

VALIDATED CONTINUATION FOR INFINITE DIMENSIONAL PROBLEMS

A Thesis
Presented to
The Academic Faculty

by

Jean-Philippe Lessard

In Partial Fulfillment
of the Requirements for the Degree
Doctor of Philosophy in the
School of Mathematics

Georgia Institute of Technology
2007

VALIDATED CONTINUATION FOR INFINITE DIMENSIONAL PROBLEMS

Approved by:

Professor Konstantin Mischaikow,
Advisor
School of Mathematics
Georgia Institute of Technology

Professor Guillermo Goldsztein
School of Mathematics
Georgia Institute of Technology

Professor Chongchun Zeng
School of Mathematics
Georgia Institute of Technology

Professor Hao Min Zhou
School of Mathematics
Georgia Institute of Technology

Professor Erik Verriest
School of Electrical and Computer
Engineering
Georgia Institute of Technology

Date Approved: June 12, 2007

À la mémoire de mon père.

ACKNOWLEDGEMENTS

First of all, I would like to thank my advisor and friend Konstantin, whose energy, generosity, enthusiasm and ideas have been essential during my five years of work with him. Always willing to talk despite an amazingly charged schedule, he gave me (and still do) great travel opportunities, fruitful international contacts, helpful financial support, hard times on racquetball courts and great Thanksgiving dinners memories. All of that made my Ph.D. a memorable time. Merci Monsieur !!!

I also want to thank my mom and sister, who were there since the very beginning and never stopped encouraging me and respecting my choices. Je vous aime.

I want to thank my research collaborators that introduced me with intelligence so many important math concepts: Jan Bouwe, for his incredible capacity to jump into details and for his great help with the math, especially toward the end of my thesis. Sarah, for her patience and support in introducing me to the fundamental and crazy world of analytic estimates. Marcio, for his ideas, which were sometimes essential in the work presented in this thesis and for his great computer skills.

This thesis would not be the same without all the short but how important math discussions I had with Luca Dieci, Alessandro Pugliese, Roger Nussbaum, John-Mallet-Paret and Yasuaki Hiraoka.

I am also wish to thank the hospitality of Rob van der Vorst (VU Amsterdam), Stanislaus Maier-Paape (RWTH Aachen), Tomasz Kaczynski (Sherbrooke),

Rob Beardmore (Imperial College), Hinke Osinga (Bristol), Hiroshi Kokubu (Kyoto), Cinzia Elia (Bari), Sarah Day (Cornell), Sebius Doedel (Concordia) and Marlène Frigon (Montréal).

I want to thank my friends of the Georgia Tech math department. Jean and Torsten, mes putains de colocos, for their taste, generosity and intelligence. Alessandro, for his humour, his typical italian flavour and for making me discover Mudcat and the Fat City Wildcats. Christel, for her great support, especially during the comps preparation. Bill, for the discussions and for the country music. Hwa Kil, for the coffees at the library fountain. Michael, for his sharing of the southern culture.

I would finally like to acknowledge the financial support of grants from the FQRNT, NSF, DOE and DARPA.

TABLE OF CONTENTS

DEDICATION	iii
ACKNOWLEDGEMENTS	iv
LIST OF FIGURES	ix
SUMMARY	xii
I INTRODUCTION	1
1.1 Continuation in Finite Dimension	4
1.2 Validated Continuation: Radii Polynomials	6
1.3 Equilibrium Solutions of PDEs	10
1.3.1 Computational Cost	11
1.3.2 Results for Swift-Hohenberg	12
1.3.3 Results for Cahn-Hilliard	12
1.4 Forcing Theorems and Chaotic Dynamics for Ordinary Differential Equations	15
1.5 Periodic Solutions of Delay Equations	20
II RADII POLYNOMIALS	24
2.1 Radii Polynomials	24
III ANALYTIC ESTIMATES	29
3.1 Background	29
3.2 Estimates for the Quadratic Nonlinearity	31
3.3 Estimates for a General Nonlinearity $p \geq 3$	32
3.4 Comparison of the General Estimates	36
3.5 Refinement of the Estimates	36
IV VALIDATED CONTINUATION FOR EQUILIBRIA OF PDES	39
4.1 Background	39
4.2 Radii polynomials	42
4.3 Computational cost	48

4.3.1	Cost of continuation	49
4.3.2	Cost of validation	51
4.3.3	Relative cost	53
4.4	Sample results with $M = m$	54
4.4.1	Cahn-Hilliard	54
4.4.2	Swift-Hohenberg	55
4.5	Sample Results using $M \geq m$	60
4.5.1	Lower Bounds for M	61
4.5.2	Computing Sums Using the Fast Fourier Transform	62
4.5.3	Results	64
4.6	Construction of the the Radii Polynomials	71
V	FORCING THEOREMS AND CHAOTIC DYNAMICS FOR ORDINARY DIFFERENTIAL EQUATIONS	79
5.1	Background	79
5.2	Proof of the Forcing Theorem	82
5.3	Topological Entropy and Chaos	89
5.4	Construction of the Radii Polynomials	92
5.4.1	Upper bounds for $Y_k(\hat{\nu})$	93
5.4.2	Upper bounds for $Z_F(r, \hat{\nu})$	95
5.4.3	Upper Bound for $Z_k(r, \hat{\nu})$ when $k \geq m$	101
5.4.4	Definition of the Radii Polynomials	104
5.5	Verification of the Geometric Hypotheses ($\mathcal{H}$)	105
VI	PERIODIC SOLUTIONS OF DELAY EQUATIONS	110
6.1	Background	110
6.2	Construction of the Radii Polynomials	112
6.2.1	Computation of the $Y_k(\alpha)$	114
6.2.2	Computation of the $Z_k(r, \alpha)$	118
6.2.3	Radii Polynomials of the Wright equation	142

VII CONCLUSION	144
REFERENCES	146

LIST OF FIGURES

1	Continuation Method	4
2	Validated Continuation	10
3	Comparison of the asymptotic ratios.	12
4	Bifurcation diagram for the Swift-Hohenberg equation (23) for some $\nu \in [0, 5.4]$. The dots indicate the points at which a numerical zero was validated.	13
5	Equilibria of (23) corresponding to the last points of each of the branches depicted in Figure 4. The colors are matching.	13
6	Some of the branches of equilibria of (23) for $0 \leq \nu \leq 10^6$. The dots indicate the points at which a numerical zero was validated. For the values $0 \leq \nu \leq 10^4$ the validation was done using interval arithmetic and hence at these points we have a mathematical proof of the existence and uniqueness of these solutions in the sets $W_{\bar{a}}(r)$. The color coding of the branches in this figure matches that of Figure 4.	14
7	Some solutions along the blue branch of the diagram on Figure 6. . .	14
8	Bifurcation diagram for (24).	15
9	Solutions along the lower branch of the diagram on Figure 8.	16
10	Sketch of the periodic solution $\tilde{u}$	17
11	Periodic solution $u_{\mathbf{a}}$ associated to $\mathbf{a} = \{243\}$	18
12	Slowly oscillating solution of the Wright's equation at $\alpha = 2.4756$. . .	21
13	Two ways that would make the conjecture false: (1) the existence of folds on $\mathcal{F}_0$, (2) the existence of isolas like $\mathcal{F}_1$	22
14	Rigorous study of a part of $\mathcal{F}_0$	23
15	Comparison of the estimates.	36
16	Comparison of the asymptotic ratios.	54
17	Validated continuation in ν for the Cahn-Hilliard equation on $[0, 1]$. .	56
18	The numerical zero $\bar{u}_F$ obtained by continuation for the Cahn-Hilliard equation at $\nu = 43.57415358799057$. Note that all even coefficients are 0. 57	
19	Validated continuation in ν for the Swift-Hohenberg equation at $L_0 = 0.65$	58

20	The numerical zero $\bar{u}_F$ obtained by continuation for the Swift-Hohenberg equation at $\nu = .6674701641462312$ and $L_0 = 0.65$. All even coefficients are 0.	58
21	Bifurcation diagram for the Swift-Hohenberg equation (73) for $0 \leq \nu \leq 5$. The dots indicate the points at which a numerical zero was validated.	65
22	Some of the branches of equilibria of (73) for $0 \leq \nu \leq 10^6$. The dots indicate the points at which a numerical zero was validated. For the values $0 \leq \nu \leq 10^4$ the validation was done using interval arithmetic and hence at these points we have a mathematical proof of the existence and uniqueness of these solutions in the sets $W_{\bar{u}}(r)$. The color coding of the branches in this figure matches that of Figure 21.	66
23	Some solutions along the blue branch of the diagram on Figure 22.	67
24	Plots of m and M along the blue branch of the diagram on Figure 22.	68
25	Plot of r along the blue branch of the diagram on Figure 22.	68
26	Bifurcation diagram for (71).	70
27	Solutions along the lower branch of the diagram on Figure 26.	70
28	(Left) The dimension of the Galerkin projection m as a function of λ along the lower branch of the diagram on Figure 26. (Right) The value of $ u_{m-2} $ as a function of λ along the same branch.	71
29	The function $h : [0, 2] \rightarrow [0, 2]$ defined by $h(x) = -\frac{3}{2}x^2 + \frac{5}{2}x + 1$ has periodic orbits of all period.	80
30	Periodic solution forcing the existence of chaos.	82
31	Left: sketch of the solution $\tilde{u}$. Right: discretized version $\{\tilde{u}_i\}_{i=1}^4$ and a shift $\{\tilde{u}_{i+2}\}_{i=1}^4$	83
32	The “up-down” setting including the oscillating tails in the local stable manifolds of ± 1	86
33	The set $U_{\mathbf{a}} = I_1 \times \cdots \times I_{18}$ associated to $\mathbf{a} = 243$	88
34	The thin (black and grey) lines denote the skeleton, where we represent u^ε and $\bar{u}^\varepsilon$ by constants for convenience. The thick free strand is in $U_{\mathbf{a}}$ for $\mathbf{a} = (4)$, $p = 4$. One can check that on the boundary of $U_{\mathbf{a}}$ the number of crossings with at least one of the skeletal strands decreases, hence the flow points outwards on the boundary $\partial U_{\mathbf{a}}$	89
35	A schematic example of a pattern in $U_{\mathbf{a}}$, with at the top the coding $\mathbf{a}$, and below the corresponding coding $\mathbf{b}$	91
36	Topological semi-conjugacy between $T : \Lambda \rightarrow \Lambda$ and $\sigma_{\mathcal{M}} : \Sigma_{\mathcal{M}} \rightarrow \Sigma_{\mathcal{M}}$	92

37	Procedure to make sure that the periodic solution $\tilde{u}$ satisfies $(\mathcal{H})$. . .	109
----	---	-----

SUMMARY

Studying the zeros of a parameter dependent operator f defined on a Hilbert space H is a fundamental problem in mathematics. When the Hilbert space is finite dimensional, continuation provides, via predictor-corrector algorithms, efficient techniques to numerically follow the zeros of f as we move the parameter. In the case of infinite dimensional Hilbert spaces, this procedure must be applied to some finite dimensional approximation which of course raises the question of validity of the output. We introduce a new technique that combines the information obtained from the predictor-corrector steps with ideas from rigorous computations and verifies that the numerically produced zero for the finite dimensional system can be used to explicitly define a set which contains a unique zero for the infinite dimensional problem $f : H \times \mathbb{R} \rightarrow Im(f)$.

We use this new *validated* continuation to study equilibrium solutions of partial differential equations, to prove the existence of chaos in ordinary differential equations and to follow branches of periodic solutions of delay differential equations. In the context of partial differential equations, we show that the cost of validated continuation is less than twice the cost of the standard continuation method alone.

CHAPTER I

INTRODUCTION

Mathematical models arising in biology, chemistry, finance and physics involve parameters. Many fundamental questions concerning these models can be reduced to the problem of finding the zeros of a specific function. Hence, a central problem in applied mathematics is the following: given a nonlinear parameter dependent function

$$f : H \times \mathbb{R} \rightarrow Im(f) \tag{1}$$

defined on a Hilbert space H , find $\mathcal{E} := \{(x, \nu) \mid f(x, \nu) = 0\}$. For many specific problems this can only be done using numerical methods. In particular, continuation provides an efficient technique for determining elements on branches of $\mathcal{E}$ by means of predictor-corrector algorithms: under the assumption that we have a numerical zero x_0 at the parameter value ν_0 , we consider a parameter value ν_1 close to ν_0 , we get a predictor $\tilde{x}_1$ at ν_1 and using a Newton-like corrector, we finally obtain another numerical zero x_1 at ν_1 . It is important to keep in mind that the corrector step relies on the convergence of an iterative scheme. If the Hilbert space H is low dimensional and if we can get a good enough representation of the function f , we have confidence about the approximate zeros coming from the continuation method. However, when the Hilbert space H is infinite dimensional, the problem of finding and continuing the zeros of (1) as we move the parameter ν is more subtle, as a finite dimensional approximation must first be considered before starting the computation. That raises the natural question of the validity of the output. To address this problem, we will introduce the concept of *validated continuation*. In reality for many applications, researchers are often interested in investigating a variety of models at a multitude of parameter values to gain scientific insight rather than an answer to a particular

question. This places a premium on minimizing computational cost, often leading to acceptance of the validity of numerical results simply based upon the reproducibility of the result at different levels of refinement. As we shall argue, the results presented in this thesis suggest that this dichotomy need not exist and we provide examples in Chapter 4 wherein it is demonstrated that by judicious use of the computations involved in the continuation method it is cheaper to *validate* the results than to re-perform the continuation at a more refined level. The concept of *validation* is quite simple: once we have a numerical zero of the finite dimensional projection, we embed it in H and construct around it a compact set of H on which we can apply the

Banach Fixed Point Theorem: *Let (Ω, d) be a complete metric space. Consider $W \subset \Omega$ and a function $T : W \rightarrow W$. If there is a constant q with $0 \leq q < 1$ such that $d(Tw, Tw') \leq q \cdot d(w, w')$ for all $w, w' \in W$ then T has a unique fixed point in W .*

Hence, in order to verify the hypotheses of the fixed point theorem, we need to construct two objects: the function T and the set W . As far as T is concerned, we propose an infinite dimensional adaptation of the finite Newton-like map of the corrector part of the continuation algorithm. The fundamental problem then becomes the construction of the set W . Many people worked on similar constructions before (e.g. see [9], [13], [42] and [43]), but their methods to build the sets W were most of the time ad hoc. What we propose here is quite different: we solve for the sets. At a given parameter value ν , we restrict our investigation to compact sets in the Hilbert space of *radius* $r > 0$ and centered at the embedded numerical zero $\bar{x}$. We denote such sets by $W_{\bar{x}}(r)$. The strategy is to solve for the sets $W_{\bar{x}}(r)$ by considering their radius as a variable and look for $r > 0$ such that the hypotheses of the Banach fixed point theorem are satisfied in a given Banach space Ω . Note that the norm of the Banach space Ω will depend on the particular choice of $W_{\bar{x}}(r)$. Denote it by $\|\cdot\|_{W_{\bar{x}}(r)}$. Details about the construction of the Banach space $(\Omega, \|\cdot\|_{W_{\bar{x}}(r)})$ are found in Chapter 2.

In order to show that $T : W_{\bar{x}}(r) \rightarrow W_{\bar{x}}(r)$ is a contraction in $(\Omega, \|\cdot\|_{W(r)})$, we construct a set of polynomials $\{p_k\}_{k \geq 0}$ and show that a sufficient condition for the existence of the desired set $W_{\bar{x}}(r)$ is that $p_k(r) < 0$ for all $k \geq 0$. These polynomials, that we call the *radii polynomials*, are the heart and the soul of this thesis. They represent sufficient conditions for the function T to act as a contraction on the set $W_{\bar{x}}(r)$. Finding a positive r making all of them simultaneously negative implies by the Banach fixed point theorem the existence of a unique fixed point of T in the set $W_{\bar{x}}(r)$ and therefore a unique zero of f in $W_{\bar{x}}(r)$ at the parameter value ν , by construction of T . Hence, for each of the applications presented in Chapters 4, 5 and 6, the main work is the construction of the coefficients of the *radii polynomials* which is essentially an analytic question. Indeed, their construction requires analytic estimates. General estimates will be presented in Chapter 3. Once the theoretical construction of the polynomials is done, we encode and solve them using the computer. Note that there are different types of arithmetic that can be used. We chose to use two of them, namely floating point arithmetic and interval arithmetic. The floating point arithmetic, being widely used, is extremely efficient and fast to use. Interval arithmetic, on the other hand, is slower to use, but it can lead to mathematical proofs. Based on interval arithmetic simulations, we will see in Chapter 4 that the floating point errors involved in the computation of the coefficients of the radii polynomials are many orders of magnitude smaller than the magnitude of the center of the interval coefficients of the radii polynomials. This strongly suggests that solving the *radii polynomials* using floating-point arithmetic provides considerable confidence about the validity of the numerical output. Therefore, recalling the necessity of computational efficiency in applied mathematics, we define the notion of *validation* as follow

Definition 1.0.1 Consider $\bar{x}$ a numerical zero and let $\{p_k\}_{k \geq 0}$ the radii polynomials computed using floating-point arithmetic. If there exists $r > 0$ such that $p_k(r) < 0$ for all $k \geq 0$, then we say that $\bar{x}$ is *validated* by the set $W_{\bar{x}}(r)$.

This being said, note that for many results presented in this thesis, we are interested in mathematical proofs, meaning that we will use the interval arithmetic version of the coefficients of the polynomials. Before introducing the different applications of validated continuation, we recall the basic notions of parameter continuation of zeros of functions defined on finite dimensional vector spaces.

1.1 Continuation in Finite Dimension

Suppose that the Hilbert space H is finite dimensional and that f in (1) is continuously differentiable. Continuation methods have been extensively developed in recent years (e.g. see [12], [23], [31]), as they provide an efficient way to numerically follow branches of zeros on $\mathcal{E} = \{(x, \nu) \mid f(x, \nu) = 0\}$. Recall that these methods involve a predictor and corrector step: given, within a prescribed tolerance, a zero x_0 at parameter value ν_0 , the predictor step produces an approximate zero $\tilde{x}_1$ at a nearby parameter value ν_1 , and the corrector step, often based on a Newton-like operator, takes $\tilde{x}_1$ as its input and produces, once again within the prescribed tolerance, a zero x_1 at ν_1 . For a geometrical interpretation, see Figure 1. Suppose that at the parameter value ν_0 ,

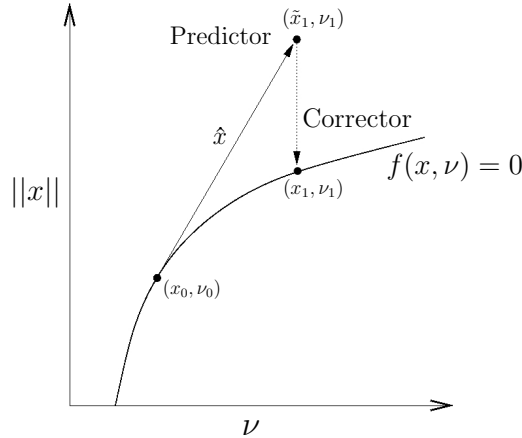


Figure 1: Continuation Method

an approximate zero x_0 and an approximate tangent vector $\hat{x}$ are found. Letting

$\nu_1 = \nu_0 + \hat{\nu}$, define the predictor by

$$\tilde{x}_1 = x_0 + \hat{\nu} \hat{x} . \quad (2)$$

For sake of simplicity of the presentation and to get the idea across, we will assume throughout this thesis that the Jacobian operator Df will always be invertible along branches of $\mathcal{E}$. By the implicit function theorem, we then have that branches on $\mathcal{E}$ can be thought as functions of ν . This does not mean that we will not go through bifurcations in the applications of validated continuation. It only means that we will not *validate* near bifurcations. This being said, suppose now that we have a good numerical approximation of $Df(\tilde{x}_1)^{-1}$ that we denote by A . The iterative scheme of the corrector part consist of computing iterations of the Newton-like map $x \mapsto x - A \cdot f(x, \nu_1)$

$$\begin{cases} x_1^{(j+1)} = x_1^{(j)} - A \cdot f(x_1^{(j)}, \nu_1) \\ x_1^{(0)} = \tilde{x}_1 \end{cases} \quad (3)$$

and the stopping criteria is when $\|f(x_1^{(j_{tol})}, \nu_1)\| \leq tol$ for some a priori fixed tolerance $tol > 0$ and for some $j_{tol} \in \mathbb{N}$. We then let $x_1 = x_1^{(j_{tol})}$.

Note that presented like this, continuation only returns numerical zeros on a discrete set of parameter values. Hence, the purpose of this thesis is to not only to generalize the ideas of parameter continuation to infinite dimensional problems, but also to develop it to get continuous range of parameter values. In order to do so, we need the notion of *radii polynomials*.

1.2 Validated Continuation: Radii Polynomials

Suppose now that the Hilbert space H is infinite dimensional. Suppose also that the original function (1) is continuously differentiable and can be expressed component-wise i.e.

$$f(x, \nu) = \begin{pmatrix} f_0(x, \nu) \\ f_1(x, \nu) \\ f_2(x, \nu) \\ \vdots \end{pmatrix},$$

where $x = (x_0, x_1, \dots)^T \in H$. We require that $x_k, f_k(x, \nu) \in \mathbb{R}^n$. In this thesis, we will only deal with the cases $n = 1, 2$. We first consider a finite dimensional approximation of (1). We use the subscript $(\cdot)_F$ to denote the nm entries corresponding to $k = 0, \dots, m-1$. We use the notation 0_∞ to denote $(0_n, 0_n, \dots)^T$, where 0_n is the zero in $\mathbb{R}^n$. Let $x_F = (x_0, \dots, x_{m-1})^T$ and $f_F = (f_0, \dots, f_{m-1})^T$ so that we can define the nm - dimensional *Galerkin projection* of f by

$$f^{(m)} : \mathbb{R}^{nm} \times \mathbb{R} \rightarrow \mathbb{R}^{nm} : (x_F, \nu) \mapsto f^{(m)}(x_F, \nu) := f_F([x_F, 0_\infty], \nu). \quad (4)$$

We now use the finite dimensional continuation method introduced in Section 1.1 to find numerical zeros of (4). At the parameter value ν_0 , assume we have numerically found an hyperbolic zero $\bar{x}_F \in \mathbb{R}^{nm}$ of $f^{(m)}$ i.e.

$$f^{(m)}(\bar{x}_F, \nu_0) \approx 0 \text{ and } Df^{(m)}(\bar{x}_F, \nu_0) \text{ is invertible.}$$

Hence, we can uniquely define the *tangent* $\hat{x}_F \in \mathbb{R}^{nm}$ by

$$Df^{(m)}(\bar{x}_F, \nu_0) \cdot \hat{x}_F = -\frac{\partial f^{(m)}}{\partial \nu}(\bar{x}_F, \nu_0).$$

We then embed $\bar{x}_F$ and $\hat{x}_F$ in H defining

$$\bar{x} = \begin{pmatrix} \bar{x}_F \\ 0_\infty \end{pmatrix} \in H \quad \text{and} \quad \hat{x} = \begin{pmatrix} \hat{x}_F \\ 0_\infty \end{pmatrix} \in H.$$

For $k \geq m$, we consider $\Lambda_k = \Lambda_k(\bar{x}, \nu_0) \in \mathbb{R}^{n \times n}$ to be such that

$$\Lambda_k \approx \frac{\partial f_k}{\partial x_k}(\bar{x}, \nu_0) \in \mathbb{R}^{n \times n}. \quad (5)$$

Let $J_{F \times F}$ the computed numerical inverse of $Df^{(m)}(\bar{x}_F, \nu_0)$ and

$$J := \begin{bmatrix} J_{F \times F} & & & 0 \\ & \Lambda_m^{-1} & & \\ & 0 & \Lambda_{m+1}^{-1} & \\ & & & \ddots \end{bmatrix} \quad (6)$$

For a parameter value $\nu \geq \nu_0$, define the operator T_ν by

$$T_\nu(x) = x - J \cdot f(x, \nu) \quad (7)$$

and considering $\hat{\nu} := \nu - \nu_0 \geq 0$, define the *predictor* x_ν by

$$x_\nu = \bar{x} + \hat{\nu} \cdot \hat{x} \in H. \quad (8)$$

Consider the set centered at $0 \in H$

$$W(r) = \prod_{k=0}^{\infty} [-w_k(r), w_k(r)]^n, \quad (9)$$

where $w_k(r) > 0$ eventually have a power decay in k and define the set $W_{x_\nu}(r)$ centered at x_ν by

$$W_{x_\nu}(r) = x_\nu + W(r). \quad (10)$$

For the different applications of validated continuation, we have different sets $W(r)$.

Example: We present three examples of $W(r)$, where r is the radius left as a variable. The first set is the one used in Chapter 4, the second set is the one we use in Chapter 5 and the third set is the one used in Chapter 6. For the first two examples, $n = 1$ and for the third one, $n = 2$. Note that in the second example, we have that the product

technically begins at $k = -1$. Fix two real numbers $s \geq 2$, $A_s > 0$.

$$1. W(r) = \prod_{k=0}^{m-1} [-r, r] \times \prod_{k=m}^{\infty} \left[-\frac{A_s}{k^s}, \frac{A_s}{k^s} \right], \quad (11)$$

$$2. W(r) = [-r, r] \times \left([-r, r] \times \prod_{k=1}^{\infty} \left[-\frac{r}{k^s}, \frac{r}{k^s} \right] \right), \quad (12)$$

$$3. W(r) = [-r, r]^2 \times \prod_{k=1}^{\infty} \left[-\frac{r}{k^s}, \frac{r}{k^s} \right]^2. \quad (13)$$

Remark 1.2.1 We note that the sets defined by (11), (12) and (13) all have the property that they eventually have a power decay. The theoretical justification for this choice of sets comes from the fact that in all the applications we consider, the zeros we are looking for are analytic. More precisely, the x_k are the coefficients of the Fourier expansion of an analytic function.

Recall again that the goal is to *validate* i.e. to prove that sets of the form (10) will uniquely contain zeros of the original problem (1) for a continuous range of parameter values $\nu \in [\nu_0, \nu_{\max}]$. To handle the cases $n \geq 1$, we introduce the following notation.

Definition 1.2.2 Let $u, v \in \mathbb{R}^n$. We denote the component-wise inequality by $\leq_{cw}$ (reps. $<_{cw}$) and say that $u \leq_{cw} v$ if $u_i \leq v_i$ (resp $u_i < v_i$), for all $i = 1, \dots, n$.

For $k \in \mathbb{N}$, we define $Y_k(\nu), Z_k(r, \nu) \in \mathbb{R}^n$ to be such that

$$|[T_\nu(x_\nu) - x_\nu]_k| \leq_{cw} Y_k(\nu) \in \mathbb{R}^n \quad (14)$$

and

$$\sup_{w, w' \in W(r)} |[DT_\nu(x_\nu + w)w']_k| \leq_{cw} Z_k(r, \nu) \in \mathbb{R}^n. \quad (15)$$

It is important to remark that since the Y_k and the Z_k are upper bounds, they are not uniquely defined.

Definition 1.2.3 Define $\mathbb{I}_n = (1, \dots, 1)^T \in \mathbb{R}^n$. For every $k \in \mathbb{N}$, choose $Y_k, Z_k \in \mathbb{R}^n$ satisfying respectively (14) and (15). We define the *radii polynomials* by

$$p_k(r, \nu) = Y_k(\nu) + Z_k(r, \nu) - w_k(r)\mathbb{I}_n, \quad k \geq 0. \quad (16)$$

For all applications of validated continuation we introduce in this thesis, there exist $M \in \mathbb{N}$ and a polynomial $\tilde{q}_M(r, \nu) \in \mathbb{R}$ such that for all $k \geq M$, we can choose

1. $Y_k = 0 \in \mathbb{R}^n$,
2. $Z_k(r, \nu) \leq_{cw} \tilde{q}_M(r, \nu) w_k(r) \mathbb{I}_n$.

Therefore the radii polynomials of (16) corresponding to the cases $k \geq M$ satisfy

$$\begin{aligned} p_k(r, \nu) &= Y_k(\nu) + Z_k(r, \nu) - w_k(r) \mathbb{I}_n \\ &\leq_{cw} [\tilde{q}_M(r, \nu) - 1] w_k(r) \mathbb{I}_n. \end{aligned}$$

Hence, if we can find $r > 0$ such that $\tilde{q}_M(r, \nu) - 1 < 0$, then $p_k(r, \nu) <_{cw} 0 \in \mathbb{R}^n$ for all $k \geq M$. We are now ready for the central ingredient of this thesis, which is proved in Chapter 2.

Theorem 1.2.4 *Let $r > 0$ and consider a set $W_{x_\nu}(r)$ centered at the predictor x_ν . Suppose that the first nM radii polynomials $\{p_k\}_{k=0, \dots, M-1}$ defined in equation (16) satisfy $p_k(r, \nu) <_{cw} 0$ for all $k \in \{0, \dots, M-1\}$ and for all $\nu \in [\nu_0, \nu_{max}]$. Suppose also that $\tilde{q}_M(r, \nu) - 1 < 0$ for all $\nu \in [\nu_0, \nu_{max}]$. Then for every fixed $\nu \in [\nu_0, \nu_{max}]$, the set $W_{x_\nu}(r)$ contains a unique zero of (1).*

For a geometrical interpretation, you may refer to Picture 2.

Definition 1.2.5 The positive r from Theorem 1.2.4 (if it exists) is called a *validation radius*. We also say that the x_ν are *validated* for all $\nu \in [\nu_0, \nu_{max}]$.

In order to get some upper bounds on the Z_k , we need some fundamental analytic estimates. This is the content of Chapter 3. In the next sections, we introduce three different applications of validated continuation in the field of dynamical systems and differential equations.

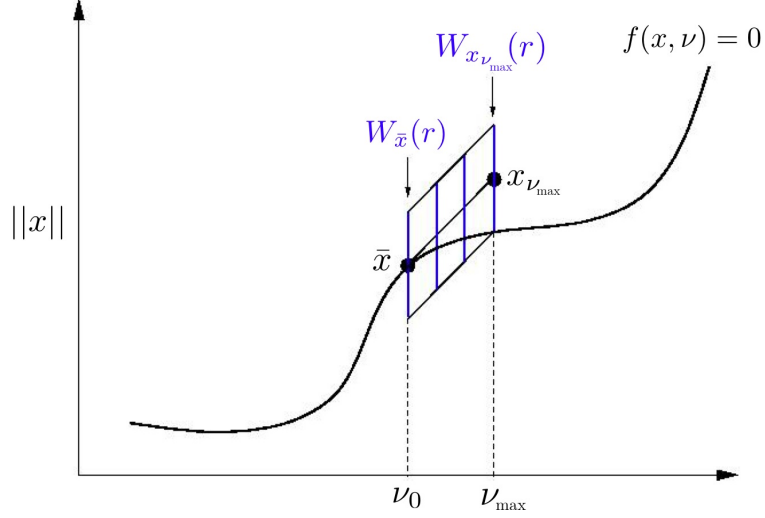


Figure 2: Validated Continuation

1.3 *Equilibrium Solutions of PDEs*

The first step in understanding the dynamics of a nonlinear parameter dependent partial differential equation

$$u_t = F(u, \nu) \quad (17)$$

on a Hilbert space is to identify the set of equilibria $\mathcal{E} := \{(u, \nu) \mid F(u, \nu) = 0\}$. To be more precise, assume that (17) takes the form

$$u_t = L(u, \nu) + \sum_{p=0}^d c_p(\nu) u^p \quad (18)$$

where $L(\cdot, \nu)$ is a linear operator at parameter value ν and d is the degree of the polynomial nonlinearity. Typically, $c_1(\nu) = 0$ since linear terms are grouped under $L(\cdot, \nu)$. Expanding (18) using an orthogonal basis chosen appropriately in terms of the eigenfunctions of the linear operator $L(\cdot, \nu)$, the particular domain and the boundary conditions, results in a countable system of differential equations on the coefficients of the expanded solution:

$$\dot{u}_k = f_k(u, \nu) := \mu_k u_k + \sum_{p=0}^d \sum_{\sum k_i=k} (c_p)_{k_0} u_{k_1} \cdots u_{k_p} \quad k = 0, 1, 2, \dots \quad (19)$$

where $\mu_k = \mu_k(\nu)$ are the parameter dependent eigenvalues of $L(\cdot, \nu)$ and $\{u_k\}$ and $\{(c_p)_k\}$ are the coefficients of the corresponding expansions of the functions u and $c_p(\nu)$ respectively with $u_k = u_{-k}$ and $(c_p)_k = (c_p)_{-k}$ for all $k \in \mathbb{N}$. Define $f = (f_k)_{k \in \mathbb{N}}$. By the a priori known regularity of the equilibria of (17), we let $H = \ell^2$. The problem of finding equilibrium solutions of (17) reduces to the one of finding zeros of

$$f : H \times \mathbb{R} \rightarrow \text{Im}(f). \quad (20)$$

1.3.1 Computational Cost

As mentioned earlier, a traditional way of studying the zeros of (17) is to consider a finite dimensional projection of (18) on which we run a predictor-corrector algorithm. This method has a computational cost that can be quite high, especially when one wants to detect bifurcations along the branch of equilibria we are following. As a strong motivation to the concept of validation, we provide a rough comparison of the cost of the traditional way of doing continuation with the cost of validated continuation for PDEs of the form

$$u_t = L(u, \nu) - u^3. \quad (21)$$

The polynomial nonlinearity of (21) is of degree $d = 3$ with coefficient functions

$$(c_p)_n = \begin{cases} -1 & p = 3 \text{ and } n = 0 \\ 0 & \text{otherwise.} \end{cases}$$

In this context, (19) then becomes

$$f_k(u, \nu) := \mu_k u_k - \sum_{\substack{k_1 + k_2 + k_3 = k \\ k_i \in \mathbb{Z}}} u_{k_1} u_{k_2} u_{k_3} \quad k = 0, 1, 2, \dots \quad (22)$$

where the μ_k 's are the parameter dependent eigenvalues of $L(\cdot, \nu)$.

Results in Chapter 4 suggests that asymptotically the ratio of the cost of validated continuation to the cost of traditional continuation is

$$\frac{26 + 3k}{20 + 3k}.$$

where k is the number of iterations performed in the corrector step. We tested this hypothesis against two fourth order partial differential equations with cubic nonlinearities, Swift-Hohenberg and Cahn-Hilliard that we introduce in the next sections. The results of the computations done are summarize in Figure 3, where m represents the dimension of the projection on which the computation was done.

PDE	m	$\frac{\# \text{ iterations}}{\# \text{ steps}}$	Experimental Ratio	Estimated Ratio $\frac{26+3k}{20+2k}$
Swift-Hohenberg	27	1.96	1.156	1.232
Cahn-Hilliard	60	1.65	1.173	1.219

Figure 3: Comparison of the asymptotic ratios.

1.3.2 Results for Swift-Hohenberg

The Swift-Hohenberg equation

$$\begin{aligned}
u_t &= \left\{ \nu - \left(1 + \frac{\partial^2}{\partial x^2} \right)^2 \right\} u - u^3, & u(\cdot, t) &\in L^2 \left(0, \frac{2\pi}{L_0} \right), \\
u(x, t) &= u \left(x + \frac{2\pi}{L_0}, t \right), & u(-x, t) &= u(x, t), \quad \nu > 0,
\end{aligned} \tag{23}$$

was originally introduced to describe the onset of Rayleigh-Bénard heat convection [35], where L_0 is a fundamental wave number for the system size $2\pi/L_0$. The parameter ν corresponds to the Rayleigh number and its increase is associated with the appearance of multiple solutions that exhibit complicated patterns. For the computations presented here we fixed $L_0 = 0.65$. For this problem, the linear operator is $L(\cdot, \nu) = \nu - (1 + \frac{\partial^2}{\partial x^2})^2$ and the eigenvalues of $L(\cdot, \nu)$ are given by $\mu_k := (\nu - 1) + 2k^2L^2 - k^4L^4$. In Figure 4, 5, 6 and 7, we present some validated results for the Swift-Hohenberg PDE (23).

1.3.3 Results for Cahn-Hilliard

The Cahn-Hilliard equation was introduced in [5] as a model for the process of phase separation of a binary alloy at a fixed temperature. On a one-dimensional domain it

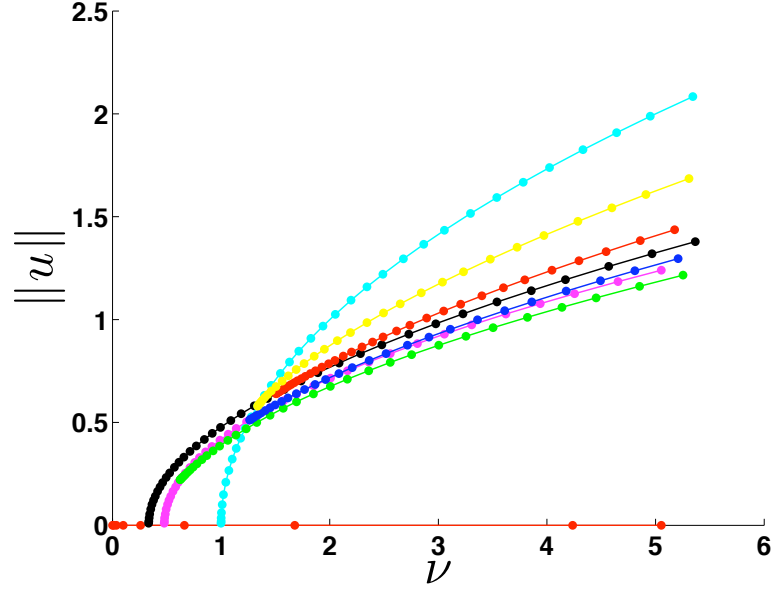


Figure 4: Bifurcation diagram for the Swift-Hohenberg equation (23) for some $\nu \in [0, 5.4]$. The dots indicate the points at which a numerical zero was validated.

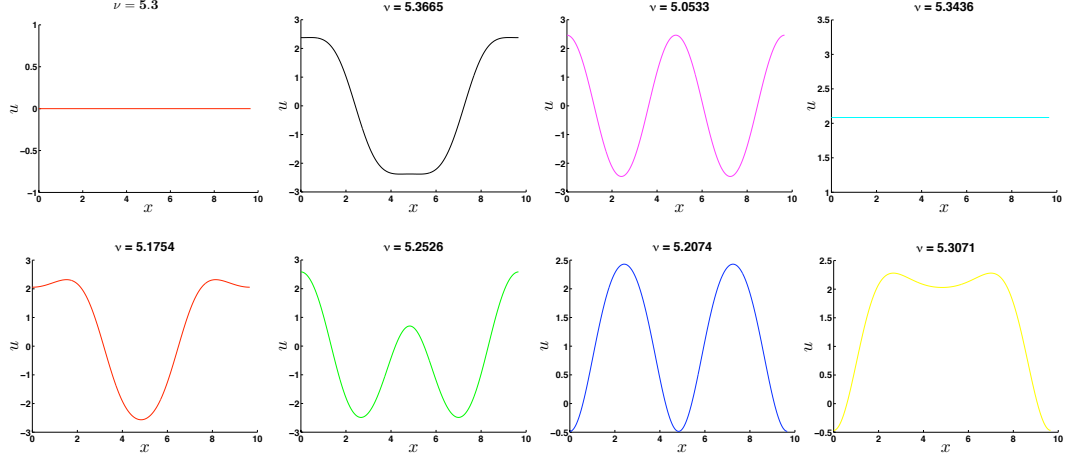


Figure 5: Equilibria of (23) corresponding to the last points of each of the branches depicted in Figure 4. The colors are matching.

takes the form

$$u_t = -\left(\frac{1}{\nu}u_{xx} + u - u^3\right)_{xx}, \quad x \in [0, 1]$$

$$u_x = u_{xxx} = 0, \quad \text{at } x = 0, 1. \quad (24)$$

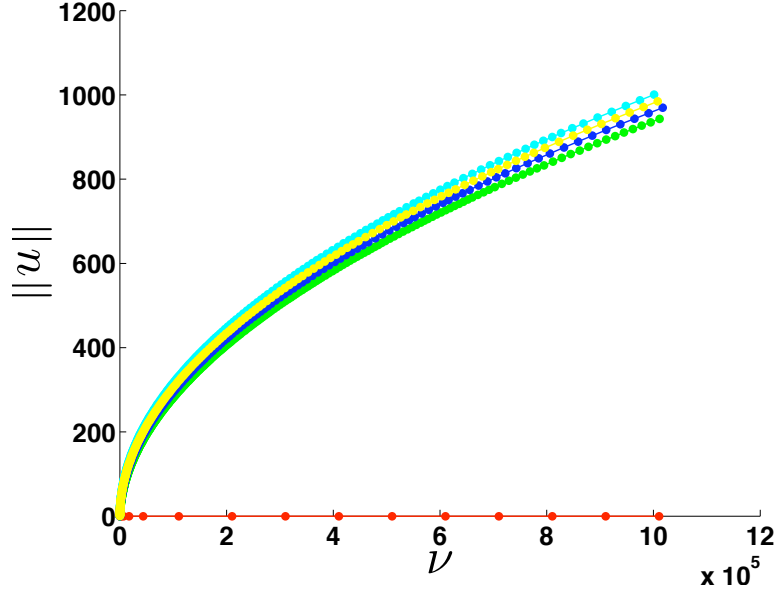


Figure 6: Some of the branches of equilibria of (23) for $0 \leq \nu \leq 10^6$. The dots indicate the points at which a numerical zero was validated. For the values $0 \leq \nu \leq 10^4$ the validation was done using interval arithmetic and hence at these points we have a mathematical proof of the existence and uniqueness of these solutions in the sets $W_{\bar{u}}(r)$. The color coding of the branches in this figure matches that of Figure 4.

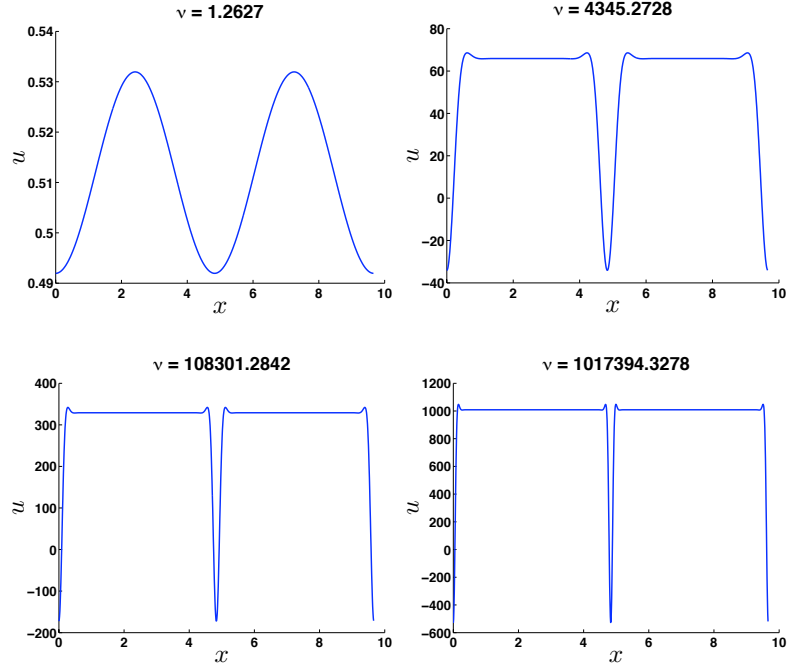


Figure 7: Some solutions along the blue branch of the diagram on Figure 6.

The assumption of an equal concentration of both alloys is formulated as

$$\int_0^1 u(x, \cdot) dx = 0 \quad (25)$$

Note that when looking for the equilibrium solutions of (24) restricted to (25), it is

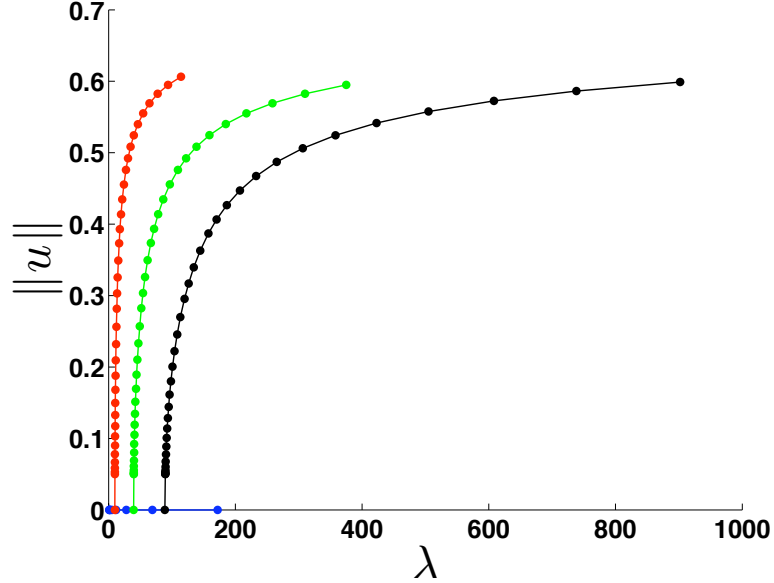


Figure 8: Bifurcation diagram for (24).

sufficient to work with the Allen-Cahn equation

$$\begin{aligned} \frac{1}{\nu} u_{xx} + u - u^3 &= c, \quad c \in \mathbb{R} \\ u_x &= 0 \quad \text{at } x = 0, 1. \end{aligned} \quad (26)$$

Letting $c = 0$, we performed validated continuation on (26). Re-writing (26) in the form of (18), the linear operator is $L(\cdot, \nu) = \frac{1}{\nu} \frac{\partial^2}{\partial x^2} + 1$. In Figure 8 and 9, we present validated results for the Allen-Cahn equation (26) when $c = 0$.

1.4 *Forcing Theorems and Chaotic Dynamics for Ordinary Differential Equations*

Getting analytic solutions of nonlinear parameter dependent ordinary differential equations is in general an extremely difficult task, most of the time impossible. The

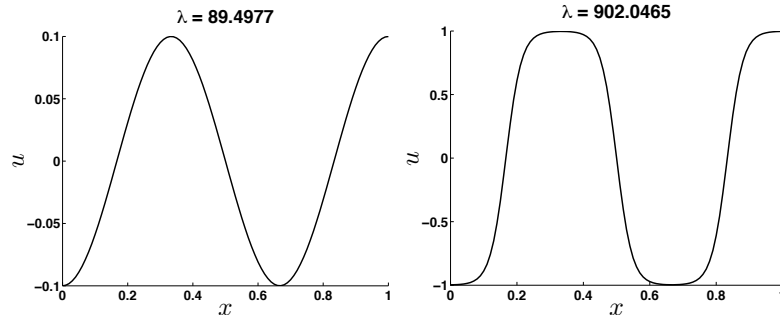


Figure 9: Solutions along the lower branch of the diagram on Figure 8.

use of numerical techniques then becomes a useful path to adopt in order to understand the dynamics of a given nonlinear ODE. People have recently realized that the numerical outputs could be used to rigorously extract coarse topological information from the systems, forcing at the same time the existence of complicated dynamics. In particular, proving the existence of chaos in nonlinear dynamical systems in such a way has become a popular topic (see [1], [10], [14], [25], [36], [37] and [38]). In some sense, we can see these results as forcing-type theorems, since a finite computable number of objects can be used to conclude about the existence of infinitely many other objects. We propose a new way to prove existence of chaos for a given class of problems, namely Lagrangian dynamical systems with a twist property. The philosophy of our proof is similar to the proofs in the above mentioned results as a finite amount of computations will be used, together with a forcing-type theorem, to prove the existence of chaos. The main difference here is that we are not doing any integration of the flow. A common feature of the proofs in [1], [14], [25] and [38] is the use of interval arithmetic to integrate the flow over sets and look for images of these rigorously integrated sets on some prescribed Poincaré sections. In contrast, our proof only requires proving the existence of a single periodic solution of a certain type. This will be done via validated continuation. A nice consequence of using validated continuation is that we can prove the existence of chaos for a continuous range

of parameter values. We focus our attention on the Swift-Hohenberg ODE

$$-u'''' - \nu u'' + u - u^3 = 0, \quad \nu > 0 \quad (27)$$

at the energy level $E = 0$, where

$$E(u, \nu) := u'''u' - \frac{1}{2}(u'')^2 + \frac{\nu}{2}(u')^2 + \frac{1}{4}(u^2 - 1)^2. \quad (28)$$

The specific periodic solution $\tilde{u}$ we are looking for has to satisfy the following geometric hypotheses

$$(\mathcal{H}) \left\{ \begin{array}{l} (1) \ \tilde{u} \text{ has exactly four monotone laps and extrema } \{\tilde{u}_i\}_{i=1}^4 \\ (2) \ \tilde{u}_1 \text{ and } \tilde{u}_3 \text{ are minima and } \tilde{u}_2 \text{ and } \tilde{u}_4 \text{ are maxima} \\ (3) \ \tilde{u}_1 < -1 < \tilde{u}_3 < 1 < \tilde{u}_2, \tilde{u}_4. \end{array} \right.$$

The following forcing result will be proved in Section 5.2.

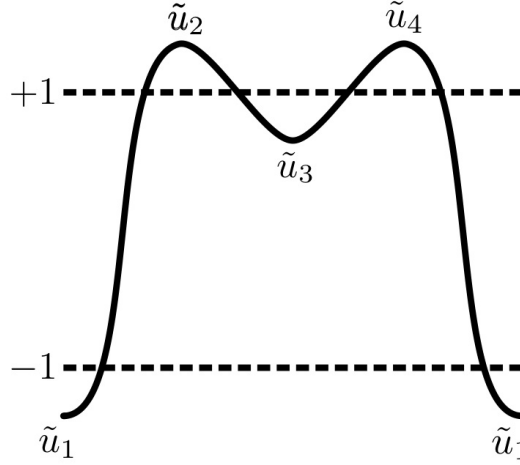


Figure 10: Sketch of the periodic solution $\tilde{u}$.

Forcing Theorem: Suppose that at the energy level $E = 0$, there exists a periodic solution $\tilde{u}$ of (27) satisfying $(\mathcal{H})$. Choose any finite, but arbitrarily long sequence $\mathbf{a} = \{\mathbf{a}_j\}_{j=1}^N$, with $\mathbf{a}_j \geq 2$, but not all equal to 2. Then there exists a periodic solution $u_{\mathbf{a}}$ of (27) at $E = 0$ that oscillates around the constant periodic solutions ± 1 as follow:

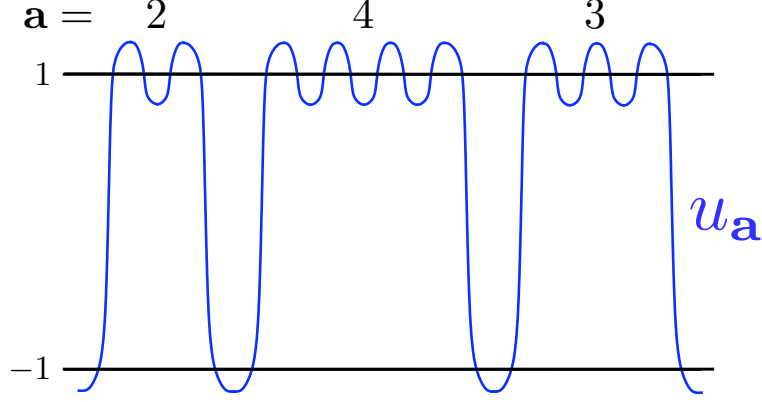


Figure 11: Periodic solution $u_{\mathbf{a}}$ associated to $\mathbf{a} = \{243\}$.

one time around -1 , $\mathbf{a}_1$ times around 1 , one time around -1 , $\mathbf{a}_2$ times around 1 , one time around -1 , $\dots$, $\mathbf{a}_N$ times around 1 and finally comes back to close at -1 .

Once we have, at a given parameter value $\nu > 0$, the existence of all these periodic orbits, we can show the following.

Corollary 1.4.1 *Suppose that at the energy level $E = 0$, there exists a periodic solution $\tilde{u}$ of (27) satisfying $(\mathcal{H})$. Then the Swift-Hohenberg equation (27) is chaotic on the energy level $E = 0$ in the sense that there exists a two-dimensional Poincaré return map which has a compact invariant set on which the topological entropy is positive.*

The definitions of topological entropy and chaos will be given in Section 5.1. The proof of Corollary 1.4.1 will be given in Section 5.3.

It is important to note that the only hypothesis that needs to be verified in order to prove the existence of chaos in (27) at $E = 0$ is the existence of the periodic solution $\tilde{u}$. Hence, we transform the problem of finding periodic solutions of (27) at $E = 0$ into the problem of finding the zeros of a specific parameter dependent function. We restrict our investigation to $\frac{2\pi}{L}$ -periodic solutions satisfying $u(y) = u(-y)$. This implies the symmetry $u(\frac{\pi}{L} - y) = u(\frac{\pi}{L} + y)$, hence $u'(0) = u'(\frac{\pi}{L}) = 0$, and similarly

for all odd derivatives. Defining

$$g(u, \nu) := -u'''' - \nu u'' + u - u^3$$

and combining this restriction with the fact that the energy E is constant along the orbits of the ODE, we have the following problem to solve

$$\begin{cases} g(u, \nu) = -u'''' - \nu u'' + u - u^3 = 0, \\ u(y + \frac{2\pi}{L}) = u(y), \quad u'(0) = u'''(0) = u'(\frac{\pi}{L}) = u'''(\frac{\pi}{L}) = 0 \\ -\frac{1}{2} (u''(0))^2 + \frac{1}{4} (u(0)^2 - 1)^2 = 0. \end{cases} \quad (29)$$

Hence, we consider the expansion of the periodic solution

$$u(y) = a_0 + 2 \sum_{k=0}^{\infty} a_k \cos kLy.$$

Plugging the expansion in (29) and taking the inner product with each $\cos kLy$, we obtain

$$\begin{aligned} -2L^2 \sum_{l=1}^{\infty} l^2 a_l - \frac{1}{\sqrt{2}} \left[a_0 + 2 \sum_{l=1}^{\infty} a_l \right]^2 + \frac{1}{\sqrt{2}} &= 0 \\ [1 + \nu L^2 k^2 - L^4 k^4] a_k - \sum_{\substack{k_1+k_2+k_3=k \\ k_i \in \mathbb{Z}}} a_{k_1} a_{k_2} a_{k_3} &= 0, \quad k \geq 0, \end{aligned}$$

since we look for solutions satisfying $u(0) < -1$ and $u''(0) > 0$ (see Figure 10). Letting $x := (L, a_0, a_1, a_2, \dots)$, we define

$$\begin{aligned} e(x) &= -2L^2 \sum_{l=1}^{\infty} l^2 a_l - \frac{1}{\sqrt{2}} \left[a_0 + 2 \sum_{l=1}^{\infty} a_l \right]^2 + \frac{1}{\sqrt{2}}, \\ g_k(x, \nu) &= [1 + \nu L^2 k^2 - L^4 k^4] a_k - \sum_{\substack{k_1+k_2+k_3=k \\ k_i \in \mathbb{Z}}} a_{k_1} a_{k_2} a_{k_3}, \quad k \geq 0. \end{aligned}$$

Letting $f = (e, g_0, g_1, \dots)$ and $H = \ell^2$, we then look for zeros of

$$f : H \times \mathbb{R} \rightarrow \text{Im}(f). \quad (30)$$

This is where validated continuation is used to get, at different parameter values ν , a set $W_{\bar{x}}(r)$ containing a periodic solution $\tilde{u}$ of (27) at $E = 0$. While performing

validated continuation on the infinite dimensional problem (30), we need to prove that the periodic solutions we find satisfy the hypotheses in $(\mathcal{H})$. If the validation radius $r > 0$ is small enough, then we have a good control on $\tilde{u}'$ and $\tilde{u}''$ which means that we can rigorously verify the hypotheses $(\mathcal{H})$. More details will be presented in Section 5.5. We are ready to state the main result.

Theorem 1.4.2 *For every $\nu \in [\frac{1}{2}, 2]$, the Swift-Hohenberg ODE (27) is chaotic at the energy level at $E = 0$.*

1.5 Periodic Solutions of Delay Equations

Another application of validated continuation is the rigorous study of periodic solutions of parameter dependent functional differential delay equations of the form

$$\dot{y}(t) = \alpha f[y(t), y(t-1)], \quad \alpha \in \mathbb{R}. \quad (31)$$

For instance, consider the famous Wright's equation

$$\dot{y}(t) = -\alpha y(t-1)[1 + y(t)], \quad \alpha > 0 \quad (32)$$

a generalization of

$$\dot{y}(t) = -(\log 2)y(t-1)[1 + y(t)]$$

that was brought to the attention of E.M. Wright, a number theorist, in the early 1950s because it played a role in probability methods applied to the distribution of prime numbers. In 1955, Wright published a paper [39] in which he studied the existence of bounded non trivial solutions of (32), for different values of $\alpha > 0$. Since then, equation (32) has been intensely studied by many mathematicians, among them, Kakutani and Markus [20], Jones [18, 19], Kaplan and Yorke [21, 22] and Nussbaum [28, 29, 30]. In particular, the following solutions of (32) have been extensively studied since the beginning of the 1960s.

Definition 1.5.1 A slowly oscillating periodic solution (*SOPS*) of (32) is a periodic solution $y(t)$ with the following property: there exist $q > 1$ and $p > q + 1$ such that, up to a time translation, $y(t) > 0$ on $(0, q)$, $y(t) < 0$ on (q, p) , and $y(t + p) = y(t)$ for all t so that p is the minimal period of $y(t)$.

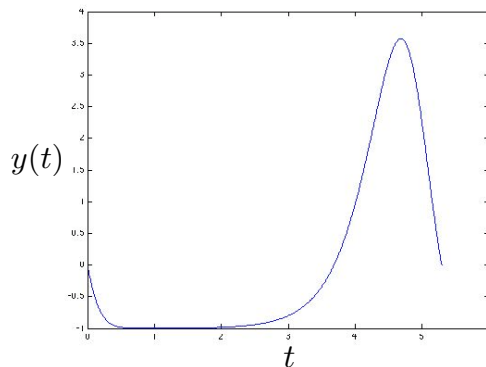


Figure 12: Slowly oscillating solution of the Wright's equation at $\alpha = 2.4756$.

In 1962, G.S. Jones proved in [19] that slowly oscillating solutions of (32) exists and remarked the following in [18]:

*The most important observable phenomenon resulting from these numerical experiments is the apparently rapid convergence of solutions of (32) to a **single** cycle fixed periodic form which seems to be independent of the initial specification on $[-1, 0]$ to within translations.*

The single cycle fixed periodic form he was referring to is in fact a slowly oscillating periodic solution. After this, people started to investigate the uniqueness of SOPS in (32). Using asymptotic estimates for large α , Xie [40, 41] proved that for $\alpha > \alpha^+ := 5.67$, (32) has a unique slowly oscillating periodic solution up to a time translation. Here is a remark he made after he stated his result on p. 97 of his thesis [41]:

The result here may be further sharpened. However, [...] the arguments here can not be used to prove the uniqueness result for SOP solutions of (32) when α is close to $\frac{\pi}{2}$.

It is known from [6] that there is an continuum of slowly oscillating periodic solutions that bifurcates (forward in α) from the trivial solution at $\alpha = \frac{\pi}{2}$. We denote this branch by $\mathcal{F}_0$. An open conjecture is then the following.

Conjecture 1.5.2 *For every $\alpha > \frac{\pi}{2}$, (32) has a unique slowly oscillating periodic solution.*

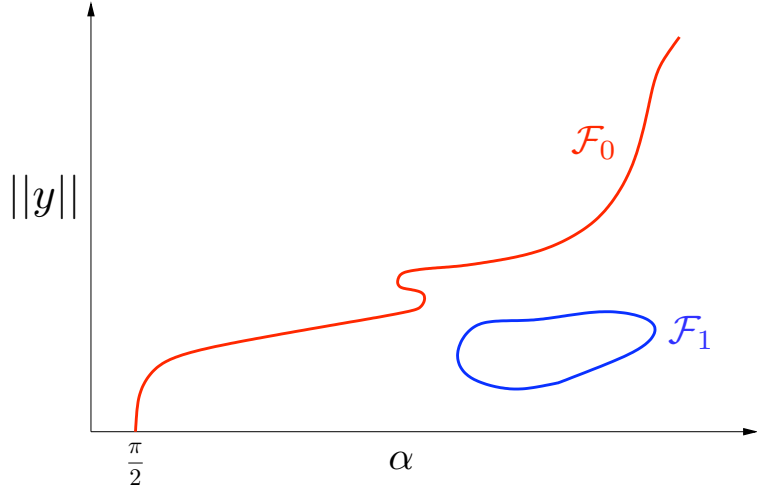


Figure 13: Two ways that would make the conjecture false: (1) the existence of folds on $\mathcal{F}_0$, (2) the existence of isolas like $\mathcal{F}_1$.

A result from [32] implies that there cannot be any secondary bifurcations from $\mathcal{F}_0$. Hence, $\mathcal{F}_0$ is a curve in the (α, y) -space. Conjecture 1.5.2 could hence fail because of: (1) the existence of folds on $\mathcal{F}_0$ (as depicted in Figure 13), (2) the existence of isolas i.e. curves of periodic solutions disconnected from $\mathcal{F}_0$ (like $\mathcal{F}_1$ in Figure 13). In this thesis, we propose to use validated continuation to rule out (1) from happening for $\alpha \in [\frac{\pi}{2} + \varepsilon, \alpha_1]$, for some $\varepsilon > 0$ and $\alpha_1 > \frac{\pi}{2} + \varepsilon$. The long term goal is to get to $\alpha_1 = \alpha^+ := 5.67$. Here is a result. For a geometrical interpretation, see Figure 14.

Validated Result 1.5.3 *Let $\varepsilon = 3.418 \times 10^{-4}$. The part of $\mathcal{F}_0$ corresponding to $\alpha \in [\frac{\pi}{2} + \varepsilon, 2.4]$ does not have any folds.*

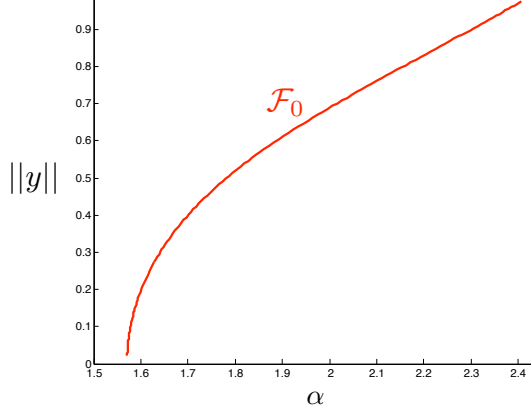


Figure 14: Rigorous study of a part of $\mathcal{F}_0$.

We obtained this result doing validated continuation on the infinite dimensional continuation problem $f : \ell^2 \times \mathbb{R} \rightarrow \text{Im}(f)$ given component-wise by

$$f_k(x, \alpha) = \begin{cases} \begin{pmatrix} a_0 + 2 \sum_{k=1}^{\infty} a_k \\ \alpha [a_0 + a_0^2 + 2 \sum_{k_1=1}^{\infty} (\cos k_1 L) (a_{k_1}^2 + b_{k_1}^2)] \end{pmatrix}, & k = 0 \\ R_k(L, \alpha) \begin{pmatrix} a_k \\ b_k \end{pmatrix} + \alpha \sum_{\substack{k_1+k_2=k \\ k_i \in \mathbb{Z}}} \Theta_{k_1}(L) \begin{pmatrix} a_{k_1} a_{k_2} - b_{k_1} b_{k_2} \\ a_{k_1} b_{k_2} + b_{k_1} a_{k_2} \end{pmatrix}, & k \geq 1 \end{cases},$$

where $x = (x_0, x_1, \dots, x_k, \dots)^T$ is given by

$$x_k = \begin{cases} [L, a_0], & k = 0 \\ [a_k, b_k], & k > 0 \end{cases},$$

and

$$R_k(L, \alpha) = \begin{pmatrix} \alpha \cos kL & -kL + \alpha \sin kL \\ kL - \alpha \sin kL & \alpha \cos kL \end{pmatrix}$$

$$\Theta_{k_1}(L) = \begin{pmatrix} \cos k_1 L & \sin k_1 L \\ -\sin k_1 L & \cos k_1 L \end{pmatrix}.$$

In Section 6.1, we show how f is constructed and why its zeros can help us proving Theorem 1.5.3. The construction of the radii polynomials is quite involved. It is presented in Section 6.2.

CHAPTER II

RADII POLYNOMIALS

The work presented in this chapter comes from joint work and helpful discussions with Jan Bouwe van den Berg, Sarah Day, Marcio Gameiro and Konstantin Mischaikow.

2.1 Radii Polynomials

Recall that our goal is to study rigorously the zeros

$$\begin{aligned} f : H \times \mathbb{R} &\rightarrow \operatorname{Im}(f) \\ (x, \nu) &\mapsto f(x, \nu) \end{aligned} \tag{33}$$

for a continuous range of parameter $[\nu_0, \nu_{\max}]$. The theoretical justification for the radii polynomials is based on a minor modification of a result of Yamamoto [42, Theorem 2.1]. A similar formulation can also be found in [13]. Recall that to apply the Banach fixed point theorem one must have a contraction mapping $T : W \rightarrow W$. With this in mind, we can state that it is appropriate to view our approach as a method by which the Newton-like iteration of the corrector step in the continuation process is used to construct a set W and some analytic estimates are used to verify that an appropriate generalization of the Newton-like operator is in fact a contraction in a specific Banach space $(\Omega, \|\cdot\|_W)$. Some of these general estimates will be presented in Chapter 3. In this section, we show how solving the radii polynomials inequalities prove that zeros of (33) can uniquely be enclosed in sets of the form

$$W_{x_\nu}(r) = x_\nu + W(r), \tag{34}$$

where $W(r) = \Pi_k[-w_k(r), w_k(r)]^n$ and $w_k(r)$ have an eventual power decay to 0. From Chapter 1, recall the predictor x_ν from (8) and the operator T_ν from (7). For

$k \in \mathbb{N}$, recall the $Y_k(\nu), Z_k(r, \nu) \in \mathbb{R}^n$ satisfying

$$|[T_\nu(x_\nu) - x_\nu]_k| \leq_{cw} Y_k(\nu) \in \mathbb{R}^n \quad (35)$$

and

$$\sup_{w, w' \in W(r)} |[DT_\nu(x_\nu + w)w']_k| \leq_{cw} Z_k(r, \nu) \in \mathbb{R}^n. \quad (36)$$

From Chapter 1, recall the fundamental existence of M : M is such that there exist a polynomial $\tilde{q}_M(r, \nu) \in \mathbb{R}$ such that for all $k \geq M$, we can set

1. $Y_k = 0 \in \mathbb{R}^n$,
2. $Z_k(r, \nu) \leq_{cw} \tilde{q}_M(r, \nu)w_k(r)\mathbb{I}_n$.

Based on this, we define the following.

Definition 2.1.1 Define $\mathbb{I}_n = (1, \dots, 1)^T \in \mathbb{R}^n$. For every $k \in \{0, \dots, M-1\}$, choose $Y_k, Z_k \in \mathbb{R}^n$ satisfying respectively (35) and (36). We define the *finite radii polynomials* by

$$p_k(r, \nu) = Y_k(\nu) + Z_k(r, \nu) - w_k(r)\mathbb{I}_n, \quad k \in \{0, \dots, M-1\} \quad (37)$$

and the *tail radii polynomial* by

$$\tilde{p}_M(r, \nu) = \tilde{q}_M(r, \nu) - 1. \quad (38)$$

We are now ready to prove the following result. Note that the proof is based on the results of Yamamoto in [42].

Theorem 2.1.2 Fix $n \in \{1, 2\}$. Let $r > 0$ and consider a set $W_{x_\nu}(r)$ centered at the predictor x_ν . Suppose that the finite radii polynomials $\{p_k\}_{k=0, \dots, M-1}$ defined by (37) satisfy $p_k(r, \nu) <_{cw} 0$ for all $k \in \{0, \dots, M-1\}$ and for all $\nu \in [\nu_0, \nu_{max}]$. Suppose also that the tail radii polynomial $\tilde{p}_M$ is such that $\tilde{p}_M(r, \nu) < 0$ for all $\nu \in [\nu_0, \nu_{max}]$. Then for every fixed $\nu \in [\nu_0, \nu_{max}]$, the set $W_{x_\nu}(r)$ contains a unique zero of (1).

Proof. The idea of the proof is to show that for $\nu \in [\nu_0, \nu_{\max}]$, T_ν contracts $W_{x_\nu}(r)$.

For $W(r) = \prod_k [-w_k(r), w_k(r)]^n$, let

$$\Omega = \left\{ b = (b_0, b_1, \dots) \mid \sup_{k \in \mathbb{N}} \frac{|b_k|_\infty}{w_k(r)} < \infty \right\}, \quad \text{where } |b_k|_\infty = \max_{i=1, \dots, n} |(b_k)_i|.$$

Then $\|b\|_{W(r)} := \sup_{k \in \mathbb{N}} \frac{|b_k|_\infty}{w_k(r)}$ is a norm on Ω . Furthermore, $(\Omega, \|\cdot\|_{W(r)})$ is a Banach space and $W(r)$ is a closed set under $\|\cdot\|_{W(r)}$. In this norm, $W(r) = B(0, 1)$ is the unit ball around 0, and $W_{x_\nu}(r) = x_\nu + W(r) = B(x_\nu, 1)$ is the unit ball around x_ν .

Fix $\nu \in [\nu_0, \nu_{\max}]$. For $x, y \in W_{x_\nu}(r)$ and for $i = 1, \dots, n$, let

$$g_{k,i}(s) := \{T_\nu[sx + (1-s)y]\}_{k,i} \in \mathbb{R}.$$

Applying the mean value theorem to $g_{k,i}$, there exists $s_{k,i} \in [0, 1]$ such that $g_{k,i}(1) - g_{k,i}(0) = g'(s_{k,i})$. The set $W_{x_\nu}(r)$ being convex, we get that $z_{k,i} := s_{k,i}x + (1-s_{k,i})y \in W_{x_\nu}(r)$. Hence, using the component-wise absolute value vector notation, we have that

$$\begin{aligned} |[T_\nu(x) - T_\nu(y)]_k| &= \left| \begin{pmatrix} [T_\nu(x) - T_\nu(y)]_{k,1} \\ \vdots \\ [T_\nu(x) - T_\nu(y)]_{k,n} \end{pmatrix} \right| \\ &= \left| \begin{pmatrix} D[T_\nu]_{k,1}(z_{k,1}) \cdot (x - y) \\ \vdots \\ D[T_\nu]_{k,n}(z_{k,n}) \cdot (x - y) \end{pmatrix} \right| \\ &= \left| \begin{pmatrix} D[T_\nu]_{k,1}(z_{k,1}) \cdot \frac{(x-y)}{\|x-y\|_{W(r)}} \\ \vdots \\ D[T_\nu]_{k,n}(z_{k,n}) \cdot \frac{(x-y)}{\|x-y\|_{W(r)}} \end{pmatrix} \right| \|x - y\|_{W(r)} \\ &\leq_{cw} \left(\begin{pmatrix} \sup_{w, w' \in W(r)} |[DT_\nu(x_\nu + w)w']_{k,1}| \\ \vdots \\ \sup_{w, w' \in W(r)} |[DT_\nu(x_\nu + w)w']_{k,n}| \end{pmatrix} \right) \|x - y\|_{W(r)} \\ &\leq_{cw} Z_k(r, \nu) \|x - y\|_{W(r)}, \end{aligned} \tag{39}$$

since by construction of $\|\cdot\|_{W(r)}$, $\frac{x-y}{\|x-y\|_{W(r)}} \in W(r)$. Let $x \in W_{x_\nu}(r)$. Then $\|x - x_\nu\|_{W(r)} \leq 1$ and for each k ,

$$\begin{aligned}
|[T_\nu(x) - x_\nu]_k| &= |[T_\nu(x) - T_\nu(x_\nu) + T_\nu(x_\nu) - x_\nu]_k| \\
&\leq_{cw} |[T_\nu(x) - T_\nu(x_\nu)]_k| + |[T_\nu(x_\nu) - x_\nu]_k| \\
&\leq_{cw} Z_k(r, \nu) \|x - x_\nu\|_{W(r)} + Y_k(\nu) \\
&= p_k(r, \nu) + w_k(r) \mathbb{I}_n \\
&<_{cw} w_k(r) \mathbb{I}_n
\end{aligned}$$

for all $\nu \in [\nu_0, \nu_{max}]$. Hence

$$\|T_\nu(x) - x_\nu\|_{W(r)} = \sup_{k \in \mathbb{N}} \frac{|[T_\nu(x) - T_\nu(y)]_k|_\infty}{w_k(r)} \leq 1.$$

Since in the norm $\|\cdot\|_{W(r)}$, $\overline{B(x_\nu, 1)} = W_{x_\nu}(r)$, we just showed that for all $\nu \in [\nu_0, \nu_{max}]$ and for all $x \in W_{x_\nu}(r)$, $T_\nu(x) - x_\nu \in W(r)$. In other words, we proved that given a $\nu \in [\nu_0, \nu_{max}]$,

$$T_\nu[W_{x_\nu}(r)] \subset W_{x_\nu}(r).$$

Now define

$$q(r, \nu) = \max \left\{ \frac{|Z_0(r, \nu)|_\infty}{w_0(r)}, \dots, \frac{|Z_{M-1}(r, \nu)|_\infty}{w_{M-1}(r)}, \tilde{q}_M(r, \nu) \right\}. \quad (40)$$

Then

$$q(r, \nu) < 1. \quad (41)$$

Indeed, since for $k = 0, \dots, M-1$, $p_k(r, \nu) <_{cw} 0$, then $\frac{Z_k(r, \nu)}{w_k(r)} <_{cw} \mathbb{I}_n$. This implies that for each $k = 0, \dots, M-1$, $\frac{|Z_k(r, \nu)|_\infty}{w_k(r)} < 1$. Also $\tilde{p}_M(r, \nu) < 0$ implies that $\tilde{q}_M(r, \nu) < 1$. That proves that $q(r, \nu) < 1$. Let $x, y \in W_{x_\nu}(r)$. Then combining (39), (41) and the fact that for all $k \geq M$, $Z_k(r, \nu) \leq_{cw} \tilde{q}_M(r, \nu) w_k(r) \mathbb{I}_n$, we have that

$$\begin{aligned}
\|T_\nu(x) - T_\nu(y)\|_{W(r)} &= \sup_{k \in \mathbb{N}} \frac{|[T_\nu(x) - T_\nu(y)]_k|_\infty}{w_k(r)} \\
&\leq_{cw} \sup_{k \in \mathbb{N}} \frac{|Z_k(r, \nu)|_\infty}{w_k(r)} \|x - y\|_{W(r)} \\
&\leq_{cw} q(r, \nu) \|x - y\|_{W(r)}.
\end{aligned}$$

Hence, $T_\nu : W_{x_\nu}(r) \rightarrow W_{x_\nu}(r)$ is a contraction. Thus, the result follows from Banach's fixed point theorem. ■

CHAPTER III

ANALYTIC ESTIMATES

3.1 *Background*

In this chapter, we introduce the fundamental estimates that will be used throughout this thesis. We present here an improvement of general estimates for infinite convolution sums with power decay of the form

$$\sum_{\substack{k_1 + \dots + k_p = k \\ k_i \in \mathbb{Z}}} a_{k_1}^{(1)} \cdots a_{k_p}^{(p)} \quad (42)$$

introduced in [7] and used in [9], [10], [11] and [15]. Most of the estimates used in the above papers are corollaries of Lemma 5.8 in [7]:

Lemma 3.1.1 [7] *Let $A > 0$ and $s \geq 2$. Let $\{a_k\}_{k \in \mathbb{Z}}$ be such that $a_{-k} = a_k$, $a_0 \in A[-1, 1]$ and $a_k \in \frac{A}{|k|^s}$ for all $k \in \mathbb{Z} \setminus \{0\}$. Let $\alpha = \frac{2}{s-1} + 2 + 3.5 \cdot 2^s$. Then*

$$\sum_{\sum n_i = k} a_{n_1} \cdots a_{n_p} \subseteq \begin{cases} \frac{\alpha^{p-1} A^p}{|k|^s} [-1, 1] & k \neq 0 \\ \alpha^{p-1} A^p [-1, 1] & k = 0. \end{cases}$$

Observe that the bounds provided by Lemma 3.1.1 grows exponentially in s since 2^s appears in the α . One reason in being interested in getting tighter analytic estimates for sums of the form (76) came from the work introduced in Chapter 5, where we use $s \geq 5$. Note that since $a_{-k} = a_k$ for all $k \in \mathbb{Z}$, we have that

$$\sum_{\substack{k_1 + \dots + k_p = -k \\ k_i \in \mathbb{Z}}} a_{k_1}^{(1)} \cdots a_{k_p}^{(p)} = \sum_{\substack{k_1 + \dots + k_p = k \\ k_i \in \mathbb{Z}}} a_{k_1}^{(1)} \cdots a_{k_p}^{(p)}.$$

Hence, we only consider the cases $k \in \mathbb{N}$. Before introducing the new general estimates, we first need the following result.

Lemma 3.1.2 *Let $s \geq 2$ and for $k \geq 2$, define*

$$\gamma_k = 2 \left[\frac{2}{k} [1 + \ln(k-1)] + \frac{\pi^2}{6} \right] \left[\frac{2}{k} + 1 \right]^{s-2}. \quad (43)$$

Then

$$\sum_{k_1=1}^{k-1} \frac{k^s}{k_1^s (k - k_1)^s} \leq \gamma_k. \quad (44)$$

Proof of Lemma 3.1.2. First observe that

$$\begin{aligned} \sum_{k_1=1}^{k-1} \frac{k^s}{k_1^s (k - k_1)^s} &= k^{s-1} \sum_{k_1=1}^{k-1} \frac{(k - k_1) + k_1}{k_1^s (k - k_1)^s} \\ &= k^{s-1} \left[\sum_{k_1=1}^{k-1} \frac{1}{k_1^s (k - k_1)^{s-1}} + \sum_{k_1=1}^{k-1} \frac{1}{k_1^{s-1} (k - k_1)^s} \right] \\ &= 2 \sum_{k_1=1}^{k-1} \frac{k^{s-1}}{k_1^{s-1} (k - k_1)^s}. \end{aligned}$$

Now define

$$\begin{aligned} \phi_k^s &:= \sum_{k_1=1}^{k-1} \frac{k^{s-1}}{k_1^{s-1} (k - k_1)^s} = k^{s-2} \sum_{k_1=1}^{k-1} \frac{(k - k_1) + k_1}{k_1^{s-1} (k - k_1)^s} \\ &= k^{s-2} \left[\sum_{k_1=1}^{k-1} \frac{1}{k_1^{s-1} (k - k_1)^{s-1}} + \sum_{k_1=1}^{k-1} \frac{1}{k_1^{s-2} (k - k_1)^s} \right] \\ &= k^{s-2} \left[\sum_{k_1=1}^{k-1} \frac{1}{k_1^{s-1} (k - k_1)^{s-1}} \right] + \left[\sum_{k_1=1}^{k-1} \frac{k^{s-2}}{k_1^{s-2} (k - k_1)^s} \right] \\ &\leq k^{s-3} \left[\sum_{k_1=1}^{k-1} \frac{(k - k_1) + k_1}{k_1^{s-1} (k - k_1)^{s-1}} \right] + \left[\sum_{k_1=1}^{k-1} \frac{k^{s-2}}{k_1^{s-2} (k - k_1)^{s-1}} \right] \\ &= \frac{1}{k} \left[\sum_{k_1=1}^{k-1} \frac{k^{s-2}}{k_1^{s-1} (k - k_1)^{s-2}} + \sum_{k_1=1}^{k-1} \frac{k^{s-2}}{k_1^{s-2} (k - k_1)^{s-1}} \right] + \phi_k^{s-1} \\ &= \frac{1}{k} [\phi_k^{s-1} + \phi_k^{s-1}] + \phi_k^{s-1} = \phi_k^{s-1} \left[\frac{2}{k} + 1 \right]. \end{aligned}$$

Hence,

$$\phi_k^s \leq \phi_k^2 \left[\frac{2}{k} + 1 \right]^{s-2},$$

where

$$\begin{aligned}
\phi_k^2 &= \sum_{k_1=1}^{k-1} \frac{k}{k_1(k-k_1)^2} = \sum_{k_1=1}^{k-1} \frac{1}{k_1(k-k_1)} + \sum_{k_1=1}^{k-1} \frac{1}{(k-k_1)^2} \\
&= \frac{2}{k} \sum_{k_1=1}^{k-1} \frac{1}{k_1} + \sum_{k_1=1}^{k-1} \frac{1}{k_1^2} \leq \frac{2}{k} [1 + \log_e(k-1)] + \frac{\pi^2}{6}.
\end{aligned}$$

We can finally conclude that

$$\begin{aligned}
\sum_{k_1=1}^{k-1} \frac{k^s}{k_1^s(k-k_1)^s} &= 2\phi_k^s \leq 2\phi_k^2 \left[\frac{2}{k} + 1 \right]^{s-2} \\
&\leq 2 \left[\frac{2}{k} [1 + \ln(k-1)] + \frac{\pi^2}{6} \right] \left[\frac{2}{k} + 1 \right]^{s-2} \\
&= \gamma_k \quad \blacksquare
\end{aligned}$$

Note that the estimates will be given via a recurrent definition in p i.e. the power of the nonlinearity. Hence, we begin by getting explicitly the estimates for the case $p = 2$. Throughout this chapter, we use $M \geq 5$ as a computational parameter.

3.2 Estimates for the Quadratic Nonlinearity

Lemma 3.2.1 (Quadratic Estimates) *Let $s \geq 2$ and $M \geq 5$. Define*

$$\alpha_k^{(2)} = \begin{cases} 4 + \frac{1}{2^{2s-1}(2s-1)}, & k = 0 \\ 2 \left[2 + \frac{1}{2^s} + \frac{1}{3^s} + \frac{1}{3^{s-1}(s-1)} \right] + \sum_{k_1=1}^{k-1} \frac{k^s}{k_1^s(k-k_1)^s}, & k \in \{1, \dots, M-1\} \\ 2 \left[2 + \frac{1}{2^s} + \frac{1}{3^s} + \frac{1}{3^{s-1}(s-1)} \right] + \gamma_k, & k \geq M \end{cases} \quad (45)$$

Let $A_1, A_2 > 0$ such that $a_0^{(i)} \in A_i[-1, 1]$ and $a_k^{(i)} \in \frac{A_i}{|k|^s}[-1, 1]$, for all $k \neq 0$ and for $i = 1, 2$. Suppose that $a_{-k}^{(i)} = a_k^{(i)}$. Then

$$\sum_{\substack{k_1+k_2=k \\ k_i \in \mathbb{Z}}} a_{k_1}^{(1)} a_{k_2}^{(2)} \in \begin{cases} \frac{\alpha_k^{(2)} A_1 A_2}{|k|^s} [-1, 1] & k \neq 0 \\ \alpha_0^{(2)} A_1 A_2 [-1, 1] & k = 0. \end{cases}$$

Proof. Let $k = 0$. Then

$$\begin{aligned}
\sum_{\substack{k_1+k_2=0 \\ k_i \in \mathbb{Z}}} a_{k_1}^{(1)} a_{k_2}^{(2)} &= \sum_{k_1 < 0} a_{k_1}^{(1)} a_{-k_1}^{(2)} + a_0^{(1)} a_0^{(2)} + \sum_{k_1 > 0} a_{k_1}^{(1)} a_{-k_1}^{(2)} \\
&= a_0^{(1)} a_0^{(2)} + 2 \sum_{k_1=1}^{\infty} a_{k_1}^{(1)} a_{k_1}^{(2)} \\
&\in A_1 A_2 \left[1 + 2 \sum_{k_1=1}^{\infty} \frac{1}{k_1^{2s}} \right] [-1, 1] \\
&\subseteq A_1 A_2 \left[4 + \frac{1}{2^{2s-1}(2s-1)} \right] [-1, 1] = \alpha_0^{(2)} A_1 A_2 [-1, 1] .
\end{aligned}$$

Now consider $k \in \{1, \dots, M-1\}$. Then

$$\begin{aligned}
\sum_{\substack{k_1+k_2=k \\ k_i \in \mathbb{Z}}} a_{k_1}^{(1)} a_{k_2}^{(2)} &= \sum_{k_1=-\infty}^{-1} a_{k_1}^{(1)} a_{k-k_1}^{(2)} + a_0^{(1)} a_k^{(2)} + \sum_{k_1=1}^{k-1} a_{k_1}^{(1)} a_{k-k_1}^{(2)} \\
&\quad + a_k^{(1)} a_0^{(2)} + \sum_{k_1=k+1}^{\infty} a_{k_1}^{(1)} a_{k-k_1}^{(2)} \\
&\in A_1 A_2 \left[\frac{2}{k^s} + 2 \sum_{k_1=1}^{\infty} \frac{1}{k_1^s (k+k_1)^s} + \sum_{k_1=1}^{k-1} \frac{k^s}{k_1^s (k-k_1)^s} \right] [-1, 1] \\
&\subseteq \frac{\alpha_k^{(2)} A_1 A_2}{k^s} [-1, 1] .
\end{aligned}$$

For the case $k \geq M$, we do the same analysis as in the case $k \in \{1, \dots, M-1\}$ and we use the upper bound γ_k from Lemma 3.1.2. ■

Remark 3.2.2 For any $k \geq M \geq 5$, we have that $\alpha_k^{(2)} \leq \alpha_M^{(2)}$. This fact will be of fundamental importance for the general estimates.

3.3 Estimates for a General Nonlinearity $p \geq 3$

Let $p \geq 3$ to be the degree of the nonlinearity, $s \geq 2$ the decay of the coefficients and $M \geq 5$ a natural number. We compute the general estimates recursively. Hence, we

first suppose that for every $k \geq 0$, we know explicitly $\alpha_k^{(p-1)} > 0$ such that

$$\sum_{\substack{k_1 + \dots + k_{p-1} = k \\ k_i \in \mathbb{Z}}} a_{k_1}^{(1)} \dots a_{k_{p-1}}^{(p-1)} \in \begin{cases} \frac{\alpha_k^{(p-1)}}{|k|^s} (\prod_{i=1}^{p-1} A_i) [-1, 1] & k \neq 0 \\ \alpha_0^{(p-1)} (\prod_{i=1}^{p-1} A_i) [-1, 1] & k = 0 \end{cases}$$

and such that $\alpha_k^{(p-1)} \leq \alpha_M^{(p-1)}$ for all $k \geq M$. We first define

$$\alpha_k^{(p)} = \begin{cases} \alpha_0^{(p-1)} + 2 \sum_{k_p=1}^{M-1} \frac{\alpha_{k_p}^{(p-1)}}{k_p^{2s}} + \frac{2\alpha_M^{(p-1)}}{(M-1)^{2s-1}(2s-1)}, & k = 0 \\ \sum_{k_p=1}^{M-k-1} \frac{\alpha_{k+k_p}^{(p-1)} k^s}{k_p^s (k+k_p)^s} + \alpha_M^{(p-1)} \left(1 + \frac{1}{2^s} + \frac{1}{3^s} + \frac{1}{3^{s-1}(s-1)} \right) \\ \quad + \alpha_k^{(p-1)} + \sum_{k_p=1}^{k-1} \frac{\alpha_{k_p}^{(p-1)} k^s}{k_p^s (k-k_p)^s} + \alpha_0^{(p-1)} + \sum_{k_p=1}^{M-1} \frac{\alpha_{k_p}^{(p-1)} k^s}{(k+k_p)^s k_p^s} \\ \quad + \frac{\alpha_M^{(p-1)}}{(M-1)^{s-1}(s-1)}, & k \in \{1, \dots, M-1\} \\ \alpha_M^{(p-1)} \left[2 + \frac{1}{2^s} + \frac{1}{3^s} + \frac{1}{3^{s-1}(s-1)} + \frac{1}{(M-1)^{s-1}(s-1)} + \gamma_k \right] \\ \quad + \alpha_0^{(p-1)} + \sum_{k_p=1}^{M-1} \frac{\alpha_{k_p}^{(p-1)}}{k_p^s} \left[1 + \frac{1}{\left[1 - \frac{k_p}{M}\right]^s} \right], & k \geq M. \end{cases} \quad (46)$$

Theorem 3.3.1 For $i = 1, \dots, p$ let $A_i > 0$ such that $a_0^{(i)} \in A_i[-1, 1]$ and $a_k^{(i)} \in \frac{A_i}{|k|^s}[-1, 1]$, for all $k \neq 0$. Suppose that $a_{-k}^{(i)} = a_k^{(i)}$. Then

$$\sum_{\substack{k_1 + \dots + k_p = k \\ k_i \in \mathbb{Z}}} a_{k_1}^{(1)} \dots a_{k_p}^{(p)} \in \begin{cases} \frac{\alpha_k^{(p)}}{|k|^s} (\prod_{i=1}^p A_i) [-1, 1] & k \neq 0 \\ \alpha_0^{(p)} (\prod_{i=1}^p A_i) [-1, 1] & k = 0. \end{cases} \quad (47)$$

Proof. Throughout the proof, we use several time the fact that $\alpha_k^{(p-1)} \leq \alpha_M^{(p-1)}$ for all $k \geq M$. For $k = 0$,

$$\begin{aligned}
\sum_{\substack{k_1+\dots+k_p=0 \\ k_i \in \mathbb{Z}}} a_{k_1}^{(1)} \dots a_{k_p}^{(p)} &= \sum_{k_p=-\infty}^{-1} a_{k_p}^{(p)} \left[\sum_{\substack{k_1+\dots+k_{p-1}=-k_p \\ k_i \in \mathbb{Z}}} a_{k_1}^{(1)} \dots a_{k_{p-1}}^{(p-1)} \right] \\
&+ a_0^{(p)} \left[\sum_{\substack{k_1+\dots+k_{p-1}=0 \\ k_i \in \mathbb{Z}}} a_{k_1}^{(1)} \dots a_{k_{p-1}}^{(p-1)} \right] + \sum_{k_p=1}^{\infty} a_{k_p}^{(p)} \left[\sum_{\substack{k_1+\dots+k_{p-1}=-k_p \\ k_i \in \mathbb{Z}}} a_{k_1}^{(1)} \dots a_{k_{p-1}}^{(p-1)} \right] \\
&\in \left(\prod_{i=1}^p A_i \right) \left[\sum_{k_p=1}^{\infty} \frac{\alpha_{k_p}^{(p-1)}}{k_p^{2s}} + \alpha_0^{(p-1)} + \sum_{k_p=1}^{\infty} \frac{\alpha_{k_p}^{(p-1)}}{k_p^{2s}} \right] [-1, 1] \\
&\subseteq \left(\prod_{i=1}^p A_i \right) \left[\alpha_0^{(p-1)} + 2 \sum_{k_p=1}^{M-1} \frac{\alpha_{k_p}^{(p-1)}}{k_p^{2s}} + \frac{2\alpha_M^{(p-1)}}{(M-1)^{2s-1}(2s-1)} \right] \\
&= \alpha_0^{(p)} \left(\prod_{i=1}^p A_i \right) [-1, 1].
\end{aligned}$$

For any $k \geq 1$,

$$\begin{aligned}
\sum_{\substack{k_1+\dots+k_p=k \\ k_i \in \mathbb{Z}}} a_{k_1}^{(1)} \dots a_{k_p}^{(p)} &= \sum_{k_p=-\infty}^{-1} a_{k_p}^{(p)} \left[\sum_{\substack{k_1+\dots+k_{p-1}=k-k_p \\ k_i \in \mathbb{Z}}} a_{k_1}^{(1)} \dots a_{k_{p-1}}^{(p-1)} \right] \\
&+ a_0^{(p)} \left[\sum_{\substack{k_1+\dots+k_{p-1}=k \\ k_i \in \mathbb{Z}}} a_{k_1}^{(1)} \dots a_{k_{p-1}}^{(p-1)} \right] + \sum_{k_p=1}^{k-1} a_{k_p}^{(p)} \left[\sum_{\substack{k_1+\dots+k_{p-1}=k-k_p \\ k_i \in \mathbb{Z}}} a_{k_1}^{(1)} \dots a_{k_{p-1}}^{(p-1)} \right] \\
&+ a_k^{(p)} \sum_{\substack{k_1+\dots+k_{p-1}=0 \\ k_i \in \mathbb{Z}}} a_{k_1}^{(1)} \dots a_{k_{p-1}}^{(p-1)} + \sum_{k_p=k+1}^{\infty} a_{k_p}^{(p)} \left[\sum_{\substack{k_1+\dots+k_{p-1}=k-k_p \\ k_i \in \mathbb{Z}}} a_{k_1}^{(1)} \dots a_{k_{p-1}}^{(p-1)} \right] \\
&\in \left(\prod_{i=1}^p A_i \right) \left[\sum_{k_p=1}^{\infty} \frac{\alpha_{k+k_p}^{(p-1)}}{k_p^s (k+k_p)^s} + \frac{\alpha_k^{(p-1)}}{k^s} + \sum_{k_p=1}^{k-1} \frac{\alpha_{k_p}^{(p-1)}}{k_p^s (k-k_p)^s} + \frac{\alpha_0^{(p-1)}}{k^s} + \sum_{k_p=1}^{\infty} \frac{\alpha_{k_p}^{(p-1)}}{(k+k_p)^s k_p^s} \right] [-1, 1].
\end{aligned}$$

Consider now $k \in \{0, \dots, M-1\}$. Since $\alpha_{k_p}^{(p-1)} \leq \alpha_M^{(p-1)}$, for all $k_p \geq M$, then

$$\begin{aligned}
\sum_{k_p=1}^{\infty} \frac{\alpha_{k+k_p}^{(p-1)}}{k_p^s (k+k_p)^s} &= \sum_{k_p=1}^{M-k-1} \frac{\alpha_{k+k_p}^{(p-1)}}{k_p^s (k+k_p)^s} + \sum_{k_p=M-k}^{\infty} \frac{\alpha_{k+k_p}^{(p-1)}}{k_p^s (k+k_p)^s} \\
&\leq \sum_{k_p=1}^{M-k-1} \frac{\alpha_{k+k_p}^{(p-1)}}{k_p^s (k+k_p)^s} + \alpha_M^{(p-1)} \sum_{k_p=M-k}^{\infty} \frac{1}{k_p^s (k+k_p)^s} \\
&\leq \sum_{k_p=1}^{M-k-1} \frac{\alpha_{k+k_p}^{(p-1)}}{k_p^s (k+k_p)^s} + \alpha_M^{(p-1)} \sum_{k_p=1}^{\infty} \frac{1}{k_p^s (k+k_p)^s} \\
&\leq \frac{1}{k^s} \left[\sum_{k_p=1}^{M-k-1} \frac{\alpha_{k+k_p}^{(p-1)} k^s}{k_p^s (k+k_p)^s} + \alpha_M^{(p-1)} \left(1 + \frac{1}{2^s} + \frac{1}{3^s} + \frac{1}{3^{s-1}(s-1)} \right) \right].
\end{aligned}$$

Similarly,

$$\sum_{k_p=1}^{\infty} \frac{\alpha_{k_p}^{(p-1)}}{(k+k_p)^s k_p^s} \leq \frac{1}{k^s} \left[\sum_{k_p=1}^{M-1} \frac{\alpha_{k_p}^{(p-1)} k^s}{(k+k_p)^s k_p^s} + \frac{\alpha_M^{(p-1)}}{(M-1)^{s-1}(s-1)} \right].$$

Recalling the definition of $\alpha_k^{(p)}$ for the cases $k \in \{1, \dots, M-1\}$, we get that

$$\sum_{\substack{k_1 + \dots + k_p = k \\ k_i \in \mathbb{Z}}} a_{k_1}^{(1)} \dots a_{k_p}^{(p)} \in \frac{\alpha_k^{(p)}}{k^s} \left(\prod_{i=1}^p A_i \right) [-1, 1].$$

Consider now $k \geq M$. Then

$$\sum_{k_p=1}^{\infty} \frac{\alpha_{k+k_p}^{(p-1)}}{k_p^s (k+k_p)^s} + \frac{\alpha_k^{(p-1)}}{k^s} \leq \frac{\alpha_M^{(p-1)}}{k^s} \left[2 + \frac{1}{2^s} + \frac{1}{3^s} + \frac{1}{3^{s-1}(s-1)} \right].$$

Recalling the definition of γ_k from (43), we get that

$$\begin{aligned}
\sum_{k_p=1}^{k-1} \frac{\alpha_{k_p}^{(p-1)}}{k_p^s (k-k_p)^s} &= \sum_{k_p=1}^{M-1} \frac{\alpha_{k_p}^{(p-1)}}{k_p^s (k-k_p)^s} + \frac{1}{k^s} \sum_{k_p=M}^{k-1} \frac{k^s \alpha_{k_p}^{(p-1)}}{k_p^s (k-k_p)^s} \\
&\leq \frac{1}{k^s} \sum_{k_p=1}^{M-1} \frac{\alpha_{k_p}^{(p-1)}}{k_p^s \left(1 - \frac{k_p}{k}\right)^s} + \frac{\alpha_M^{(p-1)}}{k^s} \sum_{k_p=M}^{k-1} \frac{k^s}{k_p^s (k-k_p)^s} \\
&\leq \frac{1}{k^s} \left[\sum_{k_p=1}^{M-1} \frac{\alpha_{k_p}^{(p-1)}}{k_p^s \left[1 - \frac{k_p}{M}\right]^s} + \alpha_M^{(p-1)} \gamma_k \right].
\end{aligned}$$

Also,

$$\sum_{k_p=1}^{\infty} \frac{\alpha_{k_p}^{(p-1)}}{(k+k_p)^s k_p^s} \leq \frac{1}{k^s} \left[\sum_{k_p=1}^{M-1} \frac{\alpha_{k_p}^{(p-1)}}{k_p^s} + \frac{\alpha_M^{(p-1)}}{(M-1)^{s-1}(s-1)} \right].$$

Combining the above inequalities, we finally have that

$$\begin{aligned}
& \sum_{\substack{k_1 + \dots + k_p = k \\ k_i \in \mathbb{Z}}} a_{k_1}^{(1)} \dots a_{k_p}^{(p)} \\
& \in \frac{1}{k^s} \left(\prod_{i=1}^p A_i \right) \left(\alpha_M^{(p-1)} \left[2 + \frac{1}{2^s} + \frac{1}{3^s} + \frac{1}{3^{s-1}(s-1)} + \frac{1}{(M-1)^{s-1}(s-1)} + \gamma_k \right] \right. \\
& \quad \left. + \alpha_0^{(p-1)} + \sum_{k_p=1}^{M-1} \frac{\alpha_{k_p}^{(p-1)}}{k_p^s} \left[1 + \frac{1}{\left[1 - \frac{k_p}{M} \right]^s} \right] \right) [-1, 1] = \frac{\alpha_k^{(p)}}{k^s} \left(\prod_{i=1}^p A_i \right) [-1, 1] . \quad \blacksquare
\end{aligned}$$

3.4 Comparison of the General Estimates

We now compare the new estimates with the ones given by Lemma 3.1.1 for different values of p and s . Since the only difference in the estimates are α^{p-1} and $\alpha_k^{(p)}$, these are the quantities we will compare. Hence, suppose that $\{a_k\}_{k \in \mathbb{Z}}$ is such that $a_0 \in [-1, 1]$ and $a_k \in \frac{1}{|k|^s}[-1, 1]$, for all $k \in \mathbb{Z} \setminus \{0\}$. For the computation, we fixed $M = 100$. In the case $p \geq 3$, increasing M would make the $\alpha_k^{(p)}$ even smaller.

p	s	k	α^{p-1}	$\alpha_k^{(p)}$
2	4	10	58.6667	7.9266
3	4	30	3.4418×10^3	45.7357
3	4	100	3.4418×10^3	37.6551
3	5	30	1.3110×10^4	43.5641
3	7	30	2.0280×10^5	43.0569
3	10	30	1.2861×10^7	44.7318
3	25	30	1.3792×10^{16}	65.1059
4	4	10	2.0192×10^5	370.3203
4	5	10	1.5011×10^6	369.0572
4	7	10	9.1328×10^7	441.7748
5	10	10	1.6541×10^{14}	6.5345×10^3
5	20	10	1.8141×10^{26}	7.4986×10^5
10	25	20	4.2497×10^{72}	5.2619×10^8
20	50	100	2.0691×10^{296}	3.5032×10^{19}

Figure 15: Comparison of the estimates.

3.5 Refinement of the Estimates

We now present a corollary of Theorem 3.3.1.

Corollary 3.5.1 *Let $p \geq 3$ the degree of the nonlinearity, $s \geq 2$ the decay of the coefficients and $M \geq 5$ a natural number. Let $k \in \{0, \dots, M-1\}$. Now consider another computational number $M_1 \geq M$. For $i = 1, \dots, p$, let $A_i > 0$ such that $a_0^{(i)} \in A_i[-1, 1]$ and $a_k^{(i)} \in \frac{A_i}{|k|^s}[-1, 1]$, for all $k \neq 0$. For each $i = 1, \dots, p$ let $|a|_{M_1}^{(i)} = (|a_0^{(i)}|, \dots, |a_{M_1-1}^{(i)}|) \in \mathbb{R}^{M_1}$. Suppose that $a_{-k}^{(i)} = a_k^{(i)}$. For $k \in \{0, \dots, M-1\}$, define*

$$\varepsilon_k^{(p)} = \frac{2\alpha_{M_1}^{(p-1)}}{(M_1 + k)^s(M_1 - 1)^{s-1}(s-1)} + \sum_{k_p=M_1}^{M_1+k-1} \frac{\alpha_{k_p-k}^{(p-1)}}{k_p^s(k_p - k)^s}. \quad (48)$$

Then we have that

$$(a^{(1)} * \dots * a^{(p)})_k \in \left[\left(|a|_{M_1}^{(1)} * \dots * |a|_{M_1}^{(p)} \right)_k + \left(\prod_{i=1}^p A_i \right) \varepsilon_k^{(p)} \right] [-1, 1], \quad (49)$$

*where $a * b$ denotes the discrete convolution between two vectors.*

Proof. First notice that

$$\begin{aligned} (a^{(1)} * \dots * a^{(p)})_k &= \sum_{\substack{k_1 + \dots + k_p = k \\ k_i \in \mathbb{Z}}} a_{k_1}^{(1)} \dots a_{k_p}^{(p)} \\ &= \sum_{\substack{k_1 + \dots + k_p = k \\ |k_i| < M_1}} a_{k_1}^{(1)} \dots a_{k_p}^{(p)} + \sum_{\substack{k_1 + \dots + k_p = k \\ \max\{|k_1|, \dots, |k_p|\} \geq M_1}} a_{k_1}^{(1)} \dots a_{k_p}^{(p)}. \end{aligned}$$

Without loss of generality, suppose that in the second sum, $|k_p| \geq M_1$. Now

$$\begin{aligned} \sum_{\substack{k_1 + \dots + k_p = k \\ \max\{|k_i|\} \geq M_1}} a_{k_1}^{(1)} \dots a_{k_p}^{(p)} &= \sum_{k_p=-\infty}^{-M_1} a_{k_p}^{(p)} \sum_{\substack{k_1 + \dots + k_{p-1} = k - k_p \\ \max\{|k_1|, \dots, |k_{p-1}|\} \geq M_1}} a_{k_1}^{(1)} \dots a_{k_{p-1}}^{(p-1)} \\ &\quad + \sum_{k_p=M_1}^{\infty} a_{k_p}^{(p)} \sum_{\substack{k_1 + \dots + k_{p-1} = k - k_p \\ \max\{|k_1|, \dots, |k_{p-1}|\} \geq M_1}} a_{k_1}^{(1)} \dots a_{k_{p-1}}^{(p-1)} \\ &\in \left(\prod_{i=1}^p A_i \right) \sum_{k_p=M_1}^{\infty} \left[\frac{\alpha_{k+k_p}^{(p-1)}}{k_p^s(k+k_p)^s} + \frac{\alpha_{k_p-k}^{(p-1)}}{k_p^s(k_p-k)^s} \right] [-1, 1] \\ &= \left(\prod_{i=1}^p A_i \right) \left[2\alpha_{M_1}^{(p-1)} \sum_{k_p=M_1}^{\infty} \frac{1}{k_p^s(k+k_p)^s} + \sum_{k_p=M_1}^{M_1+k-1} \frac{\alpha_{k_p-k}^{(p-1)}}{k_p^s(k_p-k)^s} \right] [-1, 1] \\ &\subseteq \left(\prod_{i=1}^p A_i \right) \left[\frac{2\alpha_{M_1}^{(p-1)}}{(M_1+k)^s(M_1-1)^{s-1}(s-1)} + \sum_{k_p=M_1}^{M_1+k-1} \frac{\alpha_{k_p-k}^{(p-1)}}{k_p^s(k_p-k)^s} \right] [-1, 1]. \end{aligned}$$

Recalling the definition of $\varepsilon_k^{(p)}$, we can conclude that

$$\left(a^{(1)} * \cdots * a^{(p)}\right)_k \in \left[\left(|a|_{M_1}^{(1)} * \cdots * |a|_{M_1}^{(p)}\right)_k + \left(\prod_{i=1}^p A_i\right) \varepsilon_k^{(p)} \right] [-1, 1] . \quad \blacksquare$$

CHAPTER IV

VALIDATED CONTINUATION FOR EQUILIBRIA OF PDES

The work presented in this chapter is a sum of results that came up from collaborations with Sarah Day, Marcio Gameiro and Konstantin Mischaikow presented in [11] and [15].

4.1 *Background*

The first step in understanding the dynamics of a nonlinear system of differential equations

$$u_t = F(u, \nu) \tag{50}$$

on a Hilbert space is to identify the set of equilibria $\mathcal{E} := \{(u, \nu) \mid F(u, \nu) = 0\}$. For many applications this can only be done using numerical methods. In particular, continuation provides an efficient technique for determining elements on branches of $\mathcal{E}$. With any numerical method there is the question of validity of the output as compared with the cost of computation. The goal of this chapter is to argue that for a large and important class of partial differential equations the cost of validating the existence and uniqueness of equilibria is small when compared to the cost of identifying potential equilibria by means of a continuation method.

To the best of our knowledge this is the first attempt to integrate the techniques of rigorous computations with a continuation method, thus we focus on a clear presentation of the ideas as opposed to presenting the results in the most general possible setting. We make use of spectral methods as they provide us with considerable control

on truncation errors. To be more precise, assume that (50) takes the form

$$u_t = L(u, \nu) + \sum_{p=0}^d c_p(\nu) u^p \quad (51)$$

where $L(\cdot, \nu)$ is a linear operator at parameter value ν and d is the degree of the polynomial nonlinearity. Typically, $c_1(\nu) = 0$ since linear terms are grouped under $L(\cdot, \nu)$. Expanding (51) using an orthogonal basis chosen appropriately in terms of the eigenfunctions of the linear operator $L(\cdot, \nu)$, the particular domain and the boundary conditions, results in a countable system of differential equations on the coefficients of the expanded solution.

To simplify the exposition, let us assume the expansion takes the form

$$\dot{u}_k = f_k(u, \nu) := \mu_k u_k + \sum_{p=0}^d \sum_{\sum n_i=k} (c_p)_{n_0} u_{n_1} \cdots u_{n_p} \quad k = 0, 1, 2, \dots \quad (52)$$

where $\mu_k = \mu_k(\nu)$ are the parameter dependent eigenvalues of $L(\cdot, \nu)$ and $\{u_n\}$ and $\{(c_p)_n\}$ are the coefficients of the corresponding expansions of the functions u and $c_p(\nu)$ respectively with $u_n = u_{-n}$ and $(c_p)_n = (c_p)_{-n}$ for all n . In order to simplify the notation, for a fixed parameter ν , we use $f(u)$ to denote $f(u, \nu)$. The continuation method is applied to the m -dimensional system of ODEs of the form

$$\dot{u}_k = \mu_k u_k + \sum_{p=0}^d \sum_{\substack{\sum n_i=k \\ |n_i| < m}} (c_p)_{n_0} u_{n_1} \cdots u_{n_p} \quad k = 0, 1, \dots, m-1. \quad (53)$$

obtained by performing a Galerkin projection on (52). It is this truncation that introduces the most substantial concern for the validity of the results of the continuation method. In Section 4.6 we present estimates that provide us with bounds on the errors. We obtain these bounds under the assumption of power decay rates in the coefficients $\{u_n\}$. Of course, such decay rates are directly related to the spatial smoothness of the equilibria which in turn is governed, at least in part, by the linear operator $L(\cdot, \nu)$.

Let $\bar{u}$ be a numerical zero obtained from (53). In the orthogonal basis used to obtain (52) consider the set $X = \bar{u} + W(r)$ of $\bar{u}$ where $W(r)$ is of the form

$$W(r) = \prod_{k=0}^{m-1} [-r, r] \times \prod_{k=m}^{\infty} \left[-\frac{A_s}{k^s}, \frac{A_s}{k^s} \right].$$

Section 4.6 provides an explicit set of formulas and steps and the assertion that their successful implementation leads to the construction of the radii polynomials. Presenting the formulae in this fashion has two advantages. First, they contain all the necessary information should the reader wish to independently code and test the techniques suggested in this chapter. Second, it allows for the presentation in Section 4.3 of the comparison of the computational costs between traditional and validated continuation.

It should be emphasized that how one should best compare the costs between the two methods of continuation is not completely clear. In the standard approach m , the dimension of the system on which continuation is performed, is fixed. Thus traditionally, a particular Galerkin projection dimension is chosen and continuation is performed. The results are checked by choosing a higher dimensional projection, re-performing the continuation and then deciding if the two calculations agree within a certain level of numerical tolerance. In validated continuation, m becomes a variable. In particular, if validation fails then one has the option of choosing a higher dimensional Galerkin projection. Equally important, failure of validation may be an indication that a higher dimensional projection is necessary. In summary, validated continuation provides an internal check of consistency on the dimension of truncation from the infinite to finite dimensional problem a feature which is not present in the traditional application of continuation methods.

With this in mind we have chosen to compare the computational costs as follows. First we restrict our attention to cubic nonlinearities. As is made clear by the formulae of Section 4.6 in this case the cost of evaluating the nonlinearities and performing Newton's method are both of order m^3 . Thus, we can obtain a rough bound on the

ratio of the cost of traditional versus validated continuation by counting the number of m^3 operations which need to be performed. These calculations suggest that for fixed m the cost of validated continuation is less than twice the cost of traditional continuation, that is *it appears that it is cheaper to perform validated continuation, than to perform traditional continuation and then check it against continuation performed on a higher dimensional projection*. In Section 4.4 this estimate is tested against actual computations for the Swift-Hohenberg equation and the Cahn-Hilliard equation. To ensure that these comparisons are fair, we employ standard floating point computations in both cases.

This last point raises an important distinction: validated continuation versus rigorous continuation. Using floating point calculations at all steps of the validated continuation, does not allow one to control for roundoff errors and hence one cannot rigorously conclude the existence of an equilibrium. Because the current computer technology treats floating point and interval arithmetic differently we chose not to make and present timed comparisons between the two for this chapter. However, if specific steps in the validation argument are performed using interval arithmetic, then one obtains rigorous results on the existence of equilibria. Results of this type are presented in Section 4.4 for a branch of equilibria of the Swift-Hohenberg equation.

Remark 4.1.1 *For the results presented in this Chapter, we did not do any continuous branches. Hence, we computed the radii polynomials with $\hat{\nu} = 0$ at every step. Because of this, we will drop the dependence in ν in the radii polynomials.*

4.2 Radii polynomials

Let m be a fixed projection dimension of (53). For $u_F := (u_0, \dots, u_{m-1}) \in \mathbb{R}^m$, define $f^{(m)} : \mathbb{R}^m \rightarrow \mathbb{R}^m$ by $f^{(m)}(u_F) = (f_0^{(m)}(u_F), \dots, f_{m-1}^{(m)}(u_F))$ where for $k = 0, \dots, m-1$,

$$f_k^{(m)}(u_F) = \mu_k u_k + \sum_{p=0}^d \sum_{\substack{\sum n_i = k \\ |n_i| < m}} (c_p)_{n_0 n_1 \dots n_p} u_{n_0} \dots u_{n_p}$$

The Galerkin projection can then be written

$$\dot{u}_F = f^{(m)}(u_F, \nu) . \quad (54)$$

This is the m -dimensional system to be studied numerically. Intuitively, we expect that if m is sufficiently large, (54) will capture the essential dynamics for the original system (52). We now present the formulae for *radii polynomials*. Let us begin by explicitly stating the information that is used to construct the coefficients.

- d is the degree of the nonlinearity of (51).
- m is the number of modes used in the Galerkin projection.
- $M \geq m$ is a computational parameter that allows for the use of explicit values for coefficients of $M - m$ additional modes to decrease truncation error bounds.
- $m_+ \geq m$ is a computational parameter that allows for the use of additional structure in the model to get tighter truncation error bounds.
- $\bar{u}_F \in \mathbb{R}^m$ is the numerical zero produced by the predictor-corrector step.
- $J_{F \times F}$ is the numerical inverse obtained from the predictor-corrector step.
- $(c_p)_n, |n| < m$ are the coefficients from the expansion (52).
- $\mu_k, k \geq 0$ are the eigenvalues for the linear operator L as expressed in (52) and

$$\bar{\mu} := \inf_{n \geq m_+} |\mu_n|.$$

Note that if $|\mu_n|$ is monotonically increasing for $n \geq m_+$, then $\bar{\mu} = |\mu_{m_+}|$.

- s and A_s are positive constants that are related to the regularity of the equilibria.

Observe that given this information we can evaluate the vector

$$f_F(\bar{u}) := \begin{bmatrix} f_0(\bar{u}) \\ \vdots \\ f_{m-1}(\bar{u}) \end{bmatrix}$$

where

$$f_n(\bar{u}) = \mu_n \bar{u}_n + \sum_{p=0}^d \sum_{\substack{n_0 + \dots + n_p = n \\ |n_1|, \dots, |n_p| < m}} (c_p)_{n_0} \bar{u}_{n_1} \cdots \bar{u}_{n_p} .$$

We can also set

$$Y_k \geq \begin{cases} |J_{F \times F} f_F(\bar{u})|_k & \text{if } 0 \leq k < m \\ \frac{|\sum_{p=2}^d (c_p \bar{u}^p)_k|}{|\mu_k|} & \text{if } k \geq m \end{cases} \quad (55)$$

where

$$(c_p \bar{u}^p)_k = \sum_{\sum n_i = k} (c_p)_{n_0} \bar{u}_{n_1} \cdots \bar{u}_{n_p} .$$

The following constants are all related to asymptotic bounds on the expansions of the numerical equilibrium $\bar{u}$, and the set $\bar{u} + W$. As such they are related to the regularity of the equilibrium and the coefficients of (51). Define

$$\begin{aligned} \alpha &:= \frac{2}{s-1} + 2 + 3.5 \cdot 2^s \\ C_p &:= \max_k \{ |(c_p)_0|, |(c_p)_k| |k|^s \} \\ \bar{A} &:= \max_{1 \leq k < m} \{ |\bar{u}_0|, |\bar{u}_k| |k|^s \} \\ A = A(r) &:= \max \{ A_s, r(m-1)^s \} \\ C(\bar{A}, A) &:= \sum_{l=1}^d \sum_{p=\max\{2, l\}}^d l \binom{p}{l} \alpha^p C_p \bar{A}^{p-l} A(r)^l \\ C_+(\bar{A}, A) &:= \begin{cases} \sum_{l=1}^d \sum_{p=2}^d l \binom{p}{l} \alpha^p C_p \bar{A}^{p-l} A^l & \text{if } Y_k, R_k = 0 \text{ for all } k \geq m_+ \\ \sum_{p=0}^d \alpha^p C_p \bar{A}^p + \sum_{l=1}^d \sum_{p=\max\{2, l\}}^d l \binom{p}{l} \alpha^p C_p \bar{A}^{p-l} A^l & \text{otherwise ,} \end{cases} \\ V_F^{(0)} &:= |J_{F \times F}| R_F \quad , \quad V_F^{(1)} := |I_{F \times F} - J_{F \times F} \cdot Df^{(m)}(\bar{u}_F)| \begin{pmatrix} 1 \\ 1 \\ \vdots \\ 1 \end{pmatrix} \end{aligned}$$

where $|\cdot|$ denotes entry-wise absolute value and for $k \in \{0, \dots, m-1\}$,

$$R_k := \sum_{\substack{\bar{n} = -\infty \\ |k - \bar{n}| \geq m}}^{\infty} \left| \sum_{p=1}^d p \sum_{\sum n_i = \bar{n}} (c_p)_{n_0} \bar{u}_{n_1} \cdots \bar{u}_{n_{p-1}} \right| \frac{A_s}{|k - \bar{n}|^s} .$$

Note that if all c_p have finite expansions, then $V_F^{(0)}$ requires only a finite computation. Observe also that the above implies that $\bar{u}_k \in \frac{\bar{A}}{k^s}[-1, 1]$ and $\mathbf{w}_k \subset \frac{A}{k^s}[-1, 1]$ for all k .

The validation procedure also requires bounds on the errors due to truncating modes $k \geq m$. These bounds come in the following form:

$$\epsilon_n := \sum_{l=1}^d \sum_{p=l}^d l \binom{p}{l} \epsilon_n(p, l, M) \quad (56)$$

where

$$\begin{aligned} \epsilon_n(p, l, M) := & \quad (57) \\ \min \left\{ \frac{p \alpha^{p-1} C_p \bar{A}^{p-l} A^l}{(M-1)^{s-1}(s-1)} \left[\frac{1}{(M-n)^s} + \frac{1}{(M+n)^s} \right], \frac{\alpha^p C_p \bar{A}^{p-l} A^l}{n^s} \right\}, \end{aligned}$$

and

$$\begin{aligned} C_n(p, j, l, M) := & \quad (58) \\ \sum_{|\bar{n}| < (p-l)(m-1)+M} \left| \sum_{\substack{\sum n_i = \bar{n} \\ |n_0| < M \\ |n_1|, \dots, |n_{p-l}| < m}} (c_p)_{n_0} \bar{u}_{n_1} \cdots \bar{u}_{n_{p-l}} \right| \left(\sum_{\substack{\sum n_i + \bar{n} = n \\ m \leq |n_1|, \dots, |n_j| < M}} \frac{A_s^j}{|n_1|^s \cdots |n_j|^s} \right). \end{aligned}$$

For notational purposes, we also define m -vectors containing these bounds for modes $n = 0, \dots, m-1$ as follows.

$$\epsilon_F := \begin{bmatrix} \epsilon_0 \\ \vdots \\ \epsilon_{m-1} \end{bmatrix}, \quad \text{and} \quad C_F(p, j, l, M) := \begin{bmatrix} C_0(p, j, l, M) \\ \vdots \\ C_{m-1}(p, j, l, M) \end{bmatrix}.$$

Note that these bounds are computable in that they require only a finite number of computations. In addition, increasing the computational parameter M has the effect of increasing the computational work in order to decrease the bounds. This will be the subject of Section 4.5.

Definition 4.2.1 *To simplify notation, the finite radii polynomials, $P_0, \dots, P_{m-1}$, are given as an m -vector $P_F(r) = (P_0(r), \dots, P_{m-1}(r))^t$. Define*

$$P_F(r) := \sum_{n=0}^d C_F(n) r^n \quad (59)$$

where the coefficients are

$$C_F(n) := \begin{cases} C_F^Y + C_F^Z(0) & n = 0 \\ C_F^Z(1) - 1 & n = 1 \\ C_F^Z(n) & n = 2, \dots, d. \end{cases}$$

The right hand terms are defined as follows. The individual terms of the vectors $C_F^Z(i)$ are chosen to satisfy

$$C_k^Z(i) \geq \left(\sum_{l=\max\{2,i\}}^d \sum_{p=l}^d l \binom{p}{l} \binom{l}{i} |J_{F \times F}| C_F(p, l-i, l, M) \right. \\ \left. + \begin{cases} |J_{F \times F}| \epsilon_F + V_F^{(0)} & i = 0 \\ V_F^{(1)} & i = 1 \\ 0 & \text{otherwise} \end{cases} \right)_k. \quad (60)$$

and similarly

$$C_F^Y = Y_F. \quad (61)$$

where $|\cdot|$ and the bounds are computed component-wise.

Observe, again, that determining these bounds require only a finite number of computations.

Definition 4.2.2 For $k \geq m$, the tail radii polynomial is

$$P_k(r) = \begin{cases} \frac{|\sum_{p=0}^d (c_p \bar{u}^p)_k|}{|\mu_k|} + \frac{C(\bar{A}, A(r))}{|\mu_k| k^s} - \frac{A_s}{k^s} & m \leq k < m_+ \\ \frac{C_+(\bar{A}, A)}{|\mu_k| k^s} - \frac{A_s}{k^s} & k \geq m_+ \end{cases}$$

where, again,

$$(c_p \bar{u}^p)_k = \sum_{\sum n_i = k} (c_p)_{n_0} \bar{u}_{n_1} \cdots \bar{u}_{n_p}.$$

We now present a procedure for computing a validation radius. In particular, this procedure describes a natural order for defining the decay constants A_s , s , and A . The constants A_s and s reflect regularity properties of the equation and should be chosen

either from numerical simulations or analysis. In this approach, we choose to treat $A = A(r)$ as a constant. The rationale for this choice is that from a computational perspective, we would like to find $r > 0$ solving simple constructions of the finite radii inequalities $P_0(r) < 0, \dots, P_{m-1}(r) < 0$ without having to simultaneously control the more complicated effects from A on the coefficients of these polynomials as well as on the tail polynomials $P_k, k \geq m$. A practical way to achieve this goal is to set $A = A_s$ at the beginning of the procedure and then check in the end that a solution $r > 0$ to $P_0(r) < 0, \dots, P_{m-1}(r) < 0$ also satisfies $r(m-1)^s \leq A_s$.

Here, for the sake of simplicity, we set $M = m$. If the truncation error bounds prove too large for the computations, then M should be increased as described in Remark 4.6.3 in Section 4.6. Finally, we add a condition which reduces the check of the tail polynomials $P_k(r) < 0, k > m$ to a finite number of computations. The following procedure outlines this approach.

Procedure 4.2.3 *Suppose that the eigenvalues μ_k are such that $|\mu_k| \rightarrow \infty$. Suppose further that we may choose $m, m_+, \bar{m} \in \mathbb{N}$, $\bar{m} \geq m_+ \geq m$, and $\bar{\mu} > 0$ such that*

1. *m is the Galerkin projection dimension used for numerical continuation,*
2. *m_+ is the parameter used in the computation of $C_+(\bar{A}, A)$, and*
3. *$\bar{m}$ measures where the tail terms are bounded from below by $\bar{\mu}$ as follows: for all $k \geq \bar{m}$, $|\mu_k| \geq |\bar{\mu}|$.*

Set $M = m$.

Remark: m should be chosen to give the expected nonzero modes along the bifurcation branch under study and $\bar{m} = m_+ = (2d+1)(m-1) + 1$ if $(c_p)_n = 0$ for all $n \neq 0$ and the eigenvalues, μ_k are monotonically increasing in magnitude after $k = (2d+1)(m-1)$.

Fix the decay constants

$$s \geq 2 \quad \text{and} \quad A_s > 0. \tag{62}$$

Remark: In practice, A_s and s should be determined by regularity properties of the equation.

Set $A := A_s$. Using the finite radii polynomials given in Definition 4.2.1, for $k = 0, \dots, m-1$, numerically compute $I_k := \{r > 0 \mid P_k(r) < 0\}$ and

$$\mathcal{I} := \bigcap_{k=0}^{m-1} I_k . \quad (63)$$

Check that $\mathcal{I} \neq \emptyset$.

Remark: If $\mathcal{I} = \emptyset$, begin the procedure again either by choosing m larger or by choosing s larger and/or A_s smaller in (62).

Check that there exists $\bar{r} \in \mathcal{I}$ such that

$$\bar{r} \leq \frac{A_s}{(m-1)^s} . \quad (64)$$

Remark: If such an $\bar{r}$ exists, then $A = A_s = \max\{A_s, \bar{r}(m-1)^s\}$. This in turn implies that component-wise $P_F(\bar{r}) < 0$. If $\bar{r}$ does not exist, then begin the procedure again either by choosing m larger or by choosing s larger and/or A_s smaller in (62).

Check the inequalities

$$P_m(\bar{r}) < 0, \dots, P_{\bar{m}-1}(\bar{r}) < 0 \text{ and } \frac{C(\bar{A}, A)}{|\bar{\mu}|} - A_s < 0.$$

Remark: If any of these inequalities fails, begin the procedure again either by choosing m larger or by choosing s larger and/or A_s smaller in (62).

4.3 Computational cost

We now provide a rough comparison of the cost of continuation with the cost of validated continuation for PDEs of the form

$$u_t = L(u, \nu) - u^3 . \quad (65)$$

Since the degree of the polynomial nonlinearity in (65) is cubic and we use a Newton-like operator in the continuation procedure, the most expensive terms of the computation involve m^3 operations, where m is the number of modes used in the Galerkin

projection

$$f_k^{(m)}(u_F, \nu) = \mu_k(\nu)u_k - \sum_{\substack{n_1+n_2+n_3=k \\ |n_i|<m}} u_{n_1}u_{n_2}u_{n_3}, \quad k = 0, \dots, m-1. \quad (66)$$

With this in mind we count the number of m^3 operations for both approaches to obtain an estimate for the asymptotic costs and conclude with statistics obtained from calculations for the Swift-Hohenberg and Cahn-Hilliard equations.

4.3.1 Cost of continuation

A traditional continuation procedure involves iteration of predictor and corrector steps to trace out branches of equilibria. Under the assumption that at some parameter $\nu = \nu_0$ we have an equilibrium solution for (54), we want to continue the equilibrium as we vary ν . We recall in details the predictor and the corrector steps.

1) Euler predictor: Given an approximate equilibrium x_0 at ν_0 , the *predictor* at $\nu_1 = \nu_0 + \Delta\nu$ is $x_1^{(0)} = x_0 + \dot{x}_0\Delta\nu$, where

$$\dot{x}_0 = -f_x^{(m)}(x_0, \nu_0)^{-1}f_\nu^{(m)}(x_0, \nu_0). \quad (67)$$

2) Quasi-Newton corrector: We now use the following quasi-Newton iterative scheme to improve our approximation at ν_1

$$x_1^{(n+1)} = x_1^{(n)} - f_x^{(m)}(x_1^{(n)}, \nu_1)^{-1}f_\nu^{(m)}(x_1^{(n)}, \nu_1) \quad (68)$$

If k is the total number of iterations of (68), then $\bar{u}_F := x_1^{(k)}$ and $f^{(m)}(\bar{u}_F, \nu_1) \approx 0$.

We decompose the analysis of the cost of continuation into four steps, assuming that we begin with an approximate zero x_0 at ν_0 .

Step 1. In order to get the Euler predictor (67), we need to evaluate the vector $-f_x^{(m)}(x_0, \nu_0)^{-1}f_\nu^{(m)}(x_0, \nu_0)$. This requires computing the m by m matrix $f_x^{(m)}(x_0^{(0)}, \nu_0)$,

where for $0 \leq i, j < m$,

$$\begin{aligned} \left[f_x^{(m)}(x_0^{(0)}, \nu_0) \right]_{i+1, j+1} &= \delta_{i,j} \mu_i - 3 \left(\sum_{\substack{n_1+n_2+j=i \\ |n_i| < m}} [x_0^{(0)}]_{|n_1|} [x_0^{(0)}]_{|n_2|} \right. \\ &\quad \left. + \sum_{\substack{n_1+n_2-j=i \\ |n_i| < m}} [x_0^{(0)}]_{|n_1|} [x_0^{(0)}]_{|n_2|} \right). \end{aligned}$$

This involves the evaluation of $2m^2$ sums demanding $2m - 1$ multiplications and $2m - 2$ additions each. Therefore, determining $f_x^{(m)}(x_0^{(0)}, \nu_0)$ requires $8m^3$ operations. Next, we compute the LU decomposition of $f_x^{(m)}(x_0^{(0)}, \nu_0)$ in order to compute the action of its inverse on $f_\nu^{(m)}(x_0, \nu_0)$. This involves $\frac{2}{3}m^3$ operations. In our case, $f_\nu^{(m)}(x_0, \nu_0) = x_0$, requiring no additional cost. The predictor is then

$$\begin{cases} x_1^{(0)} = x_0 - \Delta \nu f_x^{(m)}(x_0, \nu_0)^{-1} x_0 \\ \nu_1 = \nu_0 + \Delta \nu. \end{cases}$$

Step 2. We now start the corrector. To construct the quasi-Newton operator (68), we need the action of the inverse of $f_x^{(m)}$ at the predictor $(x_1^{(0)}, \nu_1)$. As seen before, it costs $8m^3$ to evaluate $f_x^{(m)}(x_1^{(0)}, \nu_1)$ and $\frac{2}{3}m^3$ to compute its inverse using LU decomposition. Note that we need to compute the LU decomposition only at the first step.

Step 3. At the j^{th} iteration of (68), we need to evaluate $f^{(m)}(x_1^{(j-1)}, \nu_1)$. Its i^{th} component is

$$\begin{aligned} [f^{(m)}(x_1^{(j-1)}, \nu_1)]_i &= \mu_i(\nu_1) [x_1^{(j-1)}]_i \\ &\quad - \sum_{\substack{n_1+n_2+n_3=i \\ |n_i| < m}} [x_1^{(j-1)}]_{|n_1|} [x_1^{(j-1)}]_{|n_2|} [x_1^{(j-1)}]_{|n_3|} \end{aligned}$$

which requires at least $3m^2$ operations to evaluate. Since $f^{(m)}$ has m components, we get a total of $3m^3$. If k is the total number of iterations of the corrector, then this step requires $3km^3$ operations.

Step 4. The corrector ends when $\|f^{(m)}(x_1^{(k)}, \nu_1)\| < \text{tolerance}$. Let $\bar{a}_F := x_1^{(k)}$.

Evaluating the function at $(\bar{u}_F, \nu_1)$ is another $3m^3$. Now, note that we have to compute the action of the inverse of $f_x^{(m)}(\bar{u}_F, \nu_1)$ to get the predictor for the next step. Recall $J_{F \times F}$ is the numerical inverse of $f_x^{(m)}(\bar{u}_F, \nu_1)$ computed as before using an LU decomposition. Explicitly computing all the coefficients in $f_x^{(m)}(\bar{u}_F, \nu_1)$ requires an extra $2m^3$ operations. We do not count the m^3 involved to get the next predictor, since that is part of the next predictor-corrector step.

Combining the costs of the four above mentioned steps suggests that the cost of one application of the predictor-corrector algorithm is on the order of $(20 + 3k)m^3$, where k is the number of iterations in the quasi-Newton corrector.

4.3.2 Cost of validation

We now show that the extra cost of performing validation for a cubic function ($d = 3$) with constant function coefficients is of the order of $6m^3$ operations where m is the projection dimension used for continuation. The additional cost comes primarily from computing the coefficients of the radii polynomials. In the following, we construct $m_+ = d(m - 1) + 1 = 3m - 2$ polynomials $P_0, \dots, P_{3m-3}$ using Procedure 4.2.3 and calculate the associated computational cost. Both to simplify the presentation and because this is what is used to perform the computations presented in Section 4.4, we set $\bar{m} = m_+ = d(m - 1) + 1$, with $|\mu_k| \geq |\mu_{\bar{m}}|$ for all $k \geq \bar{m}$, and $M = m$. As described in Procedure 4.2.3, $A = A_s$ and we consider fixed $s > 2$ and $A_s > 0$.

The only nonlinear term of (65) is a monomial of degree 3. Thus, if $p \neq 3$, then $C_k(p, j, l, M) = 0$. In addition, we have set $M = m$. Hence, if $j \neq 0$, then $C_k(p, j, l, M) = 0$ (see Remark 4.6.3). Therefore, the only nonzero terms of this form are

$$C_k(3, 0, l, m) = \left| \sum_{\substack{n_1 + n_2 + n_3 = k \\ |n_1|, |n_2|, |n_3| < m}} \bar{u}_{n_1} \cdots \bar{u}_{n_{3-l}} \right|. \quad (69)$$

Hence, by (60) we set

$$C_k^Z(0) \geq (|J_{F \times F}| \epsilon_F)_k + V_k^{(0)} \quad (70)$$

for $0 \leq k < m$ and $|\cdot|$ denotes the component-wise absolute value. Note that it is possible to get an analytic upper bound on $V_k^{(0)}$ using Lemma 4.6.2 in which case computing $V_k^{(0)}$ doesn't require any m^3 operations. Hence, all necessary computations for $C_F^Z(0)$ are of order less than m^3 . Using (60),

$$C_k^Z(1) \geq V_k^{(1)}$$

for $0 \leq k < m$ and evaluating $V_F^{(1)}$ does not require any m^3 operations.

Finally, combining (60) and (69)

$$C_F^Z(2) \geq 6|J_{F \times F}|C_F(3, 0, 2, m)$$

where $C_n(3, 0, 2, m) = |\bar{u}_n|$ and

$$C_F^Z(3) \geq 3|J_{F \times F}|C_F(3, 0, 3, m)$$

where $C_n(3, 0, 3, m) = 1$.

The last coefficient to compute to get all the finite radii polynomials (61) is

$$C_F^Y \geq |J_{F \times F} f_F(\bar{u})|$$

where again $|\cdot|$ denotes the component-wise absolute value. This comes with no extra m^3 cost since $f_F(\bar{u}) = f^{(m)}(\bar{u}_F, \nu_1)$ was computed in Step 4 of the predictor-corrector algorithm.

The next step in Procedure 4.2.3 is checking for the existence of a validation radius $r > 0$. This requires finding the numerical zeros of each of the cubic polynomials $P_0, \dots, P_{m-1}$, constructing $I_0, \dots, I_{m-1}$ where I_k are closed intervals such that $I_k \subsetneq \{r > 0 | P_k(r) < 0\}$, and finally checking for a non-empty intersection $\mathcal{I} = \cap_{k=0}^{m-1} I_k$. All of these steps are of order less than m^3 .

Assuming there exists a positive $\bar{r} \in \mathcal{I}$ such that $\bar{r}(m-1)^s \leq A_s$, we construct and evaluate the tail radii polynomials $P_m, \dots, P_{3m-1}$ at $\bar{r}$. We compute Y_k using (55) which requires $6m^3$ operations since we need to evaluate $f_k(\bar{u})$ for $k = m, \dots, 3m-3$.

Using Definition 4.2.2 and the assumption that $A = A_s$ we compute

$$C(\bar{A}, A) = \sum_{l=1}^3 l \binom{3}{l} \alpha^3 \bar{A}^{3-l} A^l = 3\alpha^3 A_s (\bar{A} + A_s)^2.$$

This latter step and the remaining computations for Procedure 4.2.3 are all of order less than m^3 .

In summary, the m^3 cost of computing the coefficients of the radii polynomials is $6m^3$. Thus the additional cost of validation is on the order of $6m^3$ operations.

4.3.3 Relative cost

Combining the results of Sections 4.3.1 and 4.3.2 suggests that asymptotically the ratio of the cost of validated continuation to the cost of traditional continuation is

$$\frac{26 + 3k}{20 + 3k}.$$

where k is the number of iterations performed in the corrector step. We tested this hypothesis again two fourth order partial differential equations with cubic nonlinearities, Swift-Hohenberg and Cahn-Hilliard. The results are discussed in greater detail in Section 4.4. For the moment we are only interested in the relative times of computation.

We performed validated continuation for 46 predictor-corrector steps involving a total of 90 quasi-Newton iterations for the cubic Swift-Hohenberg equation. We repeated the computations without validation. The ratio of elapsed time for validated continuation to the time used for continuation alone was ≈ 1.156 . Given that we had an average of $90/46$ iterations per predictor-corrector step, this is close to the rough estimate of $\frac{26+3 \cdot 90/46}{20+3 \cdot 90/46} \approx 1.232$ given by the above arguments.

Similarly, we performed validated continuation for 15 predictor-corrector steps involving a total of 37 quasi-Newton iterations for Cahn-Hilliard. Again, we repeated

the computations without validation. The ratio of elapsed time for validated continuation to the time used for continuation alone was ≈ 1.173 . Given that we had an average of $37/15$ iterations per predictor-corrector step, the asymptotic ratio is $\frac{26+3 \cdot 37/15}{20+3 \cdot 37/15} \approx 1.219$.

The results of these computations are summarize in Figure 16.

PDE	m	$\frac{\# \text{ iterations}}{\# \text{ steps}}$	Experimental Ratio	Estimated Ratio $\frac{26+3k}{20+2k}$
S-H	27	1.96	1.156	1.232
C-H	60	1.65	1.173	1.219

Figure 16: Comparison of the asymptotic ratios.

4.4 *Sample results with $M = m$*

To demonstrate the practical applicability of validated continuation we turn to two model problems, Cahn-Hilliard and Swift-Hohenberg. In both cases we follow a branch of equilibria and validate at each parameter value of the continuation. In the case of Swift-Hohenberg we also use interval arithmetic to evaluate the radii polynomials, thus allowing us to rigorously verify the existence and uniqueness of the equilibria.

4.4.1 Cahn-Hilliard

The Cahn-Hilliard equation was introduced in [5] as a model for the process of phase separation of a binary alloy at a fixed temperature. On a one-dimensional domain it takes the form

$$\begin{aligned}
 u_t &= -\left(\frac{1}{\nu}u_{xx} + u - u^3\right)_{xx}, \quad x \in [0, 1] \\
 u_x &= u_{xxx} = 0, \quad \text{at } x = 0, 1.
 \end{aligned} \tag{71}$$

The assumption of an equal concentration of both alloys is formulated as

$$\int_0^1 u(x, \cdot) dx = 0$$

Note that when looking for the equilibrium solutions of (71), it is sufficient to work with the Allen-Cahn equation

$$\begin{aligned}\frac{1}{\nu}u_{xx} + u - u^3 &= 0 \\ u_x &= 0 \quad \text{at } x = 0, 1.\end{aligned}\tag{72}$$

Re-writing (72) in the form of (51), the linear operator is $L(\cdot, \nu) = \frac{1}{\nu} \frac{\partial^2}{\partial x^2} + 1$ and the polynomial nonlinearity is of degree $d = 3$ with coefficient functions

$$(c_p)_n = \begin{cases} -1 & p = 3 \text{ and } n = 0 \\ 0 & \text{otherwise.} \end{cases}$$

Applying Procedure 4.2.3 with $M = m = 60$, $s = 3$, and $A_s = 0.01$, results in the branch of equilibria indicated in Figure 17 where each point represents the center of the infinite dimensional validation set of the form $\bar{u} + W(\bar{r})$, containing a unique equilibrium of (71). These are the points used to obtain the cost estimates presented in Figure 16. To avoid drowning the reader in large lists of numbers, we only provide the detailed numerical output at one parameter value.

Validated Result 4.4.1 *Let $\nu = 43.57415358799057$. Then,*

$$\bar{r} = 4.846104201261526 \times 10^{-8}$$

is a validation radius for the numerical zero $\bar{u}_F$ given in Figure 18. Thus, there exists a unique equilibrium for (71) in the validation set

$$(\bar{u}_F, 0) + \prod_{k=0}^{59} [-\bar{r}, \bar{r}] \times \prod_{k=60}^{\infty} \left[-\frac{0.01}{k^3}, \frac{0.01}{k^3} \right].$$

4.4.2 Swift-Hohenberg

The Swift-Hohenberg equation

$$\begin{aligned}u_t &= f(u, \nu) = \left\{ \nu - \left(1 + \frac{\partial^2}{\partial x^2} \right)^2 \right\} u - u^3, & u(\cdot, t) &\in L^2 \left(0, \frac{2\pi}{L_0} \right), \\ u(x, t) &= u \left(x + \frac{2\pi}{L_0}, t \right), & u(-x, t) &= u(x, t), & \nu &> 0,\end{aligned}\tag{73}$$

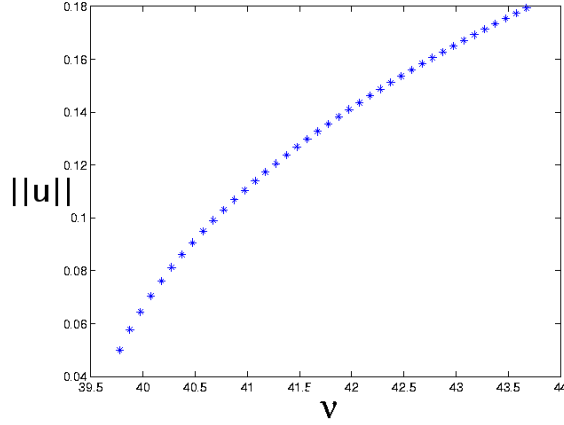


Figure 17: Validated continuation in ν for the Cahn-Hilliard equation on $[0, 1]$.

was originally introduced to describe the onset of Rayleigh-Bénard heat convection [35], where L_0 is a fundamental wave number for the system size $2\pi/L_0$. The parameter ν corresponds to the Rayleigh number and its increase is associated with the appearance of multiple solutions that exhibit complicated patterns. For the computations presented here we fixed $L_0 = 0.65$.

Re-writing (73) in the form of (51), the linear operator is $L(\cdot, \nu) = \nu - (1 + \frac{\partial^2}{\partial x^2})^2$ and the polynomial nonlinearity is of degree $d = 3$ with coefficient functions

$$(c_p)_n = \begin{cases} -1 & p = 3 \text{ and } n = 0 \\ 0 & \text{otherwise.} \end{cases}$$

Applying Procedure 4.2.3 with $M = m = 27$, $s = 4$, and $A_s = 0.002$, results in the branch of equilibria indicated in Figure 19 where each point represents the center of the infinite dimensional validation set of the form $\bar{u} + W(\bar{r})$, containing a unique equilibrium of (73). Again, these are the points used to obtain the cost estimates presented in Figure 16.

As in the case of the Cahn-Hilliard equation, we only include the output at one point on the branch of the Figure 19.

k	$\bar{u}_k$
1	$1.773844149032812 \times 10^{-1}$
3	$-7.601617928785714 \times 10^{-4}$
5	$3.271672072176762 \times 10^{-6}$
7	$-1.408100160017936 \times 10^{-8}$
9	$6.060344382471457 \times 10^{-11}$
11	$-2.608320515803233 \times 10^{-13}$
13	$1.122598345048980 \times 10^{-15}$
15	$-4.831561184682242 \times 10^{-18}$
17	$2.079457485469691 \times 10^{-20}$
19	$-8.949770271275235 \times 10^{-23}$
21	$3.851880360024139 \times 10^{-25}$
23	$-1.657801422354123 \times 10^{-27}$
25	$7.134947464114615 \times 10^{-30}$
27	$-3.070770234245256 \times 10^{-32}$
29	$1.321605495419571 \times 10^{-34}$
31	$-5.687926883858248 \times 10^{-37}$
33	$2.447955395983479 \times 10^{-39}$
35	$-1.053537452697732 \times 10^{-41}$
37	$4.534120813401209 \times 10^{-44}$
39	$-1.951337823193323 \times 10^{-46}$
41	$8.397842606319005 \times 10^{-49}$
43	$-3.614086242431264 \times 10^{-51}$
45	$1.555336697148314 \times 10^{-53}$
47	$-6.693373497802139 \times 10^{-56}$
49	$2.880447985844179 \times 10^{-58}$
51	$-1.239563989182517 \times 10^{-60}$
53	$5.334225825486573 \times 10^{-63}$
55	$-2.295445428599939 \times 10^{-65}$
57	$9.877687199770852 \times 10^{-68}$
59	$-4.250458946966345 \times 10^{-70}$
≥ 60	0

Figure 18: The numerical zero $\bar{u}_F$ obtained by continuation for the Cahn-Hilliard equation at $\nu = 43.57415358799057$. Note that all even coefficients are 0.

Validated Result 4.4.2 *Let $\nu = .6674701641462312$. Then*

$$\bar{r} = 1.998167170445973 \times 10^{-9}$$

is a validation radius for the numerical zero $\bar{u}_F$ whose coefficient values are indicated in Figure 20. Thus, there exists a unique equilibrium solution for (73) in the validation set

$$(\bar{u}_F, 0) + \prod_{k=0}^{26} [-\bar{r}, \bar{r}] \times \prod_{k=27}^{\infty} \left[-\frac{0.002}{k^4}, \frac{0.002}{k^4} \right].$$

Observe that in all the above mentioned calculations floating point round-off errors have not been controlled, thus at this point one cannot claim that the validation

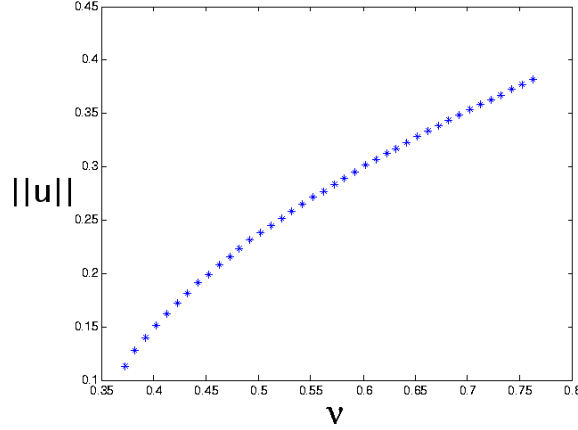


Figure 19: Validated continuation in ν for the Swift-Hohenberg equation at $L_0 = 0.65$.

k	$\bar{u}_k$
1	$-3.359998711939212 \times 10^{-1}$
3	$4.824376413178060 \times 10^{-3}$
5	$-1.761066797314072 \times 10^{-5}$
7	$7.535865329757206 \times 10^{-8}$
9	$-2.790895103063484 \times 10^{-10}$
11	$9.411109491227775 \times 10^{-13}$
13	$-3.113936321690645 \times 10^{-15}$
15	$1.007016979585499 \times 10^{-17}$
17	$-3.200410295859874 \times 10^{-20}$
19	$1.003878817132397 \times 10^{-22}$
21	$-3.114244522738206 \times 10^{-25}$
23	$9.573156964813860 \times 10^{-28}$
25	$-2.920394630491221 \times 10^{-30}$
≥ 26	0

Figure 20: The numerical zero $\bar{u}_F$ obtained by continuation for the Swift-Hohenberg equation at $\nu = .6674701641462312$ and $L_0 = 0.65$. All even coefficients are 0.

results presented above are rigorous. However, with additional computational effort a computer-assisted proof can be obtain. To be more precise, our technique relies on the existence of a validation radius $\bar{r}$ making all radii polynomials strictly negative. Hence, rigorous validation follows if the inequalities are satisfied when one includes bounds to control the possible of floating point errors. The first step in checking these inequalities on this level is to obtain floating point outer bounds for the coefficients of the polynomials. This can be done by defining each entry of

$$\bar{u}_F, f^{(m)}(\bar{u}_F, \nu), J_{F \times F}, f_x^{(m)}(\bar{u}_F, \nu), \mu_k(\nu), A_s, \text{ and } s$$

to be an interval and then computing (60), (61) and the quantities in Definition 4.2.2 using interval arithmetic. The resulting radii polynomials, which we denote by $\tilde{P}_k$, have interval coefficients. Let $\bar{r}$ be the smallest representable number such that using interval arithmetic, the corresponding finite radii polynomials may be shown to be strictly contained in $(-\infty, 0)$. Assume such an $\bar{r}$ exists. If, again using interval arithmetic, $\bar{r}(m-1) - A_s \subset (-\infty, 0)$ and the intervals obtained from evaluating tail radii polynomials at $\bar{r}$ are strictly contained in $(-\infty, 0)$, i.e. $\tilde{P}_k(\bar{r}) \subset (-\infty, 0)$ for all $k \geq m$, then the radii polynomials are simultaneously satisfied and we obtain a proof.

The above mentioned computations were performed using the interval arithmetic package in *Matlab*. Thus, we can state the following theorem.

Theorem 4.4.3 *Each point in Figure 19 represents the center of an infinite dimensional set of the form*

$$\bar{u}_F + \prod_{k=0}^{26} [-\bar{r}, \bar{r}] \times \prod_{k=27}^{\infty} \left[-\frac{0.002}{k^4}, \frac{0.002}{k^4} \right]$$

containing a unique equilibrium to (73).

The actual values for the various numerical zeros and validation radii are of limited interest and thus not presented. Of greater interest is understanding how large are the errors induced by the floating point computations as opposed to the magnitudes of the floating point computations of $P_k(\bar{r})$, $k \geq 0$, where $\bar{r}$ is the validation radius.

Let us restrict our attention to the equilibrium described by Validated Result 4.4.2. Following Procedure 4.2.3 at this parameter value, beginning using radii polynomials with interval coefficients and performing the computations with interval arithmetic leads to an interval of potential validation radii

$$\mathcal{I} = [3.373873850437414 \times 10^{-9}, 9.003755731999980 \times 10^{-4}].$$

Hence, we choose $\bar{r} = 3.373873850437415 \times 10^{-9}$. There are 53 inclusions that need to be satisfied, those arising from the $2m - 2 = 52$ tail radii polynomials with interval coefficients and the one associated with the inequality (64). The fact that the

inclusions are satisfied leads to the conclusion of Theorem 4.4.3 at this parameter value. Again, rather than listing all 53 inclusions let us focus on the two extremes, the interval closest to 0

$$\tilde{P}_{27}(\bar{r}) = -3.191484496597115 \times 10^{-11} \pm 7.037497555236307 \times 10^{-24}$$

and the interval the farthest from 0

$$-1.973098298147102 \times 10^{-3} \pm 8.673617379884037 \times 10^{-19}$$

corresponding to the inequality (64). Observe that in both cases, the width of the interval induced by the floating point errors is more than ten orders of magnitude smaller than the value of the center. Furthermore, this behavior is typical for all the validation computations that were performed. This suggests that it is reasonably safe to assume that a validated equilibrium is a true equilibrium.

4.5 *Sample Results using $M \geq m$*

We turn to two of these issues in this section.

1. As is mentioned above, the truncation of $W_{\bar{u}}(r)$ to $\prod_{k=0}^{m-1}[-r, r]$ introduces errors that must be overcome in order to solve for a validation radius. The simple assumption that $|u_k| \leq \frac{A_s}{k^s}$ for all $k \geq m$ provides a computationally cheap, but large, bound on the error. Though computationally more expensive, the bounds can be improved by using explicit constraints on $|u_k|$ for $k = m, \dots, M$ for some $M \geq m$. For the sake of clarity the computations performed in earlier sections were restricted to $M = m$. In this section we exploit the computational parameter M to carry out continuation for large ranges of parameter values. In Section 4.5.1 we provide a lower bound on the choice of M .
2. Observe that if (51) has a polynomial nonlinearity of order d , then straightforward evaluation of the nonlinear term in (53) involves on the order of m^d

operations. This computational cost can be reduced by making use of Fast Fourier Transform (FFT) techniques. This is the subject of Section 4.5.2. We will use this theory to compute all sums defined in (58).

4.5.1 Lower Bounds for M

The reason why we can get an a priori lower bound for M comes from the fact that the *tail term* is independent of the *validation radius* $r > 0$. Indeed, supposing that $M \geq d(m-1)$ the tail term inequality of Procedure 4.2.3

$$\frac{C(\bar{A}, A)}{|\mu|} - A_s = \frac{C(\bar{A}, A)}{|\mu_M|} - A_s < 0 . \quad (74)$$

Rather than obscuring the point in an abstract computation, observe that in the context of the Swift-Hohenberg equation (73), we have

$$C(\bar{A}, A) = 3\alpha(s)^3 A(\bar{A} + A)^2$$

and

$$\mu_M = \nu - (1 - M^2 L^2)^2 .$$

Since $A = A_s$, (74) becomes

$$3\alpha(s)^3 A_s (\bar{A} + A_s)^2 < A_s |\nu - (1 - M^2 L^2)^2| .$$

Supposing that $(1 - M^2 L^2)^2 > \nu$ and dividing on both sides by $A_s > 0$, we get that

$$(M^2 L^2 - 1)^2 > 3\alpha(s)^3 (\bar{A} + A_s)^2 + \nu .$$

Finally, supposing $M^2 L^2 > 1$, we get

$$M > \gamma(L, \nu, s, \bar{u}_F, A_s) := \frac{1}{L} \sqrt{1 + \sqrt{\nu + 3\alpha(s)^3 (\bar{A}(\bar{u}_F) + A_s)^2}} \quad (75)$$

Note that this lower bound only depends on the a priori information. Indeed, before starting the validation, we get all the quantities : L_0 , ν and $\bar{u}_F$ from the continuation and s and A_s a priori given. Hence, before starting the validation process, we fix M to be at least γ .

4.5.2 Computing Sums Using the Fast Fourier Transform

In this section, we address the use of the FFT algorithm to compute sums of the form

$$\sum_{\substack{l_1 + \dots + l_p = l \\ |l_1|, \dots, |l_p| < M}} a_{l_1}^1 \cdots a_{l_p}^p, \quad (76)$$

where $a^1 := (a_{-M+1}^1, \dots, a_{M-1}^1), \dots, a^p := (a_{-M+1}^p, \dots, a_{M-1}^p) \in \mathbb{R}^{2M-1}$. Note that we are not the first to use the FFT to compute sums of the form (76). In [17], the authors gave an explicit way to compute (76) for the cases $p = 3$ and $p = 5$. Here, we present the theory for a general $p \in \mathbb{N}$.

Definition 4.5.1 Let $b = (b_0, \dots, b_{2M-2}) \in \mathbb{R}^{2M-1}$. Its *Discrete Fourier Transform* $\mathcal{F}(b)$ is given by

$$a_l = \mathcal{F}(b)|_l := \sum_{j=0}^{2M-2} b_j e^{-2\pi i \left(\frac{jl}{2M-1}\right)}, \quad \text{for } l \in \{-M+1, \dots, M-1\}$$

Definition 4.5.2 Let $a = (a_{-M+1}, \dots, a_{M-1}) \in \mathbb{R}^{2M-1}$. Its *Inverse Discrete Fourier Transform* $\mathcal{F}^{-1}(a)$ is given by

$$b_j = \mathcal{F}^{-1}(a)|_j := \sum_{l=-M+1}^{M-1} a_l e^{2\pi i \left(\frac{jl}{2M-1}\right)}, \quad \text{for } j \in \{0, \dots, 2M-2\}$$

Let $\delta := \frac{p+1}{2}$, if p is odd and $\delta := \frac{p+2}{2}$ if p is even. Given $a^i = (a_{-M+1}^i, \dots, a_{M-1}^i) \in \mathbb{R}^{2M-1}$, define $\tilde{a}^i \in \mathbb{R}^{2\delta M-1}$ by

$$\tilde{a}_j^i = \begin{cases} a_j^i & \text{for } -M < j < M \\ 0 & \text{for } -\delta M + 1 \leq j \leq -M \text{ and } M \leq j \leq \delta M - 1 \end{cases} \quad (77)$$

For $j \in \{0, \dots, 2\delta M - 2\}$, set

$$\tilde{b}_j^i := \mathcal{F}^{-1}(\tilde{a}^i)|_j = \sum_{l=-\delta M+1}^{\delta M-1} \tilde{a}_l^i e^{2\pi i \left(\frac{jl}{2\delta M-1}\right)}. \quad (78)$$

For $l = -\delta M + 1, \dots, \delta M - 1$,

$$\begin{aligned} \mathcal{F}(\tilde{b}^1 * \dots * \tilde{b}^p)|_l &= \sum_{j=0}^{2\delta M-2} \tilde{b}_j^1 \dots \tilde{b}_j^p e^{-2\pi i \left(\frac{jl}{2\delta M-1}\right)} \\ &= \sum_{j=0}^{2\delta M-2} \left[\sum_{l_1=-\delta M+1}^{\delta M-1} \tilde{a}_{l_1}^1 e^{2\pi i \left(\frac{jl_1}{2\delta M-1}\right)} \right] \dots \left[\sum_{l_p=-\delta M+1}^{\delta M-1} \tilde{a}_{l_p}^p e^{2\pi i \left(\frac{jl_p}{2\delta M-1}\right)} \right] e^{-2\pi i \left(\frac{jl}{2\delta M-1}\right)} \end{aligned}$$

where

$$(\tilde{b}^1 * \cdots * \tilde{b}^p)_j := \tilde{b}_j^1 \cdots \tilde{b}_j^p . \quad (79)$$

Defining

$$\begin{aligned} S(j) &:= \prod_{i=1}^p \left[\sum_{l_i=-\delta M+1}^{\delta M-1} \tilde{a}_{l_i}^i e^{2\pi i \left(\frac{j l_i}{2\delta M-1} \right)} \right] e^{-2\pi i \left(\frac{j l}{2\delta M-1} \right)} \\ &= \sum_{\substack{l_1+\cdots+l_p=l \\ |l_1|, \dots, |l_p| < M}} a_{l_1}^1 \cdots a_{l_p}^p + \sum_{k=1}^p \left(\sum_{\substack{l_1+\cdots+l_p=l \pm k(2\delta M-1) \\ |l_1|, \dots, |l_p| < M}} a_{l_1}^1 \cdots a_{l_p}^p \right) \\ &\quad + \sum_{\substack{l_1+\cdots+l_p \notin \{l \pm k(2\delta M-1) | k=0, \dots, p\} \\ |l_1|, \dots, |l_p| < M}} a_{l_1}^1 \cdots a_{l_p}^p e^{2\pi i \left(\frac{l_1+\cdots+l_p-l}{2\delta M-1} \right) j} , \end{aligned}$$

we obtain

$$\begin{aligned} \mathcal{F}(\tilde{b}^1 * \cdots * \tilde{b}^p)|_l &= \sum_{j=0}^{2\delta M-2} S(j) \\ &= (2\delta M-1) \sum_{\substack{l_1+\cdots+l_p=l \\ |l_1|, \dots, |l_p| < M}} a_{l_1}^1 \cdots a_{l_p}^p \\ &\quad + (2\delta M-1) \sum_{k=1}^p \left(\sum_{\substack{l_1+\cdots+l_p=l \pm k(2\delta M-1) \\ |l_1|, \dots, |l_p| < M}} a_{l_1}^1 \cdots a_{l_p}^p \right) \\ &\quad + \sum_{\substack{l_1+\cdots+l_p \notin \{l \pm k(2\delta M-1) | k=0, \dots, p\} \\ |l_1|, \dots, |l_p| < M}} a_{l_1}^1 \cdots a_{l_p}^p \left[\sum_{j=0}^{2\delta M-2} e^{2\pi i \left(\frac{l_1+\cdots+l_p-l}{2\delta M-1} \right) j} \right] . \end{aligned} \quad (80)$$

Euler's formula gives that for $l_1 + \cdots + l_p - l \not\equiv 0 \pmod{2\delta M-1}$,

$$\sum_{j=0}^{2\delta M-2} e^{2\pi i \left(\frac{l_1+\cdots+l_p-l}{2\delta M-1} \right) j} = 0 .$$

Hence, the third sum in (80) is zero. Turning to the second sum in (80), observe that

$|l_1|, \dots, |l_p| < M$ and $l \in \{0, \dots, M-1\}$ implies that

$$l_1 + \cdots + l_p - l \in \{-(p+1)(M-1), \dots, p(M-1)\} .$$

Hence, given the above mentioned choice of δ , the second sum of (80) is zero. Therefore, we can conclude that

$$\sum_{\substack{l_1 + \dots + l_p = l \\ |l_1|, \dots, |l_p| < M}} a_{l_1}^1 \dots a_{l_p}^p = \frac{1}{2\delta M - 1} \cdot \mathcal{F}(\tilde{b}^1 * \dots * \tilde{b}^p)|_l. \quad (81)$$

The discrete Fourier transforms required in the computations of (78) and (81) are computed using the FFT algorithm (e.g. see [4]).

4.5.3 Results

In this section we present some computations for the one-dimensional Swift-Hohenberg and the one-dimensional Cahn-Hilliard equations. This is meant both to show the practicality of the method of validated continuation and to highlight its current limitations.

The starting point for our computations is the trivial solution, $u_0 \equiv 0$, at a particular value of the continuation parameter, and an arbitrarily chosen Galerkin projection dimension.

The iteration of validated continuation proceeds as follows. As is indicated in the Introduction, we use a standard predictor-corrector numerical method to find a numerical solution at the next parameter value. That is, given a numerical zero of the Galerkin projection at ν_0 , we find a new numerical zero $\bar{u}_F$ at the parameter value $\nu_1 = \nu_0 + \Delta\nu$. We then proceed with the validation step. We choose M to be the smallest integer satisfying

$$M \geq \max \{d(m-1), 2\gamma\}, \quad (82)$$

where γ is given by (75), and check the inequalities of Procedure 4.2.3. If the inequalities are satisfied, then Procedure 4.2.3 applies, we have validated the solution $\bar{u}_F$ at ν_1 , and we proceed to the next step; that is, we increment ν and repeat the process. If validation fails we increase m by 2, recompute the numerical zero $\bar{u}_F$ at ν_1 and try to validate it. This procedure is repeated until the numerical zero $\bar{u}_F$ at ν_1 is

validated or a maximum number of trials is reached. We remark for future reference that for Swift-Hohenberg our procedure always resulted in validation of the numerical zero.

At each step we monitor the determinant of the Jacobian to detect bifurcations. So starting with the trivial branch ($u \equiv 0$) we find branches that bifurcate from it, and then find branches that bifurcate from the newly found branches, and so on. In the case of Swift-Hohenberg we followed multiple branches. In each case we started with a low dimensional Galerkin projection, $m = 7$, and allowed the validation procedure to determine an appropriate value for m .

It is important to mention that we do not compute continuous branches of equilibria. The dots on Figures 21, 22, and 26, represent the points where we computed and validated equilibrium solutions. Notice also that the step size from one step to the next is not constant, but changes along each branch according to the formula $\Delta\nu := 2^{(4-k)/3}\Delta\nu$, where k is the number of iterations needed for the Newton method during the continuation step.

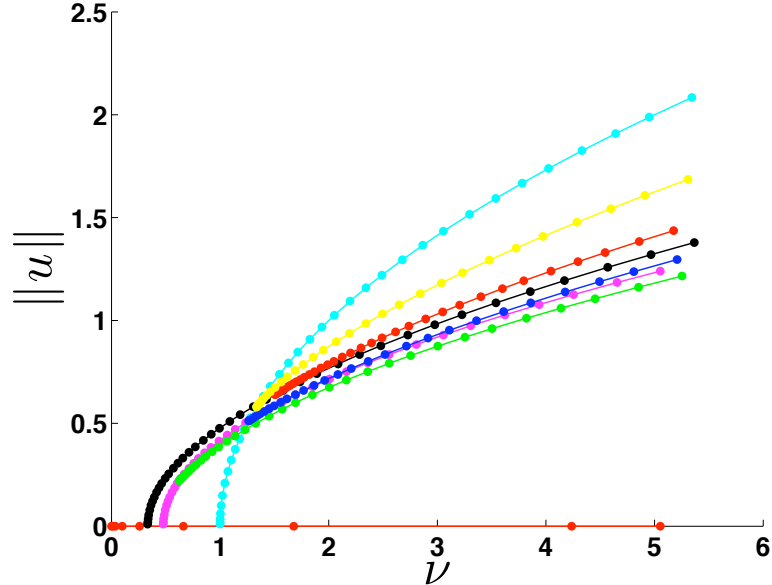


Figure 21: Bifurcation diagram for the Swift-Hohenberg equation (73) for $0 \leq \nu \leq 5$. The dots indicate the points at which a numerical zero was validated.

4.5.3.1 Swift-Hohenberg

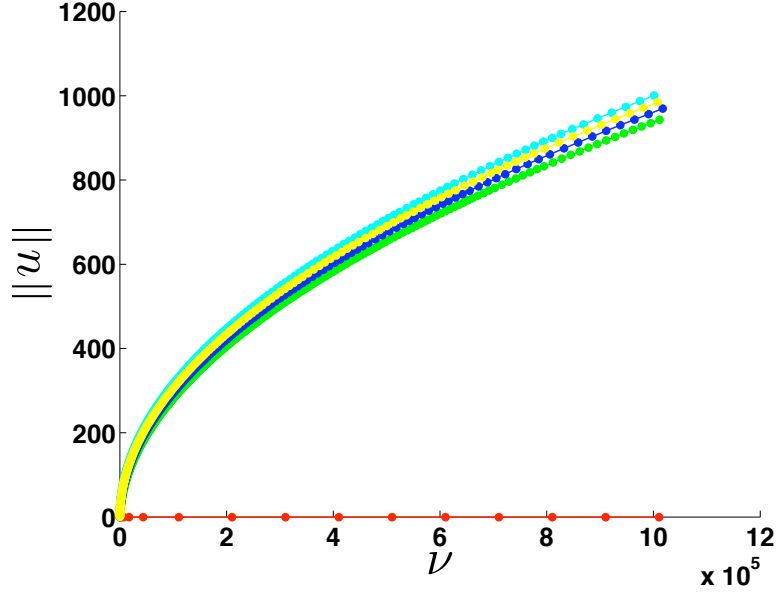


Figure 22: Some of the branches of equilibria of (73) for $0 \leq \nu \leq 10^6$. The dots indicate the points at which a numerical zero was validated. For the values $0 \leq \nu \leq 10^4$ the validation was done using interval arithmetic and hence at these points we have a mathematical proof of the existence and uniqueness of these solutions in the sets $W_{\bar{u}}(r)$. The color coding of the branches in this figure matches that of Figure 21.

As is indicated in the Introduction, we view the set $W_{\bar{u}}(r)$ as a function of r . This implies that s and A_s are considered to be constants. For (73) we set $s = 4$ and $A_s = 1$.

We computed what we believe are all the branches of equilibria for $0 \leq \nu \leq 5$ and followed some of the branches up to $\nu \approx 10^6$. The diagrams are shown on Figure 21 and Figure 22. We validated all the branches up to $\nu \approx 10^4$ in Figure 22 using interval arithmetic to control floating point errors and thus rigorously verified that the inequalities of Procedure 4.2.3 are satisfied. This implies that we have mathematically proven the existence and uniqueness within the sets $W_{\bar{u}}(r)$ of the equilibria for Swift-Hohenberg at those values of $\nu \leq 10^4$ indicated by the dots in Figure 22.

To describe some of the details and implications of these computations we focus on a branch from Figure 22. We choose the blue one and note that the results for the other branches are similar. Plots of some of the solutions along the blue branch are presented in Figure 23. The computational cost of validating these branches are determined by m and M . Observe that m plays a significant role in the cost of the continuation step - the Newton step requires an approximation of the inverse of the Jacobian. The use of the FFT implies that the size of M determines the cost of the computation of the coefficients of the radii polynomials. Figure 24 indicates how m and M varies as a function of ν , though the reader should recall that in this setting given m , M is chosen according to (82).

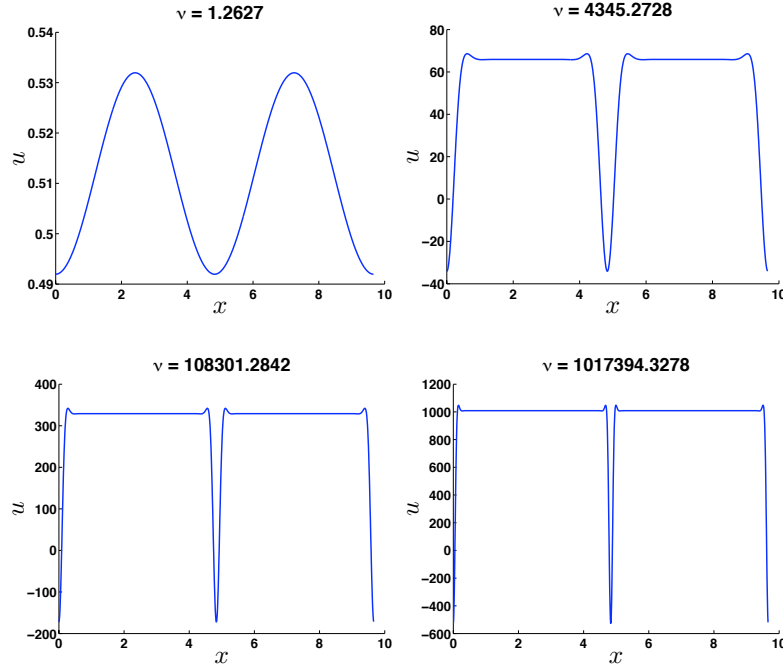


Figure 23: Some solutions along the blue branch of the diagram on Figure 22.

At the risk of being redundant, what Figure 22 indicates are the points in parameter space at which we have found a set of the form

$$W_{\bar{u}}(r) = \bar{u} + \prod_{k=0}^{m-1} [-r, r] \times \prod_{k=m}^{\infty} \left[-\frac{1}{k^4}, \frac{1}{k^4} \right]$$

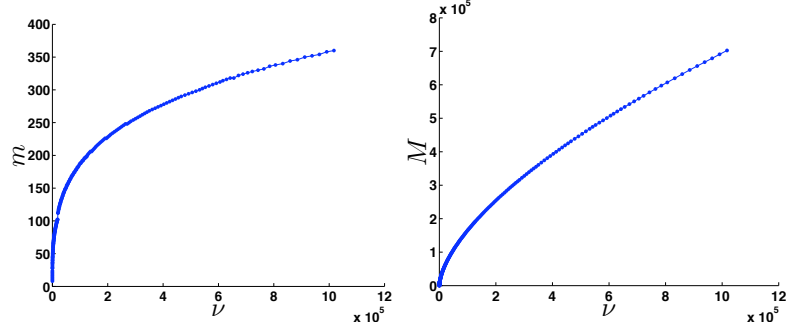


Figure 24: Plots of m and M along the blue branch of the diagram on Figure 22.

in which there exists a unique equilibrium of (73). $\bar{u}$ is determined by the continuation method. m as a function of ν is given in Figure 24 and r as a function of ν is given in Figure 25. Observe that the knowledge that the equilibrium lies inside of $W_{\bar{u}}(r)$ gives very tight bounds. In particular, the true equilibrium of (73) at $\nu = 1017394.3278$ differs from that shown in Figure 23 by less than 10^{-10} in the L^2 norm. Thus, the peaks in the solution are not numerical artifacts.

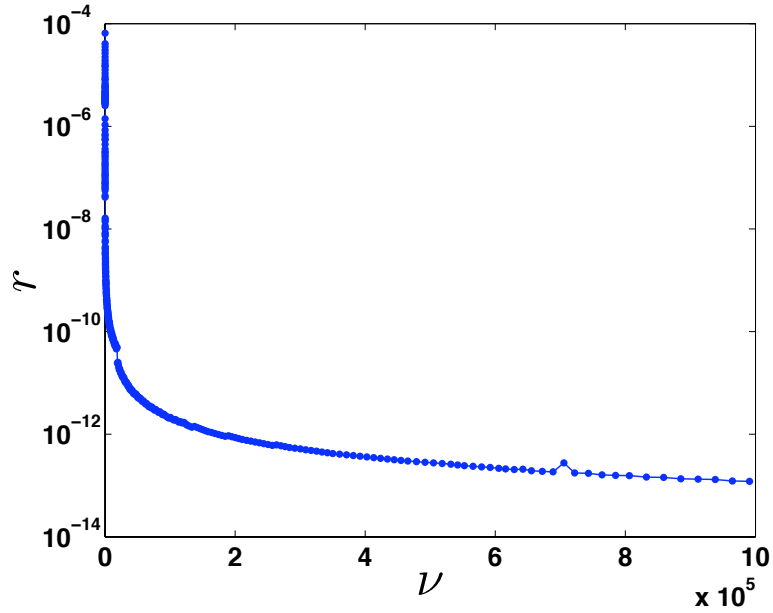


Figure 25: Plot of r along the blue branch of the diagram on Figure 22.

The computation time for the blue branch for ν up to $\nu \approx 10^4$ was 6.5 minutes

without interval arithmetic and 9.19 hours with interval arithmetic. The computation for the whole branch (up to $\nu \approx 10^6$) was 11.67 hours without interval arithmetic. The computation times for the other branches were similar.

4.5.3.2 Cahn-Hilliard

For this equation we use $\lambda = 1/\epsilon^2$ as the continuation parameter. For (72) we use the Fourier basis $\{\cos(k\pi x) \mid k = 0, 1, 2, \dots\}$, then

$$u(x, t) = u_0(t) + 2 \sum_{k=1}^{\infty} u_k(t) \cos(k\pi x).$$

So (72) takes the form

$$\dot{u}_k = \mu_k u_k - \sum_{k_1+k_2+k_3=k} u_{k_1} u_{k_2} u_{k_3},$$

where

$$\mu_k = 1 - \frac{\pi^2 k^2}{\lambda}, \quad (83)$$

is the eigenvalue of the linear operator in (72). Choosing $s = 3$ and $A_s = 0.01$ led to the branches indicated in Figure 26. In particular, equilibria associated with the black branch are indicated in Figure 27.

The branches in Figure 26 terminate because the above mentioned procedure failed. To be more precise, we declare that our method fails when validation fails for 40 consecutive times at the same value of λ (recall that each time validation fails we increase m by 2, recompute the equilibrium and try to validate it again). Figure 28 indicates the rapid increase in m as a function of λ for the black branch in Figure 26. Observe that trying to validate a solution for 40 consecutive times is equivalent to increasing the dimension of the Galerkin projection by 80, recomputing the equilibrium and trying to validate it. In all the cases the reason for failure was that we were unable to find an r satisfying condition (1) of Procedure 4.2.3. In fact, it appears that the failure is due to the fact that at least one of the finite radii

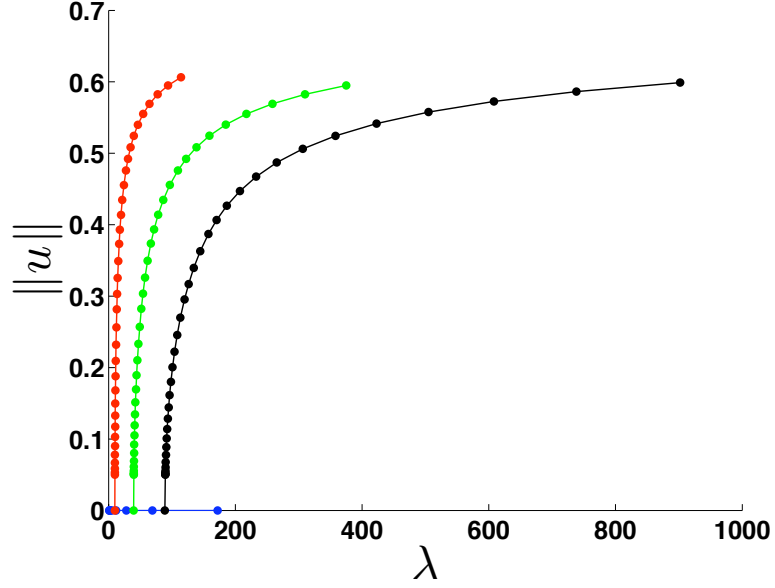


Figure 26: Bifurcation diagram for (71).

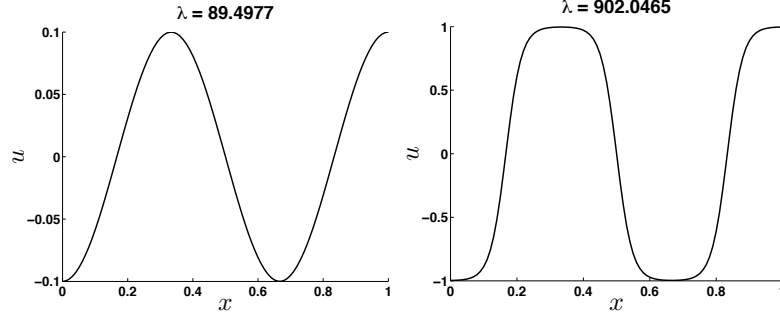


Figure 27: Solutions along the lower branch of the diagram on Figure 26.

polynomials fails to have any positive roots. Since $P_k(0) > 0$, this implies that there is no positive solution to $P_k(r) < 0$.

As is indicated at the beginning of Section 4.5, there are only a few free constants involved in the definition of the radii polynomials: m , the dimensional of the Galerkin projection; M , a computational parameter; s , the decay rate; and A_s an a priori bound on the size of the Fourier coefficients. As is described above, failure of the procedure implies that m has been increased by 80. As one may expect and as the results in Figure 28 corroborates, this implies values of u_k for k close to m are essentially zero.

Thus, further increase of the Galerkin projection at this point has little effect on the validation procedure.

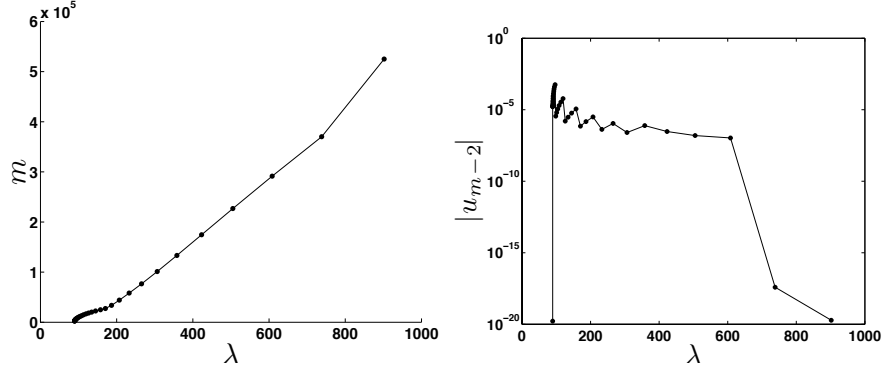


Figure 28: (Left) The dimension of the Galerkin projection m as a function of λ along the lower branch of the diagram on Figure 26. (Right) The value of $|u_{m-2}|$ as a function of λ along the same branch.

We tried to increase the value of M , since this results in better control on the tail errors. In particular, all the results indicated in Figure 26 were obtained using M equals twice the lower bound given by (75). We tried the same computations, from the beginning, using M equals four, six and ten times the lower bound in (75). In each case we were able to continue the branches in Figure 26 a bit further. However, in each case the procedure failed in the same way as before; there was no positive solution to the finite radii polynomial inequalities. This suggests that just increasing M does not provide an adequate solution to the problem.

We have no good heuristics for the choice of s and A_s . Random choices did not produce any significantly better results than $s = 3$ and $A_s = 0.01$.

4.6 Construction of the the Radii Polynomials

In order to construct the radii polynomials, we need Y_n and K_n as defined by (14) and (15) respectively. Let $J_{F \times F}$ be the numerical inverse of $Df^{(m)}(\bar{u}_F, \nu_1)$ and define the Newton-like operator T by

$$T(u) = u - Jf(u) \quad (84)$$

where

$$J := \begin{bmatrix} J_{F \times F} & & 0 \\ & \mu_m^{-1} & \\ 0 & & \mu_{m+1}^{-1} \\ & & & \ddots \end{bmatrix}$$

is the block diagonal matrix which we expect to be close to $(Df(\bar{u}, \nu_1))^{-1}$. Note that T , J , and f all depend on the parameter ν . Using a Taylor expansion of the Newton-like operator $T(u) = u - Jf(u)$ around the numerical equilibrium $\bar{u} = (\bar{u}_F, 0, 0, \dots)$ leads to

$$\begin{aligned} DT(\bar{u} + w')w &= [I - J \cdot Df(\bar{u} + w')]w \\ &= \left(I - J \left(Df(\bar{u}) + D^2f(\bar{u})(w') + \dots + \frac{D^l f(\bar{u})}{(l-1)!} (w')^{l-1} + \dots + \frac{D^d f(\bar{u})}{(d-1)!} (w')^{d-1} \right) \right) \\ &= [I - J \cdot Df(\bar{u})]w - J \left(\sum_{l=2}^d \frac{D^l f(\bar{u})}{(l-1)!} (w')^{l-1} \right) w \\ &= [I - J \cdot Df(\bar{u})]w - J \left(\sum_{l=2}^d \sum_{p=l}^d \frac{p! c_p \bar{u}^{p-l} (w')^{l-1}}{(l-1)!(p-l)!} \right) w \\ &= [I - J \cdot Df(\bar{u})]w - J \left(\sum_{l=2}^d \sum_{p=l}^d l \binom{p}{l} c_p \bar{u}^{p-l} (w')^{l-1} \right) w . \end{aligned}$$

In the rest of the section, we will make use of the discrete convolution of bi-infinite vectors i.e. considering two bi-infinite vectors $(a_j)_{j \in \mathbb{Z}}$, $(b_j)_{j \in \mathbb{Z}}$, we define their convolution by

$$(a * b)_k = \sum_{n=-\infty}^{\infty} a_n b_{k-n} = \sum_{\substack{k_1 + k_2 = k \\ k_i \in \mathbb{Z}}} a_{k_1} b_{k_2} , \quad k \in \mathbb{Z} .$$

Expanding into Fourier modes, we can write the nonlinear part in terms of convolution

$$\begin{aligned} DT(\bar{u} + w')w &= [I - J \cdot Df(\bar{u})]w - J \left(\sum_{l=2}^d \sum_{p=l}^d l \binom{p}{l} c_p \bar{u}^{p-l} (w')^{l-1} \right) * w \\ &= [I - J \cdot Df(\bar{u})]w - J \left(\sum_{l=2}^d \sum_{p=l}^d l \binom{p}{l} (c_p \bar{u}^{p-l}) * (w')^{l-1} * w \right) \quad (85) \end{aligned}$$

Thus,

$$(c_p \bar{u}^{p-l}) * ((w')^{l-1}) * w = \left[\sum_{\bar{n}} \left(\sum_{\sum n_i = \bar{n}} (c_p)_{n_0} \bar{u}_{n_1} \cdots \bar{u}_{n_{p-l}} \right) \left(\sum_{\sum n_i = n - \bar{n}} w'_{n_1} \cdots w'_{n_{l-1}} w_{n_l} \right) \right]_n .$$

Here, $[\cdot]_n$ denotes the bi-infinite vector indexed by $n \in \mathbb{Z}$ and $(\cdot)_k$ denotes the entry at index k . We use this expansion to compute the bounds

$$\begin{aligned} Z_k(r) &\geq \max_{w, w' \in W(r)} |(DT(\bar{u} + w')w)_k| \\ &\geq \max \left| [I - J \cdot Df(\bar{u})] \mathbf{w} - J \left(\sum_{l=2}^d \sum_{p=l}^d l \binom{p}{l} (c_p \bar{u}^{p-l}) * \mathbf{w}^l \right) \right| . \end{aligned}$$

The block-diagonal structure of J allows us to decompose (85) into a finite, m -dimensional piece and the infinite dimensional tail terms. For the following, we adopt the notation $[\cdot]_F$ to denote the m -vector whose n th entry is computed at index value $n - 1$ for $1 \leq n \leq m$, the subscript $\tilde{F}$ to denote the bi-infinite vector in which the k th entries for $|k| \geq m$ are set equal to 0, and the subscript $\tilde{I}$ to denote the bi-infinite vector in which the k th entries for $|k| < m$ are set equal to 0. We begin with the following decomposition of the finite part of the linear term.

$$\begin{aligned} \{[I - J \cdot Df(\bar{u})]w\}_F &= w_F - [J \cdot Df(\bar{u})w]_F \\ &= w_F - J_{F \times F} [Df(\bar{u})w]_F \\ &= w_F - J_{F \times F} \cdot Df_F(\bar{u})w \\ &= w_F - J_{F \times F} \cdot [Df^{(m)}(\bar{u}_F)w_F + R_F(\bar{u}, w)] \\ &= [I_{F \times F} - J_{F \times F} \cdot Df^{(m)}(\bar{u}_F)] w_F \\ &\quad - J_{F \times F} \cdot R_F(\bar{u}, w) , \end{aligned} \tag{86}$$

where for $k \in \{0, \dots, m-1\}$,

$$\begin{aligned} R_k(\bar{u}, w) &:= \sum_{i=m}^{\infty} \frac{\partial f_k}{\partial u_i}(\bar{u}) w_i \\ &= \sum_{\substack{\bar{n}=-\infty \\ |k-\bar{n}| \geq m}}^{\infty} \left| \sum_{p=1}^d p \sum_{\sum n_i = \bar{n}} (c_p)_{n_0} \bar{u}_{n_1} \cdots \bar{u}_{n_{p-1}} \right| \frac{A_s}{|k - \bar{n}|^s} . \end{aligned} \tag{87}$$

It follows that for all $w, w' \in W(r)$,

$$\begin{aligned} [DT(\bar{u} + w')w]_F &\subseteq [I_{F \times F} - J_{F \times F} \cdot Df^{(m)}(\bar{u}_F)] \mathbf{w}_F - J_{F \times F} \cdot R_F(\bar{u}, w) \\ &\quad - \left(J_{F \times F} \sum_{l=2}^d \sum_{p=l}^d l \binom{p}{l} [(c_p \bar{u}^{p-l}) * \mathbf{w}^l]_F \right). \end{aligned} \quad (88)$$

For $k \geq m$,

$$(DT(\bar{u} + w')w)_k \subseteq -J(k, k) \sum_{l=1}^d \sum_{p=l}^d l \binom{p}{l} ((c_p \bar{u}^{p-l}) * \mathbf{w}^l)_k. \quad (89)$$

We now focus on finding bounds on the terms given in (88) and (89). First consider

$$((c_p \bar{u}^{p-l}) * \mathbf{w}^l)_k = \sum_{\bar{n}} \left(\sum_{\sum n_i = \bar{n}} (c_p)_{n_0} \bar{u}_{n_1} \cdots \bar{u}_{n_{p-l}} \right) \left(\sum_{\sum n_i + \bar{n} = k} \mathbf{w}_{n_1} \cdots \mathbf{w}_{n_l} \right) \quad (90)$$

where p is the degree of the original monomial term of f and $l \in \{1, \dots, p\}$ is the order of the derivative being taken. One upper bound for (90) is given in the following lemma.

Lemma 4.6.1 *Let $\alpha = \frac{2}{s-1} + 2 + 3.5 \cdot 2^s$, $\bar{u}_k \in \frac{\bar{A}}{k^s}[-1, 1]$, $(c_p)_k \in \frac{C_p}{k^s}[-1, 1]$, and $\mathbf{w}_k \subset \frac{A}{k^s}[-1, 1]$ for all k . Then*

$$((c_p \bar{u}^{p-l}) * \mathbf{w}^l)_k \subseteq \begin{cases} \frac{\alpha^p C_p \bar{A}^{p-l} A^l}{|k|^s} [-1, 1] & k \neq 0 \\ \alpha^p C_p \bar{A}^{p-l} A^l [-1, 1] & k = 0. \end{cases}$$

Proof. Note that

$$\begin{aligned} \sum_{\bar{n}} \left(\sum_{\sum n_i = \bar{n}} (c_p)_{n_0} \bar{u}_{n_1} \cdots \bar{u}_{n_{p-l}} \right) \left(\sum_{\sum n_i + \bar{n} = k} \mathbf{w}_{n_1} \cdots \mathbf{w}_{n_l} \right) \\ \subseteq \sum_{\sum n_i = k} (c_p)_{n_0} \bar{u}_{n_1} \cdots \bar{u}_{n_{p-l}} \mathbf{w}_{n_{p-l+1}} \cdots \mathbf{w}_{n_p} \\ \subseteq \sum_{\sum n_i = k} \frac{C_p}{|n_0|^s} \frac{\bar{A}}{|n_1|^s} \cdots \frac{\bar{A}}{|n_{p-l}|^s} \frac{A}{|n_{p-l+1}|^s} \cdots \frac{A}{|n_p|^s} [-1, 1] \end{aligned}$$

The remainder of the proof is a modification of [7, Lemma 5.8].

In most cases, especially when l is small relative to p , this bound will be too large to use for the low modes. In particular, $\bar{u}$ may be far from zero, resulting in a large constant $\bar{A}$. By taking k sufficiently large, the contraction given by $J(k, k) \approx \mu_k^{-1}$ will overcome the large bound. A more practical approach for obtaining bounds for the low modes is given by the following lemma. For flexibility in balancing numerical computations (requiring a finite number of operations) with analysis (to obtain truncation bounds), we choose $M \geq m$ to be the dimension used to split these sums.

Lemma 4.6.2 *For $M \geq m$,*

$$((c_p \bar{u}^{p-l}) * \mathbf{w}^l)_k \subseteq \left(\sum_{j=0}^l \binom{l}{j} C_k(p, j, l, M) r^{l-j} + \epsilon_k(p, l, M) \right) [-1, 1].$$

Proof. This lemma is a modification of [7, Lemma 5.10] combined with Lemma 4.6.1.

In [7, Lemma 5.10], the bound is split into finite sums and the tail term, bounded by

$$\frac{p\alpha^{p-1}C_p\bar{A}^{p-l}A^l}{(M-1)^{s-1}(s-1)} \left[\frac{1}{(M-k)^s} + \frac{1}{(M+k)^s} \right] [-1, 1].$$

We obtain a polynomial in r by rewriting the finite sums as follows:

$$\begin{aligned} & \sum_{\bar{n}} \left(\sum_{\substack{\sum n_i = \bar{n} \\ |n_i| < M}} (c_p)_{n_0} \bar{u}_{n_1} \cdots \bar{u}_{n_{p-l}} \right) \left(\sum_{\substack{\sum n_i + \bar{n} = k \\ |n_i| < M}} \mathbf{w}_{n_1} \cdots \mathbf{w}_{n_l} \right) \\ &= \sum_{\bar{n}} \left(\sum_{\substack{\sum n_i = \bar{n} \\ |n_1|, \dots, |n_{p-l}| < m \\ |n_0| < M}} (c_p)_{n_0} \bar{u}_{n_1} \cdots \bar{u}_{n_{p-l}} \right) \left(\sum_{\substack{\sum n_i + \bar{n} = k \\ |n_i| < M}} \mathbf{w}_{n_1} \cdots \mathbf{w}_{n_l} \right) \\ &= \sum_{\bar{n}} \left(\sum_{\substack{\sum n_i = \bar{n} \\ |n_1|, \dots, |n_{p-l}| < m \\ |n_0| < M}} (c_p)_{n_0} \bar{u}_{n_1} \cdots \bar{u}_{n_{p-l}} \right) \left(\sum_{j=0}^l \binom{l}{j} \sum_{\substack{\sum n_i + \bar{n} = k \\ m \leq |n_1|, \dots, |n_j| < M \\ |n_{j+1}|, \dots, |n_l| < m}} \mathbf{w}_{n_1} \cdots \mathbf{w}_{n_l} \right) \\ &= \sum_{\bar{n}} \left(\sum_{\substack{\sum n_i = \bar{n} \\ |n_1|, \dots, |n_{p-l}| < m \\ |n_0| < M}} (c_p)_{n_0} \bar{u}_{n_1} \cdots \bar{u}_{n_{p-l}} \right) \left(\sum_{j=0}^l \binom{l}{j} r^{l-j} [-1, 1] \sum_{\substack{\sum n_i + \bar{n} = k \\ m \leq |n_1|, \dots, |n_j| < M \\ |n_{j+1}|, \dots, |n_l| < m}} \frac{A_s^j}{|n_1|^s \cdots |n_j|^s} \right) \end{aligned}$$

$$= \sum_{j=0}^l \binom{l}{j} r^{l-j} \sum_{|\bar{n}| < (p-l)(m-1)+M} [-1, 1] \left| \sum_{\substack{\sum n_i = \bar{n} \\ |n_1|, \dots, |n_{p-l}| < m \\ |n_0| < M}} (c_p)_{n_0} \bar{u}_{n_1} \cdots \bar{u}_{n_{p-l}} \right| \left(\sum_{\substack{\sum n_i + \bar{n} = k \\ m \leq |n_1|, \dots, |n_j| < M \\ |n_{j+1}|, \dots, |n_l| < m}} \frac{A_s^j}{|n_1|^s \cdots |n_j|^s} \right).$$

Remark 4.6.3 Note that in Lemma 4.6.2, $C_k(p, j, l, M)$ captures the contribution to the $(l-j)$ th polynomial coefficient from the l -th derivative of the p -th monomial term of f in the Taylor expansion. If $M = m$, then $C_k(p, j, l, M) = 0$ for all $j > 0$ and

$$C_k(p, 0, l, m) = \left| \sum_{\substack{n_0 + \dots + n_{p-l} = k \\ |n_0|, \dots, |n_{p-l}| < m}} (c_p)_{n_0} \bar{u}_{n_1} \cdots \bar{u}_{n_{p-l}} \right|.$$

For $M > m$ there is also a (small) contribution to the coefficients of higher degrees of r in the polynomials, while simultaneously decreasing the ϵ_k term. This offers a method for using additional computations to decrease the bound ϵ_k if this bound proves to be too large for the validation procedure.

For notational purposes, set ϵ_F , $C_F(p, j, l, M)$, $V_F^{(0)}$ and $V_F^{(1)}$ to be the m -vectors as defined in Section 4.2. For $0 \leq k < m$, we substitute the bounds from Lemma 4.6.2 into (88),

$$\begin{aligned} (DT(\bar{u} + W)W)_k &\subseteq rV_k^{(1)}[-1, 1] + V_k^{(0)}[-1, 1] \\ &\quad + \left(-J_{F \times F} \sum_{l=2}^d \sum_{p=l}^d l \binom{p}{l} \left(\sum_{j=0}^l \binom{l}{j} (C_F(p, j, l, M) r^{l-j} + \epsilon_F(p, l, M)) \right) \right)_k [-1, 1] \\ &= (|J_{F \times F}| \epsilon_F)_k [-1, 1] + rV_k^{(1)}[-1, 1] + V_k^{(0)}[-1, 1] \\ &\quad + \left(\sum_{l=2}^d \sum_{p=l}^d \sum_{j=0}^l r^{l-j} l \binom{p}{l} \binom{l}{j} |J_{F \times F}| C_F(p, j, l, M) \right)_k [-1, 1] \\ &= \left(|J_{F \times F}| \epsilon_F + V_F^{(0)} \right)_k [-1, 1] + rV_k^{(1)}[-1, 1] \\ &\quad + \left(\sum_{i=0}^d r^i \sum_{l=\max\{2, i\}}^d \sum_{p=l}^d l \binom{p}{l} \binom{l}{i} |J_{F \times F}| C_F(p, l-i, l, M) \right)_k [-1, 1] \end{aligned}$$

where $|\cdot|$ denotes entry-wise absolute value. For $0 \leq k < m$, set

$$Z_k(r) := \sum_{i=0}^d C_k^Z(i) r^i \geq \sup_{w, w' \in W(r)} |(DT(\bar{u} + w')w)_k|$$

where $C_k^Z(i)$ satisfies (60).

To finish the construction of the radii polynomials, we need the bounds for Y_k . Recall that

$$\begin{aligned}
Y_k &\geq |(T(\bar{u}) - \bar{u})_k| \\
&= |[-Jf(\bar{u})]_k| \\
&= \left| \left(-J \left[\mu_n \bar{u}_n + \sum_{p=0}^d \sum_{\substack{n_0+\dots+n_p=n \\ |n_1|, \dots, |n_p| < m}} (c_p)_{n_0} \bar{u}_{n_1} \cdots \bar{u}_{n_p} \right] \right)_n \right|_k. \tag{91}
\end{aligned}$$

Therefore, for $k < m$, set $Y_k = C_k^Y$ where C_k^Y is given by (61). Note that these terms involve the Galerkin projection of f at $\bar{u}$ onto the first m modes and, therefore, are expected to be small.

For $0 \leq k < m$, we now combine our bounds for Y_k with the bounds for Z_k to compute the coefficients of the polynomials $P_k(r)$. This leads us to the definition of the finite radii polynomials presented in Definition 4.2.1.

In modes $k \geq m$, we use Lemma 4.6.1 and (89) to obtain that for every $w, w' \in W(r)$,

$$\begin{aligned}
(DT(\bar{u} + w')w)_k &\subseteq -J(k, k) \sum_{l=1}^d \sum_{p=\max\{2, l\}}^d l \binom{p}{l} ((c_p \bar{u}^{p-l}) * \mathbf{w}^l)_k \\
&\subseteq \frac{1}{|\mu_k| k^s} \sum_{l=1}^d \sum_{p=\max\{2, l\}}^d l \binom{p}{l} \alpha^p C_p \bar{A}^{p-l} A^l [-1, 1].
\end{aligned} \tag{92}$$

Therefore, set $Z_k(r)$, $k \geq m$, such that

$$Z_k(r) \geq \frac{C(\bar{A}, A)}{|\mu_k| k^s}. \tag{93}$$

Recall (91). For $k \geq m$, choose Y_k (Compare with (55)) such that

$$\begin{aligned}
Y_k &\geq |(T(\bar{u}) - \bar{u})_k| \\
&= |[-J(k, k)(f_k(\bar{u}))]| \\
&= \frac{|\sum_{p=2}^d (c_p \bar{u}^p)_k|}{|\mu_k|}. \tag{94}
\end{aligned}$$

Using Lemma 4.6.1,

$$\frac{|\sum_{p=2}^d (c_p \bar{u}^p)_k|}{|\mu_k|} \subseteq \sum_{p=2}^d \frac{\alpha C_p \bar{A}^p}{|\mu_k| |k|^s} [-1, 1] \quad . \quad (95)$$

These bounds are overestimates and should only be used for large k . In fact, if the coefficient functions c_p have finite Fourier expansions (as in the examples we consider in Section 4.4) then $Y_k = 0$ for k sufficiently large.

Suppose the bounds Y_k are numerically or analytically computed for $m \leq k < m_+$. Then for $k \geq m$, the tail radii polynomial (see Definition 4.2.2) satisfies

$$\begin{aligned} P_k(r) &= Y_k + Z_k(r) - \frac{A_s}{k^s} \\ &= \begin{cases} \frac{|\sum_{p=2}^d (c_p \bar{u}^p)_k|}{|\mu_k|} + \frac{C(\bar{A}, A)}{|\mu_k| k^s} - \frac{A_s}{k^s} & m \leq k < m_+ \\ \frac{C_+(\bar{A}, A)}{|\mu_k| k^s} - \frac{A_s}{k^s} & k \geq m_+. \end{cases} \end{aligned}$$

Checking that $P_k < 0$ for $k \geq m$ reduces to checking the inequalities $P_m < 0, \dots, P_{m_+-1} < 0$ and, by rearranging terms,

$$C_+(\bar{A}, A) < |\mu_k| A_s. \quad (96)$$

Therefore, the assumption that $|\mu_k|$ is growing in k ensures that (96) may be verified for all $k \geq m$ with only a finite number of checks. More explicitly, computing a lower bound on $|\mu_k|$, $k \geq m_+$ would allow us to verify all inequalities of type (96), $k \geq m_+$, in one step. Indeed, since $\frac{C_+(\bar{A}, A)}{|\bar{\mu}|} - A_s < 0$ and $f_k(\bar{u}) = 0$ and $|\mu_k| \geq |\bar{\mu}|$ for all $k \geq \bar{m} \geq m_+$,

$$\begin{aligned} P_k(\bar{r}) &= Y_k + Z_k - \frac{A_s}{k^s} \\ &= \frac{C_+(\bar{A}, A)}{|\mu_k| k^s} - \frac{A_s}{k^s} \\ &\leq \frac{C_+(\bar{A}, A)}{|\bar{\mu}| k^s} - \frac{A_s}{k^s} \\ &< 0. \end{aligned}$$

CHAPTER V

FORCING THEOREMS AND CHAOTIC DYNAMICS FOR ORDINARY DIFFERENTIAL EQUATIONS

The work presented in this chapter is joint work with Jan Bouwe van den Berg.

5.1 *Background*

As mentioned in the introduction, we introduce here a new way to prove the existence of chaos in nonlinear ordinary differential equations. In some sense, this new result belongs to the class of forcing theorems. An example of a forcing theorem in discrete dynamical systems is given by Sarkovskii's theorem [34]

Theorem 5.1.1 *Consider a continuous function $h : \mathbb{R} \rightarrow \mathbb{R}$ and consider the following ordering of the natural numbers*

$$\begin{aligned} 3 < 5 < 7 < 9 < \dots < 2 \cdot 3 < 2 \cdot 5 < 2 \cdot 7 < \dots < 2^2 \cdot 3 < 2^2 \cdot 5 < 2^2 \cdot 7 \\ \dots < 2^k \cdot 3 < 2^k \cdot 5 < 2^k \cdot 7 < \dots < 2^4 < 2^3 < 2^2 < 2 < 1. \end{aligned}$$

If h has a periodic point of period p and $p < q$ in the above ordering, then h has also a periodic point of period q .

Example: Consider $h : [0, 2] \rightarrow [0, 2]$ defined by $h(x) = -\frac{3}{2}x^2 + \frac{5}{2}x + 1$. Observe that $h(0) = 1$, $h(1) = 2$ and $h(2) = 0$. This means that $x_0 = 0$ is a periodic point of period 3. By Sarkovskii's theorem, h has periodic orbits of all period. With a little more work, we can show that $h : [0, 2] \rightarrow [0, 2]$ is chaotic in the sense that it has positive topological entropy. The notion of topological entropy will be defined in Section 5.3. Observe that proving the existence of a single periodic orbit of a certain type forces the existence of chaos.

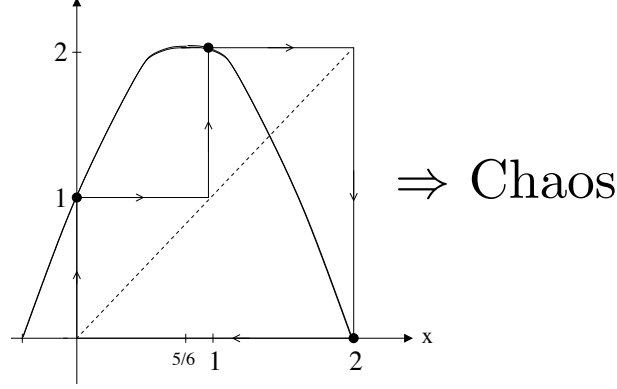


Figure 29: The function $h : [0, 2] \rightarrow [0, 2]$ defined by $h(x) = -\frac{3}{2}x^2 + \frac{5}{2}x + 1$ has periodic orbits of all period.

We adopt the philosophy of the above example to prove the existence of chaos in the Swift-Hohenberg equation

$$-u'''' - \nu u'' + u - u^3 = 0, \quad \nu > 0 \quad (97)$$

at the energy level $E = 0$, where

$$E(u, \nu) := u'''u' - \frac{1}{2}(u'')^2 + \frac{\nu}{2}(u')^2 + \frac{1}{4}(u^2 - 1)^2. \quad (98)$$

As mentioned earlier, we look for a particular solution. The periodic solution we are looking for has to satisfy the following geometric hypotheses

$$(\mathcal{H}) \left\{ \begin{array}{l} (1) \ \tilde{u} \text{ has exactly four monotone laps and extrema } \{\tilde{u}_i\}_{i=1}^4 \\ (2) \ \tilde{u}_1 \text{ and } \tilde{u}_3 \text{ are minima and } \tilde{u}_2 \text{ and } \tilde{u}_4 \text{ are maxima} \\ (3) \ \tilde{u}_1 < -1 < \tilde{u}_3 < 1 < \tilde{u}_2, \tilde{u}_4 \end{array} \right. .$$

Recall from the introduction that

$$f = (e, g_0, g_1, \dots), \quad (99)$$

where for $x := (L, a_0, a_1, a_2, \dots)$,

$$e(x) = -2L^2 \sum_{l=1}^{\infty} l^2 a_l - \frac{1}{\sqrt{2}} \left[a_0 + 2 \sum_{l=1}^{\infty} a_l \right]^2 + \frac{1}{\sqrt{2}},$$

$$g_k(x, \nu) = [1 + \nu L^2 k^2 - L^4 k^4] a_k - \sum_{\substack{k_1 + k_2 + k_3 = k \\ k_i \in \mathbb{Z}}} a_{k_1} a_{k_2} a_{k_3}, \quad k \geq 0.$$

From what was done in the introduction, we rewrite the forcing theorem as follows

Theorem 5.1.2 (Forcing Theorem) *Suppose that at the parameter value $\nu > 0$, there exist $x = (L, a_0, a_1, a_2, \dots)$ such that $f(x, \nu) = 0$ and $\tilde{u}$ given by $\tilde{u}(y) := a_0 + 2 \sum_{k=1}^{\infty} a_k \cos(kLy)$ satisfies the geometric hypotheses $(\mathcal{H})$. Choose any finite, but arbitrarily long sequence $\mathbf{a} = \{\mathbf{a}_j\}_{j=1}^N$, with $\mathbf{a}_j \geq 2$ not all equal to 2. Then there exists a periodic solution $u_{\mathbf{a}}$ of (97) at $E = 0$ that oscillates around the constant periodic solutions ± 1 as follow: $\mathbf{a}_1$ times around 1, one time around -1 , $\mathbf{a}_2$ times around 1, one time around -1 , $\dots$, $\mathbf{a}_N$ times around 1 and finally one time around -1 .*

The proof will be presented in Section 5.2. We now define the notions of topological entropy and chaos. The following definition is taken from [8].

Definition 5.1.3 Consider $X \subset \mathbb{R}^m$ compact and d a distance in $\mathbb{R}^m$. Let $f : X \rightarrow X$ be a continuous map. A set $W \subset X$ is called (n, ϵ, f) -separated if for any two different points $x, y \in W$ there is an integer j with $0 \leq j < n$ so that the $d[f^j(x), f^j(y)] > \epsilon$. Let $s(n, \epsilon, f)$ be the maximum cardinality of any (n, ϵ, f) -separated set. The *topological entropy* of f is the number

$$h_{top}(f) = \lim_{\epsilon \rightarrow 0} \limsup_{n \rightarrow \infty} \frac{\log[s(n, \epsilon, f)]}{n}. \quad (100)$$

We say that a map $f : X \rightarrow X$ is *chaotic* if $h_{top}(f) > 0$.

The following will be proved in Section 5.3

Corollary 5.1.4 *Suppose that at the parameter value $\nu > 0$, there exist*

$x = (L, a_0, a_1, a_2, \dots)$ such that $f(x, \nu) = 0$ and $\tilde{u}$ given by

$\tilde{u}(y) := a_0 + 2 \sum_{k=1}^{\infty} a_k \cos(kLy)$ satisfies the geometric hypotheses $(\mathcal{H})$. Then the Swift-Hohenberg equation (97) is chaotic on the energy level $E = 0$ in the sense that there exists a 2-D Poincaré return map T such that $h_{top}(T) > 0$.

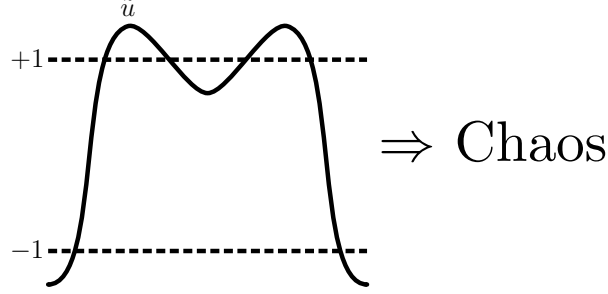


Figure 30: Periodic solution forcing the existence of chaos.

The hypotheses of Corollary 5.1.4 imply that we need to study the zeros of the parameter dependent function (99). As pointed out in the introduction, we do this via validated continuation. Hence, we have to construct the radii polynomials. This will be done in Section 5.4. The details of how rigorously verify the hypotheses $(\mathcal{H})$ are given in Section 5.5.

We combine validated continuation and Corollary 5.1.4 to get the main result.

Theorem 5.1.5 *For every $\nu \in [\frac{1}{2}, 2]$, the Swift-Hohenberg ODE (97) is chaotic at the energy level at $E = 0$.*

5.2 Proof of the Forcing Theorem

Suppose that at the parameter value $\nu > 0$, there exist $x = (L, a_0, a_1, a_2, \dots)$ such that $f(x, \nu) = 0$ and $\tilde{u}$ given by $\tilde{u}(y) := a_0 + 2 \sum_{k=1}^{\infty} a_k \cos(kLy)$ satisfies the geometric hypotheses $(\mathcal{H})$. The idea of the proof is that we will code (discretize) periodic solutions u of (97) at $E = 0$ by their extrema (see Figure 31). If $u' = 0$ then by (98), $u'' = \pm \frac{1}{\sqrt{2}}(u^2 - 1)$. Hence extrema are nondegenerate except at $u = \pm 1$, and we are going to avoid those values, so we may for the moment assume all extrema to be non degenerate.

Lemma 5.2.1 *Let $\nu > 0$. There exist nonlinear functions $\mathcal{R}_i : \mathbb{R}^3 \rightarrow \mathbb{R}$ such that $\mathcal{R}_{i+2} = \mathcal{R}_i$ (so there are really only two different functions in play) and $\mathcal{R}_i \in C^1(\Omega_i; \mathbb{R})$*

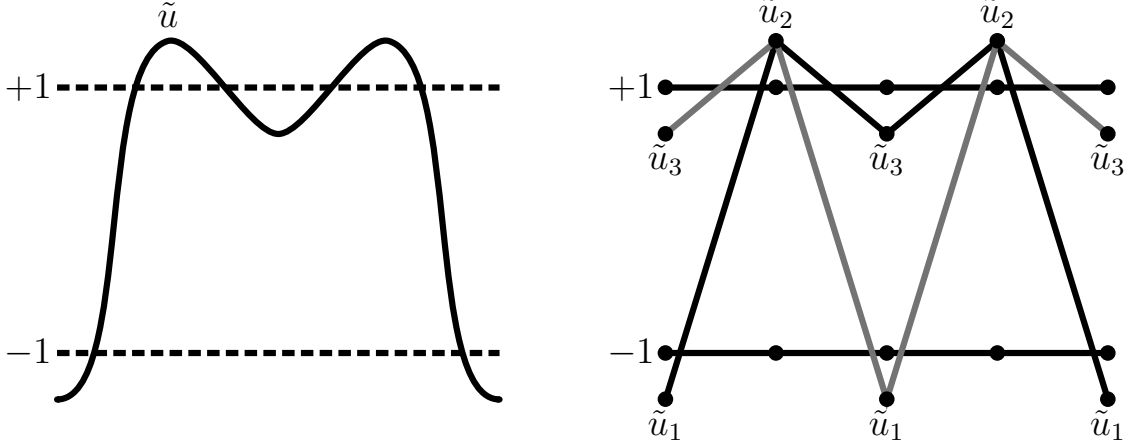


Figure 31: Left: sketch of the solution $\tilde{u}$. Right: discretized version $\{\tilde{u}_i\}_{i=1}^4$ and a shift $\{\tilde{u}_{i+2}\}_{i=1}^4$.

with domains

$$\Omega_i = \{(u, v, w) \in \mathbb{R}^3 \mid (-1)^i u < (-1)^i v, (-1)^i w < (-1)^i v, \text{ and } u, v, w \neq \pm 1\}$$

satisfying the following two properties:

- (1) Consider any (non degenerate) periodic solution of (97) at $E = 0$ and discretize it to get a sequence of non degenerate extrema $\{u_i\}_{i \in \mathbb{Z}}$, where u_i represents a local minimum for odd i and a local maximum for even i . Then $\mathcal{R}_i(u_{i-1}, u_i, u_{i+1}) = 0$.
- (2) $(\mathcal{R}_i)_{i \in \mathbb{Z}}$ is a parabolic recurrence relation, i.e. it has the monotonicity property

$$\partial_{u_{i-1}} \mathcal{R}_i > 0 \quad \text{and} \quad \partial_{u_{i+1}} \mathcal{R}_i > 0. \quad (101)$$

Proof. See [3] for all details. The *idea* is that there is a unique monotone solution with energy $E = 0$ going from the extremum u_i to the next extremum u_{i+1} . The functions $\mathcal{R}_i$ can then be defined/constructed with the help of a return map, which turns out to have the Twist property. ■

For convenience we define

$$\Omega = \{(u_i)_{i \in \mathbb{Z}} \mid (u_{i-1}, u_i, u_{i+1}) \in \Omega_i \text{ for all } i\}.$$

The connection between the functions $\mathcal{R}_i$ and the original ODE is that (see [3] and [16, Th. 37]) any $2p$ -periodic sequence $(u_i)_{i \in \mathbb{Z}} \in \Omega$ that satisfies

$$\mathcal{R}_i(u_{i-1}, u_i, u_{i+1}) = 0 \quad \text{for all } i,$$

corresponds to a periodic solution u at energy level $E = 0$ with extrema u_i . We want to exploit the fact that $\{E = 0\}$ contains the equilibria $u = \pm 1$. However, these solutions do not correspond to a proper sequence of extrema. The linearisation around the equilibria is going to help us resolve this issue. Namely, for $-\sqrt{8} < \nu < \sqrt{8}$ the equilibria ± 1 are saddle-foci, and this leads to the following fact (formulated here for the equilibrium $+1$).

Lemma 5.2.2 *Let $-\sqrt{8} < \nu < \sqrt{8}$. For any $\varepsilon > 0$ there exists a sequence $\{u_i^\varepsilon\}_{i=1}^\infty$,*

$$0 < (-1)^i(u_i^\varepsilon - 1) < \varepsilon$$

which satisfies

$$\mathcal{R}_i(u_{i-1}^\varepsilon, u_i^\varepsilon, u_{i+1}^\varepsilon) = 0 \quad \text{for } i \geq 2.$$

Note that it obviously does not hold that $\mathcal{R}_1(u_0^\varepsilon, u_1^\varepsilon, u_2^\varepsilon) = 0$, since we did not even define u_0^ε .

Proof. The idea is that the u_i^ε are the extrema of an orbit in the stable manifold of $+1$. The fact that $u_i^\varepsilon - 1$ alternates sign follows from the fact that the equilibrium $+1$ is a saddle-focus: it is easy to check that for $-\sqrt{8} < \nu < \sqrt{8}$ the *linearised* equation (i.e., $u = 1 + v$ with $v'''' + \nu v'' + 2v + O(v^2) = 0$) has solutions of the form

$$1 + Ce^{-\lambda_r x} \cos(\lambda_i x + \phi),$$

with C and ϕ arbitrary (with λ_r and λ_i depending on ν). In particular, the stable manifold intersects the hyperplane $\{u' = 0\}$ in the line

$$\ell = \{(1 + v, 0, -\sqrt{2}v, \sqrt{2}\lambda_r v) \mid v \in \mathbb{R}\}.$$

For the nonlinear equation we need to invoke the stable manifold theorem. Let us denote the stable manifold by $W^s(+1)$ and the local stable manifold by $W_{\text{loc}}^s = W^s(+1) \cap B_{\varepsilon_0}(+1)$ for $\varepsilon_0 > 0$ chosen sufficiently small for the following arguments to hold. We conclude that the local stable manifold intersects the hyperplane $\{u' = 0\}$ in a curve tangent to ℓ , and thus

$$W_{\text{loc}}^s \cap \{u' = 0\} \subset \{(1 + v, 0, -\sqrt{2}v + O(v^2), \sqrt{2}\lambda_r v + O(v^2)) \mid v \in \mathbb{R}\} \cap B_{\varepsilon_0}(+1).$$

In particular, in the local stable manifold, if $u' = 0$ and $u > 1$ then $u'' < 0$, whereas if $u' = 0$ and $u < 1$ then $u'' > 0$. This shows that all solutions in the local stable manifold have successive extrema on either side of $u = 1$. Now pick one orbit in the local stable manifold and denote its extrema by $\{u_i^{\varepsilon_0}\}_{i=1}^\infty$. Then $0 < (-1)^i(u_i^{\varepsilon_0} - 1) < \varepsilon_0$, and $u_i^{\varepsilon_0} \rightarrow 1$ as $i \rightarrow \infty$ (exponentially fast in fact). For all $\varepsilon < \varepsilon_0$ we may choose $u_i^\varepsilon = u_{i+2n(\varepsilon)}^{\varepsilon_0}$ for some $n(\varepsilon) \in \mathbb{N}$ sufficiently large. ■

Obviously, we can use the symmetry to obtain an analogous result near -1 . To be explicit, $\bar{u}_i^\varepsilon = -u_{i+1}^\varepsilon$ satisfies $0 < (-1)^i(\bar{u}_i^\varepsilon + 1) < \varepsilon$. For “technical” reasons to become clear later, we will need to shift this solution, modulo the $2p$ -periodicity:

$$\bar{\bar{u}}_i^\varepsilon = \bar{u}_{i-2 \bmod 2p}^\varepsilon.$$

See Figure 32 for an illustration of u_i^ε and $\bar{\bar{u}}_i^\varepsilon$. Notice that $\bar{\bar{u}}_i^\varepsilon$ does not “close” at $i = 3$. Nevertheless, this will not stop us from putting it to use below.

To study solutions of $\mathcal{R}_i = 0$ we introduce an artificial new time variable s and consider $u_i(s)$ evolving according to the flow $u'_i = \mathcal{R}_i$. Clearly, we want to find stationary points, and we are going to construct isolating neighborhoods for the flow (any $p \in \mathbb{N}$)

$$u'_i = \mathcal{R}_i(u_{i-1}, u_i, u_{i+1}), \quad i = 1 \dots 2p, \quad (102)$$

where we identify $u_0 = u_{2p}$. The monotonicity property (101) implies that this flow has the decreasing-intersection-number property: if two solutions are represented as

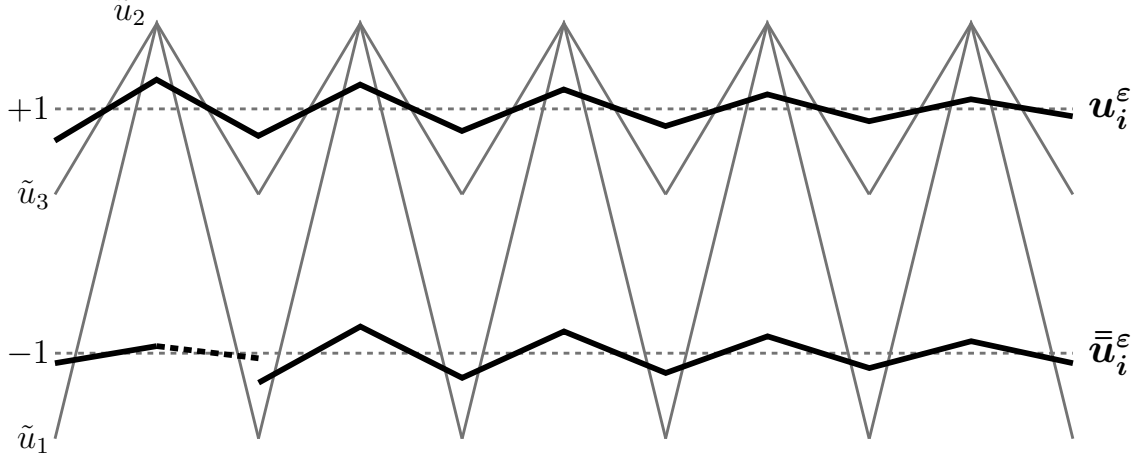


Figure 32: The “up-down” setting including the oscillating tails in the local stable manifolds of ± 1 .

piecewise linear functions (as in most of the figures), then the number of intersections can only decrease as time s increases.

Consider now the solution $\tilde{u}$ associated to the parameter value $\nu \in \mathcal{S}$. In particular, we have that

$$\mathcal{R}_1(\tilde{u}_2, \tilde{u}_1, \tilde{u}_2) = 0,$$

$$\mathcal{R}_2(\tilde{u}_1, \tilde{u}_2, \tilde{u}_3) = 0,$$

$$\mathcal{R}_1(\tilde{u}_2, \tilde{u}_1, \tilde{u}_2) = 0,$$

$$\mathcal{R}_2(\tilde{u}_3, \tilde{u}_2, \tilde{u}_1) = 0.$$

Next, we choose

$$\varepsilon = \frac{1}{2} \max\{-1 - \tilde{u}_1, \tilde{u}_2 - 1, 1 - \tilde{u}_3\}.$$

Although not strictly necessary for understanding the arguments that follow, it is worth mentioning that in the setting of discretized braids described in [16], we are going to use a skeleton consisting of four strands (see Figure 31, right, and Figure 32): $v_i^1 = \tilde{u}_i$ and $v_i^2 = \tilde{u}_{i+2}$, and $v_i^3 = u_i^\varepsilon$ and $v_i^4 = \bar{u}_i^\varepsilon$. To be precise, both v^1 and v^2 are defined for all $i \in \mathbb{Z}$ and are 4-periodic. Furthermore, v^3 is defined for all $i \geq 1$ (though not periodic), while v^4 is defined for $i = 0, \dots, 2p + 1$, with $v_0^4 = v_{2p}^4$ and

$v_{2p+1}^4 = v_1^4$. All four strands satisfy

$$\mathcal{R}_i(v_{i-1}, v_i, v_{i+1}) = 0 \quad \text{for } i = 1, \dots, 2p,$$

with the *exception* of v^4 at $i = 2, 3$ and v^3 at $i = 1$. In the construction below we will make sure that these points do not come into play in the construction of isolating neighborhoods. Recall the finite, but arbitrarily long sequence

$$\mathbf{a} = \{\mathbf{a}_j\}_{j=1}^N, \quad \mathbf{a}_j \geq 2,$$

with at least one of the $\mathbf{a}_j$ satisfying $\mathbf{a}_j > 2$. Let the period of the sequences (u_i) be $p = \sum_{j=1}^N \mathbf{a}_j$ and define the set of partial sums

$$\mathcal{A} = \left\{ \sum_{j=1}^{n-1} \mathbf{a}_j \mid n = 1, \dots, N \right\}.$$

Note that $0 \in \mathcal{A}$. Now define the neighborhood $U \subset \mathbb{R}^{2p}$ as a product of intervals

$$U_{\mathbf{a}} = \{u_i \in I_i, i = 1, \dots, 2p\}$$

where the intervals are given by

$$\begin{aligned} I_i &= [u_i^\varepsilon, \tilde{u}_2] & \text{if } i \text{ is even,} \\ I_i &= [\tilde{u}_3, u_i^\varepsilon] & \text{if } i \text{ is odd and } \frac{i-1}{2} \notin \mathcal{A}, \\ I_i &= [\tilde{u}_1, \bar{u}_i^\varepsilon] & \text{if } i \text{ is odd and } \frac{i-1}{2} \in \mathcal{A}. \end{aligned}$$

Notice that $U_{\mathbf{a}}$ is contained in the domain of definition Ω of $\mathcal{R}_i$, since ± 1 are not in any of the intervals I_i , and the “up-down” criterion is also satisfied, since the intervals I_i for odd i are strictly below those for even i . It is useful to review the intervals in the context of Figure 32, and to look at Figure 33 for an example with $\mathbf{a} = 243$.

We now prove that every $U_{\mathbf{a}}$ contains an equilibrium of (102). It follows from the general theory in [16] that $U_{\mathbf{a}}$ is an isolating block for the flow in the sense of the Conley index and that the flow points outwards everywhere on the boundary. In fact,

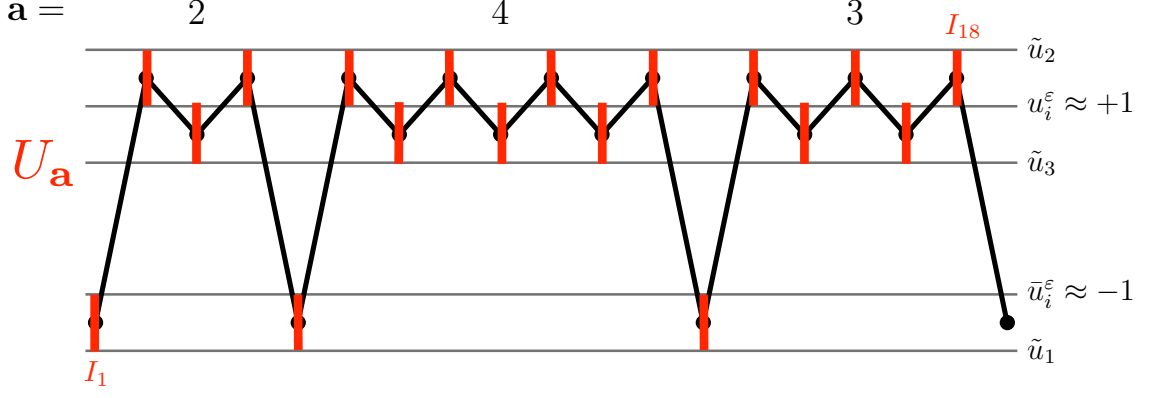


Figure 33: The set $U_{\mathbf{a}} = I_1 \times \cdots \times I_{18}$ associated to $\mathbf{a} = 243$.

it is easy to check this on the co-dimension 1 boundaries of $U_{\mathbf{a}}$, i.e., exactly one of the u_i lies on the boundary of I_i , while all the others are in the interior (for the higher co-dimension boundaries, see [16]). For the following arguments it may be helpful for the reader to consult Figure 34.

Let us consider one of the sides of the $2p$ -cube $U_{\mathbf{a}}$, for example $u_i = u_i^\varepsilon$ for some even i , i.e., u_i is on the lower boundary of I_i . Since $u_{i-1} < u_{i-1}^\varepsilon$, and $u_{i+1} < u_{i+1}^\varepsilon$ on the co-dimension 1 piece of this side, we infer from the monotonicity (101) that

$$u'_i = R_i(u_{i-1}, u_i, u_{i+1}) < R_i(u_{i-1}^\varepsilon, u_i^\varepsilon, u_{i+1}^\varepsilon) = 0.$$

Hence the flow points outwards. And when $u_i = \tilde{u}_2$ for some even i (the upper boundary point of I_i), then, since $\mathbf{a}_j \geq 2$, either $\frac{i-1}{2} \notin \mathcal{A}$ or $\frac{i+1}{2} \notin \mathcal{A}$, or both. Let us consider the case $\frac{i-1}{2} \notin \mathcal{A}$ (the other case is analogous), then $u_{i-1} > \tilde{u}_3$ and $u_{i+1} > \tilde{u}_1$ (assuming again that $(u_i)_{i=1}^{2p}$ is in a co-dimension 1 boundary), hence

$$u'_i = R_i(u_{i-1}, u_i, u_{i+1}) > R_2(\tilde{u}_3, \tilde{u}_2, \tilde{u}_1) = 0,$$

and thus the flow points outwards again. All other (co-dimension 1) boundaries can be dealt with analogously. We should note that, by construction of the neighborhoods in combination with the definition of u^ε and $\bar{u}^\varepsilon$, we avoid the three points where the skeleton does not satisfy the recurrence relation. In particular, no part of the boundary $\partial U_{\mathbf{a}}$ lies in the hyperplanes $u_1 = u_1^\varepsilon$ (since $u_1 < -1$) or $u_2 = \bar{u}_2^\varepsilon$ or $u_3 = \bar{u}_3^\varepsilon$

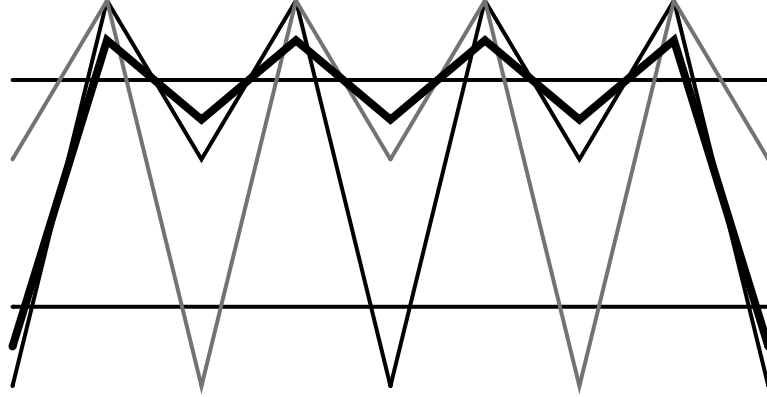


Figure 34: The thin (black and grey) lines denote the skeleton, where we represent u^ε and $\bar{u}^\varepsilon$ by constants for convenience. The thick free strand is in $U_{\mathbf{a}}$ for $\mathbf{a} = (4)$, $p = 4$. One can check that on the boundary of $U_{\mathbf{a}}$ the number of crossings with at least one of the skeletal strands decreases, hence the flow points outwards on the boundary $\partial U_{\mathbf{a}}$.

(since $a_1 \geq 2$, hence $u_2, u_3 > \tilde{u}_3$). We leave the remaining details to the reader. As said before, for the higher co-dimension boundaries we refer to [16, Prop. 11, Th. 15]. We can now conclude that since $U_{\mathbf{a}}$ is a $2p$ -cube and the flow points outwards on $\partial U_{\mathbf{a}}$, its Conley index is homotopic to a $2p$ -sphere, and the non-vanishing of its Euler characteristic implies that there has to be a stationary point inside [16, Lem. 36]. This in fact follows because the invariant set of a discrete parabolic flow consists of stationary points, periodic orbits, and connecting orbits only (i.e., no strange attractors). That concludes the proof of the forcing theorem.

5.3 Topological Entropy and Chaos

In this section, we give the proof of Corollary 5.1.4. Suppose that at the parameter value $\nu > 0$, there exist $x = (L, a_0, a_1, a_2, \dots)$ such that $f(x, \nu) = 0$ and $\tilde{u}$ given by $\tilde{u}(y) := a_0 + 2 \sum_{k=1}^{\infty} a_k \cos(kLy)$ satisfies the geometric hypotheses $(\mathcal{H})$.

By Forcing Theorem 5.1.2, we know that given any finite, but arbitrarily long sequence $\mathbf{a} = \{\mathbf{a}_j\}_{j=1}^N$, with $\mathbf{a}_j \geq 2$ not all equal to 2, there exists a periodic solution $u_{\mathbf{a}}$ of (97) that oscillates around the constant periodic solutions ± 1 as follow: $\mathbf{a}_1$

times around 1, one time around -1 , $\mathbf{a}_2$ times around 1, one time around -1 , $\dots$, $\mathbf{a}_N$ times around 1 and finally one time around -1 .

To examine the entropy of the system, we first we look at an alternative coding. To any sequence $\mathbf{a} = \{\mathbf{a}_j\}_{j=1}^N$, with $\mathbf{a}_j \geq 2$ not all equal to 2 will correspond a unique new sequence $\mathbf{b}$ defined on two symbols, say 0 and 1. Such a sequence consists of 1's interspersed by 0's, i.e., a 0 can only be followed by a 1, but a 1 can be followed by a 0 or a 1. Consider a p -periodic sequence $\mathbf{b} = b_1 b_2 \dots b_p$ of this form, then it can be written as $\mathbf{b} = 01^{d_1} 01^{d_2} 0 \dots 01^{d_N}$ for some $d_1, \dots, d_N \geq 1$, with periodic extension, and $p = N + \sum_{i=1}^N d_i$. There is a one-to-one correspondence between sequences $\mathbf{a}$ described above and $\mathbf{b}$ via the identification $\mathbf{a}_i = d_i + 1$. We denote this correspondence $\mathbf{a} \simeq \mathbf{b}$. In terms of $\mathbf{b}$ the intervals are given by

$$\begin{aligned} I_i &= [u_i^\varepsilon, \tilde{u}_2] && \text{if } i \text{ is even,} \\ I_i &= [\tilde{u}_3, u_i^\varepsilon] && \text{if } i \text{ is odd and } b_{\frac{i+1}{2}} = 0, \\ I_i &= [\tilde{u}_1, \bar{u}_i^\varepsilon] && \text{if } i \text{ is odd and } b_{\frac{i+1}{2}} = 1. \end{aligned}$$

For any sequence $\mathbf{b}$ ($\simeq \mathbf{a}$), let $u_{\mathbf{b}} = u_{\mathbf{a}}$ be the solutions of (97) at $E = 0$ corresponding to the stationary points in $U_{\mathbf{b}} = U_{\mathbf{a}}$. The sets of all orbits (varying over all possible $\mathbf{a} \simeq \mathbf{b}$) is uniformly bounded. Taking the closure of this set, we obtain a compact invariant set $\mathcal{C} \subset \{E = 0\} \subset \mathbb{R}^4$ for the ODE (note that it may include $u = \pm 1$ as well as $\tilde{u}$). Let us now look at the entropy of a return map associated to the flow in this invariant set.

The sequence $\mathbf{b}$ codes the position of the minima u_i of the stationary point in $U_{\mathbf{b}}$. The energy level $\{E = 0\}$ is a three-dimensional subset of the phase-space $\mathbb{R}^4$. A local minimum in $\{E = 0\}$ is defined by the values of u and u''' , since $u'' = \frac{1}{\sqrt{2}}|u^2 - 1|$. Let us consider the map T going from one minimum to the next (it may degenerate

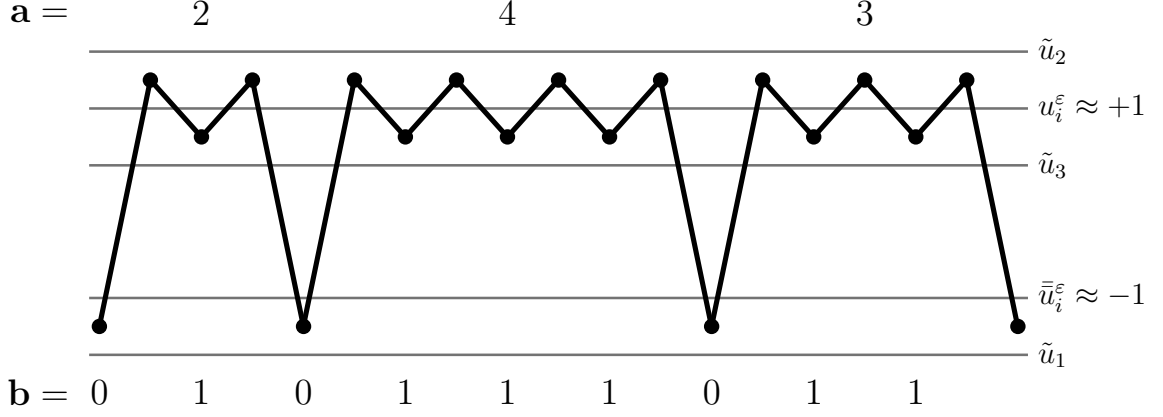


Figure 35: A schematic example of a pattern in $U_{\mathbf{a}}$, with at the top the coding $\mathbf{a}$, and below the corresponding coding $\mathbf{b}$.

at $u = \pm 1$, but that is not important here). It is thus a return map on the two-dimensional subset

$$\mathcal{P} = \left\{ (u, 0, \frac{1}{\sqrt{2}}|u^2 - 1|, u''') \mid u, u''' \in \mathbb{R} \right\} \subset \{E = 0\} \subset \mathbb{R}^4.$$

By construction, the return map T , defined on $\mathcal{P}$, has an invariant set $\Lambda = \mathcal{P} \cap \mathcal{C}$.

We will show that the map $T : \Lambda \rightarrow \Lambda$ is such that $h_{top}(T) > 0$.

Define the adjacency matrix

$$\mathcal{M} = \begin{pmatrix} m_{00} & m_{01} \\ m_{10} & m_{11} \end{pmatrix} = \begin{pmatrix} 0 & 1 \\ 1 & 1 \end{pmatrix}$$

and consider the symbol space

$$\Sigma_{\mathcal{M}} := \{s = (s_0 s_1 s_2 \cdots) \mid m_{s_k s_{k+1}} = 1, \text{ for all } k\}.$$

Consider now the *shift map* $\sigma_{\mathcal{M}} : \Sigma_{\mathcal{M}} \rightarrow \Sigma_{\mathcal{M}}$ defined

$$\sigma_{\mathcal{M}}(s) := s' \quad , \quad \text{where } s'_i = s_{i+1}.$$

A theorem from [33] implies that $h_{top}(\sigma_{\mathcal{M}}) = \log(sp(\mathcal{M}))$, where

$$sp(\mathcal{M}) = \max \{|\lambda| \mid \lambda \text{ is an eigenvalue of } \mathcal{M}\}$$

is the spectral radius of the adjacency matrix $\mathcal{M}$.

By construction of Λ , we have that to any $x \in \Lambda$ corresponds a unique $\mathbf{b}_x \in \Sigma_{\mathcal{M}}$. Define then $\rho : \Lambda \rightarrow \Sigma_{\mathcal{M}}$ by $\rho(x) = \mathbf{b}_x$. Note that $\rho : \Lambda \rightarrow \Sigma_{\mathcal{M}}$ is a continuous surjective map.

Definition 5.3.1 A continuous map $\rho : X \rightarrow Y$ is a *topological semi-conjugacy* between $f : X \rightarrow X$ and $g : Y \rightarrow Y$ if $\rho \circ f = g \circ \rho$ and if ρ is surjective.

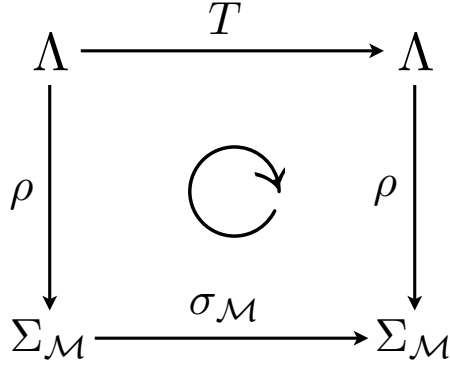


Figure 36: Topological semi-conjugacy between $T : \Lambda \rightarrow \Lambda$ and $\sigma_{\mathcal{M}} : \Sigma_{\mathcal{M}} \rightarrow \Sigma_{\mathcal{M}}$

Proposition 5.3.2 $h_{top}(T) \geq h_{top}(\sigma_{\mathcal{M}})$.

Proof. First note that $\rho : \Lambda \rightarrow \Sigma_{\mathcal{M}}$ is a topological semi-conjugacy between $T : \Lambda \rightarrow \Lambda$ and $\sigma_{\mathcal{M}} : \Sigma_{\mathcal{M}} \rightarrow \Sigma_{\mathcal{M}}$. Hence, the result follows from Theorem 2.6 in [8]. ■

Finally, since $sp(\mathcal{M}) = \frac{1+\sqrt{5}}{2}$, we can conclude by Proposition 5.3.2 that $h_{top}(T) \geq h_{top}(\sigma_{\mathcal{M}}) = \log\left(\frac{1+\sqrt{5}}{2}\right)$, and hence that the ODE is chaotic at energy level $E = 0$.

5.4 Construction of the Radii Polynomials

To construct the radii polynomials, we need the Y_k from (14) and the Z_k from (15). Since we use rigorous numerical methods to find (x, ν) such that $f(x, \nu) = 0$, we need to consider a finite dimensional projection of (99). Define

$$x_F = (x_{-1}, x_0, \dots, x_{m-1}) = (L, a_0, \dots, a_{m-1}) \in \mathbb{R}^{m+1},$$

$$e^{(m)}(x_F) = -2L^2 \sum_{l=1}^{m-1} l^2 a_l - \frac{1}{\sqrt{2}} \left[a_0 + 2 \sum_{l=1}^{m-1} a_l \right]^2 + \frac{1}{\sqrt{2}}$$

and

$$g^{(m)}(x_F, \nu) = [g_0(x_F, \nu), \dots, g_{m-1}(x_F, \nu)]^T.$$

The *Galerkin Projection* of (99) is defined by

$$f^{(m)}(x_F, \nu) = \begin{bmatrix} e^{(m)}(x_F) \\ g^{(m)}(x_F, \nu) \end{bmatrix}. \quad (103)$$

Suppose now that at the parameter ν_0 , we found numerically $\bar{x}_F, \hat{x}_F \in \mathbb{R}^{m+1}$ such that

$$f^{(m)}(\bar{x}_F, \nu_0) \approx 0 \quad \text{and} \quad Df^{(m)}(\bar{x}_F, \nu_0)\hat{x}_F + \frac{\partial f^{(m)}}{\partial \nu}(\bar{x}_F, \nu_0) \approx 0.$$

Denote $\hat{x}_F = (\hat{L}, \hat{a}_0, \hat{a}_1, \dots, \hat{a}_{m-1})$ and define $\mu_k(L, \nu) = 1 + \nu L^2 k^2 - L^4 k^4$, $J_{m \times m}$ the computed numerical inverse of $Df^{(m)}(\bar{x}_F, \nu)$ and

$$A = \begin{bmatrix} J_{m \times m} & & 0 \\ & \mu_m(\bar{L}, \nu_0)^{-1} & \\ 0 & & \mu_{m+1}(\bar{L}, \nu_0)^{-1} \\ & & & \ddots \end{bmatrix}. \quad (104)$$

Denote $0_\infty = (0, 0, \dots) \in \mathbb{R}^\infty$. Letting $\bar{x} = (\bar{x}_F, 0_\infty)$, $\hat{x} = (\hat{x}_F, 0_\infty)$ and fixing $s \geq 4$, we define

$$W(r) = [-r, r]^2 \times \prod_{k=1}^{\infty} \left[-\frac{r}{k^s}, \frac{r}{k^s} \right]. \quad (105)$$

Recall that $x_\nu = \bar{x} + \hat{\nu}\hat{x}$.

5.4.1 Upper bounds for $Y_k(\hat{\nu})$

Recalling (7) and (14), we have

$$Y_k(\hat{\nu}) \geq |[-A \cdot f(x_\nu, \nu)]_k|. \quad .$$

Define

$$\begin{aligned}
\hat{e}_1 &= -2\bar{L}^2 \sum_{l=1}^{m-1} l^2 \hat{a}_l - 4\bar{L}\hat{L} \sum_{l=1}^{m-1} l^2 \bar{a}_l - \sqrt{2} \left(\bar{a}_0 + 2 \sum_{l=1}^{m-1} \bar{a}_l \right) \left(\hat{a}_0 + 2 \sum_{l=1}^{m-1} \hat{a}_l \right), \\
\hat{e}_2 &= -4\bar{L}\hat{L} \sum_{l=1}^{m-1} l^2 \hat{a}_l - 2\hat{L}^2 \sum_{l=1}^{m-1} l^2 \bar{a}_l - \frac{1}{\sqrt{2}} \left(\hat{a}_0 + 2 \sum_{l=1}^{m-1} \hat{a}_l \right)^2, \\
\hat{e}_3 &= -2\hat{L}^2 \sum_{l=1}^{m-1} l^2 \hat{a}_l
\end{aligned}$$

and $\hat{e}_4 = \hat{e}_5 = 0$.

Given $a_F = (a_0, \dots, a_{m-1})$, $b_F = (b_0, \dots, b_{m-1})$ and $c_F = (c_0, \dots, c_{m-1})$, we use the discrete convolution notation

$$(a_F * b_F * c_F)_k = \sum_{\substack{k_1+k_2+k_3=k \\ |k_i| < m}} a_{k_1} b_{k_2} c_{k_3},$$

where we consider $a_{-k} = a_k$, $b_{-k} = b_k$ and $c_{-k} = c_k$ in evaluating the sum. Let $\bar{a}_F = (\bar{a}_0, \dots, \bar{a}_{m-1})$ and $\hat{a}_F = (\hat{a}_0, \dots, \hat{a}_{m-1})$. For $k = 0, \dots, m-1$, define

$$\begin{aligned}
\hat{g}_{k,1} &= \left(2k^2 \nu_0 \bar{L} \hat{L} + k^2 \bar{L}^2 - 4\bar{L}^3 \hat{L} k^4 \right) \bar{a}_k + (1 + \nu_0 \bar{L}^2 k^2 - \bar{L}^4 k^4) \hat{a}_k - 3(\bar{a}_F * \bar{a}_F * \hat{a}_F)_k, \\
\hat{g}_{k,2} &= \left(2k^2 \nu_0 \bar{L} \hat{L} + k^2 \bar{L}^2 - 4\bar{L}^3 \hat{L} k^4 \right) \hat{a}_k + \left(k^2 \nu_0 \hat{L}^2 + 2k^2 \bar{L} \hat{L} - 6\bar{L}^2 \hat{L}^2 k^4 \right) \bar{a}_k - 3(\bar{a}_F * \hat{a}_F * \hat{a}_F)_k, \\
\hat{g}_{k,3} &= \left(k^2 \nu_0 \hat{L}^2 + 2k^2 \bar{L} \hat{L} - 6\bar{L}^2 \hat{L}^2 k^4 \right) \hat{a}_k + (k^2 \hat{L}^2 - 4\bar{L} \hat{L}^3 k^4) \bar{a}_k - (\hat{a}_F * \hat{a}_F * \hat{a}_F)_k, \\
\hat{g}_{k,4} &= (k^2 \hat{L}^2 - 4\bar{L} \hat{L}^3 k^4) \hat{a}_k - \hat{L}^4 k^4 \bar{a}_k, \\
\hat{g}_{k,5} &= -\hat{L}^4 k^4 \hat{a}_k.
\end{aligned}$$

For $j = 1, \dots, 5$, define

$$\hat{f}_j = (\hat{e}_j \ \hat{g}_{0,j} \ \dots \ \hat{g}_{k,j} \ \dots \ \hat{g}_{m-1,j})^T \in \mathbb{R}^{m+1}. \quad (106)$$

Hence,

$$f_F^{(m)}(x_\nu, \nu_0 + \hat{\nu}) = f^{(m)}(\bar{x}_F, \nu_0) + \hat{\nu} \hat{f}_1 + \hat{\nu}^2 \hat{f}_2 + \hat{\nu}^3 \hat{f}_3 + \hat{\nu}^4 \hat{f}_4 + \hat{\nu}^5 \hat{f}_5. \quad (107)$$

For the cases $k \in \{-1, 0, 1, \dots, m-1\}$, we then let

$$\begin{aligned} Y_F(\hat{\nu}) &= |J_{m \times m} f^{(m)}(\bar{x}_F, \nu_0)| + \hat{\nu} |J_{m \times m} \hat{f}_1| + \hat{\nu}^2 |J_{m \times m} \hat{f}_2| \\ &\quad + \hat{\nu}^3 |J_{m \times m} \hat{f}_3| + \hat{\nu}^4 |J_{m \times m} \hat{f}_4| + \hat{\nu}^5 |J_{m \times m} \hat{f}_5|. \end{aligned} \quad (108)$$

Since for $k \geq m$,

$$\begin{aligned} f_k(x_\nu, \nu) &= -(\bar{a}_F * \bar{a}_F * \bar{a}_F)_k - 3\hat{\nu}(\bar{a}_F * \bar{a}_F * \hat{a}_F)_k \\ &\quad - 3\hat{\nu}^2(\bar{a}_F * \hat{a}_F * \hat{a}_F)_k - \hat{\nu}^3(\hat{a}_F * \hat{a}_F * \hat{a}_F)_k, \end{aligned}$$

we let

$$\begin{aligned} Y_k(\hat{\nu}) &= \frac{|(\bar{a}_F * \bar{a}_F * \bar{a}_F)_k|}{|\mu_k(\bar{L}, \nu_0)|} + 3\hat{\nu} \frac{|(\bar{a}_F * \bar{a}_F * \hat{a}_F)_k|}{|\mu_k(\bar{L}, \nu_0)|} \\ &\quad + 3\hat{\nu}^2 \frac{|(\bar{a}_F * \hat{a}_F * \hat{a}_F)_k|}{|\mu_k(\bar{L}, \nu_0)|} + \hat{\nu}^3 \frac{|(\hat{a}_F * \hat{a}_F * \hat{a}_F)_k|}{|\mu_k(\bar{L}, \nu_0)|}. \end{aligned} \quad (109)$$

Note that if $k \geq 3m-2$, then $Y_k = 0$.

5.4.2 Upper bounds for $Z_F(r, \hat{\nu})$

In this section, we fix $M \geq 3m-2$, we define $\mathbf{1} = [-1, 1]$ and for $j \geq 1$ we define $\mathbf{r}^j = [-r^j, r^j]$, where r comes from $W(r)$. Fix $s \geq 4$. Let $w, w' \in W(r)$. Fix $k \in \{-1, 0, \dots, m-1\}$ and let $h_k(t) = [DT_\nu(\bar{x} + t(w' + \hat{\nu}\hat{x}))w]_k$. By the mean value theorem, there exists $t_k \in [0, 1]$ such that $h_k(1) - h_k(0) = h'_k(t_k)$. Hence,

$$\begin{aligned} [DT_\nu(w' + x_\nu)w]_k &= [DT_\nu(\bar{x})w]_k \\ &\quad + [D^2T_\nu[\bar{x} + t_k(w' + \hat{\nu}\hat{x})](w' + \hat{\nu}\hat{x})w]_k. \end{aligned} \quad (110)$$

Recall that the subscript F denotes the entries $k \in \{-1, 0, 1, \dots, m-1\}$. Define R_F such that

$$Df_F(\bar{x}, \nu)w = Df^{(m)}(\bar{x}_F, \nu_0)w_F + R_F.$$

We then have from (104) that

$$[DT_\nu(\bar{x})w]_F = [(I - A \cdot Df(\bar{x}, \nu))w]_F$$

$$\begin{aligned}
&= w_F - J_{m \times m} \cdot [Df(\bar{x}, \nu)w]_F \\
&= w_F - J_{m \times m} \cdot Df_F(\bar{x}, \nu)w \\
&= w_F - J_{m \times m} \cdot [Df^{(m)}(\bar{x}_F, \nu_0)w_F + R_F] \\
&= [I_{m \times m} - J_{m \times m} Df^{(m)}(\bar{x}_F, \nu_0)]w_F - J_{m \times m} \cdot R_F
\end{aligned}$$

It's important to note that since $J_{m \times m}$ is the numerical inverse of $D\mathcal{F}^{(m)}(\bar{x}_F, \nu_0)$, the matrix $I_{m \times m} - J_{m \times m} Df^{(m)}(\bar{x}_F, \nu_0)$ should be close to $0 \in \mathbb{R}^{(m+1) \times (m+1)}$. The quantity left to compute is then $R_F \in \mathbb{R}^{m+1}$. For $k = -1$, we have

$$\begin{aligned}
Df_{-1}(\bar{x}, \nu)w &= \sum_{i=-1}^{\infty} \frac{\partial f_{-1}}{\partial x_i}(\bar{x}, \nu)w_i \\
&= \frac{\partial f_{-1}}{\partial L}(\bar{x}, \nu)w_{-1} + \frac{\partial f_{-1}}{\partial a_0}(\bar{x}, \nu)w_0 + \sum_{i=1}^{\infty} \frac{\partial f_{-1}}{\partial a_i}(\bar{x}, \nu)w_i \\
&= \left[-4\bar{L} \sum_{l=1}^{m-1} l^2 \bar{a}_l \right] w_{-1} - \sqrt{2} \left[\bar{a}_0 + 2 \sum_{l=1}^{m-1} \bar{a}_l \right] w_0 \\
&\quad + \sum_{i=1}^{\infty} \left[-2\bar{L}^2 i^2 - 2\sqrt{2} \left(\bar{a}_0 + 2 \sum_{l=1}^{m-1} \bar{a}_l \right) \right] w_i \\
&= Df_{-1}^{(m)}(\bar{x}_F, \nu_0)w_F + R_{-1} ,
\end{aligned}$$

where

$$R_{-1} = \sum_{i=m}^{\infty} \left[-2\bar{L}^2 i^2 - 2\sqrt{2} \left(\bar{a}_0 + 2 \sum_{l=1}^{m-1} \bar{a}_l \right) \right] w_i .$$

To simplify the presentation, let

$$\begin{aligned}
fs_1 &= \sum_{i=m}^{M-1} \frac{1}{i^s} , \quad is_1 = \frac{1}{(M-1)^{s-1}(s-1)} , \\
fs_2 &= \sum_{i=m}^{M-1} \frac{1}{i^{s-2}} , \quad is_2 = \frac{1}{(M-1)^{s-3}(s-3)} .
\end{aligned}$$

It's clear that

$$\sum_{i=M}^{\infty} \frac{1}{i^s} < is_1 \quad \text{and} \quad \sum_{i=M}^{\infty} \frac{1}{i^{s-2}} < is_2 .$$

Therefore, we have that for every $w \in W(r)$

$$R_{-1} \in \left(2\bar{L}^2(fs_2 + is_2) + 2\sqrt{2} \left| \bar{a}_0 + 2 \sum_{k=1}^{m-1} \bar{a}_k \right| (fs_1 + is_1) \right) \mathbf{r} .$$

Define $|\bar{a}|_M = (|\bar{a}_0|, \dots, |\bar{a}_{m-1}|, 0, \dots, 0), v_{0,\{m,M\}} = \left(0, \dots, 0, \frac{1}{m^s}, \dots, \frac{1}{(M-1)^s}\right) \in \mathbb{R}^M$. Fixing $k \in \{0, \dots, m-1\}$ and recalling that $\nu = \nu_0 + \hat{\nu}$,

$$\begin{aligned} Df_k(\bar{x}, \nu)w &= \frac{\partial f_k}{\partial L}(\bar{x}, \nu)w_{-1} + \sum_{i=0}^{\infty} \frac{\partial f_k}{\partial a_i}(\bar{x}, \nu)w_i \\ &= [2(\nu_0 + \hat{\nu})\bar{L}k^2 - 4\bar{L}^3k^4]\bar{a}_kw_{-1} + [1 + (\nu_0 + \hat{\nu})\bar{L}^2k^2 - \bar{L}^4k^4]w_k \\ &\quad - 3 \sum_{k_1+k_2+k_3=k} \bar{a}_{k_1}\bar{a}_{k_2}w_{k_3} \\ &= Df_k^{(m)}(\bar{x}_F, \nu_0)w_F + R_k, \end{aligned}$$

where

$$R_k = -3 \sum_{\substack{k_1+k_2+k_3=k \\ |k_1|, |k_2| < m \leq |k_3| < M}} \bar{a}_{k_1}\bar{a}_{k_2}w_{k_3} + \hat{\nu} [2\bar{L}k^2\bar{a}_kw_{-1} + \bar{L}^2k^2w_k].$$

Hence, recalling that $\mathbf{w}_0 = [-r, r]$ and that $\mathbf{w}_k = [-\frac{r}{k^s}, \frac{r}{k^s}]$ for $k \geq 1$, we get that

$$R_0 \in 3(|\bar{a}|_M^2 * v_{0,\{m,M\}})_0 \mathbf{r}$$

and for $k \in \{1, \dots, m-1\}$

$$R_k \in \left[3(|\bar{a}|_M^2 * v_{0,\{m,M\}})_k + \hat{\nu}|\bar{L}|k^2 \left(2|\bar{a}_k| + \frac{|\bar{L}|}{k^s} \right) \right] \mathbf{r}.$$

Define $v_F^{(0)}, v_F^{(1)} \in \mathbb{R}^{m+1}$ by

$$v_k^{(0)} = \begin{cases} 2\bar{L}^2(fs_2 + is_2) + 2\sqrt{2}|\bar{a}_0 + 2\sum_{l=1}^{m-1}\bar{a}_l|(fs_1 + is_1), & k = -1 \\ 3(|\bar{a}|_M^2 * v_{0,\{m,M\}})_k, & k \in \{0, \dots, m-1\} \end{cases}$$

and

$$v_k^{(1)} = \begin{cases} 0, & k = -1, 0 \\ |\bar{L}|k^2 \left(2|\bar{a}_k| + \frac{|\bar{L}|}{k^s} \right), & k \in \{1, \dots, m-1\}. \end{cases}$$

Defining $\mathbb{I}_F = [1, 1, \dots, 1]^T \in \mathbb{R}^{m+1}$, let

$$\begin{aligned} V_F^{(0)} &= |I_{m \times m} - J_{m \times m} Df^{(m)}(\bar{x}_F, \nu_0)| \mathbb{I}_F + |J_{m \times m}| \cdot v_F^{(0)} \\ V_F^{(1)} &= |J_{m \times m}| v_F^{(1)}. \end{aligned}$$

Hence, for every $w \in W(r)$

$$[DT_\nu(\bar{x})w]_F \in \left[V_F^{(0)} + \hat{\nu}V_F^{(1)} \right] \mathbf{r} . \quad (111)$$

We now need to compute a set enclosure of $[D^2T_\nu[\bar{x} + t_k(w' + \hat{\nu}\hat{x})](w' + \hat{\nu}\hat{x})w]_k$ for every $k \in \{-1, 0, \dots, m-1\}$. We begin by considering the case $k = -1$.

Lemma 5.4.1 *Define*

$$\begin{aligned} fs_3 &= \sum_{l=1}^{M-1} \frac{1}{l^{s-2}} , \quad fs_4 = \sum_{l=1}^{m-1} l^2 |\bar{a}_l| , \quad fs_5 = \sum_{l=1}^{m-1} l^2 |\hat{a}_l| , \quad fs_6 = \sum_{l=1}^{M-1} \frac{1}{l^s} \\ e^{(3)} &= 12(fs_3 + is_2) \\ e^{(2)} &= 4 \left([fs_4 + \hat{\nu}fs_5] + \hat{\nu}|\hat{L}|(fs_3 + is_2) \right) + 8(fs_3 + is_2) \left(|\bar{L}| + 2\hat{\nu}|\hat{L}| \right) \\ &\quad + \sqrt{2} [1 + 4(fs_6 + is_1) + 4(fs_6 + is_1)^2] \\ e^{(1)} &= 4\hat{\nu}|\hat{L}|[fs_4 + \hat{\nu}fs_5] + 8(fs_3 + is_2) (|\bar{L}| + \hat{\nu}|\bar{L}|) \hat{\nu}|\hat{L}| \\ &\quad + \hat{\nu}\sqrt{2}(1 + 2fs_6 + 2is_1) \left[|\hat{a}_0| + 2 \sum_{i=1}^{m-1} |\hat{a}_i| \right] . \end{aligned}$$

Then

$$\begin{aligned} &[D^2f[\bar{x} + t_{-1}(w' + \hat{\nu}\hat{x}), \nu](w' + \hat{\nu}\hat{x})w]_{-1} \\ &\in e^{(3)}\mathbf{r}^3 + e^{(2)}\mathbf{r}^2 + e^{(1)}\mathbf{r} . \end{aligned} \quad (112)$$

Proof. First

$$\begin{aligned} &[D^2f[\bar{x} + t_{-1}(w' + \hat{\nu}\hat{x}), \nu](w' + \hat{\nu}\hat{x})w]_{-1} \\ &= \sum_{i=-1}^{\infty} \sum_{j=-1}^{\infty} \frac{\partial^2 e}{\partial x_i \partial x_j} [\bar{x} + t_{-1}(w' + \hat{\nu}\hat{x})] (w' + \hat{\nu}\hat{x})_i w_j \\ &= \frac{\partial^2 e}{\partial L^2} [\bar{x} + t_{-1}(w' + \hat{\nu}\hat{x})] (w'_{-1} + \hat{\nu}\hat{L}) w_{-1} \\ &\quad + 2 \sum_{j=0}^{\infty} \frac{\partial^2 e}{\partial L \partial a_j} [\bar{x} + t_{-1}(w' + \hat{\nu}\hat{x})] (w'_{-1} + \hat{\nu}\hat{L}) w_j \\ &\quad + \sum_{i=0}^{\infty} \sum_{j=0}^{\infty} \frac{\partial^2 e}{\partial a_i \partial a_j} [\bar{x} + t_{-1}(w' + \hat{\nu}\hat{x})] (w'_i + \hat{\nu}\hat{a}_i) w_j . \end{aligned}$$

The result follows from computing upper bounds for each of the three sums in the above expansion and by expressing the resulting upper bounds in powers of $\mathbf{r}$. Indeed

$$\begin{aligned}
& \frac{\partial^2 e}{\partial L^2} [\bar{x} + t_{-1}(w' + \hat{\nu} \hat{x})] (w'_{-1} + \hat{\nu} \hat{L}) w_{-1} \\
& \in 4(f s_3 + i s_2) \mathbf{r}^3 + 4 \left([f s_4 + \hat{\nu} f s_5] + \hat{\nu} |\hat{L}| (f s_3 + i s_2) \right) \mathbf{r}^2 + 4 \hat{\nu} |\hat{L}| [f s_4 + \hat{\nu} f s_5] \mathbf{r} \\
& 2 \sum_{j=0}^{\infty} \frac{\partial^2 e}{\partial L \partial a_j} [\bar{x} + t_{-1}(w' + \hat{\nu} \hat{x})] (w'_{-1} + \hat{\nu} \hat{L}) w_j \\
& \in 8(f s_3 + i s_2) \left[\mathbf{r}^3 + \left(|\bar{L}| + 2 \hat{\nu} |\hat{L}| \right) \mathbf{r}^2 + \left(|\bar{L}| + \hat{\nu} |\bar{L}| \right) \hat{\nu} |\hat{L}| \mathbf{r} \right]
\end{aligned}$$

and

$$\begin{aligned}
& \sum_{i=0}^{\infty} \sum_{j=0}^{\infty} \frac{\partial^2 e}{\partial a_i \partial a_j} (\cdot) (w'_i + \hat{\nu} \hat{a}_i) w_j \in \sqrt{2} \left[1 + 4(f s_6 + i s_1) + 4(f s_6 + i s_1)^2 \right] \mathbf{r}^2 \\
& + \hat{\nu} \sqrt{2} (1 + 2 f s_6 + 2 i s_1) \left[|\hat{a}_0| + 2 \sum_{i=1}^{m-1} |\hat{a}_i| \right] \mathbf{r} . \quad \blacksquare
\end{aligned}$$

Consider $k \in \{0, \dots, m-1\}$ and recall that $\nu = \nu_0 + \hat{\nu}$. Then

$$\begin{aligned}
& \sum_{i=-1}^{\infty} \sum_{j=-1}^{\infty} \frac{\partial^2 f_k}{\partial x_i \partial x_j} (\bar{x} + t_k(w' + \hat{\nu} \hat{x}), \nu) (w'_i + \hat{\nu} \hat{x}_i) w_j \\
& = \frac{\partial^2 f_k}{\partial L^2} (\bar{x} + t_{-1}(w' + \hat{\nu} \hat{x}), \nu) (w'_{-1} + \hat{\nu} \hat{L}) w_{-1} \\
& + 2 \sum_{j=0}^{\infty} \frac{\partial^2 f_k}{\partial L \partial a_j} (\bar{x} + t_k(w' + \hat{\nu} \hat{x}), \nu) (w'_{-1} + \hat{\nu} \hat{L}) w_j \\
& + \sum_{i=0}^{\infty} \sum_{j=0}^{\infty} \frac{\partial^2 f_k}{\partial a_i \partial a_j} (\bar{x} + t_k(w' + \hat{\nu} \hat{x}), \nu) (w'_i + \hat{\nu} \hat{a}_i) w_j \\
& = \left[2 \nu k^2 - 12 \left(\bar{L} + t_{-1}(w'_{-1} + \hat{\nu} \hat{L}) \right)^2 k^4 \right] [\bar{a}_k + t_k(w'_k + \hat{\nu} \hat{a}_k)] [w'_{-1} + \hat{\nu} \hat{L}] w_{-1} \\
& + 2 \left[2 \nu \left(\bar{L} + t_k(w'_{-1} + \hat{\nu} \hat{L}) \right) k^2 - 4 \left(\bar{L} + t_k(w'_{-1} + \hat{\nu} \hat{L}) \right)^3 k^4 \right] [w'_{-1} + \hat{\nu} \hat{L}] w_k \\
& - 6 \sum_{\substack{k_1 + k_2 + k_3 = k \\ k_i \in \mathbb{Z}}} [\bar{a}_{k_1} + t_k(w'_{k_1} + \hat{\nu} \hat{a}_{k_1})] [w'_{k_2} + \hat{\nu} \hat{a}_{k_2}] w_{k_3} .
\end{aligned}$$

Denote $0_n = (0, \dots, 0) \in \mathbb{R}^n$, $0_\infty = (0, 0, \dots) \in \mathbb{R}^\infty$ and let

$$v = \left(1, 1, \frac{1}{2^s}, \dots, \frac{1}{k^s}, \dots \right) , \quad v_M = \left(1, 1, \frac{1}{2^s}, \dots, \frac{1}{(M-1)^s} \right)$$

$$|\bar{a}| = (|\bar{a}_0|, \dots, |\bar{a}_{m-1}|, 0_\infty) \ , \ |\bar{a}|_M = (|\bar{a}_0|, \dots, |\bar{a}_{m-1}|, 0_{M-m})$$

$$|\hat{a}| = (|\hat{a}_0|, \dots, |\hat{a}_{m-1}|, 0_\infty) \ , \ |\hat{a}|_M = (|\hat{a}_0|, \dots, |\hat{a}_{m-1}|, 0_{M-m})$$

$$\bar{A} = \max_{k=1, \dots, m-1} \{|\bar{a}_0|, |\bar{a}_k| k^s\} \ , \ \hat{A} = \max_{k=1, \dots, m-1} \{|\hat{a}_0|, |\hat{a}_k| k^s\} \ .$$

Remark that for all $k \geq -1$, $w_k \in v_k \mathbf{r}$. For the case $p = 3$, recall $\varepsilon_k^{(p)} = \varepsilon_k^{(3)}$ from (48).

By Corollary 3.5.1,

$$\begin{aligned} & \sum_{\substack{k_1+k_2+k_3=k \\ k_i \in \mathbb{Z}}} [\bar{a}_{k_1} + t_k (w'_{k_1} + \hat{v} \hat{a}_{k_1})] [w'_{k_2} + \hat{v} \hat{a}_{k_2}] w_{k_3} \\ & \in (v^3)_k \mathbf{r}^3 + [(|\bar{a}| * v^2)_k + 2\hat{v}(|\hat{a}| * v^2)_k] \mathbf{r}^2 \\ & \quad + [\hat{v}(|\bar{a}| * |\hat{a}| * v)_k + \hat{v}^2(|\hat{a}|^2 * v)_k] \mathbf{r} \\ & \subseteq [(v_M^3)_k + \varepsilon_k^{(3)}] \mathbf{r}^3 \\ & \quad + [(|\bar{a}|_M * v_M^2)_k + 2\hat{v}(|\hat{a}|_M * v_M^2)_k + (\bar{A} + 2\hat{v}\hat{A}) \varepsilon_k^{(3)}] \mathbf{r}^2 \\ & \quad + [\hat{v}(|\bar{a}|_M * |\hat{a}|_M * v_M)_k + \hat{v}^2(|\hat{a}|_M^2 * v_M)_k + (\hat{v}\bar{A}\hat{A} + \hat{v}^2\hat{A}^2) \varepsilon_k^{(3)}] \mathbf{r} \ . \end{aligned}$$

Hence, for $k = 0$,

$$\begin{aligned} & \sum_{i=-1}^{\infty} \sum_{j=-1}^{\infty} \frac{\partial^2 f_k}{\partial x_i \partial x_j} (\bar{x} + t_k(w' + \hat{v}\hat{x}), \nu) (w'_i + \hat{v}\hat{x}_i) w_j \\ & \in [(v_M^3)_0 + \varepsilon_0^{(3)}] \mathbf{r}^3 \\ & \quad + [(|\bar{a}|_M * v_M^2)_0 + 2\hat{v}(|\hat{a}|_M * v_M^2)_0 + (\bar{A} + 2\hat{v}\hat{A}) \varepsilon_0^{(3)}] \mathbf{r}^2 \\ & \quad + [\hat{v}(|\bar{a}|_M * |\hat{a}|_M * v_M)_0 + \hat{v}^2(|\hat{a}|_M^2 * v_M)_0 + (\hat{v}\bar{A}\hat{A} + \hat{v}^2\hat{A}^2) \varepsilon_0^{(3)}] \mathbf{r} \ . \end{aligned}$$

Let $c_0^{(5)} = c_0^{(4)} = 0$, $c_0^{(3)} = (v_M^3)_0 + \varepsilon_0^{(3)}$ and

$$\begin{aligned} c_0^{(2)} &= (|\bar{a}|_M * v_M^2)_0 + 2\hat{v}(|\hat{a}|_M * v_M^2)_0 + (\bar{A} + 2\hat{v}\hat{A}) \varepsilon_0^{(3)} \\ c_0^{(1)} &= \hat{v}(|\bar{a}|_M * |\hat{a}|_M * v_M)_0 + \hat{v}^2(|\hat{a}|_M^2 * v_M)_0 + (\hat{v}\bar{A}\hat{A} + \hat{v}^2\hat{A}^2) \varepsilon_0^{(3)} \ . \end{aligned}$$

Now, for $k \in \{1, \dots, m-1\}$, let $\delta_1 = |\bar{L}| + \hat{v}|\hat{L}|$, $\delta_2 = |\bar{a}_k| + \hat{v}|\hat{a}_k|$ and define

$$c_k^{(5)} = \frac{20}{k^{s-4}} \ ,$$

$$\begin{aligned}
c_k^{(4)} &= 12k^4\delta_2 + \frac{48\delta_1 + 20\hat{\nu}|\hat{L}|}{k^{s-4}}, \\
c_k^{(3)} &= 12k^4\delta_2 \left(\hat{\nu}|\hat{L}| + 2\delta_1 \right) + \frac{1}{k^s} \left[6\nu k^2 + 36\delta_1^2 k^4 + 48\hat{\nu}\delta_1 k^4 |\hat{L}| \right] + (v_M^3)_k + \varepsilon_k^{(3)}, \\
c_k^{(2)} &= 2\nu k^2\delta_2 + 12\delta_1\delta_2 k^4 \left(\delta_1 + 2\hat{\nu}|\hat{L}| \right) \\
&\quad + \frac{1}{k^s} \left[2\nu k^2 \left(2\delta_1 + 3\hat{\nu}|\hat{L}| \right) + 4k^4\delta_1^2 \left(2\delta_1 + 9\hat{\nu}|\hat{L}| \right) \right] \\
&\quad + (|\bar{a}|_M * v_M^2)_k + 2\hat{\nu}(|\hat{a}|_M * v_M^2)_k + \left(\bar{A} + 2\hat{\nu}\hat{A} \right) \varepsilon_k^{(3)}, \\
c_k^{(1)} &= \hat{\nu} \left(2\nu k^2 + 12k^4\delta_1^2 \right) \delta_2 |\hat{L}| + 2\delta_1 \hat{\nu} |\hat{L}| \frac{1}{k^s} \left(2\nu k^2 + 4k^4\delta_1^2 \right) \\
&\quad + \hat{\nu}(|\bar{a}|_M * |\hat{a}|_M * v_M)_k + \hat{\nu}^2(|\hat{a}|_M^2 * v_M)_k + \left(\hat{\nu}\bar{A}\hat{A} + \hat{\nu}^2\hat{A}^2 \right) \varepsilon_k^{(3)}.
\end{aligned}$$

Then we have that for $k \in \{0, \dots, m-1\}$

$$\begin{aligned}
&\sum_{i=-1}^{\infty} \sum_{j=-1}^{\infty} \frac{\partial^2 f_k}{\partial x_i \partial x_j} (\bar{x} + t_k(w' + \hat{\nu}\hat{x}), \nu) (w'_i + \hat{\nu}\hat{x}_i) w_j \\
&\in c_k^{(5)} \mathbf{r}^5 + c_k^{(4)} \mathbf{r}^4 + c_k^{(3)} \mathbf{r}^3 + c_k^{(2)} \mathbf{r}^2 + c_k^{(1)} \mathbf{r}.
\end{aligned}$$

Let $e^{(5)} = e^{(4)} = 0$. For $i = 1, 2, 3, 4, 5$, define $c_F^{(i)} = \left(e^{(i)}, c_0^{(i)}, c_1^{(i)}, \dots, c_{m-1}^{(i)} \right)^T$. Let $C_F^{(1)} = V_F^{(0)} + \hat{\nu}V_F^{(1)} + |J_{m \times m}|c_F^{(i)}$ and for $i = 2, 3, 4, 5$ define $C_F^{(i)} = |J_{m \times m}|c_F^{(i)}$. We then proved that

$$[DT_\nu(w' + x_\nu)w]_F \in C_F^{(5)} \mathbf{r}^5 + C_F^{(4)} \mathbf{r}^4 + C_F^{(3)} \mathbf{r}^3 + C_F^{(2)} \mathbf{r}^2 + C_F^{(1)} \mathbf{r}.$$

Definition 5.4.2 For the cases $k \in \{-1, 0, 1, \dots, m-1\}$, we define

$$Z_F(r, \hat{\nu}) = C_F^{(5)} r^5 + C_F^{(4)} r^4 + C_F^{(3)} r^3 + C_F^{(2)} r^2 + C_F^{(1)} r. \quad (113)$$

5.4.3 Upper Bound for $Z_k(r, \hat{\nu})$ when $k \geq m$

Now consider $k \geq m$. Then

$$[DT_\nu(w' + x_\nu)w]_k = w_k - \frac{1}{\mu_k(\bar{L}, \nu_0)} Df_k(w' + x_\nu, \nu) w,$$

where

$$Df_k(w' + x_\nu, \nu) w = \mu_k(w'_{-1} + \bar{L} + \hat{\nu}\hat{L}, \nu) w_k$$

$$-3 \sum_{\substack{k_1+k_2+k_3=k \\ k_i \in \mathbb{Z}}} (w' + x_\nu)_{k_1} (w' + x_\nu)_{k_2} w_{k_3} .$$

Define

$$\mu_k^* = \mu_k(w'_{-1} + \bar{L} + \hat{\nu}\hat{L}, \nu) - \mu_k(\bar{L}, \nu_0) .$$

Then

$$\begin{aligned} \mu_k^* \in & k^4 \mathbf{r}^4 + \left[4(|\bar{L}| + \hat{\nu}|\hat{L}|)k^4 \right] \mathbf{r}^3 + \left[\nu k^2 + 6(|\bar{L}| + \hat{\nu}|\hat{L}|)k^4 \right] \mathbf{r}^2 \\ & + \left[2\nu k^2(|\bar{L}| + \hat{\nu}|\hat{L}|) + 4k^4(|\bar{L}| + \hat{\nu}|\hat{L}|)^3 \right] \mathbf{r} \\ & + \left[\hat{\nu} k^2 \left(2\nu|\hat{L}\bar{L}| + \bar{L}^2 + \nu\hat{\nu}|\hat{L}| \right) \right. \\ & \left. + \hat{\nu}|\hat{L}|k^4 \left(4|\bar{L}|^3 + 6\bar{L}^2\hat{\nu}|\hat{L}| + 4|\bar{L}|\hat{\nu}^2\hat{L}^2 + \hat{\nu}^3|\hat{L}|^3 \right) \right] \mathbf{1} . \end{aligned}$$

Note that

$$[DT_\nu(w' + x_\nu)w]_k = -\frac{1}{\mu_k(\bar{L}, \nu_0)} [\mu_k^* w_k + 3((w' + x_\nu)^2 * w)_k] .$$

Now,

$$\begin{aligned} ((w' + x_\nu)^2 * w)_k \in & (v^3)_k \mathbf{r}^3 + 2[(|\bar{a}| * v^2)_k + \hat{\nu}(|\hat{a}| * v^2)_k] \mathbf{r}^2 \\ & + [(|\bar{a}|^2 * v)_k + 2\hat{\nu}(|\bar{a}| * |\hat{a}| * v)_k + \hat{\nu}^2(|\hat{a}|^2 * v)_k] \mathbf{r} \end{aligned}$$

Consider now the cases $k \in \{m, \dots, M-1\}$ and recall that $w_k \in \frac{1}{k^s} \mathbf{r}$. Consider the case $p = 3$ and recall the definition of $\varepsilon_k^{(p)} = \varepsilon_k^{(3)}$ from (48). By Corollary 3.5.1,

$$\begin{aligned} ((w' + x_\nu)^2 * w)_k \in & \left[(v_M^3)_k + \varepsilon_k^{(3)} \right] \mathbf{r}^3 \\ & + 2 \left[(|\bar{a}|_M * v_M^2)_k + \hat{\nu}(|\hat{a}|_M * v_M^2)_k + \left(\bar{A} + \hat{\nu}\hat{A} \right) \varepsilon_k^{(3)} \right] \mathbf{r}^2 \\ & + [(|\bar{a}|_M^2 * v_M)_k + 2\hat{\nu}(|\bar{a}|_M * |\hat{a}|_M * v_M)_k \\ & + \hat{\nu}^2(|\hat{a}|_M^2 * v_M)_k + \left(\bar{A} + \hat{\nu}\hat{A} \right)^2] \mathbf{r} . \end{aligned}$$

Recall that $\delta_1 = (|\bar{L}| + \hat{\nu}|\hat{L}|)$. For every $k \in \{m, \dots, M-1\}$, define

$$C_k^{(5)} = \frac{1}{k^{s-4} |\mu_k(\bar{L}, \nu_0)|} ,$$

$$\begin{aligned}
C_k^{(4)} &= \frac{4\delta_1}{k^{s-4}|\mu_k(\bar{L}, \nu_0)|} , \\
C_k^{(3)} &= \frac{1}{|\mu_k(\bar{L}, \nu_0)|} \left[\frac{\nu k^2 + 6\delta_1 k^4}{k^s} + 3(v_M^3)_k + 3\varepsilon_k^{(3)} \right] , \\
C_k^{(2)} &= \frac{1}{|\mu_k(\bar{L}, \nu_0)|} \left[\frac{2\nu k^2 \delta_1 + 4k^4 \delta_1^3}{k^s} \right. \\
&\quad \left. + 2(|\bar{a}|_M * v_M^2)_k + 2\hat{\nu}(|\hat{a}|_M * v_M^2)_k + 2\left(\bar{A} + \hat{\nu}\hat{A}\right)\varepsilon_k^{(3)} \right] , \\
C_k^{(1)} &= \frac{1}{|\mu_k(\bar{L}, \nu_0)|} \left[\frac{\hat{\nu}k^2}{k^s} \left(2\nu|\hat{L}\bar{L}| + \bar{L}^2 + \nu\hat{\nu}|\hat{L}| \right) \right. \\
&\quad \left. + \frac{\hat{\nu}|\hat{L}|k^4}{k^s} \left(4|\bar{L}|^3 + 6\bar{L}^2\hat{\nu}|\hat{L}| + 4|\bar{L}|\hat{\nu}^2\hat{L}^2 + \hat{\nu}^3|\hat{L}|^3 \right) \right. \\
&\quad \left. + 3(|\bar{a}|_M^2 * v_M)_k + 6\hat{\nu}(|\bar{a}|_M * |\hat{a}|_M * v_M)_k + 3\hat{\nu}^2(|\hat{a}|_M^2 * v_M)_k + 3\left(\bar{A} + \hat{\nu}\hat{A}\right)^2\varepsilon_k^{(3)} \right] .
\end{aligned}$$

We then proved that for every $k \in \{m, \dots, M-1\}$,

$$[DT_\nu(w' + x_\nu)w]_k \in C_k^{(5)}\mathbf{r}^5 + C_k^{(4)}\mathbf{r}^4 + C_k^{(3)}\mathbf{r}^3 + C_k^{(2)}\mathbf{r}^2 + C_k^{(1)}\mathbf{r} .$$

Definition 5.4.3 For $k \in \{m, \dots, M-1\}$, define

$$Z_k(r, \hat{\nu}) = C_k^{(5)}r^5 + C_k^{(4)}r^4 + C_k^{(3)}r^3 + C_k^{(2)}r^2 + C_k^{(1)}r . \quad (114)$$

Choose M large enough so that, given $\bar{L}, \nu_0 > 0$, we have that

$$\frac{\nu_0}{\bar{L}^2 k^2} - \frac{1}{\bar{L}^4 k^4} \leq \frac{1}{2} ,$$

for all $k \geq M$. In this case, $|\mu_k(\bar{L}, \nu_0)| = \bar{L}^4 k^4 [1 - (\frac{\nu_0}{\bar{L}^2 k^2} - \frac{1}{\bar{L}^4 k^4})]$, for all $k \geq M$.

Hence, we have that

$$\frac{1}{|\mu_k(\bar{L}, \nu_0)|} \leq \frac{2}{\bar{L}^4 k^4}$$

and then

$$\begin{aligned}
\frac{\mu_k^* w_k}{|\mu_k(\bar{L}, \nu_0)|} &\in \frac{1}{k^s} \left\{ \frac{2}{\bar{L}^4} \mathbf{r}^5 + \frac{8}{\bar{L}^4} \left(|\bar{L}| + \hat{\nu}|\hat{L}| \right) \mathbf{r}^4 + \frac{2}{\bar{L}^4} \left[\frac{\nu}{M^2} + 6 \left(|\bar{L}| + \hat{\nu}|\hat{L}| \right) \right] \mathbf{r}^3 \right. \\
&\quad \left. + \frac{4}{\bar{L}^4} \left[\frac{\nu}{M^2} \left(|\bar{L}| + \hat{\nu}|\hat{L}| \right) + 2 \left(|\bar{L}| + \hat{\nu}|\hat{L}| \right)^3 \right] \mathbf{r}^2 \right. \\
&\quad \left. + \left[\frac{2\hat{\nu}}{\bar{L}^4 M^2} \left(2\nu|\hat{L}\bar{L}| + \bar{L}^2 + \nu\hat{\nu}|\hat{L}| \right) \right] \mathbf{r} \right\}
\end{aligned}$$

$$+\frac{2\hat{\nu}|\hat{L}|}{\bar{L}^4} \left(4|\bar{L}|^3 + 6\bar{L}^2\hat{\nu}|\hat{L}| + 4|\bar{L}|\hat{\nu}^2\hat{L}^2 + \hat{\nu}^3|\hat{L}|^3 \right) \mathbf{r} \Big\} .$$

Recall Theorem 3.3.1 and (46) for $p = 3$. Then, for $k \geq M$, we get that

$$\begin{aligned} ((w' + x_\nu)^2 * w)_k &\in (v^3)_k \mathbf{r}^3 + 2 \left[(|\bar{a}| * v^2)_k + \hat{\nu}(|\hat{a}| * v^2)_k \right] \mathbf{r}^2 \\ &\quad + \left[(|\bar{a}|^2 * v)_k + 2\hat{\nu}(|\bar{a}| * |\hat{a}| * v)_k + \hat{\nu}^2(|\hat{a}|^2 * v)_k \right] \mathbf{r} \\ &\subseteq \frac{\alpha_k^{(3)}}{k^s} \left[\mathbf{r}^3 + 2 \left(\bar{A} + \hat{\nu}\hat{A} \right) \mathbf{r}^2 + \left(\bar{A} + \hat{\nu}\hat{A} \right) \mathbf{r} \right] \\ &\subseteq \frac{1}{k^s} \left[\alpha_M^{(3)} \mathbf{r}^3 + 2\alpha_M^{(3)} \left(\bar{A} + \hat{\nu}\hat{A} \right) \mathbf{r}^2 + \alpha_M^{(3)} \left(\bar{A} + \hat{\nu}\hat{A} \right)^2 \mathbf{r} \right] . \end{aligned}$$

Define

$$\begin{aligned} C_M^{(5)} &= \frac{2}{\bar{L}^4} , \quad C_M^{(4)} = \frac{8\delta_1}{\bar{L}^4} , \quad C_M^{(3)} = \frac{2}{\bar{L}^4} \left[\frac{\nu}{M^2} + 6\delta_1 \right] + \frac{2\alpha_M^{(3)}}{\bar{L}^4 M^4} , \\ C_M^{(2)} &= \frac{4}{\bar{L}^4} \left[\frac{\nu}{M^2} \delta_1 + 2\delta_1^3 \right] + \frac{4\alpha_M^{(3)}}{\bar{L}^4 M^4} \left(\bar{A} + \hat{\nu}\hat{A} \right) , \\ C_M^{(1)} &= \frac{2\hat{\nu}}{\bar{L}^4 M^2} \left(2\nu|\hat{L}\bar{L}| + \bar{L}^2 + \nu\hat{\nu}|\hat{L}| \right) \\ &\quad + \frac{2\hat{\nu}|\hat{L}|}{\bar{L}^4} \left(4|\bar{L}|^3 + 6\bar{L}^2\hat{\nu}|\hat{L}| + 4|\bar{L}|\hat{\nu}^2\hat{L}^2 + \hat{\nu}^3|\hat{L}|^3 \right) + \frac{2\alpha_M^{(3)}}{\bar{L}^4 M^4} \left(\bar{A} + \hat{\nu}\hat{A} \right)^2 . \end{aligned}$$

We then proved that if M is large enough, then for every $k \geq M$

$$[DT_\nu(w' + x_\nu)w]_k \in \frac{1}{k^s} \left[C_M^{(5)} \mathbf{r}^5 + C_M^{(4)} \mathbf{r}^4 + C_M^{(3)} \mathbf{r}^3 + C_M^{(2)} \mathbf{r}^2 + C_M^{(1)} \mathbf{r} \right] .$$

Definition 5.4.4 For $k \geq M$, define

$$Z_k(r, \hat{\nu}) = \frac{1}{k^s} \left[C_M^{(5)} r^5 + C_M^{(4)} r^4 + C_M^{(3)} r^3 + C_M^{(2)} r^2 + C_M^{(1)} r \right] . \quad (115)$$

Note that defined like this the Z_k satisfies

$$Z_k(r, \hat{\nu}) \leq Z_M(r, \hat{\nu}) , \quad k \geq M . \quad (116)$$

5.4.4 Definition of the Radii Polynomials

We are finally ready for the following.

Definition 5.4.5 Recalling (108), (109), (113) and (114), we define the *finite radii polynomials* $\{p_k\}_{k=-1, \dots, M-1}$ by

$$p_k(r, \hat{\nu}) = C_k^{(5)} r^5 + C_k^{(4)} r^4 + C_k^{(3)} r^3 + C_k^{(2)} r^2 + \left[C_k^{(1)} - \frac{1}{k^s} \right] r + Y_k(\hat{\nu}) . \quad (117)$$

We define the *tail radii polynomial* p_M by

$$\tilde{p}_M(r, \hat{\nu}) = C_M^{(5)} r^4 + C_M^{(4)} r^3 + C_M^{(3)} r^2 + C_M^{(2)} r + C_M^{(1)} - 1 . \quad (118)$$

Combining (115) and (116), we have that

$$p_M(r, \hat{\nu}) < 0 \implies Y_k(\hat{\nu}) + Z_k(r, \hat{\nu}) < \frac{r}{k^s} , \quad k \geq M .$$

5.5 Verification of the Geometric Hypotheses ($\mathcal{H}$)

For a fixed $s \geq 4$, suppose that using the radii polynomials, we found a set

$$W_{x_\nu}(r) = x_\nu + \left([-r, r]^2 \times \prod_{k=1}^{\infty} \left[-\frac{r}{k^s}, \frac{r}{k^s} \right] \right)$$

such that for each $\nu \in [\nu_0, \nu_0 + \hat{\nu}]$, $W_{x_\nu}(r)$ contains a unique zero of (99) at the parameter value ν . Recall that

$$(\mathcal{H}) \quad \begin{cases} (1) \ \tilde{u} \text{ has exactly four monotone laps and extrema } \{\tilde{u}_i\}_{i=1}^4 \\ (2) \ \tilde{u}_1 \text{ and } \tilde{u}_3 \text{ are minima and } \tilde{u}_2 \text{ and } \tilde{u}_4 \text{ are maxima} \\ (3) \ \tilde{u}_1 < -1 < \tilde{u}_3 < 1 < \tilde{u}_2 = \tilde{u}_4. \end{cases}$$

We need to make sure that the unique zero of f in W_{x_ν} satisfies the hypotheses of ($\mathcal{H}$). The following will help simplifying the verification.

Proposition 5.5.1 *Suppose that $\tilde{u}_{\nu_0}$ is a periodic solution of (97) at the energy level $E = 0$ when $\nu = \nu_0$. Suppose also that $\tilde{u}_{\nu_0}$ satisfies ($\mathcal{H}$). If the set $\{\tilde{u}_\nu | \nu \in [\nu_0, \nu_{\max}]\}$ is a continuous branch of periodic solutions of (97) at $E = 0$, then automatically, $\tilde{u}_\nu$ satisfies ($\mathcal{H}$) for all $\nu \in [\nu_0, \nu_{\max}]$.*

Proof. Denote by $\tilde{u}_2(\nu)$ the moving local maximum as we change $\nu \geq \nu_0$ and such that $\tilde{u}_2(\nu_0) = \tilde{u}_2$. Then $\tilde{u}_2(\nu)$ does not cross the line $u = 1$, since otherwise we would get the existence of $\nu \in [\nu_0, \nu_{\max}]$ such that $\tilde{u}'_2(\nu) = \tilde{u}''_2(\nu) = 0$ (since $E = 0$) and $\tilde{u}'''_2(\nu) = 0$ (otherwise it is no longer the maximum) which would lead to a contradiction since uniqueness of the initial value problem for the ODE then says that $u(y) = 1$ for all y (which it isn't). Similarly the minima $\tilde{u}_1(\nu)$ and $\tilde{u}_3(\nu)$ cannot cross $u = -1$ or $u = 1$, since then $u' = 0$, $u'' = 0$ (since $E = 0$), and $u''' = 0$ (by symmetry) and the contradiction follows again. At these extrema, we have that $u' = 0$ and hence, the energy is $E(u, \nu) = -\frac{1}{2}(u'')^2 + \frac{1}{4}(u^2 - 1)^2 = 0$. Since $\tilde{u}_i \neq \pm 1$, then $\tilde{u}''_i \neq 0$ and by the implicit function theorem, we get that extrema vary continuously as we move $\nu \in [\nu_0, \nu_{\max}]$ and, as already said, they cannot cross ± 1 .

We now prove that there can't be any other extrema popping up at some $\nu \in [\nu_0, \nu_{\max}]$. We argue by contradiction. Suppose for some ν there is an additional extremum. Then there is a smallest $\nu_* > \nu_0$ for which there is an additional extremum. In particular, there are no additional extrema for $\nu < \nu_*$.

For $\nu = \nu_*$, there is a point $y_* \in (0, \pi/L)$ with $u'_{\nu_*}(y_*) = 0$, and not one of the usual extrema (u_1, u_2, u_3) . If $u''(y_*) \neq 0$ then by the implicit function theorem this extremum persists for $\nu < \nu_*$, a contradiction. Hence it must be that $u''(y_*) = 0$, and thus $u(y_*) = \pm 1$ since $E = 0$. Finally, $u'''(y_*) \neq 0$ for the same reason as before. Let us consider the case $u(y_*) = 1$ and $u'''(y_*) > 0$. All other (three) cases are analogous.

We thus have

$$u_{\nu_*}(y_*) = 1, \quad u'_{\nu_*}(y_*) = 0, \quad u''_{\nu_*}(y_*) = 0, \quad u'''_{\nu_*}(y_*) > 0. \quad (119)$$

Clearly $u'_{\nu_*}(y) > 0$ for y sufficiently close to y_* . Let $\nu_n = \nu_* - 1/n$ be a sequence approaching ν_* from below. Then by the implicit function theorem, for large enough n , there exists points y_n such that $\lim_{n \rightarrow \infty} y_n = y_*$ and $u''_{\nu_n}(y_n) = 0$, and $u'_{\nu_n}(y_n) \neq 0$ by the assumption that ν_* is the smallest value for which there is an additional extremum; in fact, for the same reason it follows that $u'_{\nu_n}(y_n) > 0$.

We conclude from $E = 0$ and $u''_{\nu_n}(y_n) = 0$ that

$$\left[u'''_{\nu_n}(y_n) + \frac{\nu_n}{2} u'_{\nu_n}(y_n) \right] u'_{\nu_n}(y_n) = -\frac{1}{4} (u_{\nu_n}(y_n)^2 - 1)^2.$$

Since $u'_{\nu_n}(y_n) > 0$, this means that

$$u'''_{\nu_n}(y_n) + \frac{\nu_n}{2} u'_{\nu_n}(y_n) \leq 0.$$

Finally, take the limit $n \rightarrow \infty$ in the above inequality to obtain

$$u'''_{\nu_*}(y_*) + \frac{\nu_*}{2} u'_{\nu_*}(y_*) \leq 0,$$

which contradicts (119). Hence, for all $\nu \in [\nu_0, \nu_{\max}]$, we have that $(\mathcal{H})$ is always satisfied. ■

Hence, we only need to show that $(\mathcal{H})$ is satisfied at $\nu = \nu_0$. Consider $\bar{x}$ and denote by $\tilde{x} = (\tilde{L}, \tilde{a}_0, \tilde{a}_1, \dots)$ the unique element of $W_{\bar{x}}$ such that $f(\tilde{x}, \nu_0) = 0$. The corresponding periodic function $\tilde{u}$ is defined by

$$\tilde{u}(y) = \tilde{a}_0 + 2 \sum_{k=1}^{\infty} \tilde{a}_k \cos(k\tilde{L}y).$$

Also, we have that

$$\begin{aligned} \tilde{u}'(y) &= -2\tilde{L} \sum_{k=1}^{\infty} k\tilde{a}_k \sin(k\tilde{L}y) \\ \tilde{u}''(y) &= -2\tilde{L}^2 \sum_{k=1}^{\infty} k^2 \tilde{a}_k \cos(k\tilde{L}y). \end{aligned}$$

Note that $\tilde{L} \in \tilde{\mathbf{L}} := [\bar{L} - r, \bar{L} + r]$ and

$$\tilde{a}_k \in \begin{cases} \tilde{\mathbf{a}}_0 := [\bar{a}_0 - r, \bar{a}_0 + r], & k = 0 \\ \tilde{\mathbf{a}}_k := [\bar{a}_k - \frac{r}{k^s}, \bar{a}_k + \frac{r}{k^s}], & k = 1, \dots, m-1 \\ \tilde{\mathbf{a}}_k := [-\frac{r}{k^s}, \frac{r}{k^s}], & k \geq m. \end{cases}$$

Consider $y \in \mathbf{y} := [y^-, y^+] \subset [0, \frac{2\pi}{\bar{L}-r}]$. Let $\mathbf{1} = [-1, 1]$. Then using interval arithmetic, we can compute rigorous interval enclosures of $\tilde{u}(y)$, $\tilde{u}'(y)$ and $\tilde{u}''(y)$:

$$\tilde{u}(y) \in \tilde{\mathbf{u}}[\mathbf{y}] := \tilde{\mathbf{a}}_0 + 2 \sum_{k=1}^{m-1} \tilde{\mathbf{a}}_k \cos(k\tilde{\mathbf{L}}\mathbf{y}) + \frac{2r}{(m-1)^{s-1}(s-1)} \mathbf{1},$$

$$\begin{aligned}\tilde{u}'(y) &\in \tilde{\mathbf{u}}'[\mathbf{y}] := -2\tilde{\mathbf{L}} \sum_{k=1}^{m-1} k\tilde{\mathbf{a}}_{\mathbf{k}} \sin(k\tilde{\mathbf{L}}\mathbf{y}) + \frac{2r}{(m-1)^{s-2}(s-2)}\tilde{\mathbf{L}}, \\ \tilde{u}(y) &\in \tilde{\mathbf{u}}''[\mathbf{y}] := 2\tilde{\mathbf{L}}^2 \sum_{k=1}^{m-1} k^2\tilde{\mathbf{a}}_{\mathbf{k}} \cos(k\tilde{\mathbf{L}}\mathbf{y}) + \frac{2r}{(m-1)^{s-3}(s-3)}\tilde{\mathbf{L}}^2.\end{aligned}$$

Note that we a priori know that $\tilde{u}$ is symmetric in the lines $y = 0$ and $y = \frac{\pi}{L}$. That will be useful in the following procedure:

Procedure 5.5.2 *To check that $(\mathcal{H})$ is verified at ν_0 , we proceed as follows.*

1. *Verify that $\tilde{\mathbf{u}}[0] \subset (-\infty, -1)$. That implies that $\tilde{u}_1 < -1$.*
2. *Find the largest $y_0 > 0$ such that $\tilde{\mathbf{u}}''[0, y_0] \subset (0, \infty)$. Hence, there is a unique extremum in $[0, y_0]$ namely the minimum $\tilde{u}_1 = 0$.*
3. *Find the largest $y_1 > y_0$ such that $\tilde{\mathbf{u}}'[y_0, y_1] \subset (0, \infty)$. Hence, the interval $[y_0, y_1]$ does not contain any extremum.*
4. *Verify that $\tilde{\mathbf{u}}[y_1] \subset (1, \infty)$.*
5. *Find the largest $y_2 > y_1$ such that $\tilde{\mathbf{u}}[y_1, y_2] \subset (1, \infty)$ and $\tilde{\mathbf{u}}''[y_1, y_2] \subset (-\infty, 0)$.*
6. *Verify that $\tilde{\mathbf{u}}'[y_2] \subset (-\infty, 0)$. That implies that there is a unique extremum in $[y_1, y_2]$ namely the maximum $\tilde{u}_2 > 1$.*
7. *Find the largest $y_3 > y_2$ such that $\tilde{\mathbf{u}}'[y_2, y_3] \subset (-\infty, 0)$. Hence, the interval $[y_2, y_3]$ does not contain any extremum.*
8. *Verify that $\tilde{\mathbf{u}}[y_3] \subset (-1, 1)$.*
9. *Find the largest $y_4 > y_3$ such that $\tilde{\mathbf{u}}[y_3, y_4] \subset (-1, 1)$ and $\tilde{\mathbf{u}}''[y_3, y_4] \subset (0, \infty)$.*
10. *Verify that $y_4 > \frac{\pi}{L-r}$. That implies that there is a unique extremum in $[y_3, y_4]$ namely the minimum $-1 < \tilde{u}_3 < 1$.*

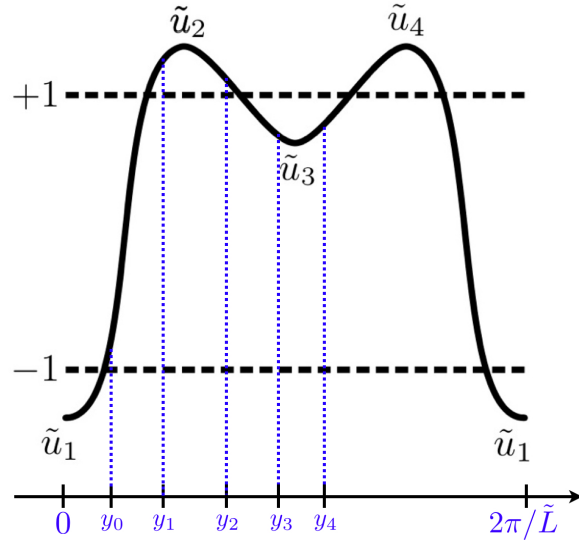


Figure 37: Procedure to make sure that the periodic solution $\tilde{u}$ satisfies $(\mathcal{H})$.

By symmetry of the periodic solution with respect to the line $y = \frac{\pi}{L}$, we can stop the procedure. Hence, if all steps of Procedure 5.5.2, then $\tilde{u}$ satisfies the hypotheses $(\mathcal{H})$.

Therefore, if Procedure 5.5.2 succeed at ν_0 , then combining Proposition 5.5.1 with Corollary 5.1.4, we get that for all $\nu \in [\nu_0, \nu_{\max}]$, the Swift-Hohenberg equation (97) is chaotic at the energy level $E = 0$.

CHAPTER VI

PERIODIC SOLUTIONS OF DELAY EQUATIONS

The work presented in this chapter was strongly motivated by helpful discussions with John-Mallet Paret and Roger Nussbaum.

6.1 *Background*

Consider the Wright's equation

$$\dot{y}(t) = -\alpha y(t-1)[1 + y(t)]. \quad (120)$$

The goal of this section is to transform the study of periodic solutions of (120) into the study of the zeros of a parameter dependent infinite dimensional problem. Since we look for periodic solutions of (120) on an a priori unknown time interval $[0, \frac{2\pi}{L}]$, we consider the expansion of the periodic solution y in Fourier series

$$y(t) = \sum_{k=-\infty}^{\infty} c_k e^{ikLt}, \quad (121)$$

where the c_k are complex numbers satisfying $c_{-k} = \overline{c_k}$, since $y(\cdot) \in \mathbb{R}$. Let $c = \{c_k\}_{k \in \mathbb{Z}}$. Substituting

$$y(t-1) = \sum_{k=-\infty}^{\infty} c_k e^{-ikL} e^{ikLt} \quad \text{and} \quad \dot{y}(t) = \sum_{k=-\infty}^{\infty} c_k ikL e^{ikLt}$$

in (120), we get that

$$\sum_{k_1=-\infty}^{\infty} [ik_1L + \alpha e^{-ik_1L}] c_{k_1} e^{ik_1Lt} + \alpha \left[\sum_{k_2=-\infty}^{\infty} c_{k_2} e^{-ik_2L} e^{ik_2Lt} \right] \left[\sum_{k_3=-\infty}^{\infty} c_{k_3} e^{ik_3Lt} \right] = 0.$$

Taking the inner product with each e^{ikLt} , we get the following countable system of equations to be satisfied

$$g_k(L, c, \alpha) := [ikL + \alpha e^{-ikL}] c_k + \alpha \sum_{k_1+k_2=k} e^{-ik_1L} c_{k_1} c_{k_2} = 0, \quad k \in \mathbb{Z}. \quad (122)$$

Since $g_{-k} = \overline{g_k}$ and $c_{-k} = \overline{c_k}$, we only need to consider the cases $k \in \mathbb{N}$ when solving for (122). Since we will not a priori know the period L of (120), we leave L as a variable. Denoting the real part and the imaginary part of c_k respectively by a_k and b_k , we get that an equivalent expansion for (121) is given by

$$y(t) = a_0 + 2 \sum_{k=1}^{\infty} [a_k \cos kLt - b_k \sin kLt]. \quad (123)$$

Note that $a_k = a_{-k}$ and $b_k = -b_{-k}$. Hence, we get that $b_0 = 0$. Given $k \in \mathbb{N}$, the real and the imaginary parts of (122) are respectively given by

$$\begin{aligned} (\kappa_k a_k + \beta_k b_k) + \alpha \sum_{k_1+k_2=k} (\cos k_1 L)(a_{k_1} a_{k_2} - b_{k_1} b_{k_2}) + (\sin k_1 L)(a_{k_1} b_{k_2} + b_{k_1} a_{k_2}) &= 0, \\ (-\beta_k a_k + \kappa_k b_k) + \alpha \sum_{k_1+k_2=k} -(\sin k_1 L)(a_{k_1} a_{k_2} - b_{k_1} b_{k_2}) + (\cos k_1 L)(a_{k_1} b_{k_2} + b_{k_1} a_{k_2}) &= 0, \end{aligned}$$

where $\kappa_k := \alpha \cos kL$ and $\beta_k := -kL + \alpha \sin kL$. Define

$$x_k = \begin{cases} [L, a_0], & k = 0 \\ [a_k, b_k], & k > 0 \end{cases}$$

and let $x = (x_0, x_1, \dots, x_k, \dots)^T$. We impose scaling condition $y(0) = 0$. Hence, define

$$f_{0,1}(x) = y(0) = a_0 + 2 \sum_{k=1}^{\infty} a_k.$$

Define $f_{0,2}(x, \alpha)$ to be the real part of $g_0(x, \alpha)$

$$f_{0,2}(x, \alpha) = \alpha \left[a_0 + a_0^2 + 2 \sum_{k_1=1}^{\infty} (\cos k_1 L) (a_{k_1}^2 + b_{k_1}^2) \right].$$

Define

$$f_0(x, \alpha) = \begin{bmatrix} f_{0,1}(x) \\ f_{0,2}(x, \alpha) \end{bmatrix} \quad (124)$$

For $k \in \mathbb{N}$ strictly positive, let

$$R_k(L, \alpha) = \begin{pmatrix} \kappa_k & \beta_k \\ -\beta_k & \kappa_k \end{pmatrix} = \begin{pmatrix} \alpha \cos kL & -kL + \alpha \sin kL \\ kL - \alpha \sin kL & \alpha \cos kL \end{pmatrix}$$

and for $k_1 \in \mathbb{Z}$, let

$$\Theta_{k_1}(L) = \begin{pmatrix} \cos k_1 L & \sin k_1 L \\ -\sin k_1 L & \cos k_1 L \end{pmatrix}.$$

For $k \geq 1$, define

$$\begin{aligned} f_k(x, \alpha) &= \begin{bmatrix} f_{k,1}(x, \alpha) \\ f_{k,2}(x, \alpha) \end{bmatrix} \\ &= R_k(L, \alpha) \begin{pmatrix} a_k \\ b_k \end{pmatrix} + \alpha \sum_{\substack{k_1+k_2=k \\ k_i \in \mathbb{Z}}} \Theta_{k_1}(L) \begin{pmatrix} a_{k_1} a_{k_2} - b_{k_1} b_{k_2} \\ a_{k_1} b_{k_2} + b_{k_1} a_{k_2} \end{pmatrix}. \end{aligned} \quad (125)$$

Finally, define the function $f : \ell^2 \times [\frac{\pi}{2}, \infty) \rightarrow \text{Im}(f) : (x, \alpha) \mapsto f(x, \alpha)$ component-wise by

$$f_k(x, \alpha) = \begin{cases} \begin{pmatrix} a_0 + 2 \sum_{k=1}^{\infty} a_k \\ \alpha [a_0 + a_0^2 + 2 \sum_{k=1}^{\infty} (\cos k_1 L) (a_{k_1}^2 + b_{k_1}^2)] \end{pmatrix}, & k = 0 \\ R_k(L, \alpha) \begin{pmatrix} a_k \\ b_k \end{pmatrix} + \alpha \sum_{\substack{k_1+k_2=k \\ k_i \in \mathbb{Z}}} \Theta_{k_1}(L) \begin{pmatrix} a_{k_1} a_{k_2} - b_{k_1} b_{k_2} \\ a_{k_1} b_{k_2} + b_{k_1} a_{k_2} \end{pmatrix}, & k \geq 1 \end{cases}, \quad (126)$$

Hence, the problem of finding periodic solutions of (120) is equivalent to finding zeros of (126). Since the periodic solutions of (120) are analytic (see [27]), it means that the Fourier coefficients a_k and b_k have a very fast decay. We are ready to do validated continuation on the infinite dimensional problem

$$f(x, \alpha) = 0. \quad (127)$$

We now have to construct the radii polynomials.

6.2 Construction of the Radii Polynomials

Since we want to do numerics on (127), we first consider a finite dimensional approximation on which we compute. Throughout this section, we use the subscript $(\cdot)_F$ to

denote the $2m$ entries corresponding to $k = 0, \dots, m-1$. Let $x_F = (x_0, \dots, x_{m-1})^T$ and $f_F = (f_0, \dots, f_{m-1})^T$ so that we can define the *Galerkin projection* of f by

$$f^{(m)} : \mathbb{R}^{2m} \times \mathbb{R} \rightarrow \mathbb{R}^{2m} : (x_F, \alpha) \mapsto f^{(m)}(x_F, \alpha) := f_F([x_F, 0], \alpha). \quad (128)$$

To be more explicit, we get that

$$f_k^{(m)}(x_F, \alpha) = \begin{cases} \begin{pmatrix} a_0 + 2 \sum_{k=1}^{m-1} a_k \\ \alpha [a_0 + a_0^2 + 2 \sum_{k_1=1}^{m-1} (\cos k_1 L) (a_{k_1}^2 + b_{k_1}^2)] \end{pmatrix}, & k = 0 \\ R_k(L, \alpha) \begin{pmatrix} a_k \\ b_k \end{pmatrix} + \alpha \sum_{\substack{k_1+k_2=k \\ |k_1|, |k_2| < m}} \Theta_{k_1}(L) \begin{pmatrix} a_{k_1} a_{k_2} - b_{k_1} b_{k_2} \\ a_{k_1} b_{k_2} + b_{k_1} a_{k_2} \end{pmatrix}, & k = 1, \dots, m-1. \end{cases}$$

Suppose that at the parameter value α_0 , we computed using the classical continuation method introduced in Section 1.1, a hyperbolic zero $\bar{x}_F \in \mathbb{R}^{2m}$ of $f^{(m)}$ i.e. a point such that

$$f^{(m)}(\bar{x}_F, \alpha_0) \approx 0 \text{ and } Df^{(m)}(\bar{x}_F, \alpha_0) \text{ is invertible.}$$

We then define the *tangent* $\hat{x}_F \in \mathbb{R}^{2m}$ by

$$Df^{(m)}(\bar{x}_F, \alpha_0) \cdot \hat{x}_F = -\frac{\partial f^{(m)}}{\partial \alpha}(\bar{x}_F, \alpha_0)$$

Let

$$\bar{x} = \begin{pmatrix} \bar{x}_F \\ 0_\infty \end{pmatrix} \text{ and } \hat{x} = \begin{pmatrix} \hat{x}_F \\ 0_\infty \end{pmatrix} \in \ell^2.$$

For $k \geq m$, define $\Lambda_k = \Lambda_k(\bar{x}, \alpha_0)$ by

$$\begin{aligned} \Lambda_k &= \frac{\partial f_k}{\partial x_k}(\bar{x}, \alpha_0) \\ &= R_k(\bar{L}, \alpha_0) + \alpha \left[[\Theta_k(\bar{L}) + \Theta_0] \begin{pmatrix} \bar{a}_0 & 0 \\ 0 & \bar{a}_0 \end{pmatrix} + [\Theta_{-k}(\bar{L}) + \Theta_{2k}(\bar{L})] \begin{pmatrix} \bar{a}_{2k} & \bar{b}_{2k} \\ \bar{b}_{2k} & -\bar{a}_{2k} \end{pmatrix} \right] \\ &= R_k(\bar{L}, \alpha_0) + \alpha_0 \bar{a}_0 [\Theta_k(\bar{L}) + \Theta_0], \end{aligned}$$

since for $k \geq m$, $\bar{a}_{2k} = \bar{b}_{2k} = 0$. Let $J_{F \times F}$ the computed numerical inverse of $Df^{(m)}(\bar{x}_F, \alpha_0)$ and

$$J := \begin{bmatrix} J_{F \times F} & & & 0 \\ & \Lambda_m^{-1} & & \\ & 0 & \Lambda_{m+1}^{-1} & \\ & & & \ddots \end{bmatrix} \quad (129)$$

For every parameter value $\alpha \geq \alpha_0$, we define the operator T_α by

$$T_\alpha(x) = x - J \cdot f(x, \alpha) \quad (130)$$

and the *predictor* x_α by

$$x_\alpha = \bar{x} + \hat{\alpha} \hat{x}, \quad (131)$$

where

$$\hat{\alpha} := \alpha - \alpha_0 \geq 0.$$

Fixing $s \geq 2$, we define the following set centered at x_α

$$\begin{aligned} W_{x_\alpha}(r) &= x_\alpha + W(r) \\ &= x_\alpha + \left\{ [-r, r]^2 \times \prod_{k=1}^{\infty} \left[-\frac{r}{k^s}, \frac{r}{k^s} \right]^2 \right\} \end{aligned} \quad (132)$$

so that a point $w \in W(r)$ can be expressed component-wise like

$$w = ([w_0^L, w_0^a], [w_1^a, w_1^b], \dots, [w_k^a, w_k^b], \dots)^T. \quad (133)$$

6.2.1 Computation of the $Y_k(\alpha)$

Recalling the definition of Y_k in (14) and equations (129) and (130), we get that

$$Y_k(\alpha) \geq |[Jf(x_\alpha, \alpha)]_k| \in \mathbb{R}^2.$$

Definition 6.2.1 Let $u, v \in \mathbb{R}^m$. We define the component-wise inequality by $\leq_{cw}$ and say that $u \leq_{cw} v$ if $u_i \leq v_i$, for all $i = 1, \dots, m$.

For the cases $k \in \{0, \dots, m-1\}$,

$$Y_F(\alpha) \geq |J_{F \times F} [f_F(x_\alpha, \alpha)]| \in \mathbb{R}^{2m} \quad (134)$$

and for a fixed $m \leq k \leq 2m-2$,

$$Y_k(\alpha) \geq |\Lambda_k(\bar{x}, \alpha_0)^{-1} \cdot f_k(x_\alpha, \alpha)| \in \mathbb{R}^2. \quad (135)$$

Now, remark that since $[x_\alpha]_k = (0, 0)^T$ for $k \geq m$ then $f_k(x_\alpha, \alpha) = (0, 0)^T$ for $k \geq 2m-1$. For $k \geq 2m-1$, we then let $Y_k(\alpha) = (0, 0)^T$. In order to construct an upper bound for Y_k , we need to compute $f_k(x_\alpha, \alpha)$, for $k \geq 0$.

Let

$$\begin{aligned} \hat{r}_{0,1} &= \hat{\alpha} \left[\hat{a}_0 + 2 \sum_{k=1}^{m-1} \hat{a}_k \right], \\ \hat{r}_{0,2} &= \alpha [\bar{a}_0 + \hat{\alpha} \hat{a}_0] + \alpha [\bar{a}_0 + \hat{\alpha} \hat{a}_0]^2 \\ &\quad + 2\alpha \sum_{k_1=1}^{m-1} \cos(k_1[\bar{L} + \hat{\alpha} \hat{L}]) \left([\bar{a}_{k_1} + \hat{\alpha} \hat{a}_{k_1}]^2 + [\bar{b}_{k_1} + \hat{\alpha} \hat{b}_{k_1}]^2 \right) \\ &\quad - \alpha_0 \left[\bar{a}_0 + \bar{a}_0^2 + 2 \sum_{k_1=1}^{m-1} \cos(k_1 \bar{L}) (\bar{a}_{k_1}^2 + \bar{b}_{k_1}^2) \right]. \end{aligned}$$

Then, we get that

$$\begin{aligned} f_{0,1}(x_\alpha) &= [\bar{a}_0 + \hat{\alpha} \hat{a}_0] + 2 \sum_{k=1}^{m-1} [\bar{a}_k + \hat{\alpha} \hat{a}_k] \\ &= f_{0,1}(\bar{x}_F) + \hat{\alpha} \left[\hat{a}_0 + 2 \sum_{k=1}^{m-1} \hat{a}_k \right] \end{aligned}$$

and

$$f_{0,2}(x_\alpha, \alpha) = f_{0,2}(\bar{x}_F, \alpha_0) + \hat{r}_{0,2}.$$

Let

$$\begin{aligned} \sigma_1 &= \sum_{k_1=1}^{m-1} \left| \bar{a}_{k_1} \hat{a}_{k_1} + \bar{b}_{k_1} \hat{b}_{k_1} \right| + \sum_{k_1=1}^{m-1} (k_1 \alpha_0 |\hat{L}| + 1) (\bar{a}_{k_1}^2 + \bar{b}_{k_1}^2), \\ \sigma_2 &= \sum_{k_1=1}^{m-1} (\hat{a}_{k_1}^2 + \hat{b}_{k_1}^2), \quad \sigma_3 = \left| \hat{a}_0 + 2 \sum_{k=1}^{m-1} \hat{a}_k \right|. \end{aligned}$$

By the mean value theorem, we get that

$$\begin{aligned} |\hat{r}_{0,2}| &\leq \hat{\alpha}^3 [\hat{a}_0^2 + 2\sigma_2] + \hat{\alpha}^2 [|\hat{a}_0| + \alpha_0 \hat{a}_0^2 + 2|\hat{a}_0 \bar{a}_0| + 4\sigma_1 + 2\alpha_0 \sigma_2] \\ &\quad + \hat{\alpha} [|\bar{a}_0| + \alpha_0 |\hat{a}_0| + \bar{a}_0^2 + 2\alpha_0 |\hat{a}_0 \bar{a}_0| + 4\alpha_0 \sigma_1]. \end{aligned}$$

Define

$$\begin{aligned} \hat{r}_0 &= (\hat{r}_{0,1}, \hat{r}_{0,2})^T, \\ \hat{r}_0^{(3)} &= (0, \hat{a}_0^2 + 2\sigma_2)^T, \\ \hat{r}_0^{(2)} &= (0, |\hat{a}_0| + \alpha_0 \hat{a}_0^2 + 2|\hat{a}_0 \bar{a}_0| + 4\sigma_1 + 2\alpha_0 \sigma_2)^T, \\ \hat{r}_0^{(1)} &= (\sigma_3, |\bar{a}_0| + \alpha_0 |\hat{a}_0| + \bar{a}_0^2 + 2\alpha_0 |\hat{a}_0 \bar{a}_0| + 4\alpha_0 \sigma_1)^T. \end{aligned}$$

Hence, we get that

$$f_0(x_\alpha, \alpha) = f_0^{(m)}(\bar{x}_F, \alpha_0) + \hat{r}_0 \quad \text{and} \quad |\hat{r}_0| \leq_{cw} \hat{\alpha}^3 \hat{r}_0^{(3)} + \hat{\alpha}^2 \hat{r}_0^{(2)} + \hat{\alpha} \hat{r}_0^{(1)}.$$

For $k \in \{1, \dots, 2m-2\}$, define

$$\begin{aligned} \hat{r}_k &= f_k(x_\alpha, \alpha) - f_k(\bar{x}, \alpha_0) \\ &= \hat{\alpha} \sum_{\substack{k_1+k_2=k \\ |k_1|, |k_2| < m}} \Theta_{k_1}(\bar{L} + \hat{\alpha} \hat{L}) \begin{pmatrix} \bar{a}_{k_1} \bar{a}_{k_2} - \bar{b}_{k_1} \bar{b}_{k_2} \\ \bar{a}_{k_1} \bar{b}_{k_2} + \bar{b}_{k_1} \bar{a}_{k_2} \end{pmatrix} \\ &\quad + \left[R_k(\bar{L} + \hat{\alpha} \hat{L}, \alpha) - R_k(\bar{L}, \alpha_0) \right] \begin{pmatrix} \bar{a}_k \\ \bar{b}_k \end{pmatrix} \\ &\quad + \hat{\alpha} R_k(\bar{L} + \hat{\alpha} \hat{L}, \alpha) \begin{pmatrix} \hat{a}_k \\ \hat{b}_k \end{pmatrix} \\ &\quad + \alpha_0 \sum_{\substack{k_1+k_2=k \\ |k_1|, |k_2| < m}} \left[\Theta_{k_1}(\bar{L} + \hat{\alpha} \hat{L}) - \Theta_{k_1}(\bar{L}) \right] \begin{pmatrix} \bar{a}_{k_1} \bar{a}_{k_2} - \bar{b}_{k_1} \bar{b}_{k_2} \\ \bar{a}_{k_1} \bar{b}_{k_2} + \bar{b}_{k_1} \bar{a}_{k_2} \end{pmatrix} \\ &\quad + \hat{\alpha} \alpha \sum_{\substack{k_1+k_2=k \\ |k_1|, |k_2| < m}} \Theta_{k_1}(\bar{L} + \hat{\alpha} \hat{L}) \begin{pmatrix} \bar{a}_{k_1} \hat{a}_{k_2} + \hat{a}_{k_1} \bar{a}_{k_2} - \bar{b}_{k_1} \hat{b}_{k_2} - \hat{b}_{k_1} \bar{b}_{k_2} \\ \bar{a}_{k_1} \hat{b}_{k_2} + \hat{a}_{k_1} \bar{b}_{k_2} + \bar{b}_{k_1} \hat{a}_{k_2} + \hat{b}_{k_1} \bar{a}_{k_2} \end{pmatrix} \end{aligned}$$

$$+\hat{\alpha}^2\alpha \sum_{\substack{k_1+k_2=k \\ |k_1|, |k_2|<m}} \Theta_{k_1}(\bar{L} + \hat{\alpha}\hat{L}) \begin{pmatrix} \hat{a}_{k_1}\hat{a}_{k_2} - \hat{b}_{k_1}\hat{b}_{k_2} \\ \hat{a}_{k_1}\hat{b}_{k_2} + \hat{b}_{k_1}\hat{a}_{k_2} \end{pmatrix}.$$

For $k \in \{1, \dots, 2m-2\}$, let

$$\begin{aligned} \hat{v}_k^{(1)} &= \begin{pmatrix} (1 + \alpha_0 k |\bar{L}|) |\bar{a}_k| + (1 + (1 + \alpha_0)k |\bar{L}|) |\bar{b}_k| \\ (1 + (1 + \alpha_0)k |\bar{L}|) |\bar{a}_k| + (1 + \alpha_0 k |\bar{L}|) |\bar{b}_k| \end{pmatrix}, \\ \hat{v}_k^{(2)} &= \begin{pmatrix} k |\bar{L} \hat{b}_k| + \alpha_0 (|\hat{a}_k| + |\hat{b}_k|) \\ k |\bar{L} \hat{a}_k| + \alpha_0 (|\hat{a}_k| + |\hat{b}_k|) \end{pmatrix}, \\ \hat{v}_k^{(3)} &= \begin{pmatrix} k |\hat{L} \hat{b}_k| + |\hat{a}_k| + |\hat{b}_k| \\ k |\hat{L} \hat{a}_k| + |\hat{a}_k| + |\hat{b}_k| \end{pmatrix}, \\ \hat{v}_k^{(4)} &= \sum_{\substack{k_1+k_2=k \\ |k_1|, |k_2|<m}} \left[1 + \alpha_0 |k_1 \hat{L}| \right] (|\bar{a}_{k_1} \bar{a}_{k_2} - \bar{b}_{k_1} \bar{b}_{k_2}| + |\bar{a}_{k_1} \bar{b}_{k_2} + \bar{b}_{k_1} \bar{a}_{k_2}|) \mathbb{I}_2, \\ \hat{v}_k^{(5)} &= \sum_{\substack{k_1+k_2=k \\ |k_1|, |k_2|<m}} \left| \bar{a}_{k_1} \hat{a}_{k_2} + \hat{a}_{k_1} \bar{a}_{k_2} - \bar{b}_{k_1} \hat{b}_{k_2} - \hat{b}_{k_1} \bar{b}_{k_2} \right| \mathbb{I}_2 \\ &\quad + \sum_{\substack{k_1+k_2=k \\ |k_1|, |k_2|<m}} \left| \bar{a}_{k_1} \hat{b}_{k_2} + \hat{a}_{k_1} \bar{b}_{k_2} + \bar{b}_{k_1} \hat{a}_{k_2} + \hat{b}_{k_1} \bar{a}_{k_2} \right| \mathbb{I}_2, \\ \hat{v}_k^{(6)} &= \sum_{\substack{k_1+k_2=k \\ |k_1|, |k_2|<m}} \left(\left| \hat{a}_{k_1} \hat{a}_{k_2} - \hat{b}_{k_1} \hat{b}_{k_2} \right| + \left| \hat{a}_{k_1} \hat{b}_{k_2} + \hat{b}_{k_1} \hat{a}_{k_2} \right| \right) \mathbb{I}_2. \end{aligned}$$

By the mean value theorem, we get that

$$\begin{aligned} |\hat{r}_k| &\leq_{cw} \hat{\alpha} \left(\hat{v}_k^{(1)} + \hat{v}_k^{(2)} + \hat{v}_k^{(4)} + \alpha_0 \hat{v}_k^{(5)} \right) \\ &\quad + \hat{\alpha}^2 \left(\hat{v}_k^{(3)} + \hat{v}_k^{(5)} + \alpha_0 \hat{v}_k^{(6)} \right) + \hat{\alpha}^3 \hat{v}_k^{(6)}. \end{aligned}$$

Note that for $k \in \{m, \dots, 2m-2\}$, we have that $\hat{v}_k^{(1)} = \hat{v}_k^{(2)} = \hat{v}_k^{(3)} = (0, 0)^T$. For every $k \in \{1, \dots, 2m-2\}$, define

$$\begin{aligned} \hat{r}_k^{(3)} &= \hat{v}_k^{(6)} \\ \hat{r}_k^{(2)} &= \hat{v}_k^{(3)} + \hat{v}_k^{(5)} + \alpha_0 \hat{v}_k^{(6)} \\ \hat{r}_k^{(1)} &= \hat{v}_k^{(1)} + \hat{v}_k^{(2)} + \hat{v}_k^{(4)} + \alpha_0 \hat{v}_k^{(5)}. \end{aligned}$$

Recalling (134), we have that

$$\begin{aligned}
|J_{F \times F} [f_F(x_\alpha, \alpha)]| &= \left| J_{F \times F} \left[f_F^{(m)}(\bar{x}_F, \alpha_0) + \hat{r}_F \right] \right| \\
&\leq_{cw} \left| J_{F \times F} \cdot f_F^{(m)}(\bar{x}, \alpha_0) \right| + |J_{F \times F} \cdot \hat{r}_F| \\
&\leq_{cw} \left| J_{F \times F} \cdot f_F^{(m)}(\bar{x}, \alpha_0) \right| + \hat{\alpha} |J_{F \times F}| \hat{r}_F^{(1)} \\
&\quad + \hat{\alpha}^2 |J_{F \times F}| \hat{r}_F^{(2)} + \hat{\alpha}^3 |J_{F \times F}| \hat{r}_F^{(3)}.
\end{aligned}$$

Hence, we let

$$Y_F(\alpha) = \left| J_{F \times F} \cdot f_F^{(m)}(\bar{x}, \alpha_0) \right| + \hat{\alpha} |J_{F \times F}| \hat{r}_F^{(1)} + \hat{\alpha}^2 |J_{F \times F}| \hat{r}_F^{(2)} + \hat{\alpha}^3 |J_{F \times F}| \hat{r}_F^{(3)}. \quad (136)$$

For a fixed $m \leq k \leq 2m - 2$,

$$\begin{aligned}
\left| \Lambda_k(\bar{x}, \alpha_0)^{-1} \cdot f_k(x_\alpha, \alpha) \right| &\leq_{cw} \left| \Lambda_k(\bar{x}, \alpha_0)^{-1} f_k(\bar{x}, \alpha_0) \right| + \hat{\alpha} \left| \Lambda_k(\bar{x}, \alpha_0)^{-1} \hat{r}_k^{(1)} \right| \\
&\quad + \hat{\alpha}^2 \left| \Lambda_k(\bar{x}, \alpha_0)^{-1} \hat{r}_k^{(2)} \right| + \hat{\alpha}^3 \left| \Lambda_k(\bar{x}, \alpha_0)^{-1} \hat{r}_k^{(3)} \right|.
\end{aligned}$$

Hence, for $k \in \{m, \dots, 2m - 2\}$, we let

$$\begin{aligned}
Y_k(\alpha) &= \left| \Lambda_k(\bar{x}, \alpha_0)^{-1} f_k(\bar{x}, \alpha_0) \right| + \hat{\alpha} \left| \Lambda_k(\bar{x}, \alpha_0)^{-1} \hat{r}_k^{(1)} \right| \\
&\quad + \hat{\alpha}^2 \left| \Lambda_k(\bar{x}, \alpha_0)^{-1} \hat{r}_k^{(2)} \right| + \hat{\alpha}^3 \left| \Lambda_k(\bar{x}, \alpha_0)^{-1} \hat{r}_k^{(3)} \right|.
\end{aligned} \quad (137)$$

Remark 6.2.2 Notice that we built the $\hat{r}_k$ component-wise monotone increasing in α which then imply that all the Y_k defined in (136) and (137) are also component-wise monotone increasing in α .

6.2.2 Computation of the $Z_k(r, \alpha)$

Recall that for $s \geq 2$ fixed, we defined

$$\begin{aligned}
W_{x_\alpha}(r) &= x_\alpha + W(r) \\
&= x_\alpha + \left\{ [-r, r]^2 \times \prod_{k=1}^{\infty} \left[-\frac{r}{k^s}, \frac{r}{k^s} \right]^2 \right\}
\end{aligned}$$

Let $w, w' \in W(r)$. Recall that in order to compute an upper bound on $Z_k(r, \alpha)$, we need to compute $[DT_\alpha(x_\alpha + w)w']_k$ and recall that the subscript F denotes the entries $k \in \{0, \dots, m-1\}$. We then have from (129) and (130) that

$$\begin{aligned}
[DT_\alpha(x_\alpha + w)w']_F &= [\{I - J \cdot Df(x_\alpha + w, \alpha)\}w']_F \\
&= w'_F - J_{F \times F} \cdot [Df(x_\alpha + w, \alpha)w']_F \\
&= w'_F - J_{F \times F} \cdot Df_F(x_\alpha + w, \alpha)w' \\
&= w'_F - J_{F \times F} \cdot [Df^{(m)}(\bar{x}_F, \alpha_0)w'_F + r_F] \\
&= [I_F - J_{F \times F} Df^{(m)}(\bar{x}_F, \alpha_0)]w_F - J_{F \times F} \cdot r_F,
\end{aligned} \tag{138}$$

where r_F will be computed later. It's important to note that since $J_{F \times F}$ is the numerical inverse of $Df^{(m)}(\bar{x}_F, \alpha_0)$, the matrix $I_F - J_{F \times F} Df^{(m)}(\bar{x}_F, \alpha_0)$ should basically be 0. For $k \geq m$, we have that

$$\begin{aligned}
[DT_\alpha(x_\alpha + w)w']_k &= [\{I - J \cdot Df(x_\alpha + w, \alpha)\}w']_k \\
&= w'_k - \Lambda_k^{-1} \cdot [Df(x_\alpha + w, \alpha)w']_k \\
&= w'_k - \Lambda_k^{-1} \cdot Df_k(x_\alpha + w, \alpha)w' \\
&= w'_k - \Lambda_k^{-1} \cdot \left[\frac{\partial f_k}{\partial x_k}(\bar{x}, \alpha_0)w'_k + r_k \right] \\
&= -\Lambda_k^{-1} r_k,
\end{aligned} \tag{139}$$

where the r_k will be computed later. In order to compute the Z_k , we first need to compute $Df_k(x_\alpha + w, \alpha)w'$. Recalling (132) and (133), we get that for $w \in W(r)$, $w_0 \in [-r, r]^2$ and $w_k \in [-\frac{r}{k^s}, \frac{r}{k^s}]$, when $k \geq 1$. Define $\xi := \hat{\alpha}\hat{x} + w$ so that $x_\alpha + w = \bar{x} + \xi$. Denote

$$\begin{aligned}
\bar{x} &= ([\bar{L}, \bar{a}_0], [\bar{a}_1, \bar{b}_1], \dots, [\bar{a}_{m-1}, \bar{b}_{m-1}], [0, 0], [0, 0], \dots)^T \\
\hat{x} &= ([\hat{L}, \hat{a}_0], [\hat{a}_1, \hat{b}_1], \dots, [\hat{a}_{m-1}, \hat{b}_{m-1}], [0, 0], [0, 0], \dots)^T \\
w' &= ([w_0^L, w_0^a], [w_1^a, w_1^b], \dots, [w_k^a, w_k^b], \dots)^T \\
\xi &= ([\xi_0^L, \xi_0^a], [\xi_1^a, \xi_1^b], \dots, [\xi_k^a, \xi_k^b], \dots)^T
\end{aligned}$$

Throughout the rest of the section, we will use the notation $\mathbf{1} = [-1, 1]$ and $\mathbf{r}^j = [-r^j, r^j]$.

Recalling that $f_{0,1}(x) = a_0 + 2 \sum_{k=1}^{\infty} a_k$, we get that

$$\begin{aligned} Df_{0,1}(\bar{x} + \xi)w' &= \sum_{i=0}^{\infty} \frac{\partial f_{0,1}}{\partial x_i}(\bar{x} + \xi)w'_i = w'_0{}^a + 2 \sum_{k=1}^{m-1} w'_k{}^a + 2 \sum_{k=m}^{\infty} w'_k{}^a \\ &= Df_{0,1}^{(m)}(\bar{x}_F)w'_F + r_{0,1}. \end{aligned} \quad (140)$$

where $r_{0,1} := 2 \sum_{k=m}^{\infty} w'_k{}^a$. Define

$$fs_1 = \sum_{k=m}^{M-1} \frac{1}{k^s}, \quad is_1 = \frac{1}{(M-1)^{s-1}(s-1)}, \quad r_{0,1}^{(1)} = 2(fs_1 + is_1). \quad (141)$$

Then we get that

$$r_{0,1} \in r_{0,1}^{(1)}\mathbf{r}. \quad (142)$$

Recalling that $f_{0,2}(x, \alpha) = \alpha [a_0 + a_0^2 + 2 \sum_{k_1=1}^{\infty} \cos(k_1 L) (a_{k_1}^2 + b_{k_1}^2)]$, we get

$$\frac{\partial f_{0,2}}{\partial L}(x, \alpha) = -2\alpha \sum_{k_1=1}^{\infty} k_1 \sin(k_1 L) (a_{k_1}^2 + b_{k_1}^2).$$

Define

$$\begin{aligned} s_{0,2,L}^{(1)} &= -2 \sum_{k_1=1}^{m-1} k_1 \sin(k_1 \bar{L}) (\bar{a}_{k_1}^2 + \bar{b}_{k_1}^2) w'_0{}^L, \\ s_{0,2,L}^{(2)} &= -2 \sum_{k_1=1}^{m-1} k_1^2 \cos(s_{k_1}) (\bar{a}_{k_1}^2 + \bar{b}_{k_1}^2) w'_0{}^L, \\ s_{0,2,L}^{(3)} &= -2 \sum_{k_1=1}^{m-1} k_1 \sin(t_{k_1}) (\hat{a}_{k_1}^2 + \hat{b}_{k_1}^2) w'_0{}^L, \\ s_{0,2,L}^{(4)} &= -2 \sum_{k_1=1}^{m-1} k_1 \sin(t_{k_1}) \left(2\bar{a}_{k_1} \hat{a}_{k_1} + 2\bar{b}_{k_1} \hat{b}_{k_1} + 2\hat{a}_{k_1} w_{k_1}^a + 2\hat{b}_{k_1} w_{k_1}^b \right) w'_0{}^L, \\ s_{0,2,L}^{(5)} &= -2 \sum_{k_1=1}^{\infty} k_1 \sin(t_{k_1}) (2\bar{a}_{k_1} w_{k_1}^a + 2\bar{b}_{k_1} w_{k_1}^b + (w_{k_1}^a)^2 + (w_{k_1}^b)^2) w'_0{}^L, \\ r_{0,2,L} &= \hat{\alpha} s_{0,2,L}^{(1)} + \alpha(\hat{\alpha} \hat{L} + w_0^L) s_{0,2,L}^{(2)} + \hat{\alpha}^2 \alpha s_{0,2,L}^{(3)} + \hat{\alpha} \alpha s_{0,2,L}^{(4)} + \alpha s_{0,2,L}^{(5)}. \end{aligned}$$

Hence,

$$\frac{\partial f_{0,2}}{\partial L}(\bar{x} + \xi, \alpha)w'_0{}^L$$

$$\begin{aligned}
&= -2(\alpha_0 + \hat{\alpha}) \sum_{k_1=1}^{m-1} k_1 \sin(k_1 \bar{L}) (\bar{a}_{k_1}^2 + \bar{b}_{k_1}^2) w_0'^L \\
&\quad - 2\alpha \sum_{k_1=1}^{m-1} k_1 [\sin(k_1 \bar{L} + k_1 \xi_0^L) - \sin(k_1 \bar{L})] (\bar{a}_{k_1}^2 + \bar{b}_{k_1}^2) w_0'^L \\
&\quad - 2\alpha \sum_{k_1=1}^{\infty} k_1 \sin(k_1 \bar{L} + k_1 \xi_0^L) [2\bar{a}_{k_1} \xi_{k_1}^a + 2\bar{b}_{k_1} \xi_{k_1}^b + (\xi_{k_1}^a)^2 + (\xi_{k_1}^b)^2] w_0'^L \\
&= \frac{\partial f_{0,2}^{(m)}}{\partial L}(\bar{x}_F, \alpha_0) w_0'^L - 2\hat{\alpha} \sum_{k_1=1}^{m-1} k_1 \sin(k_1 \bar{L}) (\bar{a}_{k_1}^2 + \bar{b}_{k_1}^2) w_0'^L \\
&\quad - 2\alpha \sum_{k_1=1}^{m-1} k_1^2 \xi_0^L \cos(s_{k_1}) (\bar{a}_{k_1}^2 + \bar{b}_{k_1}^2) w_0'^L \\
&\quad - 2\alpha \sum_{k_1=1}^{\infty} k_1 \sin(t_{k_1}) [2\bar{a}_{k_1} \xi_{k_1}^a + 2\bar{b}_{k_1} \xi_{k_1}^b + (\xi_{k_1}^a)^2 + (\xi_{k_1}^b)^2] w_0'^L \\
&= \frac{\partial f_{0,2}^{(m)}}{\partial L}(\bar{x}_F, \alpha_0) w_0'^L + r_{0,2,L}.
\end{aligned}$$

Let

$$\begin{aligned}
\Sigma_{0,2,L}^{(1)} &= 2 \sum_{k_1=1}^{m-1} k_1 (\bar{a}_{k_1}^2 + \bar{b}_{k_1}^2), \quad \Sigma_{0,2,L}^{(2)} = 2 \sum_{k_1=1}^{m-1} k_1^2 (\bar{a}_{k_1}^2 + \bar{b}_{k_1}^2) \\
\Sigma_{0,2,L}^{(3)} &= 2 \sum_{k_1=1}^{m-1} k_1 (\hat{a}_{k_1}^2 + \hat{b}_{k_1}^2), \quad \Sigma_{0,2,L}^{(4)} = 4 \sum_{k_1=1}^{m-1} k_1 \left| \bar{a}_{k_1} \hat{a}_{k_1} + \bar{b}_{k_1} \hat{b}_{k_1} \right|, \\
\Sigma_{0,2,L}^{(5)} &= 4 \sum_{k_1=1}^{m-1} \frac{|\hat{a}_{k_1}| + |\hat{b}_{k_1}|}{k_1^{s-1}}, \quad \Sigma_{0,2,L}^{(6)} = 4 \sum_{k_1=1}^{m-1} \frac{|\bar{a}_{k_1}| + |\bar{b}_{k_1}|}{k_1^{s-1}}, \\
fs_2 &= \sum_{k_1=1}^{M-1} \frac{1}{k_1^{s-1}}, \quad is_2 = \frac{1}{(M-1)^{s-2}(s-2)}
\end{aligned} \tag{143}$$

and define

$$\begin{aligned}
r_{0,2,L}^{(3)} &= 4\alpha(fs_2 + is_2) \\
r_{0,2,L}^{(2)} &= \alpha\Sigma_{0,2,L}^{(2)} + \hat{\alpha}\alpha\Sigma_{0,2,L}^{(5)} + \alpha\Sigma_{0,2,L}^{(6)} \\
r_{0,2,L}^{(1)} &= \hat{\alpha}\Sigma_{0,2,L}^{(1)} + \alpha\hat{\alpha}|\hat{L}|\Sigma_{0,2,L}^{(2)} + \hat{\alpha}^2\alpha\Sigma_{0,2,L}^{(3)} + \hat{\alpha}\alpha\Sigma_{0,2,L}^{(4)}.
\end{aligned} \tag{144}$$

Then

$$r_{0,2,L} \in r_{0,2,L}^{(3)} \mathbf{r}^3 + r_{0,2,L}^{(2)} \mathbf{r}^2 + r_{0,2,L}^{(1)} \mathbf{r}. \tag{145}$$

Now $\frac{\partial f_{0,2}}{\partial a_0}(x, \alpha) = \alpha(1 + 2a_0)$. Define

$$\begin{aligned} r_{0,2,a_0} &= [2\alpha_0 w_0^a + \hat{\alpha}(2\alpha_0 \hat{a}_0 + 1 + 2\bar{a}_0 + 2w_0^a) + \hat{\alpha}^2(2\hat{a}_0)] w_0'^a \\ r_{0,2,a_0}^{(2)} &= 2\alpha, \quad r_{0,2,a_0}^{(1)} = \hat{\alpha}(1 + 2|\bar{a}_0|) + 2\alpha\hat{\alpha}|\hat{a}_0|. \end{aligned} \quad (146)$$

Hence

$$\begin{aligned} \frac{\partial f_{0,2}}{\partial a_0}(\bar{x} + \xi, \alpha) w_0'^a &= (\alpha_0 + \hat{\alpha})(1 + 2\bar{a}_0 + 2\xi_0^a) w_0'^a \\ &= \frac{\partial f_{0,2}^{(m)}}{\partial a_0}(\bar{x}_F, \alpha_0) w_0'^a + r_{0,2,a_0} \end{aligned}$$

and

$$r_{0,2,a_0} \in r_{0,2,a_0}^{(2)} \mathbf{r}^2 + r_{0,2,a_0}^{(1)} \mathbf{r}. \quad (147)$$

For $i \geq 1$, we have that $\frac{\partial f_{0,2}}{\partial x_i}(x, \alpha) = 4\alpha \cos(iL)[a_i, b_i]$. By the mean value theorem, there exist $s_i, t_i \in [0, 1]$ such that

$$\begin{aligned} \sum_{i=1}^{\infty} \frac{\partial f_{0,2}}{\partial x_i}(\bar{x} + \xi, \alpha) w_i' &= 4\alpha \sum_{i=1}^{\infty} \cos(i\bar{L} + i\xi_0^L) [\bar{a}_i + \xi_i^a, \bar{b}_i + \xi_i^b] \begin{pmatrix} w_i'^a \\ w_i'^b \end{pmatrix} \\ &= 4(\alpha_0 + \hat{\alpha}) \sum_{i=1}^{m-1} \cos(i\bar{L} + i\xi_0^L) [\bar{a}_i, \bar{b}_i] \begin{pmatrix} w_i'^a \\ w_i'^b \end{pmatrix} \\ &\quad + 4\alpha \sum_{i=1}^{\infty} \cos(i\bar{L} + i\xi_0^L) [\xi_i^a, \xi_i^b] \begin{pmatrix} w_i'^a \\ w_i'^b \end{pmatrix} \\ &= 4(\alpha_0 + \hat{\alpha}) \sum_{i=1}^{m-1} \cos(i\bar{L}) [\bar{a}_i w_i'^a + \bar{b}_i w_i'^b] \\ &\quad + 4\alpha \sum_{i=1}^{m-1} [\cos(i\bar{L} + i\xi_0^L) - \cos(i\bar{L})] [\bar{a}_i w_i'^a + \bar{b}_i w_i'^b] \\ &\quad + 4\alpha \sum_{i=1}^{\infty} \cos(i\bar{L} + i\xi_0^L) [\xi_i^a w_i'^a + \xi_i^b w_i'^b] \\ &= \sum_{i=1}^{m-1} \frac{\partial f_{0,2}^{(m)}}{\partial x_i}(\bar{x}_F, \alpha_0) w_i' + r_{0,2,\infty}. \end{aligned}$$

where $r_{0,2,\infty}$ is defined by the following

$$s_{0,2}^{(1)} = \sum_{i=1}^{m-1} \cos(i\bar{L}) [\bar{a}_i w_i'^a + \bar{b}_i w_i'^b], \quad s_{0,2}^{(2)} = \sum_{i=1}^{m-1} -i \sin(s_i) [\bar{a}_i w_i'^a + \bar{b}_i w_i'^b]$$

$$\begin{aligned}
s_{0,2}^{(3)} &= \sum_{i=1}^{m-1} \cos(t_i) \left[\hat{a}_i w_i'^a + \hat{b}_i w_i'^b \right], \quad s_{0,2}^{(4)} = \sum_{i=1}^{\infty} \cos(t_i) \left[w_i^a w_i'^a + w_i^b w_i'^b \right], \\
r_{0,2,\infty} &= 4\hat{\alpha} s_{0,2}^{(1)} + 4\alpha(\hat{\alpha}\hat{L} + w_0^L) s_{0,2}^{(2)} + 4\alpha\hat{\alpha} s_{0,2}^{(3)} + 4\alpha s_{0,2}^{(4)}.
\end{aligned}$$

Let

$$\begin{aligned}
\Sigma_{0,2}^{(1)} &= \sum_{i=1}^{m-1} \frac{|\bar{a}_i| + |\bar{b}_i|}{i^s}, \quad \Sigma_{0,2}^{(2)} = \sum_{i=1}^{m-1} \frac{|\bar{a}_i| + |\bar{b}_i|}{i^{s-1}}, \quad \Sigma_{0,2}^{(3)} = \sum_{i=1}^{m-1} \frac{|\hat{a}_i| + |\hat{b}_i|}{i^s} \\
f s_3 &= \sum_{i=1}^{M-1} \frac{1}{i^{2s}}, \quad i s_3 = \frac{1}{(M-1)^{2s-1}(2s-1)}
\end{aligned} \tag{148}$$

and define

$$\begin{aligned}
r_{0,2,\infty}^{(2)} &= 8\alpha(f s_3 + i s_3) + 4\alpha \Sigma_{0,2}^{(2)} \\
r_{0,2,\infty}^{(1)} &= 4\hat{\alpha} \Sigma_{0,2}^{(1)} + 4\alpha\hat{\alpha}|\hat{L}| \Sigma_{0,2}^{(2)} + 4\alpha\hat{\alpha} \Sigma_{0,2}^{(3)}.
\end{aligned} \tag{149}$$

Then

$$r_{0,2,\infty} \in r_{0,2,\infty}^{(2)} \mathbf{r}^2 + r_{0,2,\infty}^{(1)} \mathbf{r}. \tag{150}$$

Defining

$$r_{0,2} = r_{0,2,L} + r_{0,2,a_0} + r_{0,2,\infty}$$

and combining (145), (147) and (150), we get that

$$\begin{aligned}
&Df_{0,2}(x_\alpha + w, \alpha)w' \\
&= \frac{\partial f_{0,2}}{\partial L}(\bar{x} + \xi, \alpha)w_0'^L + \frac{\partial f_{0,2}}{\partial a_0}(\bar{x} + \xi, \alpha)w_0'^a + \sum_{i=1}^{\infty} \frac{\partial f_{0,2}}{\partial x_i}(\bar{x} + \xi, \alpha)w_i' \\
&= \frac{\partial f_{0,2}^{(m)}}{\partial L}(\bar{x}_F, \alpha_0)w_0'^L + r_{0,2,L} + \frac{\partial f_{0,2}^{(m)}}{\partial a_0}(\bar{x}_F, \alpha_0)w_0'^a + r_{0,2,a_0} \\
&\quad + \sum_{i=1}^{m-1} \frac{\partial f_{0,2}^{(m)}}{\partial x_i}(\bar{x}_F, \alpha_0)w_i' + r_{0,2,\infty} \\
&= Df_{0,2}(\bar{x}_F, \alpha_0)w_F' + r_{0,2}.
\end{aligned}$$

Recalling (141), (144), (146) and (149), we let

$$r_0 = (r_{0,1}, r_{0,2})^T, \quad r_0^{(1)} = \left(r_{0,1}^{(1)}, r_{0,2,L}^{(1)} + r_{0,2,a_0}^{(1)} + r_{0,2,\infty}^{(1)} \right)^T$$

$$r_0^{(2)} = \left(0, r_{0,2,L}^{(2)} + r_{0,2,a_0}^{(2)} + r_{0,2,\infty}^{(2)}\right)^T, \quad r_0^{(3)} = \left(0, r_{0,2,L}^{(3)}\right)^T, \quad (151)$$

we get that

$$Df_0(x_\alpha + w, \alpha)w' = Df_0^{(m)}(\bar{x}_F, \alpha_0)w'_F + r_0. \quad (152)$$

and

$$r_0 \in r_0^{(3)}\mathbf{r}^3 + r_0^{(2)}\mathbf{r}^2 + r_0^{(1)}\mathbf{r}. \quad (153)$$

In what follows, we will need the following.

Lemma 6.2.3 *Suppose that $k \geq M \geq 5$ and let $s \geq 2$. Then*

$$\sum_{k_1=1}^{k-1} \frac{1}{k_1^{s-1}(k-k_1)^s} \leq \frac{2}{k^{s-1}} \left[\frac{2}{M} [1 + \ln(M-1)] + \frac{\pi^2}{6} \right] \left[\frac{2}{M} + 1 \right]^{s-2}. \quad (154)$$

Proof. See the proof Lemma 3.1.2. $\blacksquare$

Consider now $k \geq 1$ and recall that in this case

$$f_k(x, \alpha) = R_k \begin{pmatrix} a_k \\ b_k \end{pmatrix} + \alpha \sum_{k_1+k_2=k} \Theta_{k_1} \begin{pmatrix} a_{k_1}a_{k_2} - b_{k_1}b_{k_2} \\ a_{k_1}b_{k_2} + b_{k_1}a_{k_2} \end{pmatrix} \in \mathbb{R}^2$$

where

$$R_k(L, \alpha) = \begin{pmatrix} \alpha \cos kL & -kL + \alpha \sin kL \\ kL - \alpha \sin kL & \alpha \cos kL \end{pmatrix}, \quad \Theta_{k_1}(L) = \begin{pmatrix} \cos k_1L & \sin k_1L \\ -\sin k_1L & \cos k_1L \end{pmatrix}.$$

For $k \geq 1$, denote

$$R'_k(L, \alpha) = \begin{pmatrix} -\alpha k \sin kL & -k + \alpha k \cos kL \\ k - \alpha k \cos kL & -\alpha k \sin kL \end{pmatrix}, \quad (155)$$

and for $k_1 \in \mathbb{Z}$, denote

$$\Theta'_{k_1}(L) = \begin{pmatrix} -k_1 \sin k_1L & k_1 \cos k_1L \\ -k_1 \cos k_1L & -k_1 \sin k_1L \end{pmatrix}. \quad (156)$$

Lemma 6.2.4 *Let $\mathbb{I}_2 = (1, 1)^T$, $k_1 \in \mathbb{Z}$, $a, b, \hat{L} \in \mathbb{R}$, $\hat{\alpha}, \bar{L} \geq 0$, $\alpha_0 \geq \pi/2$, $\alpha = \alpha_0 + \hat{\alpha}$, $w'_k \in \frac{\mathbf{r}}{k^s} \mathbb{I}_2$, $\xi = \hat{\alpha} \hat{L} + w_0^L$ with $w_0^L \in \mathbf{r} = [-r, r]$. Let $M \geq 2m - 1$ and recall that $\mathbf{1} = [-1, 1]$. For $k \in \{1, \dots, M - 1\}$, define*

$$\begin{aligned}
\Sigma_{k,L}^{(1)} &= \sum_{k_1+k_2=k} |k_1| (|\bar{a}_{k_1} \bar{a}_{k_2} - \bar{b}_{k_1} \bar{b}_{k_2}| + |\bar{a}_{k_1} \bar{b}_{k_2} + \bar{b}_{k_1} \bar{a}_{k_2}|) \mathbb{I}_2 \\
\Sigma_{k,L}^{(2)} &= \sum_{k_1+k_2=k} k_1^2 (|\bar{a}_{k_1} \bar{a}_{k_2} - \bar{b}_{k_1} \bar{b}_{k_2}| + |\bar{a}_{k_1} \bar{b}_{k_2} + \bar{b}_{k_1} \bar{a}_{k_2}|) \mathbb{I}_2 \\
\Sigma_{k,L}^{(3)} &= \sum_{k_1+k_2=k} |k_1| (|\hat{a}_{k_1} \hat{b}_{k_2} - \hat{b}_{k_1} \hat{b}_{k_2}| + |\hat{a}_{k_1} \hat{b}_{k_2} + \hat{b}_{k_1} \hat{a}_{k_2}|) \mathbb{I}_2 \\
\Sigma_{k,L}^{(4)} &= \sum_{k_1+k_2=k} |k_1| (|\bar{a}_{k_1} \hat{a}_{k_2} + \hat{a}_{k_1} \bar{a}_{k_2} - \bar{b}_{k_1} \hat{b}_{k_2} - \hat{b}_{k_1} \bar{b}_{k_2}|) \mathbb{I}_2 \\
&\quad + \sum_{k_1+k_2=k} |k_1| (|\bar{a}_{k_1} \hat{b}_{k_2} + \hat{a}_{k_1} \bar{b}_{k_2} + \bar{b}_{k_1} \hat{a}_{k_2} + \hat{b}_{k_1} \bar{a}_{k_2}|) \mathbb{I}_2 \\
\Sigma_{k,L}^{(5)} &= \sum_{k_1=-m+1}^{m-1} \frac{|k_1| + |k - k_1|}{|\widehat{k - k_1}|^s} (|\hat{a}_{k_1}| + |\hat{b}_{k_1}|) \mathbb{I}_2 \\
\Sigma_{k,L}^{(6)} &= \sum_{k_1=-m+1}^{m-1} \frac{|k_1| + |k - k_1|}{|\widehat{k - k_1}|^s} (|\bar{a}_{k_1}| + |\bar{b}_{k_1}|) \mathbb{I}_2 \\
\Sigma_{k,L}^{(7)} &= \left[\sum_{k_1=1}^{M-1} \frac{k + 2k_1}{k_1^s (k + k_1)^s} + \frac{1}{[k(M-1) + (M-1)^2]^{s-1} (s-1)} + \sum_{k_1=1}^k \frac{1}{k_1^{s-1} (\widehat{k - k_1})^s} \right] \mathbb{I}_2.
\end{aligned}$$

For $k \in \{1, \dots, m - 1\}$, define

$$\begin{aligned}
r_{k,L} &= [R'_k(\bar{L} + \xi_0^L, \alpha) - R'_k(\bar{L}, \alpha_0)] \begin{pmatrix} \bar{a}_k \\ \bar{b}_k \end{pmatrix} w_0'^L + R'_k(\bar{L} + \xi_0^L, \alpha) \begin{pmatrix} \xi_k^a \\ \xi_k^b \end{pmatrix} w_0'^L \\
&\quad + \sum_{k_1+k_2=k} [\alpha \Theta'_{k_1}(\bar{L} + \xi_0^L) - \alpha_0 \Theta'_{k_1}(\bar{L})] \begin{pmatrix} \bar{a}_{k_1} \bar{a}_{k_2} - \bar{b}_{k_1} \bar{b}_{k_2} \\ \bar{a}_{k_1} \bar{b}_{k_2} + \bar{b}_{k_1} \bar{a}_{k_2} \end{pmatrix} w_0'^L \\
&\quad + \alpha \sum_{k_1+k_2=k} \Theta'_{k_1}(\bar{L} + \xi_0^L) \begin{pmatrix} \bar{a}_{k_1} \xi_{k_2}^a + \xi_{k_1}^a \bar{a}_{k_2} + \xi_{k_1}^a \xi_{k_2}^a - \bar{b}_{k_1} \xi_{k_2}^b - \xi_{k_1}^b \bar{b}_{k_2} - \xi_{k_1}^b \xi_{k_2}^b \\ \bar{a}_{k_1} \xi_{k_2}^b + \xi_{k_1}^a \bar{b}_{k_2} + \xi_{k_1}^a \xi_{k_2}^b + \bar{b}_{k_1} \xi_{k_2}^a + \xi_{k_1}^b \bar{a}_{k_2} + \xi_{k_1}^b \xi_{k_2}^a \end{pmatrix} w_0'^L
\end{aligned} \tag{157}$$

and

$$r_{k,L}^{(3)} = 4\alpha \Sigma_{k,L}^{(7)} \tag{158}$$

$$r_{k,L}^{(2)} = 2\hat{\alpha} \alpha \Sigma_{k,L}^{(5)} + \frac{2\alpha + 1}{k^{s-1}} \mathbb{I}_2 + 2\alpha \Sigma_{k,L}^{(6)} + \alpha_0 \left[(|\bar{a}_k| + |\bar{b}_k|) k^2 \mathbb{I}_2 + \Sigma_{k,L}^{(2)} \right] \tag{159}$$

$$\begin{aligned}
r_{k,L}^{(1)} &= \hat{\alpha}^2 \alpha \Sigma_{k,L}^{(3)} + \hat{\alpha} \alpha \Sigma_{k,L}^{(4)} + \hat{\alpha}^2 k \left(|\hat{a}_k| + |\hat{b}_k| \right) \mathbb{I}_2 + \hat{\alpha} \Sigma_{k,L}^{(1)} + \hat{\alpha} \alpha_0 |\hat{L}| \Sigma_{k,L}^{(2)} \\
&\quad + \hat{\alpha} (|\bar{a}_k| + |\bar{b}_k|) (\alpha_0 k^2 |\hat{L}| + k) \mathbb{I}_2 + \hat{\alpha} k \begin{pmatrix} \alpha_0 |\hat{a}_k| + (1 + \alpha_0) |\hat{b}_k| \\ (1 + \alpha_0) |\hat{a}_k| + \alpha_0 |\hat{b}_k| \end{pmatrix} \quad (160)
\end{aligned}$$

Then, for $k \in \{1, \dots, m-1\}$, we have that

$$\frac{\partial f_k}{\partial L}(\bar{x} + \xi, \alpha) w_0'^L = \frac{\partial f_k}{\partial L}(\bar{x}_F, \alpha_0) w_0'^L + r_{k,L} \quad (161)$$

and

$$r_{k,L} \in r_{k,L}^{(3)} \mathbf{r}^3 + r_{k,L}^{(2)} \mathbf{r}^2 + r_{k,L}^{(1)} \mathbf{r}. \quad (162)$$

For $k \in \{m, \dots, M-1\}$, we have that

$$\begin{aligned}
\frac{\partial f_k}{\partial L}(\bar{x} + \xi, \alpha) w_0'^L &\in \left[\alpha \Sigma_{k,L}^{(1)} + \hat{\alpha}^2 \alpha \Sigma_{k,L}^{(3)} + \hat{\alpha} \alpha \Sigma_{k,L}^{(4)} \right] \mathbf{r} \\
&\quad + \left[2\hat{\alpha} \alpha \Sigma_{k,L}^{(5)} + 2\alpha \Sigma_{k,L}^{(6)} + \frac{2\alpha + 1}{k^{s-1}} \mathbb{I}_2 \right] \mathbf{r}^2 + 4\alpha \Sigma_{k,L}^{(7)} \mathbf{r}^3. \quad (163)
\end{aligned}$$

For $k \geq M$, define

$$\begin{aligned}
\Sigma_{M,L}^{(5)} &= \left[\frac{1}{M} \sum_{k_1=1}^{m-1} k_1 \left(1 + \frac{1}{[1 - \frac{k_1}{M}]^s} \right) (|\hat{a}_{k_1}| + |\hat{b}_{k_1}|) \right. \\
&\quad \left. + |\hat{a}_0| + |\hat{b}_0| + \sum_{k_1=1}^{m-1} \left(1 + \frac{1}{[1 - \frac{k_1}{M}]^{s-1}} \right) (|\hat{a}_{k_1}| + |\hat{b}_{k_1}|) \right] \mathbb{I}_2 \quad (164)
\end{aligned}$$

$$\begin{aligned}
\Sigma_{M,L}^{(6)} &= \left[\frac{1}{M} \sum_{k_1=1}^{m-1} k_1 \left(1 + \frac{1}{[1 - \frac{k_1}{M}]^s} \right) (|\bar{a}_{k_1}| + |\bar{b}_{k_1}|) \right. \\
&\quad \left. + |\bar{a}_0| + |\bar{b}_0| + \sum_{k_1=1}^{m-1} \left(1 + \frac{1}{[1 - \frac{k_1}{M}]^{s-1}} \right) (|\bar{a}_{k_1}| + |\bar{b}_{k_1}|) \right] \mathbb{I}_2 \quad (165)
\end{aligned}$$

$$\begin{aligned}
\Sigma_{M,L}^{(7)} &= \left[2 + \frac{2}{M} + \frac{1}{s-1} + 2 \left[\frac{2}{M} [1 + \ln(M-1)] + \frac{\pi^2}{6} \right] \left[\frac{2}{M} + 1 \right]^{s-2} \right] \mathbb{I}_2 \quad (166)
\end{aligned}$$

Then for $k \geq M$, we have that

$$\begin{aligned}
\frac{\partial f_k}{\partial L}(\bar{x} + \xi, \alpha) w_0'^L &\in \frac{1}{k^{s-1}} \left[4\alpha \Sigma_{M,L}^{(7)} \mathbf{r}^3 + \left(2\hat{\alpha} \alpha \Sigma_{M,L}^{(5)} + (2\alpha + 1) \mathbb{I}_2 + 2\alpha \Sigma_{M,L}^{(6)} \right) \mathbf{r}^2 \right]. \quad (167)
\end{aligned}$$

Proof. Consider any $k \geq 1$.

$$\frac{\partial f_k}{\partial L}(x, \alpha) = R'_k(L, \alpha) \begin{pmatrix} a_k \\ b_k \end{pmatrix} + \alpha \sum_{k_1+k_2=k} \Theta'_{k_1}(L) \begin{pmatrix} a_{k_1}a_{k_2} - b_{k_1}b_{k_2} \\ a_{k_1}b_{k_2} + b_{k_1}a_{k_2} \end{pmatrix}.$$

Hence

$$\begin{aligned} \frac{\partial f_k}{\partial L}(\bar{x} + \xi, \alpha) w_0'^L &= R'_k(\bar{L} + \xi_0^L, \alpha) \begin{pmatrix} \bar{a}_k + \xi_k^a \\ \bar{b}_k + \xi_k^b \end{pmatrix} w_0'^L \\ &\quad + \alpha \sum_{k_1+k_2=k} \Theta'_{k_1}(\bar{L} + \xi_0^L) \begin{pmatrix} [\bar{a}_{k_1} + \xi_{k_1}^a][\bar{a}_{k_2} + \xi_{k_2}^a] - [\bar{b}_{k_1} + \xi_{k_1}^b][\bar{b}_{k_2} + \xi_{k_2}^b] \\ [\bar{a}_{k_1} + \xi_{k_1}^a][\bar{b}_{k_2} + \xi_{k_2}^b] + [\bar{b}_{k_1} + \xi_{k_1}^b][\bar{a}_{k_2} + \xi_{k_2}^a] \end{pmatrix} w_0'^L \\ &= R'_k(\bar{L} + \xi_0^L, \alpha) \begin{pmatrix} \bar{a}_k \\ \bar{b}_k \end{pmatrix} w_0'^L + R'_k(\bar{L} + \xi_0^L, \alpha) \begin{pmatrix} \xi_k^a \\ \xi_k^b \end{pmatrix} w_0'^L \\ &\quad + \alpha \sum_{k_1+k_2=k} \Theta'_{k_1}(\bar{L} + \xi_0^L) \begin{pmatrix} \bar{a}_{k_1}\bar{a}_{k_2} - \bar{b}_{k_1}\bar{b}_{k_2} \\ \bar{a}_{k_1}\bar{b}_{k_2} + \bar{b}_{k_1}\bar{a}_{k_2} \end{pmatrix} w_0'^L \\ &\quad + \alpha \sum_{k_1+k_2=k} \Theta'_{k_1}(\bar{L} + \xi_0^L) \begin{pmatrix} \bar{a}_{k_1}\xi_{k_2}^a + \xi_{k_1}^a\bar{a}_{k_2} + \xi_{k_1}^a\xi_{k_2}^a - \bar{b}_{k_1}\xi_{k_2}^b - \xi_{k_1}^b\bar{b}_{k_2} - \xi_{k_1}^b\xi_{k_2}^b \\ \bar{a}_{k_1}\xi_{k_2}^b + \xi_{k_1}^a\bar{b}_{k_2} + \xi_{k_1}^a\xi_{k_2}^b + \bar{b}_{k_1}\xi_{k_2}^a + \xi_{k_1}^b\bar{a}_{k_2} + \xi_{k_1}^b\xi_{k_2}^a \end{pmatrix} w_0'^L. \end{aligned}$$

Consider the case $k \in \{1, \dots, m-1\}$.

$$\begin{aligned} \frac{\partial f_k}{\partial L}(\bar{x} + \xi, \alpha) w_0'^L &= \left[R'_k(\bar{L}, \alpha_0) \begin{pmatrix} \bar{a}_k \\ \bar{b}_k \end{pmatrix} + \alpha_0 \sum_{k_1+k_2=k} \Theta'_{k_1}(\bar{L}) \begin{pmatrix} \bar{a}_{k_1}\bar{a}_{k_2} - \bar{b}_{k_1}\bar{b}_{k_2} \\ \bar{a}_{k_1}\bar{b}_{k_2} + \bar{b}_{k_1}\bar{a}_{k_2} \end{pmatrix} \right] w_0'^L + r_{k,L} \\ &= \frac{\partial f_k}{\partial L}(\bar{x}_F, \alpha_0) w_0'^L + r_{k,L}. \end{aligned}$$

In order to compute a set enclosure of $r_{k,L}$, it is sufficient to observe that

$$\begin{aligned} &[R'_k(\bar{L} + \xi_0^L, \alpha) - R'_k(\bar{L}, \alpha_0)] \begin{pmatrix} \bar{a}_k \\ \bar{b}_k \end{pmatrix} w_0'^L \\ &\in \hat{\alpha} \left[(|\bar{a}_k| + |\bar{b}_k|)(\alpha_0 k^2 |\hat{L}| + k) \right] \mathbf{r} + (|\bar{a}_k| + |\bar{b}_k|) \alpha_0 k^2 \mathbf{r}^2, \end{aligned}$$

$$R'_k(\bar{L} + \xi_0^L, \alpha) \begin{pmatrix} \xi_k^a \\ \xi_k^b \end{pmatrix} w_0'^L \in (2\alpha + 1) \frac{1}{k^{s-1}} \mathbb{I}_2 \mathbf{r}^2 \\ + \left[\hat{\alpha}^2 k \left(|\hat{a}_k| + |\hat{b}_k| \right) \mathbb{I}_2 + \hat{\alpha} k \begin{pmatrix} \alpha_0 |\hat{a}_k| + (1 + \alpha_0) |\hat{b}_k| \\ (1 + \alpha_0) |\hat{a}_k| + \alpha_0 |\hat{b}_k| \end{pmatrix} \right] \mathbf{r},$$

$$\sum_{k_1+k_2=k} [\alpha \Theta'_{k_1}(\bar{L} + \xi_0^L) - \alpha_0 \Theta'_{k_1}(\bar{L})] \begin{pmatrix} \bar{a}_{k_1} \bar{a}_{k_2} - \bar{b}_{k_1} \bar{b}_{k_2} \\ \bar{a}_{k_1} \bar{b}_{k_2} + \bar{b}_{k_1} \bar{a}_{k_2} \end{pmatrix} w_0'^L \\ \in [\hat{\alpha} \Sigma_{k,L}^{(1)} + \hat{\alpha} \alpha_0 |\hat{L}| \Sigma_{k,L}^{(2)}] \mathbf{r} + \alpha_0 \Sigma_{k,L}^{(2)} \mathbf{r}^2,$$

$$\alpha \sum_{k_1+k_2=k} \Theta'_{k_1}(\bar{L} + \xi_0^L) \begin{pmatrix} \bar{a}_{k_1} \xi_{k_2}^a + \xi_{k_1}^a \bar{a}_{k_2} + \xi_{k_1}^a \xi_{k_2}^a - \bar{b}_{k_1} \xi_{k_2}^b - \xi_{k_1}^b \bar{b}_{k_2} - \xi_{k_1}^b \xi_{k_2}^b \\ \bar{a}_{k_1} \xi_{k_2}^b + \xi_{k_1}^a \bar{b}_{k_2} + \xi_{k_1}^a \xi_{k_2}^b + \bar{b}_{k_1} \xi_{k_2}^a + \xi_{k_1}^b \bar{a}_{k_2} + \xi_{k_1}^b \xi_{k_2}^a \end{pmatrix} w_0'^L \\ \in [\hat{\alpha}^2 \alpha \Sigma_{k,L}^{(3)} + \hat{\alpha} \alpha \Sigma_{k,L}^{(4)}] \mathbf{r} + [2\hat{\alpha} \alpha \Sigma_{k,L}^{(5)} + 2\alpha \Sigma_{k,L}^{(6)}] \mathbf{r}^2 + 4\alpha \Sigma_{k,L}^{(7)} \mathbf{r}^3.$$

Consider now the case $k \in \{m, \dots, M-1\}$. Then

$$\frac{\partial f_k}{\partial L}(\bar{x} + \xi, \alpha) w_0'^L \\ = R'_k(\bar{L} + \xi_0^L, \alpha) \begin{pmatrix} w_k^a \\ w_k^b \end{pmatrix} w_0'^L + \alpha \sum_{k_1+k_2=k} \Theta'_{k_1}(\bar{L} + \xi_0^L) \begin{pmatrix} \bar{a}_{k_1} \bar{a}_{k_2} - \bar{b}_{k_1} \bar{b}_{k_2} \\ \bar{a}_{k_1} \bar{b}_{k_2} + \bar{b}_{k_1} \bar{a}_{k_2} \end{pmatrix} w_0'^L \\ + \alpha \sum_{k_1+k_2=k} \Theta'_{k_1}(\bar{L} + \xi_0^L) \begin{pmatrix} \bar{a}_{k_1} \xi_{k_2}^a + \xi_{k_1}^a \bar{a}_{k_2} + \xi_{k_1}^a \xi_{k_2}^a - \bar{b}_{k_1} \xi_{k_2}^b - \xi_{k_1}^b \bar{b}_{k_2} - \xi_{k_1}^b \xi_{k_2}^b \\ \bar{a}_{k_1} \xi_{k_2}^b + \xi_{k_1}^a \bar{b}_{k_2} + \xi_{k_1}^a \xi_{k_2}^b + \bar{b}_{k_1} \xi_{k_2}^a + \xi_{k_1}^b \bar{a}_{k_2} + \xi_{k_1}^b \xi_{k_2}^a \end{pmatrix} w_0'^L \\ \in \left[\frac{2\alpha + 1}{k^{s-1}} \mathbb{I}_2 \right] \mathbf{r}^2 + \alpha \Sigma_{k,L}^{(1)} \mathbf{r} \\ + [\hat{\alpha}^2 \alpha \Sigma_{k,L}^{(3)} + \hat{\alpha} \alpha \Sigma_{k,L}^{(4)}] \mathbf{r} + [2\hat{\alpha} \alpha \Sigma_{k,L}^{(5)} + 2\alpha \Sigma_{k,L}^{(6)}] \mathbf{r}^2 + 4\alpha \Sigma_{k,L}^{(7)} \mathbf{r}^3.$$

Consider finally the case $k \geq M$. Then

$$\frac{\partial f_k}{\partial L}(\bar{x} + \xi, \alpha) w_0'^L = R'_k(\bar{L} + \xi_0^L, \alpha) \begin{pmatrix} w_k^a \\ w_k^b \end{pmatrix} w_0'^L$$

$$\begin{aligned}
& +\alpha \sum_{k_1+k_2=k} \Theta'_{k_1}(\bar{L} + \xi_0^L) \begin{pmatrix} \bar{a}_{k_1} w_{k_2}^a + w_{k_1}^a \bar{a}_{k_2} + w_{k_1}^a w_{k_2}^a - \bar{b}_{k_1} w_{k_2}^b - w_{k_1}^b \bar{b}_{k_2} - w_{k_1}^b w_{k_2}^b \\ \bar{a}_{k_1} w_{k_2}^b + w_{k_1}^a \bar{b}_{k_2} + w_{k_1}^a w_{k_2}^b + \bar{b}_{k_1} w_{k_2}^a + w_{k_1}^b \bar{a}_{k_2} + w_{k_1}^b w_{k_2}^a \end{pmatrix} w_0'^L \\
& \in \frac{2\alpha+1}{k^{s-1}} \mathbb{I}_2 \mathbf{r}^2 + 2\alpha \sum_{k_1+k_2=k} |k_1| \left[(|\bar{a}_{k_1}| + |\bar{b}_{k_1}|) \mathbf{w}_{k_2} + \mathbf{w}_{k_1} (|\bar{a}_{k_2}| + |\bar{b}_{k_2}|) + 2\mathbf{w}_{k_1} \mathbf{w}_{k_2} \right] \mathbb{I}_2 \mathbf{r} \\
& + 2\alpha \hat{\alpha} \sum_{k_1+k_2=k} |k_1| \left[(|\hat{a}_{k_1}| + |\hat{b}_{k_1}|) \mathbf{w}_{k_2} + \mathbf{w}_{k_1} (|\hat{a}_{k_2}| + |\hat{b}_{k_2}|) \right] \mathbb{I}_2 \mathbf{r}.
\end{aligned}$$

Now,

$$\begin{aligned}
& \sum_{k_1+k_2=k} |k_1| \left[(|\bar{a}_{k_1}| + |\bar{b}_{k_1}|) \mathbf{w}_{k_2} + \mathbf{w}_{k_1} (|\bar{a}_{k_2}| + |\bar{b}_{k_2}|) \right] \\
& = \sum_{k_1=-m+1}^{m-1} |k_1| (|\bar{a}_{k_1}| + |\bar{b}_{k_1}|) \frac{\mathbf{r}}{|k-k_1|^s} + \sum_{k_2=-m+1}^{m-1} |k-k_2| \frac{\mathbf{r}}{|k-k_2|^s} (|\bar{a}_{k_2}| + |\bar{b}_{k_2}|) \\
& = \sum_{k_1=1}^{m-1} k_1 (|\bar{a}_{k_1}| + |\bar{b}_{k_1}|) \left[\frac{1}{(k+k_1)^s} + \frac{1}{(k-k_1)^s} \right] \mathbf{r} + \frac{\mathbf{r}}{k^{s-1}} (|\bar{a}_0| + |\bar{b}_0|) \\
& + \sum_{k_1=1}^{m-1} (|\bar{a}_{k_1}| + |\bar{b}_{k_1}|) \left[\frac{1}{(k+k_1)^{s-1}} + \frac{1}{(k-k_1)^{s-1}} \right] \mathbf{r} \\
& \subseteq \frac{1}{k^{s-1}} \left[\frac{1}{M} \sum_{k_1=1}^{m-1} k_1 \left(1 + \frac{1}{[1-\frac{k_1}{M}]^s} \right) (|\bar{a}_{k_1}| + |\bar{b}_{k_1}|) \right. \\
& \quad \left. + |\bar{a}_0| + |\bar{b}_0| + \sum_{k_1=1}^{m-1} \left(1 + \frac{1}{[1-\frac{k_1}{M}]^{s-1}} \right) (|\bar{a}_{k_1}| + |\bar{b}_{k_1}|) \right] \mathbf{r}.
\end{aligned}$$

Using in part Lemma 6.2.3, we get that

$$\begin{aligned}
\sum_{k_1+k_2=k} |k_1| \mathbf{w}_{k_1} \mathbf{w}_{k_2} & = \sum_{k_1=1}^{\infty} (2k_1+k) \mathbf{w}_{k_1} \mathbf{w}_{k+k_1} + \sum_{k_1=1}^k k_1 \mathbf{w}_{k_1} \mathbf{w}_{k-k_1} \\
& = \left[\sum_{k_1=1}^{\infty} \frac{2k_1+k}{k_1^s (k+k_1)^s} + \frac{1}{k^{s-1}} + \sum_{k_1=1}^{k-1} \frac{1}{k_1^{s-1} (k-k_1)^s} \right] \mathbf{r}^2 \\
& \subseteq \frac{1}{k^{s-1}} \left[2 + \frac{2}{M} + \frac{1}{s-1} + 2 \left[\frac{2}{M} [1 + \ln(M-1)] + \frac{\pi^2}{6} \right] \left[\frac{2}{M} + 1 \right]^{s-2} \right] \mathbf{r}^2.
\end{aligned}$$

Hence, we finally get that

$$\frac{\partial f_k}{\partial L}(\bar{x} + \xi, \alpha) w_0'^L \in \frac{1}{k^{s-1}} \left[4\alpha \Sigma_{M,L}^{(7)} \mathbf{r}^3 + \left(2\hat{\alpha} \alpha \Sigma_{M,L}^{(5)} + (2\alpha+1) \mathbb{I}_2 + 2\alpha \Sigma_{M,L}^{(6)} \right) \mathbf{r}^2 \right]. \quad \blacksquare$$

Lemma 6.2.5 For $k \in \{1, \dots, m-1\}$, define

$$\begin{aligned} r_{k,a_0} &= (\hat{\alpha}\Theta_0 + \alpha\Theta_k(\bar{L} + \xi_0^L) - \alpha_0\Theta_k(\bar{L})) \begin{pmatrix} \bar{a}_k \\ \bar{b}_k \end{pmatrix} w_0'^a \\ &\quad + \alpha [\Theta_0 + \Theta_k(\bar{L} + \xi_0^L)] \begin{pmatrix} \hat{\alpha}\hat{a}_k + w_k^a \\ \hat{\alpha}\hat{b}_k + w_k^b \end{pmatrix} w_0'^a \end{aligned} \quad (168)$$

and let

$$r_{k,a_0}^{(2)} = \frac{3\alpha}{k^s} \mathbb{I}_2 + \alpha_0 k (|\bar{a}_k| + |\bar{b}_k|) \mathbb{I}_2 \quad (169)$$

$$\begin{aligned} r_{k,a_0}^{(1)} &= \hat{\alpha}\alpha \begin{pmatrix} 2|\hat{a}_k| + |\hat{b}_k| \\ |\hat{a}_k| + 2|\hat{b}_k| \end{pmatrix} \\ &\quad + \hat{\alpha} \left[\begin{pmatrix} |\bar{a}_k| \\ |\bar{b}_k| \end{pmatrix} + (1 + \alpha_0 k |\hat{L}|) (|\bar{a}_k| + |\bar{b}_k|) \mathbb{I}_2 \right] \end{aligned} \quad (170)$$

Then,

$$\frac{\partial f_k}{\partial a_0}(\bar{x} + \xi, \alpha) w_0'^a = \frac{\partial f_k}{\partial a_0}(\bar{x}_F, \alpha_0) w_0'^a + r_{k,a_0} \quad (171)$$

and

$$r_{k,a_0} \in r_{k,a_0}^{(2)} \mathbf{r}^2 + r_{k,a_0}^{(1)} \mathbf{r}. \quad (172)$$

For $k \geq m$, define

$$r_{k,a_0}^{(2)} = \alpha \frac{3}{k^s} \mathbb{I}_2.$$

We get that

$$\frac{\partial f_k}{\partial a_0}(\bar{x} + \xi, \alpha) w_0'^a \in r_{k,a_0}^{(2)} \mathbf{r}^2. \quad (173)$$

Proof. For any $k \geq 1$, we have that

$$\frac{\partial f_k}{\partial a_0}(x, \alpha) = \alpha [\Theta_0 + \Theta_k(L)] \begin{pmatrix} a_k \\ b_k \end{pmatrix}.$$

Consider the case $k \in \{1, \dots, m-1\}$,

$$\frac{\partial f_k}{\partial a_0}(\bar{x} + \xi, \alpha) w_0'^a = \alpha [\Theta_0 + \Theta_k(\bar{L} + \xi_0^L)] \begin{pmatrix} \bar{a}_k + \xi_k^a \\ \bar{b}_k + \xi_k^b \end{pmatrix} w_0'^a$$

$$\begin{aligned}
&= \alpha_0 [\Theta_0 + \Theta_k(\bar{L})] \begin{pmatrix} \bar{a}_k \\ \bar{b}_k \end{pmatrix} w_0'^a + (\hat{\alpha}\Theta_0 + \alpha\Theta_k(\bar{L} + \xi_0^L) - \alpha_0\Theta_k(\bar{L})) \begin{pmatrix} \bar{a}_k \\ \bar{b}_k \end{pmatrix} w_0'^a \\
&\quad + \alpha [\Theta_0 + \Theta_k(\bar{L} + \xi_0^L)] \begin{pmatrix} \hat{\alpha}\hat{a}_k + w_k^a \\ \hat{\alpha}\hat{b}_k + w_k^b \end{pmatrix} w_0'^a \\
&= \frac{\partial f_k}{\partial a_0}(\bar{x} + \xi, \alpha) w_0'^a + r_{k,a_0}.
\end{aligned}$$

To obtain the set enclosure of r_{k,a_0} , it is sufficient to notice that

$$\begin{aligned}
&[\hat{\alpha}\Theta_0 + \alpha\Theta_k(\bar{L} + \xi_0^L) - \alpha_0\Theta_k(\bar{L})] \begin{pmatrix} \bar{a}_k \\ \bar{b}_k \end{pmatrix} w_0'^a \\
&\in \hat{\alpha} \left[\begin{pmatrix} |\bar{a}_k| \\ |\hat{b}_k| \end{pmatrix} + (1 + \alpha_0 k |\hat{L}|) (|\bar{a}_k| + |\bar{b}_k|) \mathbb{I}_2 \right] \mathbf{r} + \alpha_0 k (|\bar{a}_k| + |\bar{b}_k|) \mathbb{I}_2 \mathbf{r}^2
\end{aligned}$$

and

$$\alpha [\Theta_0 + \Theta_k(\bar{L} + \xi_0^L)] \begin{pmatrix} \hat{\alpha}\hat{a}_k + w_k^a \\ \hat{\alpha}\hat{b}_k + w_k^b \end{pmatrix} w_0'^a \in \hat{\alpha}\alpha \begin{pmatrix} 2|\hat{a}_k| + |\hat{b}_k| \\ |\hat{a}_k| + 2|\hat{b}_k| \end{pmatrix} \mathbf{r} + \frac{3\alpha}{k^s} \mathbb{I}_2 \mathbf{r}^2. \quad \blacksquare$$

Lemma 6.2.6 *Let $\mathbb{I}_2 = (1, 1)^T$, $a, b, \hat{L} \in \mathbb{R}$, $\hat{\alpha}, \bar{L} \geq 0$, $\alpha_0 \geq \pi/2$, $\alpha = \alpha_0 + \hat{\alpha}$, $w_k' \in \frac{\mathbf{r}}{k^s} \mathbb{I}_2$ for $k \geq 1$, $\xi = \hat{\alpha}\hat{L} + w_0^L$ with $w_0^L \in \mathbf{r} = [-r, r]$. Recall that $\mathbf{1} = [-1, 1]$. For $k \in \{1, \dots, m-1\}$, define*

$$\begin{aligned}
\Sigma_k^{(1)} &= \sum_{i=1}^{k+m-1} \frac{i + |k-i|}{i^s} (|\bar{a}_{k-i}| + |\bar{b}_{k-i}|) \mathbb{I}_2, \quad \Sigma_k^{(2)} = \sum_{i=1}^{k+m-1} \frac{(|\bar{a}_{k-i}| + |\bar{b}_{k-i}|)}{i^s} \mathbb{I}_2, \\
\Sigma_k^{(3)} &= \sum_{i=m}^{k+m-1} \frac{(|\bar{a}_{k-i}| + |\bar{b}_{k-i}|)}{i^s} \mathbb{I}_2, \quad \Sigma_k^{(4)} = \sum_{i=1}^{m-k-1} \frac{(k+2i)}{i^s} (|\bar{a}_{k+i}| + |\bar{b}_{k+i}|) \mathbb{I}_2, \\
\Sigma_k^{(5)} &= \sum_{i=1}^{m-k-1} \frac{(|\bar{a}_{k+i}| + |\bar{b}_{k+i}|)}{i^s} \mathbb{I}_2, \quad \Sigma_k^{(6)} = \sum_{i=1}^{k+m-1} \frac{(|\hat{a}_{k-i}| + |\hat{b}_{k-i}|)}{i^s} \mathbb{I}_2, \\
\Sigma_k^{(7)} &= \sum_{i=1}^{m-k-1} \frac{(|\hat{a}_{k+i}| + |\hat{b}_{k+i}|)}{i^s} \mathbb{I}_2, \\
\Sigma_k^{(8)} &= \left[\sum_{k_1=1}^{k-1} \frac{1}{k_1^s (k-k_1)^s} + \frac{1}{k^s} + \sum_{k_1=1}^{M-1} \frac{2}{k_1^s (k+k_1)^s} + \frac{2}{(k+M)^s (M-1)^{s-1} (s-1)} \right] \mathbb{I}_2.
\end{aligned}$$

Consider $k \in \{1, \dots, m-1\}$ and define in this case

$$\begin{aligned}
\rho_k &= [R_k(\bar{L} + \xi_0^L, \alpha) - R_k(\bar{L}, \alpha_0)] w'_k \\
&+ \alpha \sum_{i=1}^{\infty} [\Theta_i(\bar{L} + \xi_0^L) + \Theta_{k-i}(\bar{L} + \xi_0^L)] \begin{pmatrix} \bar{a}_{k-i} & -\bar{b}_{k-i} \\ \bar{b}_{k-i} & \bar{a}_{k-i} \end{pmatrix} w'_i \\
&- \alpha_0 \sum_{i=1}^{m-1} [\Theta_i(\bar{L}) + \Theta_{k-i}(\bar{L})] \begin{pmatrix} \bar{a}_{k-i} & -\bar{b}_{k-i} \\ \bar{b}_{k-i} & \bar{a}_{k-i} \end{pmatrix} w'_i \\
&+ \alpha \sum_{i=1}^{\infty} [\Theta_{-i}(\bar{L} + \xi_0^L) + \Theta_{k+i}(\bar{L} + \xi_0^L)] \begin{pmatrix} \bar{a}_{k+i} & -\bar{b}_{k+i} \\ \bar{b}_{k+i} & \bar{a}_{k+i} \end{pmatrix} w'_i \\
&- \alpha_0 \sum_{i=1}^{m-1} [\Theta_{-i}(\bar{L}) + \Theta_{k+i}(\bar{L})] \begin{pmatrix} \bar{a}_{k+i} & -\bar{b}_{k+i} \\ \bar{b}_{k+i} & \bar{a}_{k+i} \end{pmatrix} w'_i \\
&+ \alpha \sum_{i=1}^{\infty} [\Theta_i(\bar{L} + \xi_0^L) + \Theta_{k-i}(\bar{L} + \xi_0^L)] \begin{pmatrix} \xi_{k-i}^a & -\xi_{k-i}^b \\ \xi_{k-i}^b & \xi_{k-i}^a \end{pmatrix} w'_i \\
&+ \alpha \sum_{i=1}^{\infty} [\Theta_{-i}(\bar{L} + \xi_0^L) + \Theta_{k+i}(\bar{L} + \xi_0^L)] \begin{pmatrix} \xi_{k+i}^a & -\xi_{k+i}^b \\ \xi_{k+i}^b & \xi_{k+i}^a \end{pmatrix} w'_i.
\end{aligned} \tag{174}$$

Then

$$\sum_{i=1}^{\infty} \frac{\partial f_k}{\partial x_i}(\bar{x} + \xi, \alpha) w'_i = \sum_{i=1}^{m-1} \frac{\partial f_k^{(m)}}{\partial x_i}(\bar{x}_F, \alpha_0) w'_i + \rho_k. \tag{175}$$

Still for the case $k \in \{1, \dots, m-1\}$, letting

$$\rho_k^{(2)} = \frac{(2\alpha_0 + 1)}{k^{s-1}} \mathbb{I}_2 + 2\alpha_0 \left[\Sigma_k^{(1)} + \Sigma_k^{(4)} \right] + 8\alpha \Sigma_k^{(8)}, \tag{176}$$

$$\begin{aligned}
\rho_k^{(1)} &= \hat{\alpha} \left[(2\alpha_0 + 1)k|\hat{L}| + 2 \right] \frac{1}{k^{s-1}} \mathbb{I}_2 + 2\alpha_0 \hat{\alpha} |\hat{L}| \left(\Sigma_k^{(1)} + \Sigma_k^{(4)} \right) \\
&+ 4\hat{\alpha} \left(\Sigma_k^{(2)} + \Sigma_k^{(5)} \right) + 4\alpha \Sigma_k^{(3)} + 4\alpha \hat{\alpha} \left(\Sigma_k^{(6)} + \Sigma_k^{(7)} \right).
\end{aligned} \tag{177}$$

we get that

$$\rho_k \in \rho_k^{(2)} \mathbf{r}^2 + \rho_k^{(1)} \mathbf{r}. \tag{178}$$

Consider now $k \geq m$. Define

$$\rho_k = [R_k(\bar{L} + \xi_0^L, \alpha) - R_k(\bar{L}, \alpha_0)] w'_k$$

$$\begin{aligned}
& +\alpha_0 \sum_{i=1}^{k-1} [\Theta_i(\bar{L} + \xi_0^L) + \Theta_{k-i}(\bar{L} + \xi_0^L)] \begin{pmatrix} \bar{a}_{k-i} + \xi_{k-i}^a & -\bar{b}_{k-i} - \xi_{k-i}^b \\ \bar{b}_{k-i} + \xi_{k-i}^b & \bar{a}_{k-i} + \xi_{k-i}^a \end{pmatrix} w'_i \\
& +\alpha_0 \bar{a}_0 [\Theta_k(\bar{L} + \xi_0^L) - \Theta_0(\bar{L})] w'_k \\
& +\alpha_0 [\Theta_k(\bar{L} + \xi_0^L) + \Theta_0(\cdot)] \begin{pmatrix} \xi_0^a & -\xi_0^b \\ \xi_0^b & \xi_0^a \end{pmatrix} w'_k \\
& +\alpha_0 \sum_{i=k+1}^{\infty} [\Theta_i(\bar{L} + \xi_0^L) + \Theta_{k-i}(\bar{L} + \xi_0^L)] \begin{pmatrix} \bar{a}_{k-i} + \xi_{k-i}^a & -\bar{b}_{k-i} - \xi_{k-i}^b \\ \bar{b}_{k-i} + \xi_{k-i}^b & \bar{a}_{k-i} + \xi_{k-i}^a \end{pmatrix} w'_i \\
& +\hat{\alpha} \sum_{i=1}^{\infty} [\Theta_i(\bar{L} + \xi_0^L) + \Theta_{k-i}(\bar{L} + \xi_0^L)] \begin{pmatrix} \bar{a}_{k-i} + \xi_{k-i}^a & -\bar{b}_{k-i} - \xi_{k-i}^b \\ \bar{b}_{k-i} + \xi_{k-i}^b & \bar{a}_{k-i} + \xi_{k-i}^a \end{pmatrix} w'_i \\
& +\alpha \sum_{i=1}^{\infty} [\Theta_{-i}(\bar{L} + \xi_0^L) + \Theta_{k+i}(\bar{L} + \xi_0^L)] \begin{pmatrix} w_{k+i}^a & -w_{k+i}^b \\ w_{k+i}^b & w_{k+i}^a \end{pmatrix} w'_i.
\end{aligned}$$

Then for $k \geq m$, we have that

$$\sum_{i=1}^{\infty} \frac{\partial f_k}{\partial x_i}(\bar{x} + \xi, \alpha) w'_i = \Lambda_k w'_k + \rho_k. \quad (179)$$

For $k \in \{m, \dots, M-1\}$, define

$$\rho_k^{(2)} = \frac{2\alpha_0 + 1}{k^{s-1}} \mathbb{I}_2 + \frac{2\alpha_0 |\bar{a}_0|}{k^{s-1}} \mathbb{I}_2 + \frac{3\alpha}{k^s} \mathbb{I}_2 \quad (180)$$

$$+ 8\alpha \left[\sum_{k_1=1}^{k-1} \frac{1}{(k-k_1)^s k_1^s} + \sum_{k_1=1}^{M-1} \frac{1}{(k+k_1)^s k_1^s} + \frac{1}{(k+M)^s (M-1)^{s-1} (s-1)} \right] \mathbb{I}_2$$

$$\rho_k^{(1)} = \left[2 + (2\alpha_0 + 1) |\hat{L}| k \right] \frac{\hat{\alpha}}{k^s} \mathbb{I}_2 + 4\alpha \sum_{k_1=1}^{m-1} (|\bar{a}_{k_1}| + |\bar{b}_{k_1}|) \left[\frac{1}{(k-k_1)^s} + \frac{1}{(k+k_1)^s} \right] \mathbb{I}_2$$

$$+ 4\alpha \hat{\alpha} \sum_{k_1=1}^{m-1} (|\hat{a}_{k_1}| + |\hat{b}_{k_1}|) \left[\frac{1}{(k-k_1)^s} + \frac{1}{(k+k_1)^s} \right] \mathbb{I}_2 \quad (181)$$

$$+ \frac{2\alpha_0}{k^{s-1}} |\bar{a}_0| \hat{\alpha} |\hat{L}| \mathbb{I}_2 + \frac{3\hat{\alpha}}{k^s} (|\bar{a}_0| + \alpha |\hat{a}_0|) \mathbb{I}_2.$$

Then for $k \in \{m, \dots, M-1\}$, we have that

$$\rho_k \in \rho_k^{(2)} \mathbf{r}^2 + \rho_k^{(1)} \mathbf{r}. \quad (182)$$

Define

$$\begin{aligned}\rho_M^{(2)} &= \left[(2\alpha_0 + 1) + 2\alpha_0|\bar{a}_0| + \frac{3\alpha}{M} \right] \mathbb{I}_2 \\ &\quad + \frac{32\alpha}{M} \left[\frac{2}{M} [1 + \ln(M-1)] + \frac{\pi^2}{6} \right] \left[\frac{2}{M} + 1 \right]^{s-2} \mathbb{I}_2 \\ &\quad + \frac{8\alpha}{M} \left[1 + \frac{1}{2^s} + \frac{1}{3^s} + \frac{1}{3^{s-1}(s-1)} \right] \mathbb{I}_2\end{aligned}\tag{183}$$

$$\begin{aligned}\rho_M^{(1)} &= \hat{\alpha} \left[\frac{2}{M} + (2\alpha_0 + 1)|\hat{L}| \right] \mathbb{I}_2 + \frac{4\alpha}{M} \sum_{k_1=1}^{m-1} (|\bar{a}_{k_1}| + |\bar{b}_{k_1}|) \left[\frac{1}{(1 - \frac{k_1}{M})^s} + 1 \right] \mathbb{I}_2 \\ &\quad + \frac{4\alpha}{M} \hat{\alpha} \sum_{k_1=1}^{m-1} (|\hat{a}_{k_1}| + |\hat{b}_{k_1}|) \left[\frac{1}{(1 - \frac{k_1}{M})^s} + 1 \right] \mathbb{I}_2 \\ &\quad + 2\alpha_0|\bar{a}_0|\hat{\alpha}|\hat{L}|\mathbb{I}_2 + \frac{3\hat{\alpha}}{M}(|\bar{a}_0| + \alpha|\hat{a}_0|)\mathbb{I}_2.\end{aligned}\tag{184}$$

Then for $k \geq M$,

$$\rho_k \in \frac{1}{k^{s-1}} \left[\rho_M^{(2)} \mathbf{r}^2 + \rho_M^{(1)} \mathbf{r} \right].\tag{185}$$

Proof. For all $k \geq 1$, we have that

$$\frac{\partial f_k}{\partial x_j}(x, \alpha) = \delta_{k,j} R_k + \alpha [\Theta_j + \Theta_{k-j}] \begin{pmatrix} a_{k-j} & -b_{k-j} \\ b_{k-j} & a_{k-j} \end{pmatrix} + \alpha [\Theta_{-j} + \Theta_{k+j}] \begin{pmatrix} a_{k+j} & b_{k+j} \\ b_{k+j} & -a_{k+j} \end{pmatrix}.$$

Hence, recalling that $\xi = \hat{\alpha}\hat{x} + w$ and still considering any $k \geq 1$,

$$\begin{aligned}&\sum_{i=1}^{\infty} \frac{\partial f_k}{\partial x_i}(\bar{x} + \xi, \alpha) w'_i \\ &= R_k(\bar{L} + \xi_0^L, \alpha) w'_k \\ &\quad + \alpha \sum_{i=1}^{\infty} [\Theta_i(\bar{L} + \xi_0^L) + \Theta_{k-i}(\bar{L} + \xi_0^L)] \begin{pmatrix} \bar{a}_{k-i} + \xi_{k-i}^a & -\bar{b}_{k-i} - \xi_{k-i}^b \\ \bar{b}_{k-i} + \xi_{k-i}^b & \bar{a}_{k-i} + \xi_{k-i}^a \end{pmatrix} w'_i \\ &\quad + \alpha \sum_{i=1}^{\infty} [\Theta_{-i}(\bar{L} + \xi_0^L) + \Theta_{k+i}(\bar{L} + \xi_0^L)] \begin{pmatrix} \bar{a}_{k+i} + \xi_{k+i}^a & -\bar{b}_{k+i} - \xi_{k+i}^b \\ \bar{b}_{k+i} + \xi_{k+i}^b & \bar{a}_{k+i} + \xi_{k+i}^a \end{pmatrix} w'_i.\end{aligned}$$

Consider now the case $k \in \{1, \dots, m-1\}$. Hence

$$\sum_{i=1}^{\infty} \frac{\partial f_k}{\partial x_i}(\bar{x} + \xi, \alpha) w'_i$$

$$\begin{aligned}
&= R_k(\bar{L}, \alpha_0)w'_k + [R_k(\bar{L} + \xi_0^L, \alpha) - R_k(\bar{L}, \alpha_0)] w'_k \\
&\quad + \alpha \sum_{i=1}^{\infty} [\Theta_i(\bar{L} + \xi_0^L) + \Theta_{k-i}(\bar{L} + \xi_0^L)] \begin{pmatrix} \bar{a}_{k-i} & -\bar{b}_{k-i} \\ \bar{b}_{k-i} & \bar{a}_{k-i} \end{pmatrix} w'_i \\
&\quad + \alpha \sum_{i=1}^{\infty} [\Theta_{-i}(\bar{L} + \xi_0^L) + \Theta_{k+i}(\bar{L} + \xi_0^L)] \begin{pmatrix} \bar{a}_{k+i} & -\bar{b}_{k+i} \\ \bar{b}_{k+i} & \bar{a}_{k+i} \end{pmatrix} w'_i \\
&\quad + \alpha \sum_{i=1}^{\infty} [\Theta_i(\bar{L} + \xi_0^L) + \Theta_{k-i}(\bar{L} + \xi_0^L)] \begin{pmatrix} \xi_{k-i}^a & -\xi_{k-i}^b \\ \xi_{k-i}^b & \xi_{k-i}^a \end{pmatrix} w'_i \\
&\quad + \alpha \sum_{i=1}^{\infty} [\Theta_{-i}(\bar{L} + \xi_0^L) + \Theta_{k+i}(\bar{L} + \xi_0^L)] \begin{pmatrix} \xi_{k+i}^a & -\xi_{k+i}^b \\ \xi_{k+i}^b & \xi_{k+i}^a \end{pmatrix} w'_i \\
&= \sum_{i=1}^{m-1} \frac{\partial f_k^{(m)}}{\partial x_i}(\bar{x}_F, \alpha_0)w'_i + \rho_k.
\end{aligned}$$

In order to compute a set enclosure of ρ_k , we apply the mean value theorem several times.

$$\begin{aligned}
&[R_k(\bar{L} + \xi_0^L, \alpha) - R_k(\bar{L}, \alpha_0)] \begin{pmatrix} w'_k{}^a \\ w'_k{}^b \end{pmatrix} \\
&\in (2\alpha_0 + 1) \frac{1}{k^{s-1}} \mathbb{I}_2 \mathbf{r}^2 + \hat{\alpha} \left[(2\alpha_0 + 1)k|\hat{L}| + 2 \right] \frac{1}{k^{s-1}} \mathbb{I}_2 \mathbf{r}, \\
&\alpha \sum_{i=1}^{\infty} [\Theta_i(\bar{L} + \xi_0^L) + \Theta_{k-i}(\bar{L} + \xi_0^L)] \begin{pmatrix} \bar{a}_{k-i} & -\bar{b}_{k-i} \\ \bar{b}_{k-i} & \bar{a}_{k-i} \end{pmatrix} w'_i \\
&\quad - \alpha_0 \sum_{i=1}^{m-1} [\Theta_i(\bar{L}) + \Theta_{k-i}(\bar{L})] \begin{pmatrix} \bar{a}_{k-i} & -\bar{b}_{k-i} \\ \bar{b}_{k-i} & \bar{a}_{k-i} \end{pmatrix} w'_i \\
&\in 2\alpha_0 \Sigma_k^{(1)} \mathbf{r}^2 + \left[2\alpha_0 \hat{\alpha} |\hat{L}| \Sigma_k^{(1)} + 4\hat{\alpha} \Sigma_k^{(2)} + 4\alpha_0 \Sigma_k^{(3)} \right] \mathbf{r}
\end{aligned}$$

and

$$\alpha \sum_{i=1}^{\infty} [\Theta_{-i}(\bar{L} + \xi_0^L) + \Theta_{k+i}(\bar{L} + \xi_0^L)] \begin{pmatrix} \bar{a}_{k+i} & -\bar{b}_{k+i} \\ \bar{b}_{k+i} & \bar{a}_{k+i} \end{pmatrix} w'_i$$

$$\begin{aligned}
& -\alpha_0 \sum_{i=1}^{m-1} [\Theta_{-i}(\bar{L}) + \Theta_{k+i}(\bar{L})] \begin{pmatrix} \bar{a}_{k+i} & -\bar{b}_{k+i} \\ \bar{b}_{k+i} & \bar{a}_{k+i} \end{pmatrix} w'_i \\
& \in 2\alpha_0 \Sigma_k^{(4)} \mathbf{r}^2 + \left[2\alpha_0 \hat{\alpha} |\hat{L}| \Sigma_k^{(4)} + 4\hat{\alpha} \Sigma_k^{(5)} \right] \mathbf{r}.
\end{aligned}$$

Finally,

$$\begin{aligned}
& \alpha \sum_{i=1}^{\infty} [\Theta_i(\bar{L} + \xi_0^L) + \Theta_{k-i}(\bar{L} + \xi_0^L)] \begin{pmatrix} \xi_{k-i}^a & -\xi_{k-i}^b \\ \xi_{k-i}^b & \xi_{k-i}^a \end{pmatrix} w'_i \\
& + \alpha \sum_{i=1}^{\infty} [\Theta_{-i}(\bar{L} + \xi_0^L) + \Theta_{k+i}(\bar{L} + \xi_0^L)] \begin{pmatrix} \xi_{k+i}^a & -\xi_{k+i}^b \\ \xi_{k+i}^b & \xi_{k+i}^a \end{pmatrix} w'_i \\
& \in 4\alpha \hat{\alpha} \left(\Sigma_k^{(6)} + \Sigma_k^{(7)} \right) \mathbf{r} + 8\alpha \Sigma_k^{(8)} \mathbf{r}^2
\end{aligned}$$

Now consider $k \geq m$. Then

$$\begin{aligned}
& \sum_{i=1}^{\infty} \frac{\partial f_k}{\partial x_i}(\bar{x} + \xi, \alpha) w'_i \\
& = R_k(\bar{L}, \alpha_0) w'_k + \alpha_0 \bar{a}_0 [\Theta_k(\bar{L}) + \Theta_0(\cdot)] w'_k \\
& + [R_k(\bar{L} + \xi_0^L, \alpha) - R_k(\bar{L}, \alpha_0)] w'_k \\
& + \alpha \sum_{i=1}^{k-1} [\Theta_i(\bar{L} + \xi_0^L) + \Theta_{k-i}(\bar{L} + \xi_0^L)] \begin{pmatrix} \bar{a}_{k-i} + \xi_{k-i}^a & -\bar{b}_{k-i} - \xi_{k-i}^b \\ \bar{b}_{k-i} + \xi_{k-i}^b & \bar{a}_{k-i} + \xi_{k-i}^a \end{pmatrix} w'_i \\
& + \alpha_0 \bar{a}_0 [\Theta_k(\bar{L} + \xi_0^L) - \Theta_k(\bar{L})] w'_k + \hat{\alpha} \bar{a}_0 [\Theta_k(\bar{L} + \xi_0^L) + \Theta_0(\cdot)] w'_k \\
& + \alpha [\Theta_k(\bar{L} + \xi_0^L) + \Theta_0(\cdot)] \begin{pmatrix} \xi_0^a & -\xi_0^b \\ \xi_0^b & \xi_0^a \end{pmatrix} w'_k \\
& + \alpha \sum_{i=k+1}^{\infty} [\Theta_i(\bar{L} + \xi_0^L) + \Theta_{k-i}(\bar{L} + \xi_0^L)] \begin{pmatrix} \bar{a}_{k-i} + \xi_{k-i}^a & -\bar{b}_{k-i} - \xi_{k-i}^b \\ \bar{b}_{k-i} + \xi_{k-i}^b & \bar{a}_{k-i} + \xi_{k-i}^a \end{pmatrix} w'_i \\
& + \alpha \sum_{i=1}^{\infty} [\Theta_{-i}(\bar{L} + \xi_0^L) + \Theta_{k+i}(\bar{L} + \xi_0^L)] \begin{pmatrix} w_{k+i}^a & -w_{k+i}^b \\ w_{k+i}^b & w_{k+i}^a \end{pmatrix} w'_i \\
& = \Lambda_k w'_k + \rho_k.
\end{aligned}$$

Still considering $k \geq m$, observe that

$$\begin{aligned}
& [R_k(\bar{L} + \xi_0^L, \alpha) - R_k(\bar{L}, \alpha_0)] w'_k \in \frac{2\alpha_0 + 1}{k^{s-1}} \mathbb{I}_2 \mathbf{r}^2 + \hat{\alpha} \left[2 + (2\alpha_0 + 1) |\hat{L}| k \right] \frac{1}{k^s} \mathbb{I}_2 \mathbf{r}, \\
& \alpha \sum_{i=1}^{k-1} [\Theta_i(\bar{L} + \xi_0^L) + \Theta_{k-i}(\bar{L} + \xi_0^L)] \begin{pmatrix} \bar{a}_{k-i} + \xi_{k-i}^a & -\bar{b}_{k-i} - \xi_{k-i}^b \\ \bar{b}_{k-i} + \xi_{k-i}^b & \bar{a}_{k-i} + \xi_{k-i}^a \end{pmatrix} w'_i \\
& + \alpha \sum_{i=k+1}^{\infty} [\Theta_i(\bar{L} + \xi_0^L) + \Theta_{k-i}(\bar{L} + \xi_0^L)] \begin{pmatrix} \bar{a}_{k-i} + \xi_{k-i}^a & -\bar{b}_{k-i} - \xi_{k-i}^b \\ \bar{b}_{k-i} + \xi_{k-i}^b & \bar{a}_{k-i} + \xi_{k-i}^a \end{pmatrix} w'_i \\
& \in 4\alpha \sum_{k_1=1}^{m-1} (|\bar{a}_{k_1}| + |\bar{b}_{k_1}|) \left[\frac{1}{(k - k_1)^s} + \frac{1}{(k + k_1)^s} \right] \mathbb{I}_2 \mathbf{r} \\
& + 4\alpha \hat{\alpha} \sum_{k_1=1}^{m-1} (|\hat{a}_{k_1}| + |\hat{b}_{k_1}|) \left[\frac{1}{(k - k_1)^s} + \frac{1}{(k + k_1)^s} \right] \mathbb{I}_2 \mathbf{r} \\
& + 8\alpha \left[\sum_{k_1=1}^{k-1} \frac{1}{(k - k_1)^s k_1^s} + \sum_{k_1=1}^{\infty} \frac{1}{(k + k_1)^s k_1^s} \right] \mathbb{I}_2 \mathbf{r}^2, \\
& \alpha_0 \bar{a}_0 [\Theta_k(\bar{L} + \xi_0^L) - \Theta_k(\bar{L})] w'_k + \hat{\alpha} \bar{a}_0 [\Theta_k(\bar{L} + \xi_0^L) + \Theta_0(\cdot)] w'_k \\
& + \alpha [\Theta_k(\bar{L} + \xi_0^L) + \Theta_0(\cdot)] \begin{pmatrix} \xi_0^a & -\xi_0^b \\ \xi_0^b & \xi_0^a \end{pmatrix} w'_k \\
& \in \left[\frac{2\alpha_0 |\bar{a}_0|}{k^{s-1}} \mathbb{I}_2 + \frac{3\alpha}{k^s} \mathbb{I}_2 \right] \mathbf{r}^2 + \left[\frac{2\alpha_0}{k^{s-1}} |\bar{a}_0| \hat{\alpha} |\hat{L}| \mathbb{I}_2 + \frac{3\hat{\alpha}}{k^s} (|\bar{a}_0| + \alpha |\hat{a}_0|) \mathbb{I}_2 \right] \mathbf{r}
\end{aligned}$$

and

$$\begin{aligned}
& \alpha \sum_{i=1}^{\infty} [\Theta_{-i}(\bar{L} + \xi_0^L) + \Theta_{k+i}(\bar{L} + \xi_0^L)] \begin{pmatrix} w_{k+i}^a & -w_{k+i}^b \\ w_{k+i}^b & w_{k+i}^a \end{pmatrix} w'_i \\
& \in 8\alpha \sum_{k_1=1}^{\infty} \frac{1}{(k + k_1)^s k_1^s} \mathbb{I}_2 \mathbf{r}^2.
\end{aligned}$$

Hence, for $k \geq m$,

$$\begin{aligned}
\rho_k & \in \left(\frac{2\alpha_0 + 1}{k^{s-1}} + 8\alpha \left[\sum_{k_1=1}^{k-1} \frac{1}{(k - k_1)^s k_1^s} + \sum_{k_1=1}^{\infty} \frac{1}{(k + k_1)^s k_1^s} \right] + \frac{2\alpha_0 |\bar{a}_0|}{k^{s-1}} + \frac{3\alpha}{k^s} \right) \mathbb{I}_2 \mathbf{r}^2 \\
& + \left(\left[2 + (2\alpha_0 + 1) |\hat{L}| k \right] \frac{\hat{\alpha}}{k^s} + 4\alpha \sum_{k_1=1}^{m-1} (|\bar{a}_{k_1}| + |\bar{b}_{k_1}|) \left[\frac{1}{(k - k_1)^s} + \frac{1}{(k + k_1)^s} \right] \right)
\end{aligned}$$

$$\begin{aligned}
& + 4\alpha\hat{\alpha} \sum_{k_1=1}^{m-1} \left(|\hat{a}_{k_1}| + |\hat{b}_{k_1}| \right) \left[\frac{1}{(k-k_1)^s} + \frac{1}{(k+k_1)^s} \right] \\
& + \frac{2\alpha_0}{k^{s-1}} |\bar{a}_0| \hat{\alpha} |\hat{L}| + \frac{3\hat{\alpha}}{k^s} (|\bar{a}_0| + \alpha |\hat{a}_0|) \Big) \mathbb{I}_2 \mathbf{r}.
\end{aligned}$$

Hence, for $k \in \{m, \dots, M-1\}$, we get that

$$\rho_k \in \rho_k^{(2)} \mathbf{r}^2 + \rho_k^{(1)} \mathbf{r}.$$

Consider now $k \geq M$. Then first observe that by Lemma 6.2.3,

$$\begin{aligned}
\sum_{k_1=1}^{k-1} \frac{k^s}{k_1^s (k-k_1)^s} &= 2 \sum_{k_1=1}^{k-1} \frac{k^{s-1}}{k_1^s (k-k_1)^s} \\
&\leq 4 \left[\frac{2}{M} [1 + \ln(M-1)] + \frac{\pi^2}{6} \right] \left[\frac{2}{M} + 1 \right]^{s-2}.
\end{aligned}$$

Hence, for $k \geq M$,

$$\sum_{k_1=1}^{k-1} \frac{1}{k_1^s (k-k_1)^s} \leq \frac{1}{k^{s-1}} \cdot \frac{4}{M} \left[\frac{2}{M} [1 + \ln(M-1)] + \frac{\pi^2}{6} \right] \left[\frac{2}{M} + 1 \right]^{s-2}.$$

Therefore, we finally get that for every $k \geq M$

$$\rho_k \in \frac{1}{k^{s-1}} \left[\rho_M^{(2)} \mathbf{r}^2 + \rho_M^{(1)} \mathbf{r} \right]. \quad \blacksquare$$

For $k \in \{1, \dots, m-1\}$, recall (157), (168), (174) and define

$$r_k = r_{k,L} + r_{k,a_0} + \rho_k. \tag{186}$$

Then

$$Df_k(x_\alpha + w, \alpha)w' = Df_k^{(m)}(\bar{x}_F, \alpha_0)w'_F + r_k \tag{187}$$

Recalling (158), (159), (160), (169), (170), (176) and (177), we define

$$\begin{aligned}
r_k^{(3)} &= r_{k,L}^{(3)} \\
r_k^{(2)} &= r_{k,L}^{(2)} + r_{k,a_0}^{(2)} + \rho_k^{(2)} \\
r_k^{(1)} &= r_{k,L}^{(1)} + r_{k,a_0}^{(1)} + \rho_k^{(1)}.
\end{aligned}$$

Recalling (162), (172) and (178), we have that

$$r_k \in r_k^{(3)} \mathbf{r}^3 + r_k^{(2)} \mathbf{r}^2 + r_k^{(1)} \mathbf{r}. \quad (188)$$

Combining (151) and (186), we define

$$r_F = [r_0, r_1, \dots, r_{m-1}]^T \in \mathbb{R}^{2m}. \quad (189)$$

Hence,

$$Df_F(x_\alpha + w)w' = Df^{(m)}(\bar{x}_F, \alpha_0)w_F + r_F. \quad (190)$$

Also, for $i = 1, 2, 3$, we define

$$r_F^{(i)} = [r_0^{(i)}, r_1^{(i)}, \dots, r_{m-1}^{(i)}]^T \in \mathbb{R}^{2m}. \quad (191)$$

Hence, by (153) and (188), we get that

$$r_F \in r_F^{(3)} \mathbf{r}^3 + r_F^{(2)} \mathbf{r}^2 + r_F^{(1)} \mathbf{r}. \quad (192)$$

Define

$$v_F = \left[(1, 1), (1, 1), \left(\frac{1}{2^s}, \frac{1}{2^s} \right), \dots, \left(\frac{1}{(m-1)^s}, \frac{1}{(m-1)^s} \right) \right]^T \in \mathbb{R}^{2m}.$$

Recalling (138), we have that

$$\begin{aligned} [DT_\alpha(x_\alpha + w)w']_F &= [I_F - J_{F \times F} Df^{(m)}(\bar{x}_F, \alpha_0)]w_F - J_{F \times F} \cdot r_F \\ &\in |I_F - J_{F \times F} Df^{(m)}(\bar{x}_F, \alpha_0)| v_F \mathbf{r} \\ &\quad + |J_{F \times F}| \left(r_F^{(3)} \mathbf{r}^3 + r_F^{(2)} \mathbf{r}^2 + r_F^{(1)} \mathbf{r} \right). \end{aligned}$$

Definition 6.2.7 For $k \in \{0, \dots, m-1\}$, we define $Z_k(r, \alpha)$ by

$$\begin{aligned} Z_F(r, \alpha) &= \left[|J_{F \times F}| r_F^{(3)} \right] r^3 + \left[|J_{F \times F}| r_F^{(2)} \right] r^2 \\ &\quad + \left[|I_F - J_{F \times F} Df^{(m)}(\bar{x}_F, \alpha_0)| v_F + |J_{F \times F}| r_F^{(1)} \right] r. \end{aligned} \quad (193)$$

For $k \geq m$, define

$$r_k = \frac{\partial f_k}{\partial L}(\bar{x} + \xi, \alpha)w_0'^L + \frac{\partial f_k}{\partial a_0}(\bar{x} + \xi, \alpha)w_0'^a + \rho_k. \quad (194)$$

Hence,

$$\begin{aligned} Df_k(x_\alpha + w, \alpha)w' &= Df_k(\bar{x} + \xi, \alpha)w' \\ &= \frac{\partial f_k}{\partial L}(\bar{x} + \xi, \alpha)w_0'^L + \frac{\partial f_k}{\partial a_0}(\bar{x} + \xi, \alpha)w_0'^a + \sum_{i=1}^{\infty} \frac{\partial f_k}{\partial x_i}(\bar{x} + \xi, \alpha)w_i' \\ &= \Lambda_k w_k' + \left[\frac{\partial f_k}{\partial L}(\bar{x} + \xi, \alpha)w_0'^L + \frac{\partial f_k}{\partial a_0}(\bar{x} + \xi, \alpha)w_0'^a + \rho_k \right] \\ &= \Lambda_k w_k' + r_k. \end{aligned} \quad (195)$$

Consider now $k \in \{m, \dots, M-1\}$. By (163), (173) and (182), we get that

$$\begin{aligned} r_k &\in 4\alpha\Sigma_{k,L}^{(7)}\mathbf{r}^3 + \left[2\hat{\alpha}\alpha\Sigma_{k,L}^{(5)} + 2\alpha\Sigma_{k,L}^{(6)} + \frac{2\alpha+1}{k^{s-1}}\mathbb{I}_2 + r_{k,a_0}^{(2)} + \rho_k^{(2)} \right] \mathbf{r}^2 \\ &\quad + \left[\alpha\Sigma_{k,L}^{(1)} + \hat{\alpha}^2\alpha\Sigma_{k,L}^{(3)} + \hat{\alpha}\alpha\Sigma_{k,L}^{(4)} + \rho_k^{(1)} \right] \mathbf{r} \end{aligned}$$

Combining (139) and (195), we get that for $k \in \{m, \dots, M-1\}$

$$\begin{aligned} [DT_\alpha(x_\alpha + w)w']_k &= -\Lambda_k^{-1}r_k \\ &\in |\Lambda_k^{-1}| \left[4\alpha\Sigma_{k,L}^{(7)} \right] \mathbf{r}^3 \\ &\quad + |\Lambda_k^{-1}| \left[2\hat{\alpha}\alpha\Sigma_{k,L}^{(5)} + 2\alpha\Sigma_{k,L}^{(6)} + \frac{2\alpha+1}{k^{s-1}}\mathbb{I}_2 + r_{k,a_0}^{(2)} + \rho_k^{(2)} \right] \mathbf{r}^2 \\ &\quad + |\Lambda_k^{-1}| \left[\alpha\Sigma_{k,L}^{(1)} + \hat{\alpha}^2\alpha\Sigma_{k,L}^{(3)} + \hat{\alpha}\alpha\Sigma_{k,L}^{(4)} + \rho_k^{(1)} \right] \mathbf{r}. \end{aligned}$$

Definition 6.2.8 For $k \in \{m, \dots, M-1\}$, we define $Z_k(r, \alpha)$ by

$$\begin{aligned} Z_k(r, \alpha) &= |\Lambda_k^{-1}| \left[4\alpha\Sigma_{k,L}^{(7)} \right] r^3 \\ &\quad + |\Lambda_k^{-1}| \left[2\hat{\alpha}\alpha\Sigma_{k,L}^{(5)} + 2\alpha\Sigma_{k,L}^{(6)} + \frac{2\alpha+1}{k^{s-1}}\mathbb{I}_2 + r_{k,a_0}^{(2)} + \rho_k^{(2)} \right] r^2 \\ &\quad + |\Lambda_k^{-1}| \left[\alpha\Sigma_{k,L}^{(1)} + \hat{\alpha}^2\alpha\Sigma_{k,L}^{(3)} + \hat{\alpha}\alpha\Sigma_{k,L}^{(4)} + \rho_k^{(1)} \right] r. \end{aligned} \quad (196)$$

Consider now $k \geq M$. In order to compute the $Z_k(r, \alpha)$, we need the following.

Lemma 6.2.9 *Let $\bar{L}, \alpha_0 > 0$ and $\bar{a}_0 \in \mathbb{R}$. Fix $m \in \mathbb{N}$, $s \geq 2$ and let $M \in \mathbb{N}$ such that $M > \frac{\alpha_0|1+\bar{a}_0|}{\bar{L}}$ and $M \geq 2m - 1$. Define*

$$C_M = \frac{M}{M\bar{L} - \alpha_0|1 + \bar{a}_0|} > 0$$

and

$$\Psi_M = \begin{pmatrix} \frac{C_M^2}{M} \alpha_0 (|\bar{a}_0| + |1 + \bar{a}_0|) & C_M \\ C_M & \frac{C_M^2}{M} \alpha_0 (|\bar{a}_0| + |1 + \bar{a}_0|) \end{pmatrix}. \quad (197)$$

Then for all $k \geq M$, we have that

$$|\Lambda_k^{-1}| \leq_{cw} \frac{1}{k} \Psi_M. \quad (198)$$

Proof. First observe that

$$\begin{aligned} \Lambda_k &= R_k(\bar{L}, \alpha_0) + \alpha_0 \bar{a}_0 [\Theta_k(\bar{L}) + \Theta_0] \\ &= \begin{pmatrix} \alpha_0 \cos k\bar{L} & -k\bar{L} + \alpha_0 \sin k\bar{L} \\ k\bar{L} - \alpha_0 \sin k\bar{L} & \alpha_0 \cos k\bar{L} \end{pmatrix} + \alpha_0 \bar{a}_0 \begin{pmatrix} \cos k\bar{L} + 1 & \sin k\bar{L} \\ -\sin k\bar{L} & \cos k\bar{L} + 1 \end{pmatrix} \\ &= \begin{pmatrix} \alpha_0 \bar{a}_0 + \alpha_0(1 + \bar{a}_0) \cos k\bar{L} & -k\bar{L} + \alpha_0(1 + \bar{a}_0) \sin k\bar{L} \\ k\bar{L} - \alpha_0(1 + \bar{a}_0) \sin k\bar{L} & \alpha_0 \bar{a}_0 + \alpha_0(1 + \bar{a}_0) \cos k\bar{L} \end{pmatrix} \\ &= \begin{pmatrix} \tau_k & \delta_k \\ -\delta_k & \tau_k \end{pmatrix} \end{aligned}$$

where $\tau_k := \alpha_0 \bar{a}_0 + \alpha_0(1 + \bar{a}_0) \cos k\bar{L}$ and $\delta_k := -k\bar{L} + \alpha_0(1 + \bar{a}_0) \sin k\bar{L}$. Then

$$\Lambda_k^{-1} = \frac{1}{\tau_k^2 + \delta_k^2} \begin{pmatrix} \tau_k & -\delta_k \\ \delta_k & \tau_k \end{pmatrix}.$$

Recalling that $M > \frac{\alpha_0|1+\bar{a}_0|}{\bar{L}}$ and that $k \geq M$, we have that

$$\begin{aligned} |\delta_k| &= k\bar{L} - \alpha_0(1 + \bar{a}_0) \sin k\bar{L} \\ &\geq k\bar{L} - \alpha_0|1 + \bar{a}_0| \\ &= k \left(\bar{L} - \frac{\alpha_0|1 + \bar{a}_0|}{k} \right) \end{aligned}$$

$$\geq k \left(\bar{L} - \frac{\alpha_0 |1 + \bar{a}_0|}{M} \right) = \frac{k}{C_M} > 0.$$

Therefore, we get that

$$\frac{1}{|\delta_k|} \leq \frac{C_M}{k}$$

which implies that

$$\left| \frac{\delta_k}{\tau_k^2 + \delta_k^2} \right| \leq \frac{|\delta_k|}{\delta_k^2} = \frac{1}{|\delta_k|} \leq \frac{1}{k} C_M.$$

Finally, since $|\tau_k| \leq \alpha_0 (|\bar{a}_0| + |1 + \bar{a}_0|)$, we get that

$$\begin{aligned} \left| \frac{\tau_k}{\tau_k^2 + \delta_k^2} \right| &\leq \frac{\alpha_0 (|\bar{a}_0| + |1 + \bar{a}_0|)}{\gamma_k^2 + \delta_k^2} \leq \frac{\alpha_0 (|\bar{a}_0| + |1 + \bar{a}_0|)}{\delta_k^2} \\ &\leq \frac{C_M^2 \alpha_0 (|\bar{a}_0| + |1 + \bar{a}_0|)}{k^2} \leq \frac{1}{k} \left[\frac{C_M^2 \alpha_0 (|\bar{a}_0| + |1 + \bar{a}_0|)}{M} \right]. \quad \blacksquare \end{aligned}$$

Recall (164), (165), (166), (183) and (184). By (168), (173) and (185), we get that for all $k \geq M$,

$$r_k \in \frac{1}{k^{s-1}} \left[4\alpha \Sigma_{M,L}^{(7)} \mathbf{r}^3 + \left(2\hat{\alpha} \alpha \Sigma_{M,L}^{(5)} + (2\alpha + 1) \mathbb{I}_2 + 2\alpha \Sigma_{M,L}^{(6)} + \frac{3\alpha}{M} \mathbb{I}_2 + \rho_M^{(2)} \right) \mathbf{r}^2 + \rho_M^{(1)} \mathbf{r} \right].$$

Combining (139), (195) and Lemma 6.2.9, we have that for any $k \geq M$

$$\begin{aligned} [DT_\alpha(x_\alpha + w)w']_k &= -\Lambda_k^{-1} r_k \\ &\in |\Lambda_k^{-1}| \frac{1}{k^{s-1}} \left[4\alpha \Sigma_{M,L}^{(7)} \mathbf{r}^3 + \left(2\hat{\alpha} \alpha \Sigma_{M,L}^{(5)} + (2\alpha + 1) \mathbb{I}_2 + 2\alpha \Sigma_{M,L}^{(6)} + \frac{3\alpha}{M} \mathbb{I}_2 + \rho_M^{(2)} \right) \mathbf{r}^2 + \rho_M^{(1)} \mathbf{r} \right] \\ &\subseteq \frac{\mathbf{r}}{k^s} \Psi_M \left[4\alpha \Sigma_{M,L}^{(7)} \mathbf{r}^2 + \left(2\hat{\alpha} \alpha \Sigma_{M,L}^{(5)} + (2\alpha + 1) \mathbb{I}_2 + 2\alpha \Sigma_{M,L}^{(6)} + \frac{3\alpha}{M} \mathbb{I}_2 + \rho_M^{(2)} \right) \mathbf{r} + \rho_M^{(1)} \mathbf{1} \right]. \end{aligned}$$

Definition 6.2.10 For $k \geq M$, we define $Z_k(r, \alpha)$ by

$$\begin{aligned} Z_k(r, \alpha) &= \frac{r}{k^s} \Psi_M \left[4\alpha \Sigma_{M,L}^{(7)} r^2 \right. \\ &\quad \left. + \left(2\hat{\alpha} \alpha \Sigma_{M,L}^{(5)} + (2\alpha + 1) \mathbb{I}_2 + 2\alpha \Sigma_{M,L}^{(6)} + \frac{3\alpha}{M} \mathbb{I}_2 + \rho_M^{(2)} \right) r + \rho_M^{(1)} \right]. \end{aligned} \quad (199)$$

6.2.3 Radii Polynomials of the Wright equation

Recall Y_F from (136). For a fixed $m \leq k \leq 2m - 2$, recall Y_k given by (137). Recall also that we fixed $Y_k = 0$, for any $k \geq 2m - 1$. Consider now $M \geq 2m - 1$ and recall the definition of the $Z_k(r, \alpha)$ given by (193), (196) and (199).

Definition 6.2.11 Consider $k \in \{0, \dots, M-1\}$. The *finite radii polynomials* of the Wright equation are given by

$$p_k(r, \hat{\alpha}) = Y_k + Z_k(r, \alpha) - \frac{r}{k^s} \mathbb{I}_2. \quad (200)$$

Consider $k \geq M$. The *tail radii polynomials* of the Wright equation are given by

$$p_k(r, \hat{\alpha}) = Z_k(r, \alpha) - \frac{r}{k^s} \mathbb{I}_2. \quad (201)$$

Remark 6.2.12 Suppose that we found an r_0 and $\hat{\alpha}$ such that

$$p_M(r_0, \hat{\alpha}) = Z_M(r_0, \alpha) - \frac{r_0}{M^s} \mathbb{I}_2 <_{cw} 0.$$

Then for any $k \geq M$, we have that

$$\begin{aligned} p_k(r_0, \hat{\alpha}) &= Z_k(r_0, \alpha) - \frac{r_0}{k^s} \mathbb{I}_2 \\ &= \frac{r_0}{k^s} \Psi_M \left[4\alpha \Sigma_{M,L}^{(7)} r_0^2 \right. \\ &\quad \left. + \left(2\hat{\alpha} \alpha \Sigma_{M,L}^{(5)} + (2\alpha + 1) \mathbb{I}_2 + 2\alpha \Sigma_{M,L}^{(6)} + \frac{3\alpha}{M} \mathbb{I}_2 + \rho_M^{(2)} \right) r + \rho_M^{(1)} \right] - \frac{r_0}{k^s} \mathbb{I}_2 \\ &= \frac{M^s}{k^s} \left\{ \frac{r_0}{M^s} \Psi_M \left[4\alpha \Sigma_{M,L}^{(7)} r_0^2 \right. \right. \\ &\quad \left. \left. + \left(2\hat{\alpha} \alpha \Sigma_{M,L}^{(5)} + (2\alpha + 1) \mathbb{I}_2 + 2\alpha \Sigma_{M,L}^{(6)} + \frac{3\alpha}{M} \mathbb{I}_2 + \rho_M^{(2)} \right) r + \rho_M^{(1)} \right] - \frac{r_0}{M^s} \mathbb{I}_2 \right\} \\ &= \frac{M^s}{k^s} p_M(r_0, \hat{\alpha}) <_{cw} 0. \end{aligned}$$

When solving for the tail radii polynomials, we only need to study p_M . Define

$$\begin{aligned} \tilde{p}_M(r, \hat{\alpha}) &:= \Psi_M \left[4\alpha \Sigma_{M,L}^{(7)} \right] r^2 \\ &\quad + \Psi_M \left[2\hat{\alpha} \alpha \Sigma_{M,L}^{(5)} + (2\alpha + 1) \mathbb{I}_2 + 2\alpha \Sigma_{M,L}^{(6)} + \frac{3\alpha}{M} \mathbb{I}_2 + \rho_M^{(2)} \right] r \\ &\quad + \Psi_M \rho_M^{(1)} - \mathbb{I}_2. \end{aligned}$$

Since we look for $(r, \hat{\alpha})$ such that $p_M(r, \hat{\alpha}) < 0$, we can modify p_M observing that

$$p_M(r, \hat{\alpha}) = \frac{r}{k^s} \tilde{p}_M(r, \hat{\alpha}).$$

Therefore, $\tilde{p}_M(r, \hat{\alpha}) <_{cw} (0, 0)^T$ implies that $p_k(r, \hat{\alpha}) <_{cw} (0, 0)^T$ for all $k \geq M$.

CHAPTER VII

CONCLUSION

The purpose of this thesis is to communicate the essential ideas of our proposed validation continuation method. As such we have presented it in a somewhat limited setting. Thus, we conclude with a range of comments, beginning with obvious generalizations, describing ongoing work, and ending with some open questions.

- We first believe that generalizing this technique to pseudo-arclength continuation should be fairly straightforward.
- As is pointed out in Section 4.4, the floating point errors are many orders of magnitude smaller than the magnitude of the radii polynomials evaluated at the validation radius. This suggests that it might be possible to compute a priori bounds on the floating point errors from which one could conclude that the validation computations are in fact rigorous computations. The techniques in [26] might prove useful for this purpose.
- The particular choice of the abstract expression for the expansion of the partial differential equation (52) was chosen because it was appropriate for the application to Cahn-Hilliard (71) and Swift-Hohenberg (73). Hopefully it is clear that a different choice of boundary conditions or symmetries does not affect the essential estimates. It is expected, but remains to be checked, that the form of the estimates can be lifted to parabolic PDEs on rectangular domains (see [?] where similar estimates were used to study the equilibria of the Cahn-Hilliard equation on the unit square) and to systems of such PDEs.
- In all the applications of validated continuation presented in this thesis, we used

Fourier expansion. We would like to develop the theory of validated continuation for problems where the discretization comes from finite element methods.

- In Chapter 6, we presented an example of rigorous continuation of periodic solution of a scalar delay equation with a state independent delay. We would like to try to apply the idea of validated continuation to delay equations with multiple delays and to delay equations with state dependent delays.

REFERENCES

- [1] GIANNI ARIOLI, AND PIOTR ZGLICZYŃSKI, *Symbolic Dynamics for the Hénon-Heiles Hamiltonian on the Critical Level*, Journal of Differential Equations, 171:173–202, 2001.
- [2] JAN BOUWE VAN DEN BERG, AND JEAN-PHILIPPE LESSARD, *Chaotic braided solutions via rigorous numerics: Chaos in the Swift-Hohenberg equations*, In preparation.
- [3] JAN BOUWE VAN DEN BERG, AND ROB VAN DER VORST, *Fourth order conservative Twist systems: simple closed characteristics*, Transactions of the AMS, 354, 1383–1420, 2002.
- [4] E. ORAN BRIGHAM, *Fast Fourier Transform and its Applications*, Prentice Hall, 1st edition, 1988.
- [5] JOHN W. CAHN, AND JOHN E. HILLIARD, *Free energy of a nonuniform system I. Interfacial free energy*, Journal of Chemical Physics, 28 (1958), pp. 258–267.
- [6] SHUI NEE CHOW, AND JOHN-MALLET PARET, *Integral averaging and bifurcation*, Journal of Differential Equations, 26 (1977), no. 1, 112–159.
- [7] SARAH DAY, *A Rigorous Numerical Method in Infinite Dimensions*, Ph.D. thesis, Georgia Institute of Technology, 2003.
- [8] SARAH DAY, R. FRONGILLO, AND R. TREVINO, *Algorithms for rigorous entropy bounds and symbolic dynamics*, submitted for publication, 2007.
- [9] SARAH DAY, YASUAKI HIRAOKA, KONSTANTIN MISCHAIKOW, AND TOSHIYUKI OGAWA, *Rigorous numerics for global dynamics: A study of the Swift-Hohenberg equation*, SIAM Journal on Applied Dynamical Systems, 4 (2005), pp. 1–31.
- [10] SARAH DAY, OLIVER JUNGE, AND KONSTANTIN MISCHAIKOW, *A rigorous numerical method for the global analysis of infinite-dimensional discrete dynamical systems*, SIAM Journal on Applied Dynamical Systems, 3(2):117–160 (electronic), 2004.
- [11] SARAH DAY, JEAN-PHILIPPE LESSARD, AND KONSTANTIN MISCHAIKOW, *Validated Continuation for Equilibria of PDEs*, SIAM Journal on Numerical Analysis, **45** : 1398–1424 (electronic), 2007.
- [12] EUSEBIUS DOEDEL, ALAN R. CHAMPNEYS, THOMAS F. FAIRGRIEVE, YURI A. KUZNETSOV, BJORN SANDSTED, AND XUEZHI WANG, *AUTO97: Continuation and bifurcation software for ordinary differential equations (with HOMCONT)*, Technical report, Concordia University, 1997.

- [13] ZBIGNIEW GALIAS, AND PIOTR ZGLICZYŃSKI, *An Interval Method for Finding Fixed Points and Periodic Orbits of Infinite Dimensional Discrete Dynamical Systems*, to appear in International Journal of Bifurcation and Chaos.
- [14] MARCIO GAMEIRO, TOMAS GEDEON, WILLIAM KALIES, HIROSHI KOKUBU, KONSTANTIN MISCHAIKOW, AND HIROE OKA, *Topological Horseshoes of Travelling Waves for a Fast-Slow Predator-Prey System*, Journal of Differential Equations, 225:242-307, 2006.
- [15] MARCIO GAMEIRO, JEAN-PHILIPPE LESSARD, AND KONSTANTIN MISCHAIKOW, *Rigorous Continuation over Long Parameter Ranges for Equilibria of PDEs*, Submitted.
- [16] ROB W. GHRIST, JAN BOUWE VAN DEN BERG, AND ROB VAN DER VORST, *Morse theory on spaces of braids and Lagrangian dynamics*, Inventiones Mathematicae, 152, 369-432, 2003.
- [17] YASUAKI HIRAOKA, AND TOSHIYUKI OGAWA, *An efficient estimate based on FFT in topological verification method*, J. Comput. Appl. Math. 199 (2007), no. 2, 238-244.
- [18] G. STEPHEN JONES, *On the Nonlinear Differential-Difference Equation $f'(x) = -\alpha f(x-1)\{1 + f(x)\}$* , Journal of Mathematical Analysis and Applications, 4 (1962) 440-469.
- [19] G. STEPHEN JONES, *The existence of periodic solutions of $f'(x) = -\alpha f(x-1)\{1 + f(x)\}$* , Journal of Mathematical Analysis and Applications, 5 (1962) 435-450.
- [20] SHIZUO KAKUTANI, AND LAWRENCE MARKUS, *On the non-linear difference-differential equation $y'(t) = [A - By(t-\tau)]y(t)$* , 1958 Contributions to the theory of nonlinear oscillations, Vol. IV pp. 1-18, Annals of Mathematics Studies, no. 41 Princeton University Press, Princeton, N.J.
- [21] JAMES L. KAPLAN, AND JAMES A. YORKE, *On the stability of a periodic solution of a differential delay equation*, SIAM Journal on Mathematical Analysis, 6 (1975), 268-282.
- [22] JAMES L. KAPLAN, AND JAMES A. YORKE, *On the nonlinear differential delay equation $x'(t) = -f(x(t), x(t-1))$* , Journal of Differential Equations, 23 (1977), no. 2, 293-314.
- [23] HERBERT B. KELLER, *Lectures on numerical methods in bifurcation problems*, Tata Institute of Fundamental Research Lectures on Mathematics and Physics, 79, Springer-Verlag, Berlin, 1987.
- [24] JOHN MALLET-PARET, AND ROGER NUSSBAUM, *Global continuation and asymptotic behaviour for periodic solutions of a differential-delay equation*, Annali di Matematica Pura ed Applicata. Series IV, (4) 145 (1986), 33-128.

- [25] KONSTANTIN MISCHAIKOW, AND MARIAN MROZEK, *Chaos in the Lorenz equations: a computer-assisted proof*, Bulletin of the AMS, 32(1):66–72, 1995.
- [26] MARIAN MROZEK, *Rigorous error analysis of numerical algorithms via symbolic computations*, Journal of Symbolic Computation, 22 (1996), pp. 435–458.
- [27] ROGER NUSSBAUM, *Periodic solutions of analytic functional differential equations are analytic*, Michigan Math. J. 20 (1973), 249–255.
- [28] ROGER NUSSBAUM, *The range of periods of periodic solutions of $x'(t) = -\alpha f(x(t-1))$* , Journal of Mathematical Analysis and Applications, 58 (1977), no. 2, 280–292.
- [29] ROGER NUSSBAUM, *Asymptotic analysis of some functional-differential equations*, Dynamical systems, II (Gainesville, Fla., 1981), 277–301, Academic Press, New York-London, 1982.
- [30] ROGER NUSSBAUM, *Wright’s equation has no solutions of period four*, Proceedings of the Royal Society of Edinburgh. Section A. Mathematics, 113 (1989), no. 3-4, 281–288.
- [31] JAMES M. ORTEGA, AND WERNER C. RHEINBOLDT, *Iterative solution of nonlinear equations in several variables*, New York, Academic Press, 1970.
- [32] BENJAMIN T. REGALA, *Periodic Solutions And Stable Manifolds Of Generic Delay Differential Equations*, Ph.D. thesis, Division of Applied Mathematics, Brown University, 1989.
- [33] CLARK ROBINSON, *Dynamical Systems: Stability, Symbolic Dynamics, and Chaos*, Studies in Advanced Mathematics, CRC Press, 1995.
- [34] O.M. SARKOVSKII, *Co-existence of cycles of a continuous mapping of the line into itself*, (Russian) Ukrain. Mat. Ž. 16 1964 61–71.
- [35] JACK B. SWIFT, AND PIERRE C. HOHENBERG, *Hydrodynamic fluctuations at the convective instability*, Physical Review A, 15:319, 1977.
- [36] ANDRZEJ SZYMCAK, *The Conley index and symbolic dynamics*, Topology, 35(2):287–299, 1996.
- [37] WARWICK TUCKER, *The Lorenz attractor exists*, Comptes Rendus de l’Académie des Sciences. Serie I. Mathématique, 328 (1999), no. 12, 1197–1202.
- [38] DANIEL WILCZAK, *Chaos in the Kuramoto-Sivashinsky equations—a computer-assisted proof*, Journal of Differential Equations, 194:433–459, 2003.
- [39] EDWARD MAITLAND WRIGHT, *A non-linear difference-differential equation*, Journal für die reine und angewandte Mathematik, 194 (1955), 66–87.

- [40] XIANWEN XIE, *Uniqueness and stability of slowly oscillating periodic solutions of delay equations with unbounded nonlinearity*, Journal of Differential Equations 103 (1993), no. 2, 350–374.
- [41] XIANWEN XIE, *Uniqueness and Stability of Slowly Oscillating Periodic Solutions of Differential Delay Equations*, Ph.D. thesis, Mathematics Department, Rutgers University, 1991.
- [42] NOBITO YAMAMOTO, *A numerical verification method for solutions of boundary value problems with local uniqueness by Banach’s fixed-point theorem*, SIAM Journal on Numerical Analysis, 35 (1998), pp. 2004–2013.
- [43] PIOTR ZGLICZYŃSKI, AND KONSTANTIN MISCHAIKOW, *Rigorous numerics for partial differential equations: The Kuramoto-Sivashinsky equation*, Foundations of Computational Mathematics, 1 (2001), pp. 255–288.