28)). One then normally has to check for the controllability of $(\xi_t)_{t\geq 0}$, in addition of the parabolic Hörmander condition (PH) for $(\xi_t)_{t\geq 0}$. While controllability is not so hard to check on a case-by-case basis, it can sometimes be fiddly and cumbersome. Fortunately, San Martin and Arnold [197] give weak and general conditions for the controllability and hence uniqueness of a stationary measure for $(\xi_t)_{t\geq 0}$ on $\mathbf{P}(\mathcal{M})$ to hold; we state their result below.

First recall that the evolution equations of $(\varphi_t)_{t\geq 0}$ and $(\xi_t)_{t\geq 0}$ are respectively given by

$$\mathrm{d}\varphi_t = X_0(\varphi_t)\mathrm{d}t + \sum_{i=1}^{\ell} X_i(\varphi_t) \circ \mathrm{d}B_t^i(\omega), \qquad \varphi_0 = x, \tag{5.32}$$

and

$$\mathrm{d}\xi_t = \tilde{X}_0(\xi_t)\mathrm{d}t + \sum_{i=1}^{\ell} \tilde{X}_i(\xi_t) \circ \mathrm{d}B_t^i, \qquad \xi_0 = (x, v), \tag{5.33}$$

where $X_0, X_1, \ldots, X_\ell$ (and thus $\tilde{X}_0, \tilde{X}_1, \ldots, \tilde{X}_\ell$) are *analytic* and complete vector fields. Then [197] asserts that if $(\varphi_t)_{t\geq 0}$ possesses a unique ergodic probability measure on $\mathcal{M}$, then it is sufficient for $(\xi_t)_{t\geq 0}$ to merely fulfil the weak Hörmander condition (WH) for it to possess a unique ergodic probability measure on $\mathbf{P}\mathcal{M}$.

Proposition 5.14. Recall that $X_0, X_1, \ldots, X_\ell$ are *analytic* and complete vector fields on $\mathcal{M}$. Assume that the Markov process $(\varphi_t)_{t\geq 0}$ possesses a unique ergodic probability measure $\mu(\mathrm{d}x) =$

$w(x)\mathrm{d}x$ on $\mathcal{M}$ and that $(\varphi_t)_{t\geq 0}$ is controllable on $C = \mathrm{supp}\mu \subset \mathcal{M}$. Then if the evolution equation (5.33) of $(\xi_t)_{t\geq 0}$ satisfies the weak Hörmander condition (WH), then there exists a unique ergodic probability measure $\tilde{\mu}$ for $(\xi_t)_{t\geq 0}$ on $\mathbf{P}\mathcal{M}$. Furthermore, denoting $\tilde{\mu}(\mathrm{d}\xi) = \tilde{w}(\xi)\mathrm{d}\xi$, then $\tilde{w}$ is smooth, $\tilde{\mathcal{L}}^*\tilde{w} = 0$ and for all $x \in \mathcal{M}$

$$w(x) = \int_{\mathbf{P}(T_x\mathcal{M})} \tilde{w}(x,s)\mathrm{d}s$$

Proof. Under these assumptions, we can combine Theorem 7 and Corollary 2 of [197] which give the uniqueness of an invariant control set $\tilde{C}$ for $(\xi_t)_{t\geq 0} = (\varphi_t, s_t)_{t\geq 0}$ on $\mathbf{P}C \subset \mathbf{P}\mathcal{M}$. Furthermore, there exists a unique smooth ergodic measure $\mathrm{d}\tilde{\mu} = \tilde{w}\mathrm{d}\xi$ for $(\xi_t)_{t\geq 0}$ on $\mathbf{P}C$ and thus on $\mathbf{P}\mathcal{M}$. This essentially follows from the Stroock–Varadhan theorem (e.g. see [128]) which asserts that invariant distributions are supported on such control sets. Note that under the weak Hörmander condition (WH), there can only exist one invariant measure on such control set [16]. □

Corollary 5.15. Assume that the Markov process $(\varphi_t)_{t\geq 0}$ possesses an invariant distribution μ on $\mathcal{M}$. Assume further that the evolution equation (5.32) of $(\varphi_t)_{t\geq 0}$ satisfies the strong Hörmander condition (SH) and the evolution equation (5.33) of $(\xi_t)_{t\geq 0}$ satisfies the weak Hörmander condition (WH). Then μ is the unique ergodic measure for $(\varphi_t)_{t\geq 0}$ and the conclusions of Proposition 5.14 hold.

As in Remark 5.12, this result can be generalised to other fibre bundles [196] such as Grassmannian bundles to obtain lower Lyapunov exponents.

5.4 The cellular flow with sinks

In this section, we first discuss the example presented in Theorem 1.10, and then treat a similar system but with multiplicative noise.

Consider again the cellular flow with sinks

$$\begin{cases} \mathrm{d}x_t &= (\cos(x_t)/2 - \cos y_t)\sin x_t \mathrm{d}t + \sigma \mathrm{d}B_t^1 \\ \mathrm{d}y_t &= (\cos(y_t)/2 + \cos x_t)\sin y_t \mathrm{d}t + \sigma \mathrm{d}B_t^2 \end{cases} \tag{5.34}$$

i.e. the corresponding vector fields on $\mathcal{M} = \mathbb{T}^2$ are

$$X_0(x,y) = \begin{pmatrix} (\cos(x)/2 - \cos y)\sin x \\ (\cos(y)/2 + \cos x)\sin y \end{pmatrix}, \qquad X_1(x,y) = \begin{pmatrix} \sigma \\ 0 \end{pmatrix}, \qquad X_2(x,y) = \begin{pmatrix} 0 \\ \sigma \end{pmatrix}.$$

Recall that it is a modification of the standard cellular flow [63], such that the deterministic dynamics of the system ($\sigma = 0$) are attracting for almost all initial conditions (see Figure 1.4a). In the case of the standard cellular flow, which is Hamiltonian, it is more straightforward to show that for any $\sigma > 0$ small enough, the Lyapunov exponent λ is positive. This chaotic behaviour can be seen as the result of a shearing effect along the level curves of the corresponding Hamiltonian. This is clearly not the case in our system which displays a negative Lyapunov exponent λ for $\sigma > 0$

close to zero. We however show that the system can be destabilised if the noise $\sigma > 0$ is increased enough (see Figure 1.4b).

5.4.1 The additive noise case

Recall that we aim to compute the Lyapunov exponent λ via the projective process $(\xi_t)_{t\geq 0} = (\varphi_t, s_t)_{t\geq 0}$ where

$$s_t = \frac{D\varphi_t v}{\|D\varphi_t v\|}, \qquad v \in T_x\mathcal{M}.$$

We can compute the random differential equation for s_t via formula (5.28). Now, identifying $\mathbf{P}(T_x\mathcal{M}) \simeq \mathbf{P}(\mathbb{R}) \simeq \mathbb{T}$ and denoting $s_t = (\cos(\theta_t/2), \sin(\theta_t/2))$, we find

$$\frac{\mathrm{d}\theta_t}{\mathrm{d}t} = \frac{1}{2}\left(\sin\theta_t(4\cos x_t \cos y_t - \cos 2x_t + \cos 2y_t) - 4\sin x_t \sin y_t\right) =: h(x_y, y_t, \theta_t), \tag{5.35}$$

and

$$\lambda = \int_{\mathbb{T}^3} Q(x,y,\theta)\tilde{\mu}(\mathrm{d}x, \mathrm{d}y, \mathrm{d}\theta)$$
$$Q(x,y,\theta) = \frac{1}{4}(\cos 2x + \cos 2y - \cos\theta(4\cos x \cos y + \cos 2y - \cos 2x)),$$

where $\tilde{\mu}$ is the unique stationary distribution of the process $(\varphi_t, \theta_t)_{t\geq 0}$. This uniqueness follows (via Corollary 5.15) from the fact that the base process $(\varphi_t)_{t\geq 0}$ is clearly ergodic and controllable on the compact state space $\mathcal{M}$ as a diffusion with additive noise and the verification of the parabolic Hörmander condition (PH) for the process $(\varphi_t, \theta_t)_{t\geq 0}$ in the file `cellular/hypoelltipticity.ipynb` at [78].

Proof of Theorem 1.10. Following the strategy laid out in Section 5.2, for the parameter $\sigma = \sqrt{2}$, we compute a numerical solution

$$\bar{u} \in \mathrm{Span}\left(\{\cos kx, \sin kx\}_{k=0}^{25} \otimes \{\cos my, \sin my\}_{m=0}^{25} \otimes \{\cos n\theta, \sin n\theta\}_{n=0}^{550}\right)$$

(which can be found in the file `cellular/ubar` [78]) to the Poisson problem

$$\tilde{\mathcal{L}}u = Q - \lambda, \tag{5.36}$$

where h is as in (5.35) and

$$\tilde{\mathcal{L}} = \left(\frac{\cos x}{2} - \cos y\right)\partial_x + \left(\frac{\cos y}{2} + \cos x\right)\partial_y + h(x,y,\theta)\partial_\theta + \frac{\sigma^2}{2}(\partial_{xx} + \partial_{yy}). \tag{5.37}$$

We define $\bar{\lambda}$ and $\bar{Q}$ as outlined in Section 5.2, i.e.,

$$\bar{\lambda} := P_0(Q - \mathcal{L}\bar{u}), \tag{5.38}$$

and

$$\bar{Q} := \mathcal{L}\bar{u} + \bar{\lambda} \approx Q. \tag{5.39}$$

Choosing $W = \tilde{W} = 1$, we find that

$$|\lambda - \bar{\lambda}| \leq \|Q - \bar{Q}\|_\infty,$$

which can be evaluated directly by summing the absolute values of the Fourier coefficients of $Q - \bar{Q}$. The proof is performed in the file `cellular/proof` at [78] □

Remark 5.16. Since the operator $\mathcal{L}$ defined in (5.37) fulfils the parabolic Hörmander condition (PH), the process $(\xi_t)_{t\geq 0}$ is strong Feller and u is expected to be of class $\mathcal{C}^\infty$. Therefore, its Fourier coefficients should decay faster than algebraically, and this is why we can get a tight enclosure of λ in Theorem 1.10. However, many more basis functions are still needed in the non-elliptic direction of the problem (the θ variable).

Remark 5.17. One can actually state [14, Theorem 4.2.6] for this two-dimensional example that for $(\mathbb{P} \times \mu)$-almost every $(\omega, x) \in \Omega \times \mathcal{M}$, there exists $v^* \in \mathbf{P}\mathcal{M}$ such that for all $v \in \mathbf{P}\mathcal{M}\backslash\{v^*\}$

$$\lim_{t\to\infty} \frac{1}{t} \log \|D\varphi_t(\omega, x)v\| = \lambda,$$

and

$$\lim_{t\to\infty} \frac{1}{t} \log \|D\varphi_t(\omega, x)v^*\| =: \lambda_2 = 2\lambda_\Sigma - \lambda,$$

where λ_Σ is as in Section 5.2.2 and λ_2 is the second Lyapunov exponent. Thus, combining (1.50) and (5.26), we obtain that

$$\lambda_2 = 2\lambda_\Sigma - \lambda = -0.11756188842594 \pm 10^{-13} < 0.$$

5.4.2 A modification with multiplicative noise

Now consider a modification of the cellular flow with sinks (5.34) where we replace the additive noise with a multiplicative one in the spirit of Baxendale [23]. We now consider the vector fields

$$\begin{aligned} X_0(x,y) &= \begin{pmatrix} (\cos(x)/2 - \cos y)\sin x \\ (\cos(y)/2 + \cos x)\sin y \end{pmatrix}, \qquad X_1(x,y) = \begin{pmatrix} \sigma \sin x \\ 0 \end{pmatrix}, \\ X_2(x,y) &= \begin{pmatrix} \sigma \cos x \\ 0 \end{pmatrix}, \qquad X_3(x,y) = \begin{pmatrix} 0 \\ \sigma \sin y \end{pmatrix}, \qquad X_4(x,y) = \begin{pmatrix} 0 \\ \sigma \cos y \end{pmatrix}. \end{aligned} \tag{5.40}$$

It turns out that the random dynamical system induced by these vector fields has the same *statistical* one-point motion as the previously considered system, i.e. they are described by the same Markov semi-group. That can be directly seen from the generator which is in both cases

$$\mathcal{L} = \left(\frac{\cos x}{2} - \cos y\right)\sin x \frac{\partial}{\partial x} + \left(\frac{\cos y}{2} + \cos x\right)\sin y \frac{\partial}{\partial y} + \frac{\sigma^2}{2}\left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2}\right).$$

We will however see that the *dynamical* properties of the stochastic flow $(\varphi_t)_{t\geq 0}$ are very different under this multiplicative noise. Indeed, we will show that the system now displays a negative Lyapunov exponent. Following [23] (with minor modifications due to our choice of variables), we find that

$$\mathrm{d}\log\varrho_t = Q(x_t,y_t,\theta_t)\mathrm{d}t + \frac{\sigma}{2}\Big[(\cos\theta_t+1)(\cos x_t\mathrm{d}B_t^1 - \sin x_t\mathrm{d}B_t^2) + (\cos\theta_t - 1)(\cos y_t\mathrm{d}B_t^3 - \sin y_t\mathrm{d}B_t^4)\Big],$$

where

$$Q(x,y,\theta) = \frac{1}{4}(\cos 2x + \cos 2y - \cos\theta(4\cos x\cos y + \cos 2y - \cos 2x)) - \frac{\sigma^2}{2}\cos^2\theta.$$

Similarly, we find that

$$\begin{aligned}\tilde{\mathcal{L}} = &\left(\frac{\cos x}{2} - \cos y\right)\sin x\partial_x + \left(\frac{\cos y}{2} + \cos x\right)\sin y\partial_y + \left(h(x,y,\theta) + \frac{\sigma^2}{2}\sin 2\theta\right)\partial_\theta \\ &+ \frac{\sigma^2}{2}\left(\partial_{xx} + \partial_{yy} + 2\sin^2\theta\partial_{\theta\theta}\right),\end{aligned}$$

where h is as in (5.35). These calculations essentially follow from the Stratonovich-to-Itô correction [189, Chapter 3.2]. Now, as discussed earlier since $\mathcal{M} = \mathbb{T}^2$, the integrability condition (5.30) clearly holds and we have that

$$\lambda = \int_{\mathbb{T}^3} Q(x,y,\theta)\tilde{\mu}(\mathrm{d}x,\mathrm{d}y,\mathrm{d}\theta).$$

Theorem 5.18. Consider the stochastic flow $(\varphi_t)_{t\geq 0}$ generated by the vector fields (5.40), with $\sigma = \sqrt{2}$, then for the corresponding Lyapunov exponent λ, there are the following bounds

$$\lambda = -0.6124 \pm 1.6\times 10^{-3} < 0.$$

Proof. The weak Hörmander condition is verified by checking that $\tilde{X}_1, \tilde{X}_2, \tilde{X}_3, \tilde{X}_4$ span $\mathbb{R}^3$ for $\theta \neq \pi/2 \pm \pi/2$ and $\tilde{X}_0, \tilde{X}_1, \tilde{X}_2, \tilde{X}_3, \tilde{X}_4, [\tilde{X}_0,\tilde{X}_2], [\tilde{X}_0,\tilde{X}_4], [[\tilde{X}_0,\tilde{X}_2],\tilde{X}_4]$ span $\mathbb{R}^3$ for $\theta = \pi/2 \pm \pi/2$. Since the generator $\mathcal{L}$ of the Markov process $(\varphi_t)_{t\geq 0}$ is uniformly elliptic, by Proposition 5.14, there indeed exists a unique stationary measure $\tilde{\mu}(\mathrm{d}\xi) = \tilde{w}(\xi)\mathrm{d}\xi$ for the projective process $(\xi_t)_{t\geq 0} = (\varphi_t, s_t)_{t\geq 0}$. The application of the adjoint method as described in Section 5.2 is available at [78] in the file `cellular/baxendale_proof`. □

5.5 The randomly forced pendulum

In this section, we discuss the example presented in Theorem 5.1, namely the randomly forced pendulum (or Josephson junction [189])

$$" \ddot{x}_t = -\kappa\sin x_t - \gamma\dot{x}_t + \sigma\dot{B}_t "$$

with gravitational acceleration $\kappa > 0$, friction coefficient $\gamma > 0$ and noise strength $\sigma > 0$. It

translates to the proper stochastic differential equation

$$\begin{cases} \mathrm{d}x_t &= y_t \mathrm{d}t \\ \mathrm{d}y_t &= -(\kappa \sin x_t + \gamma y_t)\mathrm{d}t + \sigma \mathrm{d}B_t \end{cases} \tag{5.41}$$

on $\mathcal{M} = \mathbb{T} \times \mathbb{R}$. Since this differential equation has $\mathcal{C}^\infty$-vector fields with bounded derivatives of all orders, it clearly induces a stochastic flow of diffeomorphisms $(\varphi_t)_{t\geq 0}$ (see [155, Chapter II.4]).

While this system is the stochastic version of a classical ordinary differential equation and also typically appears in applications related to superconductors [145], its study from a mathematically rigorous point of view is so far limited.

Analogously to the previous example, this system can also be seen as an attracting version of a Hamiltonian pendulum (when the friction $\gamma = 0$). We are thus interested in the possible chaotic behaviour of the system when $\sigma > 0$. Note however that the mechanisms inducive of chaos for the randomly forced pendulum are not so clear: From Theorem 5.1, chaos appears as a consequence of the large noise σ in the y-direction. However, this allows trajectories to spend more time away from the x-axis, where most of the dynamics seem to be happening from the deterministic point of view (see Figure 5.1a) and does not a priori push trajectories into more expanding regions of the system. The large noise may though act as a catalyst for a stretch-and-fold mechanism when the system crosses the x-axis (see Figure 5.1b).

5.5.1 Ergodicity of the projective process

In this section, we verify the ergodicity of the projective process. We achieve this by following Section 5.3.2 and first proving the ergodicity of the base process $(\varphi_t)_{t\geq 0}$ (Steps 1–3) and then showing that the projective process $(\xi_t)_{t\geq 0} = (\varphi_t, s_t)_{t\geq 0}$ satisfies the weak Hörmander condition (WH). As usual [85, 127], the former is shown via the construction of a judicious Lyapunov function, proving the process is Feller via the parabolic Hörmander condition (PH) and showing the controllability of $(\varphi_t)_{t\geq 0}$ on $\mathcal{M} = \mathbb{T} \times \mathbb{R}$.

Step 1 (Choice of a Lyapunov function)**.** Recall that here the generator of the process $(\varphi_t)_{t\geq 0}$ is given by

$$\mathcal{L} = y\frac{\partial}{\partial x} - (\kappa \sin x + \gamma y)\frac{\partial}{\partial y} + \frac{\sigma^2}{2}\frac{\partial^2}{\partial y^2} = y\frac{\partial}{\partial x} - \kappa \sin x \frac{\partial}{\partial y} + L_y,$$

where

$$L_y = -\gamma y \frac{\partial}{\partial y} + \frac{\sigma^2}{2}\frac{\partial^2}{\partial y^2} \tag{5.42}$$

is the generator of an Ornstein–Uhlenbeck process with stationary density $e^{-\gamma y^2/\sigma^2}$ [189]. Thus, a natural choice for a Lyapunov function is $W(x, y) = e^{\gamma y^2/(2\sigma^2)}$; we have

$$\begin{aligned} \mathcal{L}W(x,y) &= \frac{\gamma}{2\sigma^2}(-\gamma y^2 + \sigma^2 - 2\kappa y \sin x)W(x,y) \\ &= -cW(x,y) + \left[\frac{\gamma}{2\sigma^2}(-\gamma y^2 + \sigma^2 - 2\kappa y \sin x) + c\right] e^{\gamma y^2/(2\sigma^2)} \\ &\leq -cW(x,y) + d\mathbb{1}_C, \end{aligned}$$

where $c > 0$ and

$$C := \left\{ y \in \mathbb{R} \,\middle|\, \frac{\gamma}{2\sigma^2}(-\gamma y^2 + \sigma^2 + 2\kappa|y|) + c > 0 \right\}$$
$$d := \sup_{y \in C} \left[\frac{\gamma}{2\sigma^2}(-\gamma y^2 + \sigma^2 + 2\kappa|y|) + c \right] e^{\gamma y^2/(2\sigma^2)}. \tag{5.43}$$

Step 2 (Parabolic Hörmander condition (PH) for the base process)**.** We have that

$$X_0(x, y, \theta) = \begin{pmatrix} y \\ -\kappa \sin x - \gamma y \end{pmatrix}, \qquad X_2(x, y, \theta) = \begin{pmatrix} 0 \\ \sigma \end{pmatrix},$$

and thus,

$$[X_2, X_0](x, y, \theta) = \begin{pmatrix} \sigma \\ -\gamma\sigma \end{pmatrix},$$

which shows that $(\varphi_t)_{t \geq 0}$ fulfils the parabolic Hörmander condition.

Step 3 (Controllability of the base process)**.** First note that from (5.41), it is clear that y is completely controllable. Now, fixing $x_0 \in \mathbb{T}$, note that for all $(\bar{x}, \bar{y}) \in \mathbb{T} \times \mathbb{R} \backslash \{(0, 0), (\pi, 0)\}$, there exists $y_0 \in \mathbb{R}$ such that $(\bar{x}, \bar{y}) \in O^+(x_{,0}, y_0)$ where $O^+(x_{,0}, y_0)$ is the forward orbit starting at (x_0, y_0) of the deterministic system (represented in Figure 5.1a). This shows the controllability and thus ergodicity of the base process $(\varphi_t)_{t \geq 0}$ on $\mathcal{M} = \mathbb{T} \times \mathbb{R}$.

Step 4 (Weak Hörmander condition for the projective process)**.** It now remains to be shown that the projective process $(\xi_t)_{t \geq 0} = (\varphi_t, s_t)_{t \geq 0}$ satisfies the weak Hörmander condition (WH) to apply Proposition 5.14. Writing $s_t = (\cos(\theta_t/2), \sin(\theta_t/2))$, we find that on $\mathbf{P}\mathcal{M} \simeq \mathbb{T} \times \mathbb{R} \times \mathbb{T}$

$$\tilde{X}_0(x, y, \theta) = \begin{pmatrix} y \\ -\gamma y - \kappa \sin x \\ -\gamma \sin\theta + \cos\theta - \kappa \cos x(\cos\theta + 1) - 1 \end{pmatrix}, \qquad \tilde{X}_2(x, y, \theta) = \begin{pmatrix} 0 \\ \sigma \\ 0 \end{pmatrix}.$$

Again, we have that

$$\left[\tilde{X}_2, \tilde{X}_0\right](x, y, \theta) = \begin{pmatrix} \sigma \\ -\gamma\sigma \\ 0 \end{pmatrix}.$$

It thus remains to show that among the remaining vector fields of the Lie algebra, some are non-zero in the direction e_3. Now

$$\left[\left[\tilde{X}_2, \tilde{X}_0\right], \tilde{X}_0\right](x, y, \theta) = \begin{pmatrix} -\gamma\sigma \\ \sigma\left(\gamma^2 - \kappa\cos x\right) \\ \kappa\sigma \sin x(\cos\theta + 1) \end{pmatrix}.$$

so that the remaining points to check are reduced to the set $\{(x, y, \theta) \in \mathbb{T} \times \mathbb{R} \times \mathbb{T} \mid \theta = \pi \text{ or } x = \pi/2 \pm \pi/2\}$. For $\theta = \pi$, we have that

$$\tilde{X}_0(x, y, \pi) = \begin{pmatrix} y \\ -\gamma y - \kappa \sin x \\ -2 \end{pmatrix}.$$

Finally, for $x = \pi/2 \pm \pi/2$, we have that

$$\left[\left[\left[\left[\tilde{X}_2, \tilde{X}_0\right], \tilde{X}_0\right], \tilde{X}_0\right], \tilde{X}_2\right](\pi/2 \pm \pi/2, y, \theta) = \mp \begin{pmatrix} 0 \\ 0 \\ \kappa\sigma^2(1 + \cos\theta) \end{pmatrix},$$

which finishes the proof of the weak Hörmander condition (WH) and thus of the ergodicity for the projective process by Proposition 5.14.

5.5.2 The adjoint method for the pendulum

In this section, we outline the proof of Theorem 5.1. Recall that we must numerically find approximate solutions $\bar{u}$ and $\bar{\lambda}$ to the Poisson problem

$$\tilde{\mathcal{L}}u = Q - \lambda, \tag{5.44}$$

where

$$\tilde{\mathcal{L}} = y\frac{\partial}{\partial x} - (1 + \gamma\sin\theta - \cos\theta + \kappa(\cos\theta + 1)\cos x)\frac{\partial}{\partial\theta} - \kappa\sin x\frac{\partial}{\partial y} + L_y \tag{5.45}$$

and

$$Q(x, y, \theta) = \frac{1}{2}(\gamma\cos\theta + \sin\theta - \gamma - \kappa\sin\theta\cos x).$$

We follow the procedure of Section 5.2 and need to choose a judicious Hilbert basis. Note that (as it is well-known from the study Ornstein–Uhlenbeck process)

$$L_y H_m(\sqrt{\gamma}y/\sigma) = -\gamma m H_m(\sqrt{\gamma}y/\sigma),$$

where the H_m's are Hermite polynomials (see [1, p. 775]) and L_y is as in (5.42). We thus naturally

use the Hilbert basis

$$\{\cos kx, \sin kx\} \otimes \{h_m(\sqrt{\gamma}y/\sigma)\} \otimes \{\cos n\theta, \sin n\theta\},$$

where we choose the normalisation $h_m = H_m/\sqrt{2^m m!}$. With respect to this basis, we compute a numerical solution $\bar{u}$ to the Poisson problem (5.44) available in the file `pendulum/ubar` at [78] for the parameters $\kappa = 2/3, \gamma = 1/4$ and $\sigma = 4$.

In the file `pendulum/compute_sups.jl` at [78], we give enclosures for

$$\sup_{y\in\mathbb{R}} \left| \frac{h_m(\sqrt{\gamma}y/\sigma)}{W(x,y)} \right| = \sup_{z\in\mathbb{R}} |h_m(z)e^{-z^2/2}|,$$

for all $m = 0, \ldots, 551$, where $W(x,y) = \tilde{W}(x,y) = e^{\gamma y^2/(2\sigma^2)}$. This is achieved by enclosing all the roots of $\partial_z(h_m(z)e^{-z^2/2})$ by combining the Fundamental Theorem of Algebra and the Intermediate Value Theorem. Finally, note that since

$$\mathcal{L}W \leq -cW + d,$$

with any $c > 0$ and d as in (5.43), we obtain the bound $\mu(W) \leq d/c$ by [175, Theorem 4.3.(ii)]. Since μ is the marginal of $\tilde{\mu}$ on $\mathcal{M} = \mathbb{T} \times \mathbb{R}$, and we also have that

$$\tilde{\mu}(W) = \int_{\mathbf{P}\mathcal{M}} W \mathrm{d}\tilde{\mu} = \int_{\mathcal{M}} W \mathrm{d}\mu \leq \frac{d}{c},$$

which is computed rigorously for a specific c in the file `pendulum/Lyapunov_bound.jl` at [78]. The proof of Theorem 5.1 is performed in the file `pendulum/proof.ipynb`, applying estimate (5.24) of Proposition 5.7.

Remark 5.19. For this problem, the most challenging part was without a doubt the computation of a good approximate solution $\bar{u}$ to the Poisson problem (5.44), which was done via the least-square problem (5.19). This difficulty stems from the very non-elliptic nature of the operator (5.45). Even accounting for the symmetry in the problem, we used $48,312,000$ basis functions just to confirm the sign of the Lyapunov exponent λ (We used $105,568,462$ for the result of Theorem 5.1). A crucial feature of our computation was to first solve the problem on a small number of basis functions and iteratively increase the number of basis functions while taking the result of the previous step as an initial guess for `LSQR` [187]. Some additional improvements to speed up our calculation would be to parallelise our matrix-vector multiplication (with several CPUs, using for instance MKL or using a GPU).

5.6 The Hopf normal form

We now come back to our motivation of Section 1.1 and studied in Chapter 4, the Hopf normal form with additive noise

$$\mathrm{d}\begin{pmatrix} x_t \\ y_t \end{pmatrix} = \left[\begin{pmatrix} \alpha & -\beta \\ \beta & \alpha \end{pmatrix} \begin{pmatrix} x_t \\ y_t \end{pmatrix} - \begin{pmatrix} a & b \\ -b & a \end{pmatrix} \begin{pmatrix} x_t \\ y_t \end{pmatrix} (x_t^2 + y_t^2) \right] \mathrm{d}t + \sigma \mathrm{d} \begin{pmatrix} B_t^1 \\ B_t^2 \end{pmatrix}. \tag{5.46}$$

for which we aim to compute the Lyapunov exponent λ_b. We will show that in contrast with the approaches of [57] and in Chapter 4, the method presented in this chapter allows to deal with the full problem on $\mathbb{R}^2$, while being much simpler. Recently, Baxendale [24], and Chemnitz and Engel [73] did prove that the Lyapunov exponent λ_b associated to (5.46) becomes positive in the asymptotic regime $b \to \infty$. In this section, we tackle the opposite (and complementary) problem for b small, and prove that $\lambda_b > 0$ for an explicit parameter range of finite and explicit values of b, while also enclosing the critical value of b at which the transition from negative to positive takes place. Note that Baxendale [24] also made use of the adjoint method in his proof, though in a quite different fashion.

5.6.1 The adjoint method for a single parameter

Recall the derivation of the Furstenberg-Khasminskii formula in Section 4.1. Before proving Theorem 1.4 in the next subsection, we first explain how to rigorously enclose the Lyapunov exponent of (5.46) for a fixed value of b.

We first need to numerically solve the Poisson problem

$$\mathcal{L}u = Q - \lambda, \tag{5.47}$$

where $\mathcal{L}$ and Q are as in Section 4.1. This equation is "polynomial" with respect to these new polar coordinates (r_t, ϑ_t). This allows us to choose a suitable basis in polar coordinates, rendering our problem sparse. Here, we use the following basis in the Hermite–Laguerre family (or a scaling of it)

$$H_n^m(r, \vartheta) := r^{|m|} L_n^{(|m|)}(r^2) \begin{cases} \sin m\vartheta & m > 0 \\ \cos m\vartheta & m \leq 0 \end{cases}$$

where $L_n^{(m)}$ denotes the generalised Laguerre polynomial of degree n and parameter m (see [1, p. 775]). We choose the normalisation convention of numerical analysis and denote $h_n^m = \sqrt{n!/(m+n)!} H_n^m$ for all $m \in \mathbb{Z}, n \in \mathbb{N}$. Note also the slight change of definition from 4.2 which will be more practical here. Though this basis is well-known to physicists and has been studied mathematically in [142, 75], it has not been used much for numerical purposes.

Remark 5.20. Note that our choice of basis does not perfectly match the "physics" of our problem. Indeed, our basis is orthogonal with respect to the Gaussian measure $e^{-r^2} r \mathrm{d}r\mathrm{d}\vartheta$. One could expect better results with a basis orthogonal with respect to the Freud weight $e^{-(\alpha r^4/2 - \alpha r^2)/\sigma^2} r \mathrm{d}r\mathrm{d}\vartheta$ which is the marginal of μ onto r. However, the construction of such a basis is beyond the scope of this work. Nevertheless, our choice of basis does not prevent the application of our method as the only rigorous computation needed is essentially the application of the operator $\mathcal{L}$ to $\bar{u}$. This is in contrast with computer-assisted proofs for the solutions of PDEs which would typically necessitate some *a priori* estimates on the inverse of some part of the operator $\mathcal{L}$ with respect to a suitable basis.

For $\alpha = a = 4, \sigma = \sqrt{2}$ and $b = 21.5381$, in the file `Hopf/proof` at [78], with respect to this basis, we compute an ansatz $\bar{u}$ to (5.47) represented in Figure 5.4 and obtained the following result.

Theorem 5.21. For the Hopf normal form with additive noise (5.46), with the parameters $\alpha = a = 4, \sigma = \sqrt{2}$ and $b = 21.5381$, the Lyapunov exponent λ is positive.

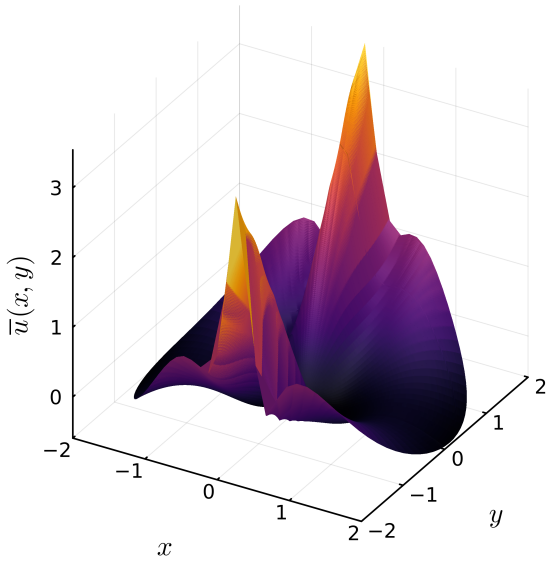


Figure 5.4: Plot of the numerical solution $\bar{u}$ to Eq. (5.47) with $a = \alpha = 4, \sigma = \sqrt{2}$ and $b = 21.5381$.

Finally, note that the choice of $W = \tilde{W}$ is quite straightforward as from (4.5), the marginal of μ on the radial direction is simply

$$\mu(\mathrm{d}r, \mathbb{T}) = \frac{re^{-(ar^4/2-\alpha r^2)/\sigma^2}}{Z}\mathrm{d}r, \qquad Z = \int_0^\infty re^{-(ar^4/2-\alpha r^2)/\sigma^2}\mathrm{d}r.$$

Therefore, choosing for instance W of the form

$$W(r) = e^{cr^4/(2\sigma^2)}, \qquad 0 < c < a,$$

we can compute the integral

$$\mu(W) = \frac{1}{Z}\int_0^\infty re^{((c-a)r^4/2+\alpha r^2)/\sigma^2}\mathrm{d}r = \frac{\sqrt{a}e^{\alpha^2 c/2a\sigma^2(a-c)}(1+\mathrm{erf}(\alpha/(\sigma\sqrt{2(a-c)})))}{\sqrt{a-c}(1+\mathrm{erf}(\alpha/(\sigma\sqrt{2a})))}, \qquad \alpha > 0,$$

where the function erf can be rigorously enclosed using `Arb` [144] which implements the evaluation of special functions in ball arithmetic. Here, we chose $c = a/2$. As in Section 5.5.2, we computed the suprema of $|H_n^m/W|$ in the file `Hopf/compute_sups.jl` at [78].

5.6.2 Continuation with respect to the shear b

We now show how our method can be combined with continuation techniques recently developed in [51], which we implement in the file `Hopf/continuation` at [78]. We now want to enclose the parameter-dependent Lyapunov exponent

$$\lambda_b = \int_{\mathbb{R}_+\times\mathbb{T}} Q_b \mathrm{d}\mu_b = \int_{\mathbb{R}_+\times\mathbb{T}} \left(\alpha - 2ar^2 + \sqrt{a^2+b^2}r^2 \sin 2\vartheta\right) \mu_b(\mathrm{d}r, \mathrm{d}\vartheta),$$

for all b in a parameter range $[b_-, b_+]$. We first define an approximate solution $\bar{u}_b$ for the Poisson problem $\mathcal{L}_b u_b = Q_b - \lambda_b$ (where these are all now parameter-dependent) for all $b \in [b_-, b_+]$ of the form

$$\bar{u}_b(r,\vartheta) = \sum_{k=0}^{K} \sum_{m,n} c_{k,m,n} T_k(b) h_n^m(r,\vartheta),$$

where T_k denotes the Cheybyshev polynomial of the first kind of degree k on $[b_-, b_+]$. This is done by computing approximate solutions for $K+1$ values of b in $[b_-, b_+]$ (taken at the Chebyshev nodes) and interpolating them.

We then need to rigorously apply $\mathcal{L}_b$ to $\bar{u}_b$, for $b \in [b_-, b_+]$. This could be done *exactly*, i.e. $\mathcal{L}_b \bar{u}_b$ would have a finite expansion in the (Hermite–Laguerre)–Chebyshev basis, except for the fact that Q_b is not polynomial in b. We therefore first build a degree K polynomial p (in the Chebyshev basis) approximating $\sqrt{a^2+b^2}$ and compute an error bound ε such that

$$\sup_{b\in[b_-,b_+]} \left| p(b) - \sqrt{a^2+b^2} \right| < \varepsilon.$$

We then denote $\hat{Q}_b := \alpha - 2ar^2 + p(b)r^2 \sin 2\vartheta$, which is now polynomial in b and should approximate Q_b well in b, and

$$\hat{\mathcal{L}}_b := (\alpha r - ar^3)\partial_r + \left(br^2 + p(b)r^2 \cos 2\vartheta\right)\partial_\vartheta + \frac{\sigma^2}{2}\Delta.$$

We now have that $\hat{\mathcal{L}}\bar{u}_b - \hat{Q}_b$ is polynomial of degree $2K$ in b and given that it is written in terms of Chebyshev coefficients, it is straightforward to give an upper bound on

$$\sup_{b\in[b_-,b_+]} \|(\hat{\mathcal{L}}_b \bar{u}_b - \hat{Q}_b + \bar{\lambda}_b)/W\|_\infty,$$

where $\bar{\lambda}_b = P_0(\hat{Q}_b - \hat{\mathcal{L}}_b \bar{u}_b)$.

We now incorporate the errors coming from approximating Q_b by $\hat{Q}_b$

$$\begin{aligned}
|\bar{\lambda}_b - \lambda_b| &\le \left| \bar{\lambda}_b - \int_{\mathbb{R}_+\times\mathbb{T}} Q_b \mathrm{d}\mu_b \right| \\
&\le \left| \bar{\lambda}_b - \int_{\mathbb{R}_+\times\mathbb{T}} \hat{Q}_b \mathrm{d}\mu_b \right| + \left| \int_{\mathbb{R}_+\times\mathbb{T}} (Q_b - \hat{Q}_b) \mathrm{d}\mu_b \right| \\
&\le \left| \int_{\mathbb{R}_+\times\mathbb{T}} (\bar{\lambda}_b - \hat{Q}_b + \hat{\mathcal{L}}\bar{u}_b) \mathrm{d}\mu_b \right| + \left| \int_{\mathbb{R}_+\times\mathbb{T}} (\hat{\mathcal{L}}\bar{u}_b) \mathrm{d}\mu_b \right| + \left| \int_{\mathbb{R}_+\times\mathbb{T}} (Q_b - \hat{Q}_b) \mathrm{d}\mu_b \right|.
\end{aligned}$$

We then have,

$$\left| \int_{\mathbb{R}_+\times\mathbb{T}} (\bar{\lambda} - \hat{Q}_b + \hat{\mathcal{L}}\bar{u}_b) \mathrm{d}\mu_b \right| \le \mu(W) \sup_b \|(\hat{\mathcal{L}}_b \bar{u}_b - \hat{Q}_b + \bar{\lambda}_b)/W\|_\infty =: \delta_1,$$

which can be bounded explicitly. Similarly, using the fact that $\mathcal{L}\bar{u}_b$ is μ_b-mean zero

$$\begin{aligned}\left|\int_{\mathbb{R}_+\times\mathbb{T}}(\hat{\mathcal{L}}\bar{u}_b)\mathrm{d}\mu_b\right| &= \left|\int_{\mathbb{R}_+\times\mathbb{T}}(\hat{\mathcal{L}}\bar{u}_b-\mathcal{L}\bar{u}_b)\mathrm{d}\mu_b\right| \\ &\leq \left|\int_{\mathbb{R}_+\times\mathbb{T}}(\sqrt{a^2+b^2}-p(b))r^2\sin(2\vartheta)\partial_\vartheta\bar{u}_b\mathrm{d}\mu_b\right| \\ &\leq \varepsilon\mu(W)\sup_{b\in[b_-,b_+]}\|(r^2\sin(2\vartheta)\partial_\vartheta\bar{u}_b)/W\|_\infty =: \delta_2,\end{aligned}$$

which also can be bounded explicitly, and finally

$$\left|\int_{\mathbb{R}_+\times\mathbb{T}}(Q_b-\hat{Q}_b)\mathrm{d}\mu_b\right| \leq \varepsilon\mu(W)\|r^2\sin(2\vartheta)/W\|_\infty =: \delta_3,$$

so that, for all $b\in[b_-,b_+]$,

$$|\lambda_b-\bar{\lambda}_b|\leq\delta_1+\delta_2+\delta_3.$$

Remark 5.22. The two important parameters of the system are α and b as the sign of the Lyapunov exponent is invariant under a proper rescaling with respect to the other parameters (see [24, Proposition 3.1] for instance). Our method could of course be naturally extended to compute a full rigorous two-parameter bifurcation diagram for the Lyapunov exponent. While this would be for a bounded parameter region, one could hope to combine it with the complementary results of [24, 73] (with a more precise treatment to make this analysis more quantitative) to obtain a diagram for $(\alpha,b)\in\mathbb{R}^2$.

5.7 Proof of chaos for the stochastic Duffing–van der Pol system

In this Section, we explain how to apply the adjoint method to system (5.13), leading to the proofs of Theorem 5.2 and Theorem 5.3. As shown in [27, p. 263], the sign of the Lyapunov exponent of the system (5.13) only depends on the quantities $\beta\nu^2/\sigma^2$ and $b\nu/a$, and we can assume without loss of generality $\nu/a=\nu/\sigma=1$. Henceforth, we thus consider the system (5.1) on $\mathcal{M}=\mathbb{R}^2\backslash\{0\}$ with the vector fields

$$\begin{aligned}X_0(x,y)&=\left(\frac{\beta}{2}-\frac{b}{8}(x^2+y^2)\right)\begin{pmatrix}x\\y\end{pmatrix}-\frac{3}{8}(x^2+y^2)\begin{pmatrix}y\\-x\end{pmatrix},\\ X_1(x,y)&=\frac{1}{2\sqrt{2}}\begin{pmatrix}x\\-y\end{pmatrix},\qquad X_2(x,y)=\frac{1}{2\sqrt{2}}\begin{pmatrix}y\\x\end{pmatrix},\qquad X_3(x,y)=\frac{1}{2}\begin{pmatrix}y\\-x\end{pmatrix},\end{aligned}\tag{5.48}$$

depending only on the parameters b and β.

Note that when this system is considered on full space $\mathbb{R}^2$, it displays a multiplicity of stationary

distributions with two ergodic components $\{0\}$ and $\mathbb{R}^2\backslash\{0\}$. However, as will become clear, this does not prevent us from applying the adjoint method. While the Lyapunov exponent associated to the system linearised at 0 can be found explicitly, finding bounds on the Lyapunov exponent for the system on $\mathbb{R}^2\backslash\{0\}$ is more challenging. Indeed, the degeneracy of the diffusion around 0 creates an additional difficulty which we remove in a rather interesting fashion.

To the best of our knowledge, the chaotic behaviour of the Duffing–van der Pol system (5.14) was previously only shown in [29] for $b = 0$ and small $\varepsilon > 0$ (and thus for small $b > 0$ by a continuity argument).

5.7.1 Derivation of the Furstenberg-Khasminskii formula

Following [27], writing the system in polar coordinates, i.e. $(x_t, y_t) = (r_t \cos\phi_t, \sin\phi_t)$ and passing to Itô integration gives

$$\begin{cases} \mathrm{d}r_t &= \left(\frac{\beta r_t}{2} - \frac{b r_t^3}{8} + \frac{3r_t}{16}\right)\mathrm{d}t + \frac{1}{2\sqrt{2}} r_t \left(\cos(2\phi_t)\mathrm{d}B_t^1 + \sin(2\phi_t)\mathrm{d}B_t^2\right), \\ \mathrm{d}\phi_t &= \frac{r_t^2}{8}\mathrm{d}t + \frac{1}{2\sqrt{2}}\left(-\sin(2\phi_t)\mathrm{d}B_t^1 + \cos(2\phi_t)\mathrm{d}B_t^2\right) - \frac{1}{2}\mathrm{d}B_t^3. \end{cases} \tag{5.49}$$

Now, taking $(\varrho_t, s_t)_{t\geq 0}$ as in (5.27) and posing $s_t = (\cos\theta_t, \sin\theta_t)$, one obtains

$$\begin{cases} \mathrm{d}\log\varrho_t &= \left(\frac{\beta}{2} + \frac{1}{8} - \frac{b r_t^2}{8} - \frac{b r^2}{4}\cos^2(\theta_t - \phi_t) + \frac{3r_t^2}{8}\sin(2\theta_t - 2\phi_t)\right)\mathrm{d}t \\ &\quad + \frac{1}{2\sqrt{2}}\left(\cos(2\theta_t)\mathrm{d}B_t^1 + \sin(2\theta_t)\mathrm{d}B_t^2\right), \\ \mathrm{d}\theta_t &= r_t^2\left(\frac{1}{8} + \frac{b}{8}\sin(2\theta_t - 2\phi_t) + \frac{3}{4}\cos^2(\theta_t - \phi_t)\right)\mathrm{d}t \\ &\quad + \frac{1}{2\sqrt{2}}\left(-\sin(2\theta_t)\mathrm{d}B_t^1 + \cos(2\theta_t)\mathrm{d}B_t^2\right) - \frac{1}{2}\mathrm{d}B_t^3. \end{cases} \tag{5.50}$$

Defining independent Brownian motions B_t^r, B_t^ϕ as

$$\mathrm{d}\begin{pmatrix} B_t^r \\ B_t^\phi \end{pmatrix} = \begin{pmatrix} \cos 2\phi_t & \sin 2\phi_t \\ -\sin 2\phi_t & \cos 2\phi_t \end{pmatrix} \mathrm{d}\begin{pmatrix} B_t^1 \\ B_t^2 \end{pmatrix},$$

and $\vartheta_t = 2(\theta_t - \phi_t)$, by subtracting (5.50) by (5.49), one obtains

$$\begin{cases} \mathrm{d}r_t &= \left(\frac{\beta r_t}{2} - \frac{b r_t^3}{8} + \frac{3r_t}{16}\right)\mathrm{d}t + \frac{1}{2\sqrt{2}} r_t \mathrm{d}B_t^r & (5.51) \\ \mathrm{d}\vartheta_t &= r_t^2\left(\frac{b}{4}\sin\vartheta_t + \frac{3}{4}(1 + \cos\vartheta)\right)\mathrm{d}t + \frac{1}{\sqrt{2}}\left(-\sin\vartheta_t \mathrm{d}B_t^r + (\cos\vartheta_t - 1)\mathrm{d}B_t^\phi\right), & (5.52) \\ \mathrm{d}\log\varrho_t &= \left(\frac{\beta}{2} + \frac{1}{8} - \frac{b r_t^2}{8}(2 + \cos\vartheta_t) + \frac{3r_t^2}{8}\sin\vartheta_t\right)\mathrm{d}t + \frac{1}{2\sqrt{2}}\left(\cos\vartheta_t \mathrm{d}B_t^r + \sin\vartheta_t \mathrm{d}B_t^\phi\right). & (5.53) \end{cases}$$

The existence and uniqueness of a stationary measure μ_β on $(0,\infty)\times\mathbb{T}$ for the process $(r_t, \vartheta_t)_{t\geq 0}$ for $\beta > -1/4$ is shown in [27]. Furthermore, note that from (5.51), the process $(r_t)_{t\geq 0}$ is now

decoupled so that the marginal of μ_β onto $\mathbb{R}_+^* := (0,\infty)$ is given by

$$\mu_\beta(\mathrm{d}r,\mathbb{T}) = \frac{1}{Z_\beta} r^{1+8\beta}\exp\left(-br^2\right), \qquad Z_\beta = \frac{1}{2}b^{-(1+4\beta)}\Gamma(1+4\beta). \tag{5.54}$$

5.7.2 An adaptation of the adjoint method

We now explain how to adapt the ideas from Section 5.2.1 to this specific problem. The generator of the process $(r_t,\vartheta_t)_{t\geq 0}$ is given by

$$\mathcal{L}_\beta = -\frac{r}{16}\left(2br^2-8\beta-3\right)\partial_r + \frac{r^2}{16}\partial_{rr} + \frac{r^2}{4}(b\sin\vartheta+3\cos\vartheta+3)\partial_\vartheta - \frac{r}{4}\sin\vartheta\partial_{r\vartheta} + \frac{1}{2}(1-\cos\vartheta)\partial_{\vartheta\vartheta},$$

and we want to approximately solve the Poisson problem

$$\mathcal{L}_\beta u = Q_\beta - \lambda_\beta, \qquad \lambda_\beta := \int_{\mathbb{R}_+^*\times\mathbb{T}} Q_\beta \mathrm{d}\mu_\beta, \tag{5.55}$$

where, from (5.53), the infinitesimal growth rate along the projective flow is

$$Q_\beta(r,\vartheta) = \frac{\beta}{2} + \frac{1}{8} - \frac{b}{8}r^2(2+\cos\vartheta) + \frac{3}{8}r^2\sin\vartheta.$$

We consider the problem for a fixed β, the continuation procedure allowing to get a control that is uniform in β being the same as in Section 5.6.2 (and even simpler in practice, since here $\mathcal{L}_\beta$ and Q_β are already polynomials in β).

A natural basis to consider in order to find an approximate solution $\bar{u}$ could be

$$\{\cos m\vartheta, \sin m\vartheta\}_{m\in\mathbb{N}} \otimes \{L_n(br^2)\}_{n\in\mathbb{N}}$$

built from the Laguerre polynomials $\{L_n\}_{n\in\mathbb{N}} = \{L_n^{(0)}\}_{n\in\mathbb{N}}$. However, one rapidly realises that such a polynomial basis is not quite suitable.

Indeed, let us first look at a simpler Poisson problem, chosen somewhat arbitrarily, namely

$$\mathcal{L}_\beta v = \frac{b}{8}r^2 - \mathcal{I}, \qquad \text{where } \mathcal{I} = \int_{\mathbb{R}_+^*\times\mathbb{T}} \frac{b}{8}r^2\mu_\beta(\mathrm{d}r,\mathrm{d}\vartheta) = \frac{\beta}{2}+\frac{1}{8} \text{ by (5.54)}.$$

Then, one can compute that the solution to this equation is given (up to an additive constant) by $v(r,\vartheta) = -\log r$. This function is singular around $r=0$, and we expect the solution u to Eq. (5.55) to have a similar behaviour near the origin, therefore it is hopeless to try to approximate u with a purely polynomial basis. However, it turns out that one can simply add this single extra log function to our basis in order to resolve the Poisson problem (5.55) numerically up to reasonable accuracy. That is, we now consider the space

$$\mathcal{V} = \{\log r\} \oplus \mathcal{H}_{M,N}, \qquad \mathcal{H}_{M,N} = \mathrm{Span}\left\{\{\cos m\vartheta, \sin m\vartheta\}_{m=0}^{M} \otimes \{L_n(br^2)\}_{n=0}^{N}\right\}.$$

Note that, even if $\mathcal{V}$ contains the singular function log, we have $\mathcal{L}(\mathcal{V}) \subset \mathcal{H}_{M+1,N+1}$. Therefore, the addition of the log allows us to obtain a more accurate approximate solution $\bar{u}$ but does not hamper the a posteriori error estimates. Indeed, once a suitable approximate solution $\bar{u} \in \mathcal{V}$ is

found, we only need to control $\mathcal{L}\bar{u}$ when using the adjoint method, which we detail below for this specific example.

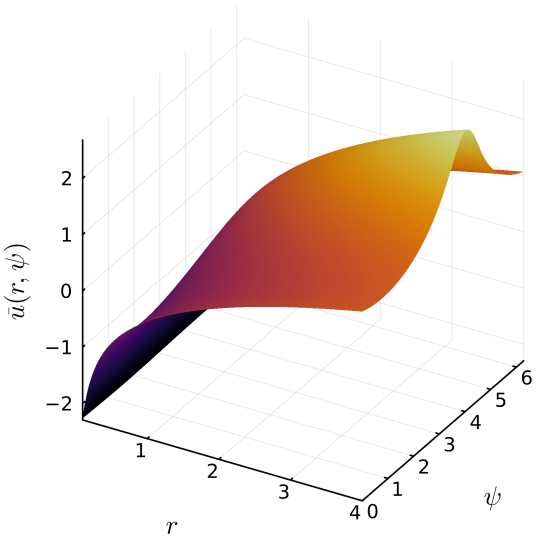


Figure 5.5: Plot of the numerical solution $\bar{u}$ to Eq. (5.55) with $b = 1.24$ and $\beta = -0.159$.

Here again $Q_\beta - \bar{Q}_\beta$ will not be bounded in L^∞, so we consider $W = \exp(br^2/2)$, for which we have $\|L_n/W\|_\infty = 1$ for all $n \in \mathbb{N}$, along with $\mu(W) = 2^{1+4\beta}$. We then take $\tilde{W} = W \log^2 r$, since for all $f \in \mathcal{V}$, $|f(r,\vartheta)|/\tilde{W}(r) \to 0$ as $|f(r,\vartheta)| \to \infty$ and

$$\mathcal{L}\tilde{W} \leq c\tilde{W}, \qquad c = \sup_{r\in\mathbb{R}_+^*} \left| \frac{\log r \left(br^2 \log r \left(-br^2 + 8\beta + 4\right) + 16\beta + 4\right) + 2}{16 \log^2 r} \right| < \infty.$$

In particular, this applies if we take $f(r,\vartheta) = \log r$ such that, by [24, Proposition B.1]

$$\int_{\mathbb{R}_+^* \times \mathbb{T}} (\mathcal{L} \log(r,\vartheta)) \mu(\mathrm{d}r, \mathrm{d}\vartheta) = 0.$$

This guarantees that we can still apply the adjoint method rigorously as described in Section 5.2.1, i.e. writing

$$(Q_\beta - \bar{Q}_\beta)(r,\vartheta) = g_0(br^2) + \sum_{m=1}^{M+1} (g_m(br^2)\cos m\vartheta + g_{-m}(br^2)\sin m\vartheta), \qquad g_m = \sum_{n=0}^{N+1} \epsilon_{mn} L_n,$$

we have the following bound on the Lyapunov exponent λ_β

$$|\lambda_\beta - \bar{\lambda}_\beta| \leq \mu_\beta(W) \|Q_\beta - \bar{Q}_\beta\|_\infty \leq 2^{1+4\beta} \sum_{|m|\leq M+1} \sum_{n=0}^{N+1} |\epsilon_{mn}|. \tag{5.56}$$

Note that while the Lyapunov exponent λ_β is not well defined at $\beta = -1/4$, as the system loses ergodicity, the quantity $\|Q_\beta - \bar{Q}_\beta\|_\infty$ is; which allows us to perform the continuation down to $\beta = -1/4$.

5.7.3 Improved error bounds

The error bound (5.56) was obtained following the general strategy exposed in Section 5.2.1, and provides a control on $|\lambda - \bar{\lambda}|$ in terms of the ℓ^1-norm of the vector $\epsilon = (\epsilon_{mn})$ describing $Q_\beta - \bar{Q}_\beta$. However, we show here that better estimates can be obtained, using the same ϵ. This is particularly relevant for this specific example, as λ itself is already quite small in magnitude (see Figure 5.2a), therefore rigorously determining its sign requires relatively tight error bounds.

For $\beta > -1/8$, instead of (5.56), we may use the following estimate:

$$\begin{aligned}
|\lambda_\beta - \bar{\lambda}_\beta| &= \left| \int_{\mathbb{R}_+^* \times \mathbb{T}} (Q_\beta - \bar{Q}_\beta)(r,\vartheta) \mu_\beta(\mathrm{d}r, \mathrm{d}\vartheta) \right|, && \text{from Eq. (5.10)}, \\
&\leq \int_{\mathbb{R}_+^* \times \mathbb{T}} \left| Q_\beta - \bar{Q}_\beta \right| (r,\vartheta) \mu_\beta(\mathrm{d}r, \mathrm{d}\vartheta) \\
&\leq \sum_{|m| \leq M+1} \int_{\mathbb{R}_+^* \times \mathbb{T}} |g_m(br^2)| \mu_\beta(\mathrm{d}r, \mathrm{d}\vartheta) && \text{using } |\cos m\vartheta|, |\sin m\vartheta| \leq 1 \\
&\leq \frac{1}{Z_\beta} \sum_{|m| \leq M+1} \int_0^\infty |g_m(br^2)| r^{1+8\beta} e^{-br^2} \mathrm{d}r \\
&\leq \frac{b^{-1-4\beta}}{2Z_\beta} \sum_{|m| \leq M+1} \int_0^\infty |g_m(z)| z^{4\beta} e^{-z} \mathrm{d}z && \text{with } z = br^2 \\
&\leq \frac{1}{\Gamma(1+4\beta)} \sum_{|m| \leq M+1} \left(\int_0^\infty |g_m(z)|^2 e^{-z} \mathrm{d}z \right)^{1/2} \left(\int_0^\infty z^{8\beta} e^{-z} \mathrm{d}z \right)^{1/2} && \text{by Cauchy–Schwarz} \\
&\leq \frac{\Gamma(1+8\beta)^{1/2}}{\Gamma(1+4\beta)} \sum_{|m| \leq M+1} \left(\int_0^\infty |g_m(z)|^2 e^{-z} \mathrm{d}z \right)^{1/2}.
\end{aligned}$$

Thus, by orthonormality of the Laguerre polynomials $\{L_n\}_{n \in \mathbb{N}}$ with respect to $e^{-z}\mathrm{d}z$, we obtain

$$\left| \lambda_\beta - \bar{\lambda}_\beta \right| \leq \frac{\Gamma(1+8\beta)^{1/2}}{\Gamma(1+4\beta)} \sum_{|m| \leq M+1} \left(\sum_{n=0}^{N+1} \epsilon_{mn}^2 \right)^{1/2}. \tag{5.57}$$

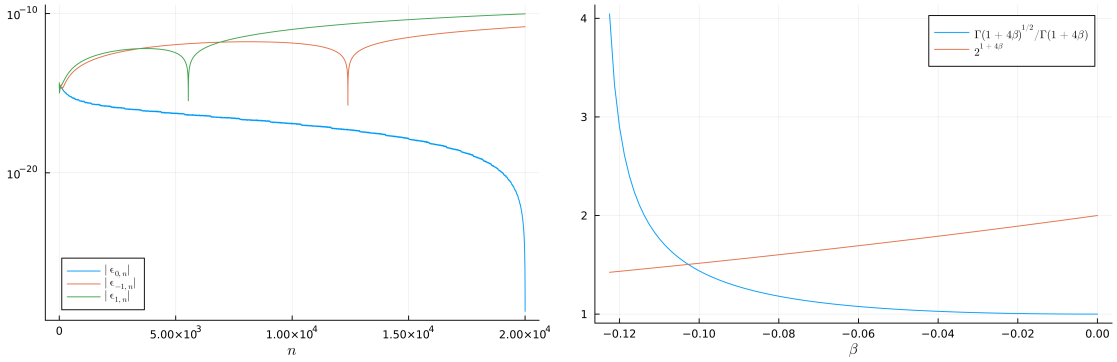
Comparing (5.56) and (5.57), we trivially have that

$$\left(\sum_{n=0}^{N+1} \epsilon_{mn}^2 \right)^{1/2} \leq \sum_{n=0}^{N+1} |\epsilon_{mn}|,$$

but the ℓ^2-norm can actually be much smaller than the ℓ^1-norm, especially when the coefficients ϵ_{mn} do not decay rapidly with n (see Figure 5.6a). For instance, in the extreme case where $\epsilon_{mn} = \epsilon_m$ does not depend on n, one has

$$\left(\sum_{n=0}^{N+1} \epsilon_{mn}^2 \right)^{1/2} \approx \frac{1}{\sqrt{N}} \sum_{n=0}^{N+1} |\epsilon_{mn}|.$$

Therefore, we expect (5.57) to give a sharper estimate than (5.56), at least when the constants $2^{1+4\beta}$ and $\Gamma(1+8\beta)^{1/2}/\Gamma(1+4\beta)$ have the same order of magnitude, which is the case as long as $\beta > -1/8$ is not too close to $-1/8$ (see Figure 5.6b).



(a) Plot of $\epsilon_{m,n}$ for $m = -1, 0, 1$ at $\beta = 0$.

(b) The two different constants.

Figure 5.6: Some of the terms involved in the error bounds (5.56) and (5.57).

The above ℓ^2 bound is limited to $\beta > -1/8$, but a similar idea can in fact be used to go past this barrier, up to using a different basis. For any $\alpha > -1$, we consider $\left\{l_n^{(\alpha)}\right\}_{n\in\mathbb{N}} = \left\{L_n^{(\alpha)}/\sqrt{\Gamma(n+\alpha+1)/n!}\right\}_{n\in\mathbb{N}}$, which forms an orthonormal with respect to $z^\alpha e^{-z}\mathrm{d}z$. We can use this basis in place of $\left\{l_n^{(0)}\right\}_{n\in\mathbb{N}} = \{L_n\}_{n\in\mathbb{N}}$ in $\mathcal{H}_{M,N}$, first in order to numerically find the approximate solution $\bar{u}$, and then to express $Q_\beta - \bar{Q}_\beta$:

$$(Q_\beta - \bar{Q}_\beta)(r,\vartheta) = g_0(br^2) + \sum_{m=1}^{M+1}(g_m(br^2)\cos m\vartheta + g_{-m}(br^2)\sin m\vartheta), \qquad g_m = \sum_{n=0}^{N+1}\epsilon_{mn}l_n^{(\alpha)}.$$

For any $\alpha > -1$, the above ℓ^2 bound now generalises for all $\beta > (\alpha-1)/8$, and yields

$$\begin{aligned}
&|\lambda_\beta - \bar{\lambda}_\beta| && (5.58)\\
\leq&\frac{b^{-1-4\beta}}{2Z_\beta}\sum_{|m|\leq M+1}\int_0^\infty |g_m(z)|z^{4\beta}e^{-z}\mathrm{d}z \qquad \text{with } z = br^2\\
\leq&\frac{1}{\Gamma(1+4\beta)}\sum_{|m|\leq M+1}\left\{\int_0^\infty |g_m(z)|^2 z^\alpha e^{-z}\mathrm{d}z\right\}^{1/2}\left\{\int_0^\infty z^{8\beta-\alpha}e^{-z}\mathrm{d}z\right\}^{1/2} \qquad \text{by Cauchy–Schwarz}\\
\leq&\frac{\Gamma(1+8\beta-\alpha)^{1/2}}{\Gamma(1+4\beta)}\sum_{|m|\leq M+1}\left\{\int_0^\infty |g_m(z)|^2 z^\alpha e^{-z}\mathrm{d}z\right\}^{1/2}\\
\leq&\frac{\Gamma(1+8\beta-\alpha)^{1/2}}{\Gamma(1+4\beta)}\sum_{|m|\leq M+1}\left\{\sum_{n=0}^{N+1}\epsilon_{mn}^2\right\}^{1/2}. && (5.59)
\end{aligned}$$

A natural choice would be to take $\alpha = 4\beta$ but this would make the continuation with respect to β more intricate, as it would make the basis functions depend on β. Instead, we split the interval $[-0.25, 0]$ into three subintervals $[\underline{\beta}, \bar{\beta}]$, and use a fixed value of α on each subinterval. The output is summarised in the first three rows of Table 5.1, and yields Theorem 5.2. In order to obtain Theorem 5.3, we refine our results by focusing close to the values of β for which λ_β vanishes, as reported in the two last rows of Table 5.1.

$[\underline{\beta}, \bar{\beta}]$	Estimate	α	$\delta > \lvert\lambda_\beta - \bar{\lambda}_\beta\rvert$	File at [78]
$[-0.25, -0.18]$	(5.56)	0	1.3×10^{-6}	`Duffing/proof_1`
$[-0.18, -0.11]$	(5.59)	$-1/2$	9.4×10^{-7}	`Duffing/proof_2`
$[-0.11, 0]$	(5.57)	0	2.2×10^{-6}	`Duffing/proof_3`
$[-0.25, -0.249]$	(5.56)	0	1.6×10^{-7}	`Duffing/proof_1bis`
$[-0.16, -0.159]$	(5.59)	$-1/2$	1.4×10^{-7}	`Duffing/proof_2bis`

Table 5.1: Error bounds resulting from the continuation with respect to the parameter β obtained with $M = 200$ and $N = 20,000$ which Theorems 5.2 and 5.3 rely upon.

5.8 Outlook

5.8.1 Application to more general random dynamical systems

It turns out that the adjoint method approach can be applied to other Markov processes such as jump diffusions and discrete-time Markov chains [123]. For instance, consider the "double-tent map" with additive noise on $[0, 1)$

$$x_{n+1} = T(x_n) + \xi_n \qquad \mod 1,$$

where the ξ_n's are independent identically distributed uniform random variables on $[-\varepsilon, \varepsilon]$ and

$$T(x) = \begin{cases} x/3 & \text{for } 0 \leq x < 1/6, \\ 1/9 - x/3 & \text{for } 1/6 \leq x < 1/3, \\ 3x - 1 & \text{for } 1/3 \leq x < 2/3, \\ 3 - 3x & \text{for } 2/3 \leq x < 1. \end{cases} \tag{5.60}$$

We chose this example as it fulfils the assumptions of [159]. This system clearly displays a negative Lyapunov exponent λ_ε for a small noise ε but one can show [158] that there exists $\varepsilon_0 < 1/2$ such that for all $\varepsilon > \varepsilon_0$, $\lambda_\varepsilon > 0$. The techniques of [158] actually provide an upper bound for ε_0. Our technique should however give a sharper estimate for ε_0. In this case, the Lyapunov exponent can be written as

$$\lambda_\varepsilon = \int_0^1 \log |T'(x)| \mu(\mathrm{d}x),$$

where μ is the unique stationary distribution of the Markov process $(x_n)_{n\in\mathbb{N}}$. Now consider the Markov semi-group $(\mathcal{P}^n)_{n\in\mathbb{N}}$ associated to $(x_n)_{n\in\mathbb{N}}$

$$\mathcal{P}u(x) = \mathbb{E}\left[u(x_1) \mid x_0 = x\right],$$

for all $u \in [0, 1) \to \mathbb{R}$ bounded-measurable. We have that for all such u

$$\int_0^1 (\mathcal{P}u)\mathrm{d}\mu = \int_0^1 u\mathrm{d}(\mathcal{P}^*\mu) = \int_0^1 u\mathrm{d}\mu,$$

and thus,

$$\int_0^1 (\mathcal{P}u - u)\mathrm{d}\mu = 0.$$

We therefore seek to solve the Poisson problem

$$(\mathcal{P} - \mathrm{id})u = \log|T'| - \lambda_\varepsilon. \tag{5.61}$$

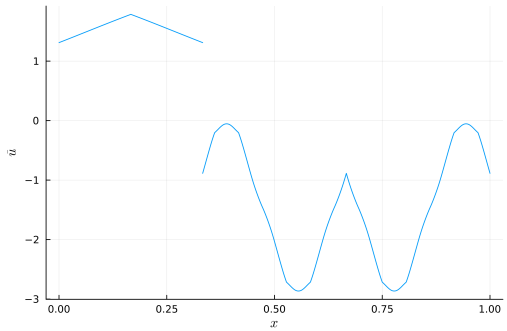
We thus consider for some large $N \in \mathbb{N}$, a piecewise constant numerical guess $\bar{u}$ for the above Poisson problem

$$\bar{u}(x) = \sum_{n=1}^{N} \bar{u}_i \mathbb{1}_{[(i-1)/N, i/N)}(x).$$

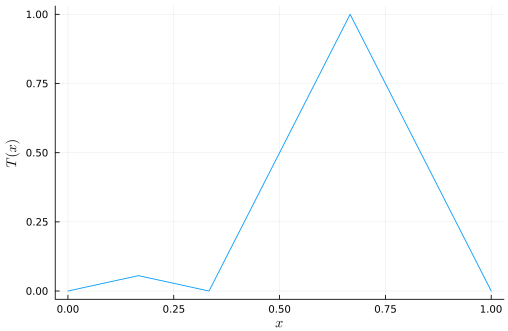
It turns out that directly solving this system led to numerical instabilities, as $(\mathcal{P} - \mathrm{id})$ is non-invertible and dense, and its kernel is not immediately straightforward to mod out. We thus instead used the formula [122]

$$u(x) = -\sum_{n=0}^{\infty} \mathbb{E}\left[\log|T'(x_n)| - \lambda_\varepsilon \mid x_0 = x\right] = -\sum_{n=0}^{\infty} (\mathcal{P}^n \log|T'| - \lambda_\varepsilon)(x).$$

By iterating $\mathcal{P}$ enough times, we find $\bar{u}$ represented in Figure 5.7a for $\varepsilon = 1/4$.



(a) Plot of a numerical solution $\bar{u}$ to the Poisson problem (5.61).



(b) Plot of $T : [0,1) \to [0,1)$ as defined in (5.60).

Figure 5.7: Plots of the functions $\bar{u}$ and T.

Thus, for the parameter $\varepsilon = 1/4$, we find that

$$\lambda_\varepsilon = 0.095547 \pm 1.4 \times 10^{-4} > 0.$$

Furthermore, the results of [159] imply that for this parameter, the random dynamical system displays a random Young tower and a random horseshoe.

Note that this approach is quite simplistic and one would expect much better results from a spectral method [230], by splitting the domain into several pieces and using Chebyshev interpolation on each subinterval for instance.

While this system can also be treated with existing methods (such as the Ulam method [77, 114]) and this naive approach simply in this form cannot at this stage handle critical points of T, we believe that it provides a more realistic framework to treat higher-dimensional systems such as the Hénon map with bounded noise (see Remark 5.8).

5.8.2 Towards the central limit theorem

If one is interested in the study of the fluctuations of the finite-time Lyapunov exponents

$$\lambda_t(\omega, x, v) = \frac{1}{t} \log \|D\varphi_t(\omega, x)v\|,$$

then one can for instance use the central limit theorem [17, Section 7]

$$\sqrt{t}(\lambda - \lambda_t) \xrightarrow[t\to\infty]{\text{law}} \mathcal{N}(0, \sigma_\lambda^2),$$

where

$$\sigma_\lambda^2 = -2 \int (Q - \lambda) u \mathrm{d}\tilde{\mu},$$

and $\mathcal{L}u = Q - \lambda$ (see also [31, 25, 36]). Note that we then have

$$\left| \sigma_\lambda^2 - 2 \int (\lambda - Q)\bar{u} \mathrm{d}\tilde{\mu} \right| \leq 2 \left| \int (Q - \lambda)(u - \bar{u}) \mathrm{d}\tilde{\mu} \right|,$$

where the integral of the left-hand side can in principle be enclosed with the techniques of the present chapter (provided we first have obtained bounds on λ). Now, for the right-hand side (assuming without loss of generality that $\tilde{\mu}(u) = \tilde{\mu}(\bar{u}) = 0$), for a suitable Lyapunov function W, one can bound the operator $\mathcal{L}^{-1}$ [122, Theorem 2.3] (see also [188]): there exists a constant $C > 0$ (depending only on $\mathcal{L}$ and W) such that

$$\left\| \frac{(u - \bar{u})}{W} \right\|_\infty \leq C \left\| \frac{(Q - \bar{Q})}{W} \right\|_\infty,$$

where $\|(Q - \bar{Q})/W\|_\infty$ is already known. In the case of diffusions, an estimate for C seems difficult to obtain (even with computer-assisted techniques) as its existence usually relies on a non-completely constructive argument (typically in the proof of the so-called coupling property). An exception is in the case of uniformly elliptic diffusions (such as in Section 5.6): one can in principle use [46] for the construction of such a bound which is however intricate and beyond the scope of this work. In the case of a uniformly elliptic diffusion on a bounded domain and in particular on the torus $\mathbb{T}^{2d-1}$, one can in principle enclose $\bar{u}$ with respect to the L^∞-norm [181]. We additionally mention [121, 135] which gives computable bounds in the case of discrete-time Markov chains, and [38] where a computer-assisted enclosure for σ_λ^2 is obtained for a very specific SDE example.

A

Appendix

A.1 Proof of Lemma 3.38

Again, without loss of generality, we consider the action of $\mathcal{J}$ on the subspace of even functions. Recall that we want to find a constant c such that

$$\|\mathcal{J}\|_{H^1\to L^2} = \|[\mathcal{J}]_{H^1\to L^2}\|_{\ell^2} = \|D^T P^{-1}\|_{\ell^2} \leq c.$$

Note that from $\{p_n\}_{n\in 2\mathbb{N}}$ to $\{p_n\}_{n\in 2\mathbb{N}+1}$, $\mathcal{J}$ has the representation

$$D^T = \begin{pmatrix} \alpha_1 & & & \\ \beta_1 & \alpha_3 & & \\ & \beta_3 & \ddots & \\ & & \ddots & \end{pmatrix}.$$

Thus,

$$\|D^T P^{-1}\|_{\ell^2} \leq \|\mathrm{Diag}(\alpha_{1:2:})P^{-1}\|_{\ell^2} + \|\mathrm{Diag}(\beta_{1:2:})P^{-1}\|_{\ell^2}.$$

For instance, we have

$$\mathrm{Diag}(\alpha_{1:2:})P^{-1} := \left(\begin{array}{c|c} \mathrm{Diag}(\alpha_{1:2:n+1})P_{\leq n}^{-1} & -\beta_n \mathrm{Diag}(\alpha_{1:2:n+1})(P_{\leq n}^{-1})_{:,-1}(D_{>n}^{-1})_{1,:} \\ \hline & \mathrm{Diag}(\alpha_{n+3:2:})D_{>n}^{-1} \end{array}\right).$$

Recall that we have that

$$\frac{\sqrt[4]{3}}{\sqrt{c^+}}n^{3/4} \leq \alpha_n \leq \frac{\sqrt[4]{3}}{\sqrt{c^-}}n^{3/4} \qquad \text{and} \qquad \beta_n \leq \frac{(c^+)^{3/2}}{3^{3/4}}.$$

Mimicking the calculations of Section 3.3.3, we find that

$$\begin{aligned} \| \left(\mathrm{Diag}(\alpha_{n+3:2:})D_{>n}^{-1}\right)_{i,:} \|_{\ell^1} &= \alpha_{n+2i+1} \sum_{j=i}^{\infty} \left| \frac{(-1)^{i-j}}{\alpha_{n+2j}} \prod_{k=i}^{j-1} \frac{\beta_{n+2k}}{\alpha_{n+2k}} \right| \\ &\leq \sqrt{\frac{c^+}{c^-}} \left(\frac{n+2i+1}{n+2i}\right)^{3/4} \sum_{j=i}^{\infty} \theta^{j-i} \\ &\leq \frac{\sqrt{c^+}}{\sqrt{c^-}(1-\theta)} \left(\frac{n+3}{n+2}\right)^{3/4}, \end{aligned}$$

and

$$\begin{aligned} \|\mathrm{Diag}(\alpha_{n+3:2:})(D_{>n}^{-1})_{:,j}\|_{\ell^1} &= \sum_{i=1}^{j} \left| \alpha_{n+2i+1} \frac{(-1)^{i-j}}{\alpha_{n+2j}} \prod_{k=i}^{j-1} \frac{\beta_{n+2k}}{\alpha_{n+2k}} \right| \\ &\leq \sqrt{\frac{c^+}{c^-}} \left(\frac{n+2+1}{n+2j}\right)^{3/4} \sum_{i=1}^{j} \theta^{j-i} \\ &\leq \frac{\sqrt{c^+}}{\sqrt{c^-}(1-\theta)} \left(\frac{n+3}{n+2}\right)^{3/4}, \end{aligned}$$

such that

$$\|\mathrm{Diag}(\alpha_{n+3:2:})D_{>n}^{-1}\|_{\ell^2} \leq \|\mathrm{Diag}(\alpha_{n+3:2:})D_{>n}^{-1}\|_{\ell^1}^{1/2} \|\mathrm{Diag}(\alpha_{n+3:2:})D_{>n}^{-1}\|_{\ell^\infty}^{1/2} \leq \frac{\sqrt{c^+}}{\sqrt{c^-}(1-\theta)} \left(\frac{n+3}{n+2}\right)^{3/4}.$$

This yields that

$$\|\mathrm{Diag}(\alpha_{1:2:})P^{-1}\|_{\ell^2} \le c_\alpha := \left\| \begin{pmatrix} \|\mathrm{Diag}(\alpha_{1:2:n+1})P_{\le n}^{-1}\|_{\ell^2} & \beta_n \|\mathrm{Diag}(\alpha_{1:2:n+1})(P_{\le n}^{-1})_{:,-1}\|_{\ell^2} \|(D_{>n}^{-1})_{1,:}\|_{\ell^2} \\ 0 & \frac{\sqrt{c^+}}{\sqrt{c^-}(1-\theta)} \left(\frac{n+3}{n+2}\right)^{3/4} \end{pmatrix} \right\|_{\ell^2},$$

where

$$\|(D_{>n}^{-1})_{1,:}\|_{\ell^2} \le \frac{1}{C_\alpha \sqrt{1-\theta^2}} \frac{1}{n^{3/4}}.$$

Similarly, we find that

$$\|\mathrm{Diag}(\beta_{n+3:2:})D_{>n}^{-1}\|_{\ell^2} \le \frac{(c^+)^2}{3(1-\theta)} \left(\frac{n+3}{n+2}\right)^{3/4},$$

such that

$$\|\mathrm{Diag}(\beta_{1:2:})P^{-1}\|_{\ell^2} \le c_\beta := \left\| \begin{pmatrix} \|\mathrm{Diag}(\beta_{1:2:n+1})P_{\le n}^{-1}\|_{\ell^2} & \beta_n \|\mathrm{Diag}(\beta_{1:2:n+1})(P_{\le n}^{-1})_{:,-1}\|_{\ell^2} \|(D_{>n}^{-1})_{1,:}\|_{\ell^2} \\ 0 & \frac{(c^+)^2}{3(1-\theta)} \left(\frac{n+3}{n+2}\right)^{3/4} \end{pmatrix} \right\|_{\ell^2}.$$

We thus choose $c := c_\alpha + c_\beta$. Now, to finalize our estimates, first note that

$$\|e^{-V/2}u\|_{L^2(\mathbb{R})}^2 = Z\|u\|_{L^2(\nu)}^2 \le \max(1, C_P)\|u\|_{H^1(\nu)}^2.$$

Then, for all $u \in H^1(\nu)$

$$\|(e^{-V/2}u)'\|_{L^2(\mathbb{R})} \le \frac{\sqrt{Z}}{2}\left(\|\mathcal{J}u\|_{L^2(\nu)} + \|u\|_{H^1(\nu)}\right) \le \frac{\sqrt{Z}}{2}\left(\|\mathcal{J}u\|_{H^1 \to L^2} + 1\right)\|u\|_{H^1(\nu)} \le \frac{\sqrt{Z}}{2}(c+1)\|u\|_{H^1(\nu)}.$$

By [61, Theorem VIII.7],

$$\begin{aligned} \|e^{-V/2}u\|_\infty &\le \sqrt{2}\|e^{-V/2}u\|_{L^2(\mathbb{R})}^{1/2}\|(e^{-V/2}u)'\|_{L^2(\mathbb{R})}^{1/2} \\ &\le \sqrt{Z(c+1)}\|u\|_{L^2(\nu)}^{1/2}\|u\|_{H^1(\nu)}^{1/2} \\ &\le \sqrt{Z(c+1)}\max(1, C_P)^{1/4}\|u\|_{H^1(\nu)}, \end{aligned}$$

which yields (3.43). Similarly,

$$\begin{aligned} \|e^{-V/2}u\|_{H^1(\mathbb{R})} :&= \left(\|e^{-V/2}u\|_{L^2(\mathbb{R})}^2 + \|(e^{-V/2}u)'\|_{L^2(\mathbb{R})}^2\right)^{1/2} \\ &\le \sqrt{Z}\left(\|e^{-V/2}u\|_{L^2(\nu)}^2 + \frac{(c+1)^2}{4}\|u\|_{H^1(\nu)}^2\right)^{1/2} \\ &\le \sqrt{Z}\left(\max(1, C_P) + \frac{(c+1)^2}{4}\right)^{1/2}\|u\|_{H^1(\nu)}, \end{aligned}$$

which yields (3.44).

In the case $\kappa = 4$, the calculation leading to an explicit value of c is performed at [79] in the file `GP_eq/embedding.ipynb`.

A.2 Quadrature

To obtain the bounds of Section 3.4.2, we need to compute rigorously many integrals of the form

$$\frac{1}{\tilde{Z}}\int_{\mathbb{R}}\left(\prod_{k=1}^{m} f_k\right)e^{-\tilde{V}}\mathrm{d}x,$$

where the f_k's are polynomials, $m = 4$ or $m = 6$, $\tilde{V}$ is a quartic potential of the form $\tilde{V} = mV/2$, and $\tilde{Z}$ is the corresponding normalisation constant. Similarly, we denote the orthonormal polynomials with respect to $e^{-\tilde{V}}$ by $\{\tilde{p}_n\}_{n\in\mathbb{N}}$ and the coefficients of their recurrence relation (3.9) by $\{\tilde{a}_n\}_{n\in\mathbb{N}}$. We achieve this integration by essentially following the method employed in 2.3 (See also [65] in the case of unweighted polynomial nonlinearities). Given some $N \in \mathbb{N}$ such that $2N-1 \geq \sum_{k=1}^{m} \deg f_k$, we denote by $(\tilde{x}_i)_{i=1}^{N}$ the roots of $\tilde{p}_N$. Then, given the weights [137, p. 390]

$$\tilde{W}_i = \frac{\tilde{a}_N}{\tilde{a}_{N-1}}\frac{\frac{1}{\tilde{Z}}\int \tilde{p}_{N-1}^2 e^{-\tilde{V}}\mathrm{d}x}{\tilde{p}'_N(\tilde{x}_i)p_{N_1}(\tilde{x}_i)} = \frac{\tilde{a}_N}{\tilde{a}_{N-1}}\frac{1}{\left(\frac{N}{\tilde{a}_N}p_{N-1}(\tilde{x}_i) + \tilde{a}_N\tilde{a}_{N-1}\tilde{a}_{N-2}p_{N-3}(\tilde{x}_i)\right)p_{N_1}(\tilde{x}_i)}$$

for $i = 1, \ldots, N$, we have that

$$\frac{1}{\tilde{Z}}\int_{\mathbb{R}}\left(\prod_{k=1}^{m} f_k\right)e^{-\tilde{V}}\mathrm{d}x = \sum_{i=1}^{N}\tilde{W}_i\left(\prod_{k=1}^{m} f_k(\tilde{x}_i)\right).$$

The $\tilde{x}_i$'s are enclosed rigorously similarly to [53] by

- finding approximate roots of $\tilde{p}_N$ by numerically finding eigenvalues of the N-dimensional (tridiagonal) Jacobi matrix constructed from $\{\tilde{a}_n\}_{n=1}^{N-1}$,
- refining these approximate roots using Newton's method in `BigFloat` arithmetic,
- and rigorously enclosing these roots via a combination of the Intermediate Value Theorem and the Fundamental Theorem of Algebra (recall that orthogonal polynomials always have simple real roots).

As in [53], in practice we will express a function u in $\Pi_n^{L^2}(L^2(\nu))$ with respect to the basis $\{p_n\}$ (orthogonal with respect to $\mathrm{d}\nu = e^{-V}\mathrm{d}x/Z$ now!), i.e.

$$u = \sum_{j=0}^{n} c_j p_j, \qquad c := (c_0, \ldots, c_n)^T,$$

such that it suffices to evaluate $p_j(\tilde{x}_i)$ via the recurrence relation

$$p_{j+1}(\tilde{x}_i) = \frac{\tilde{x}_i p_j(\tilde{x}_i) - a_j p_{j-1}(\tilde{x}_i)}{a_{j+1}} \qquad i = 1, \ldots, N.$$

This defines a pseudo-Vandermonde matrix $M = (p_j(\tilde{x}_i))$. As in Chapter 2, we regularise M by replacing it by $\bar{M} = \mathrm{Diag}(W)^{1/m}M$ which can be stored in lower precision. For instance, we then

have that the finite-dimensional projection of the a cubic nonlinearity can be handled by the matrix

$$G_{ij} = \langle p_i, e^{-V} u^2 p_j \rangle,$$

which can be written as $G = \bar{M}^T \mathrm{Diag}(\bar{M}c)^2 \bar{M}$.

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