Coexistence of hexagons and rolls

Jan Bouwe van den Berg [*] Andréa Deschênes [†]
Jean-Philippe Lessard[‡] Jason D. Mireles James[§]

Abstract

In this work we introduce a rigorous computational method for finding heteroclinic solutions of a system of two second order differential equations. These solutions correspond to standing waves between rolls and hexagonal patterns of a two-dimensional pattern formation PDE model. After reformulating the problem as a projected boundary value problem (BVP) with boundaries in the stable/unstable manifolds, we compute the local manifolds using the Parameterization Method and solve the BVP using Chebyshev series and the radii polynomial approach. Our results settle a conjecture by Doelman et al. [European J. Appl. Math., **14** (1), 85–110 (2003)] about the coexistence of hexagons and rolls.

1 Introduction

The analysis of pattern formation phenomena is often hampered by the inherent complexity of nonlinearities. On the one hand, nonlinear dynamics is usually the fundamental drive for the patterns to form, while on the other hand the nonlinear character of the equations obstructs the rigorous mathematical analysis of its solutions.

In many pattern formation problems one can exploit some asymptotic regime in which the problem simplifies through a rigorous reduction (e.g. center manifolds, Lyapunov-Schmidt reduction, averaging, normal forms). This reduces the governing partial differential equation to a less complicated one, or even to a system of ordinary differential equations, describing certain coherent structures that govern much of the dynamics. However, in all but the simplest cases, even the reduced, simplified problem is nonlinear and still cannot be fully analyzed rigorously.

In this paper we demonstrate how novel advances in rigorous computer-assisted analysis of dynamical systems can overcome this obstacle. In particular, we consider the pattern formation model [1]

$$\partial_t \mathrm{U} = -(1+\Delta)^2 \mathrm{U} + \mu \mathrm{U} - \beta |\nabla \mathrm{U}|^2 - \mathrm{U}^3 \tag{1.1}$$

in the plane, i.e., $\mathrm{U} = \mathrm{U}(t,x) \in \mathbb{R}$, $t \geq 0$, $x \in \mathbb{R}^2$. This equation generalizes the Swift-Hohenberg equation [2]. The additional term $\beta|\nabla \mathrm{U}|^2$, reminiscent of the Kuramoto-Sivashinsky equation [3, 4], breaks the up-down symmetry $\mathrm{U} \mapsto -\mathrm{U}$ for $\beta \neq 0$. The

*VU University Amsterdam, Department of Mathematics, De Boelelaan 1081, 1081 HV Amsterdam, The Netherlands. janbouwe@few.vu.nl
†Université Laval, Département de Mathématiques et de Statistique, 1045 avenue de la Médecine, Québec, QC, G1V0A6, Canada. andrea.deschenes.1@ulaval.ca.
‡Université Laval, Département de Mathématiques et de Statistique, 1045 avenue de la Médecine, Québec, QC, G1V0A6, Canada. jean-philippe.lessard@mat.ulaval.ca.
§Florida Atlantic University, Department of Mathematical Sciences, Science Building, Room 234, 777 Glades Road, Boca Raton, Florida, 33431 , USA. jmirelesjames@fau.edu .

Swift-Hohenberg equation acts as a phenomenological model for pattern formation in Rayleigh-Bénard convection, with $\beta \neq 0$ corresponding to a free boundary at the top of the convection cell, rather than a fixed one for the symmetric case $\beta = 0$ [5]. The parameter μ is related to the distance to the onset of convection rolls. For $\mu < 0$ the trivial equilibrium $\mathrm{U} \equiv 0$ is locally stable, whereas for $\mu > 0$ it is unstable.

Depending on the parameter values the dynamics generated by (1.1) exhibit a variety of patterns besides simple convection rolls (a stripe pattern); in particular, hexagonal spot patterns are observed. In [6] it is shown that stable hexagonal patterns with small amplitude can be found for $\beta < 0$ only. In [1] the interplay between hexagons and rolls near onset (small μ) is examined using a weakly nonlinear analysis. Introducing a small parameter $\varepsilon > 0$, the parameters are scaled as

$$\mu = \varepsilon^2 \tilde{\mu}, \qquad \beta = \varepsilon \tilde{\beta}.$$

In the asymptotic regime $\varepsilon \ll 1$, one can describe the roll and hexagonal patterns via amplitude equations. The seminal result in [1], based on spatial dynamics and geometric singular perturbation theory, is that heteroclinic solutions of the system

$$\begin{cases} 4B_1'' + \tilde{c}B_1' + \tilde{\mu}B_1 - \tilde{\beta}B_2^2 - 3B_1^2 - 12B_1B_2^2 = 0 \\ B_2'' + \tilde{c}B_2' + \tilde{\mu}B_2 - \tilde{\beta}B_1B_2 - 9B_1^2 - 6B_1^2B_2 = 0 \end{cases} \tag{1.2}$$

correspond to modulated front solutions, travelling at (rescaled) speed $\tilde{c}$.

The variables B_1 and B_2 represent amplitudes of certain wave modes (slowly varying in the original variables). We refer to [1] for the details and the rigorous justification of the derivation. The dynamical system (1.2) has up to seven stationary points:

$$\begin{array}{ll} (B_1, B_2) = (0, 0) & \text{trivial state} \\ (B_1, B_2) = (B_{\mathrm{rolls}}, 0) & \text{“positive” rolls} \\ (B_1, B_2) = (-B_{\mathrm{rolls}}, 0) & \text{“negative” rolls} \\ (B_1, B_2) = (B^+_{\mathrm{hex}}, B^+_{\mathrm{hex}}) & \text{hexagons} \\ (B_1, B_2) = (B^-_{\mathrm{hex}}, B^-_{\mathrm{hex}}) & \text{“false” hexagons} \\ (B_1, B_2) = (-\tilde{\beta}/3, B^{\pm}_{\mathrm{mm}}) & \text{two “mixed mode” states.} \end{array} \tag{1.3}$$

Here $B_{\mathrm{rolls}} = \sqrt{\tilde{\mu}/3}$ and $B^{\pm}_{\mathrm{hex}} = \frac{-\tilde{\beta} \pm \sqrt{\tilde{\beta}^2 + 60\tilde{\mu}}}{30}$ and $B^{\pm}_{\mathrm{mm}} = \pm\frac{1}{3}\sqrt{\tilde{\mu} - \tilde{\beta}^2/3}$. Due to symmetry, there are two equilibria corresponding to rolls. We refer to [1] for a full discussion of all states and their stability properties. In this paper we consider the interplay between hexagons and rolls (both positive and negative).

While the weakly nonlinear analysis in [1] provided a vast reduction in complexity from (1.1) to (1.2), one outstanding issue remained: the heteroclinic solutions are difficult to analyse rigorously due to the nonlinear nature of the equations (1.2). In the limit $\tilde{c} \to \infty$ various connections could be found through a further asymptotic reduction [1], but for finite wave speeds the analysis of (1.2) was out of reach. In the present paper we introduce a computer-assisted, rigorous method for finding heteroclinic solutions for $\tilde{c} = 0$, i.e. standing waves. In particular we find connections between hexagons and rolls with *zero* propagation speed, i.e., the two patterns coexist.

The system (1.2) is gradient-like for $\tilde{c} \neq 0$, while it is Hamiltonian for $\tilde{c} = 0$, see Section 2.1. Hence, for hexagons and rolls to coexist their free energy must be equal, a situation that occurs when $\tilde{\mu} = \frac{7+3\sqrt{6}}{30}\tilde{\beta}^2$. We prove the following theorem, which settles the conjecture in [1] about the coexistence of hexagons and rolls:

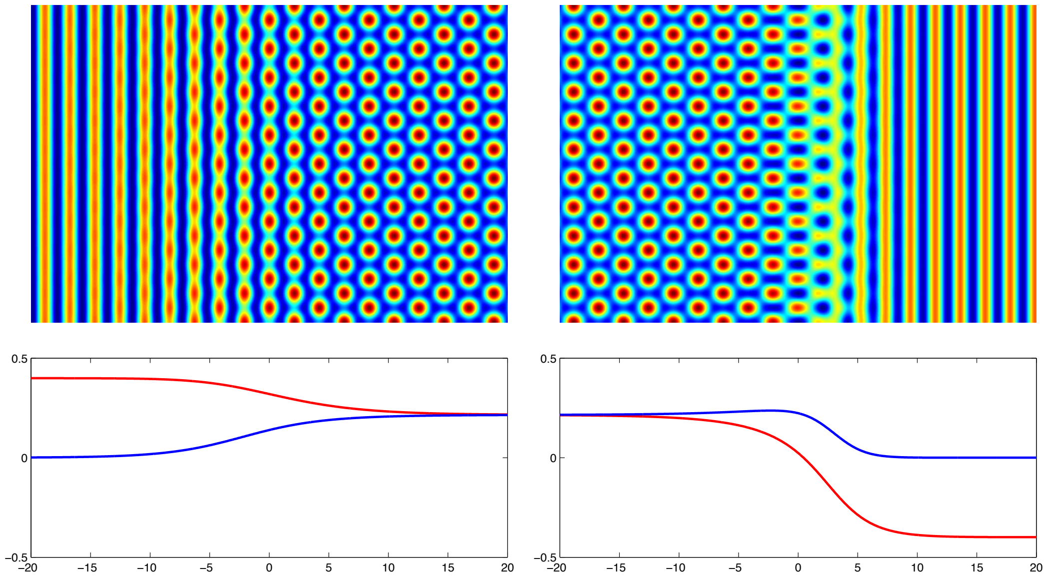

Figure 1: At the bottom are graphs of B_1 (red) and B_2 (blue) representing heteroclinic solutions of (1.2) that connect the hexagon state to the positive rolls (on the left) and negative rolls (and the right). The parameter values are $\tilde{c} = 0$, $\tilde{\mu} = \frac{7+3\sqrt{6}}{30}$ and $\tilde{\beta} = 1$, corresponding to the assumptions in Theorem 1. At the top are the corresponding stationary patterns of (1.1). We note that the two phase transitions from rolls to hexagons have distinctive features. On the left, the stripes ("positive" rolls) undergo pearling, which gradually leads to separation into spots (hexagons). On the right, the stripes ("negative" rolls) develop transverse waves, which break up into a block structure that then transforms into hexagonal spots.

Theorem 1. *For parameter values $\tilde{\mu} = \frac{7+3\sqrt{6}}{30}\tilde{\beta}^2$ and $\tilde{c} = 0$ there exists a heteroclinic orbit of* (1.2) *between the hexagons and positive rolls, see* (1.3)*, as well as a heteroclinic orbit between the hexagons and negative rolls.*

The heteroclinic solutions are depicted in Figure 1, together with the corresponding patterns of the PDE (1.1). These orbits thus represent two types of stationary domain walls between hexagons and rolls (spots and stripes). While each heteroclinic connection exists on a parabola in the $(\tilde{\beta}, \tilde{\mu})$ parameter plane, a parameter scaling reduces this to a single connecting orbit, see Section 2.1.

Our method, which builds on foundations laid in [7, 8, 9, 10], is summarized as follows. At the center of the method is an approximate solution u_{num}, obtained through a numerical calculation. We then construct an operator which has as its fixed points the heteroclinic solutions, and we set out to prove that this operator is a contraction mapping on a small ball around u_{num} in an appropriate Banach space. The ball should be small enough for the estimates to be sufficiently strong to prove contraction, but large enough to include both u_{num} (the center of the ball) and the solution (the fixed point). Qualitatively, considering the numerical approximations of solutions depicted as graphs in Figure 1, we can choose the radius of the ball so small that the solution is guaranteed to lie within the thickness of the lines. A mathematically precise, quantitative statement can be found in Section 5.

We can distinguish several components in the computer-assisted proof of Theorem 1. Since we are looking for solutions of (1.2) on an unbounded domain, we first reduce the problem to a finite domain by parameterizing the local stable and unstable manifolds of the equilibria, see Section 3.2. This leaves us with a boundary value problem, which we approach using a Chebyshev series expansion, see Section 2.2. In particular, we construct a fixed point operator in a Banach space of Chebyshev coefficients that decay at exponential rate. This analytic setting leads to somewhat simpler estimates than the ones derived in [10] for spaces of algebraically decaying coefficients, see Section 3.1.

The fact that the method is based on the Banach contraction theorem essentially implies local uniqueness and robustness of the solution. Note that because of the Hamiltonian nature of the problem the heteroclinic solution is not a transversal intersection of stable and unstable manifolds, hence not robust in a dynamical systems sense. Therefore, we carefully adapt the construction to incorporate the conserved quantity, see Section 2.1 (Lemma 2). All errors due to truncation are estimated analytically, see Section 4, with all bounds expressed explicitly in terms of analytically known constants and in terms of the data of u_{num}. In these estimates we keep the radius of the ball as a parameter (as in [8, 11, 12, 13, 14, 15]) in order to retain the flexibility to tune the radius. With the assistance of the computer we then check that the operator is indeed a contraction on balls with small (but not too small) radius, see Section 2.3, leading to a unique fixed point, hence a unique heteroclinic solution in a small neighborhood around u_{num}.

The crux of the present paper is the presentation of a novel, computer-assisted, rigorous technique for solving nonlinear analysis problems in pattern formation. The coexistence between hexagons and rolls (spots and stripes) as described by heteroclinic solutions of (1.2) features as a showcase to convey the general idea. We want to touch upon two alternatives to our approach. First, for $\tilde{c} = 0$ the system (1.2) can be formulated in a variational setting, which gives a handle for a very different strategy to prove Theorem 1, although it is not a straightforward task to complete this variational route. Second, a distinct type of phase-space oriented, topological computer-assisted approach, see [16, 17, 18, 19] and the references therein, could be applied to prove the existence of the connections. Such methods have been used successfully to find connecting orbits in a variety of nonlinear systems [20, 21, 22, 23, 24], and they are especially adept for low regularity settings. In the present paper on the other hand, by combining a functional analytic setting and a parameterization method, we exploit the high regularity of solutions in the (parabolic) pattern formation problem. It thus complements the lower regularity phase-space techniques nicely.

To conclude this introduction, we remark on extensions and future work. While we focus on coexistence of patterns in this paper, more generally problem (1.2) represents a (modulated) travelling wave problem, where the invasion/propagation velocity $\tilde{c}$ is nonzero and a priori unknown. We are confident that our method can be adjusted to this case, which we are exploring in current research. In this context it is also natural to consider the continuation problem where one seeks to establish a continuous curve of heteroclinic orbits parameterized by a parameter. Finally, to find a connection for $\tilde{c} = 0$ between the hexagons and the trivial state (the appropriate parameter value for coexistence is $\tilde{\mu} = -\frac{2}{135}\tilde{\beta}^2$), one needs to deal with resonances between eigenvalues in the spectrum of the trivial state, which is once again subject of an ongoing project.

2 The rigorous computational method

We begin by reformulating the problem (1.2) in more convenient variables:

$$u(\tau) = -\sqrt{2}\tilde{\beta}^{-1} B_1\big(\tilde{\beta}^{-1}\tau\big), \qquad v(\tau) = -\tilde{\beta}^{-1} B_2\big(\tilde{\beta}^{-1}\tau\big),$$

and we introduce the (single) parameter $\gamma = \frac{\tilde{\mu}}{\tilde{\beta}^2}$. This transforms (1.2) into

$$\begin{cases} u'' = g_1(u,v) \stackrel{\text{def}}{=} -\frac{\gamma}{4}u - \frac{\sqrt{2}}{4}v^2 + \frac{3}{8}u^3 + 3uv^2, \\ v'' = g_2(u,v) \stackrel{\text{def}}{=} -\gamma v - \frac{\sqrt{2}}{2}uv + 9v^3 + 3u^2 v. \end{cases} \tag{2.1}$$

The nontrivial equilibria that we are interested in are now given by

$$\begin{aligned} &(u,v) = (\sqrt{2\gamma/3}, 0) && \text{positive rolls,} \\ &(u,v) = (-\sqrt{2\gamma/3}, 0) && \text{negative rolls,} \\ &(u,v) = (\sqrt{2}v^*, v^*) && \text{hexagons,} \end{aligned}$$

where $v^* \stackrel{\text{def}}{=} \frac{1+\sqrt{1+60\gamma}}{30}$ solves the equation $15v^2 - v - \gamma = 0$.

The Hamiltonian associated to (2.1) is

$$\mathcal{H}(u,u',v,v') \stackrel{\text{def}}{=} \frac{1}{2}(u')^2 + \frac{1}{2}(v')^2 + \mathcal{V}(u,v), \tag{2.2}$$

with potential energy

$$\mathcal{V}(u,v) \stackrel{\text{def}}{=} \frac{\gamma}{8}u^2 + \frac{\gamma}{2}v^2 - \frac{3}{32}u^4 - \frac{9}{4}v^4 + \frac{\sqrt{2}}{4}uv^2 - \frac{3}{2}u^2v^2.$$

We note that for

$$\gamma = \gamma_* \stackrel{\text{def}}{=} \frac{7+3\sqrt{6}}{30}$$

the hexagonal and the (positive and negative) roll states have the same energy. For hexagons and rolls to coexist, the patterns being separated by a stationary domain wall (see Figure 1) corresponding to a heteroclinic solution of (2.1), we must thus fix $\gamma = \gamma_*$.

2.1 Derivation of the functional equation

We now introduce a functional equation whose zeroes correspond to connecting orbits of (2.1). Consider a time scaling factor $L > 0$ and set

$$U(t) = (U_1(t), U_2(t), U_3(t), U_4(t)) \stackrel{\text{def}}{=} (u(Lt), u'(Lt), v(Lt), v'(Lt)).$$

We rewrite (2.1) as a vector field

$$U'(t) = \Psi(U(t)), \quad t \in [-1,1], \tag{2.3}$$

where

$$\Psi(U) \stackrel{\text{def}}{=} L \begin{pmatrix} U_2 \\ g_1(U_1,U_3) \\ U_4 \\ g_2(U_1,U_3) \end{pmatrix}. \tag{2.4}$$

Next, consider two stationary solutions U_- and U_+ of the system (2.3), which we can write as $U_\pm = (u_\pm, 0, v_\pm, 0)$. Naturally, we choose U_- and U_+ to correspond to rolls and hexagons. Denote by $W^u(U_-)$ the unstable manifold of U_- and by $W^s(U_+)$ the stable manifold of U_+. Hence, a heteroclinic orbit connecting U_- and U_+ corresponds to a solution of the boundary value problem

$$\begin{cases} U'(t) = \Psi(U(t)), \quad t \in [-1,1], \\ U(-1) \in W^u(U_-), \\ U(1) \in W^s(U_+). \end{cases} \tag{2.5}$$

Note that $\dim W^u(U_-) = \dim W^s(U_+) = 2$. Let us assume that $P : \mathbb{R}^2 \to \mathbb{R}^4$ is a parameterization of the local stable manifold of U_+ and that $Q : \mathbb{R}^2 \to \mathbb{R}^4$ is a parameterization of the local unstable manifold of U_-. A solution of (2.5) can then be identified with a triple (θ, ϕ, U), where $\theta, \phi \in \mathbb{R}^2$ and $U = (U_1, U_2, U_3, U_4)$, that solves the boundary value problem

$$\begin{cases} U'(t) = \Psi(U(t)), \quad t \in [-1,1], \\ U(-1) = Q(\phi), \\ U(1) = P(\theta). \end{cases} \tag{2.6}$$

By integrating the differential equation in (2.6) on the interval $[-1, t]$ and by using the first boundary condition, we obtain

$$U(t) - Q(\phi) - \int_{-1}^{t} \Psi(U(s))\, ds = 0.$$

Combining this with the second boundary condition in (2.6) leads us to define the operator

$$\widehat{F}(\theta, \phi, U)(t) \stackrel{\text{def}}{=} \begin{pmatrix} U(1) - P(\theta) \\ U(t) - Q(\phi) - \displaystyle\int_{-1}^{t} \Psi(U(s))\, ds \end{pmatrix}.$$

Zeroes of $\widehat{F}$ correspond to the solutions of the boundary value problem (2.6) and consequently to the heteroclinic orbits of (2.1).

Every translation of a heteroclinic solution is a heteroclinic solution. To remove this degeneracy we add the *phase condition* that fixes the radius ρ of the ball in the local parameterization of the stable manifold, that is $\theta = \theta(\psi) \stackrel{\text{def}}{=} (\rho \cos \psi, \rho \sin \psi)$, with $\psi \in \mathbb{R}$ the angle variable and $\rho > 0$ fixed. Hence, $\psi \in \mathbb{R}$ replaces $\theta \in \mathbb{R}^2$ as an unknown.

Furthermore, since the problem is Hamiltonian, the intersections between stable and unstable manifolds are not transversal in phase space. In particular, intersections must be viewed geometrically within a fixed energy level. We refer to [25] for a general discussion of such phenomena and their resolution. Here we take a direct approach, which is suitable because we have chosen a functional analytic setting that is distant from the geometric (phase space) point of view. We simply exclude one of the boundary conditions and define the operator

$$F(\psi, \phi, U)(t) \stackrel{\text{def}}{=} \begin{pmatrix} U_1(1) - P_1(\theta(\psi)) \\ U_3(1) - P_3(\theta(\psi)) \\ U_4(1) - P_4(\theta(\psi)) \\ U(t) - Q(\phi) - \displaystyle\int_{-1}^{t} \Psi(U(s))\, ds \end{pmatrix}, \tag{2.7}$$

which *leaves out* the final boundary condition

$$U_2(1) - P_2(\theta(\psi)) = 0. \tag{2.8}$$

We thus need to show that this boundary condition is fulfilled *automatically* by zeroes of F. Lemma 2 below guarantees (provided equation (2.10) holds) that this final boundary condition is satisfied.

Since the Hamiltonian (2.2) is constant along solutions of the differential equation, we infer that $\mathcal{H}(U(1)) = \mathcal{V}(u_-, v_-)$ and $\mathcal{H}(P(\theta)) = \mathcal{V}(u_+, v_+)$. Furthermore, since $\gamma = \gamma_*$, the equilibria have the same energy: $\mathcal{V}(u_-, v_-) = \mathcal{V}(u_+, v_+)$. Given that $U_k(1) = P_k(\theta)$ for $k = 1, 3, 4$, and that $P(\theta)$ and $U(1)$ lie in the same energy level, we infer that the two numbers $U_2(1)$ and $P_2(\theta)$ both satisfy the equation

$$\frac{1}{2}x^2 = \mathcal{E} - \frac{1}{2}U_4(1)^2 - \mathcal{V}\big(U_1(1), U_3(1)\big), \tag{2.9}$$

where $\mathcal{E} = \mathcal{V}(u_-, v_-) = \mathcal{V}(u_+, v_+)$ is the energy of the equilibria $(u_\pm, v_\pm)$. There are only two solutions (of opposite sign) to this equation, hence if we show that $U_2(1)$ and $P_2(\theta)$ have the same sign, then we can conclude that $U_2(1) = P_2(\theta)$, i.e., the final boundary condition (2.8) is satisfied. This argument is stated more formally in the next lemma.

Lemma 2. *Let $\gamma = \gamma_*$ and let (ψ, ϕ, U) be a zero of F, defined in* (2.7)*. If*

$$\operatorname{sign}(U_2(1)) = \operatorname{sign}(P_2(\theta(\psi))), \tag{2.10}$$

then $U_2(1) = P_2(\theta(\psi))$, hence U represents a heteroclinic orbit between U_- and U_+.

We summarize what we have achieved so far. We have introduced the operator F defined by (2.7) whose zeroes correspond, in case hypothesis (2.10) of Lemma 2 is verified, to the desired heteroclinic connections. We incorporated in the operator F a phase condition that eliminates arbitrary time shifts. This implies isolation of the solutions. The philosophy of the approach is then to compute a numerical approximation u_{num} and to apply the contraction mapping theorem on a set centered at u_{num}. u_{num} is obtained using Chebyshev series. Since solutions of analytic vector fields are analytic, the Chebyshev coefficients of the solution decays exponentially fast to zero. This motivates the choice of the Banach space on which the contraction mapping argument is performed.

2.2 Chebyshev series and the choice of Banach space

Definition 1. *The Chebyshev polynomials $T_k : [-1, 1] \to \mathbb{R}$ are defined by $T_0(t) = 1$, $T_1(t) = t$ and $T_{k+1}(t) = 2tT_k(t) - T_{k-1}(t)$ for $k \geq 1$. Equivalently, $T_k(t) = \cos(k \arccos t)$.*

Since $\Psi(U)$ defined by (2.4) is analytic, a solution U to the BVP (2.6) is analytic. Each component U_i of U therefore admits a unique Chebyshev series representation $U_i(t) = (a_i)_0 + 2\sum_{k\geq 1}(a_i)_k T_k(t)$ whose coefficients $a_i \stackrel{\text{def}}{=} \{(a_i)_k\}_{k=0}^{\infty}$ decay to zero exponentially fast [26]. This motivates the definition of the following Banach space. For any $\nu > 1$ we define the ν-weighted ℓ^1-norm on sequences of real numbers $a = \{a_n\}_{n=0}^{\infty}$ by

$$\|a\|_\nu \stackrel{\text{def}}{=} \sum_{n=0}^{\infty} |a_n| \nu^n,$$

and let

$$\ell_\nu^1 \stackrel{\text{def}}{=} \left\{ a = \{a_n\}_{n=0}^{\infty} : \|a\|_\nu < \infty \right\}.$$

Given two sequences $a, b \in \ell_\nu^1$, denote by $a * b$ the discrete convolution

$$(a * b)_k = \sum_{\substack{k_1 + k_2 = k \\ k_i \in \mathbb{Z}}} a_{|k_1|} b_{|k_2|}. \tag{2.11}$$

An important property of ℓ^1_ν is that it is a Banach space and an algebra under discrete convolutions.

Lemma 3. *For $a, b \in \ell^1_\nu$, $\|a * b\|_\nu \leq 4\|a\|_\nu \|b\|_\nu$.*

Proof. We estimate

$$\begin{aligned}
\|a * b\|_\nu &= \sum_{k\geq 0} |(a*b)_k|\nu^k = \sum_{k\geq 0} \left| \sum_{\substack{k_1+k_2=k \\ k_i\in\mathbb{Z}}} a_{|k_1|} b_{|k_2|} \right| \nu^k \\
&\leq \sum_{k\geq 0} \sum_{\substack{k_1+k_2=k \\ k_i\in\mathbb{Z}}} |a_{|k_1|}||b_{|k_2|}|\nu^k \leq \sum_{k_i\in\mathbb{Z}} |a_{|k_1|}||b_{|k_2|}|\nu^{k_1}\nu^{k_2} \\
&\leq 4 \sum_{k_i\geq 0} |a_{k_1}|\nu^{k_1}|b_{k_2}|\nu^{k_2} = 4\left(\sum_{k_1\geq 0}|a_{k_1}|\nu^{k_1}\right)\left(\sum_{k_2\geq 0}|b_{k_2}|\nu^{k_2}\right) = 4\|a\|_\nu\|b\|_\nu. \qquad \square
\end{aligned}$$

We write

$$U(t) = a^{(0)} + 2\sum_{k\geq 1} a^{(k)} T_k(t)$$

where $a^{(k)} = ((a_1)_k, (a_2)_k, (a_3)_k, (a_4)_k) \in \mathbb{R}^4$ and $a_i = \{(a_i)_k\}_{k=0}^\infty \in \ell^1_\nu$ for $i = 1, 2, 3, 4$. The Chebyshev series representation of $\Psi(U)$ defined in (2.4) is written as

$$\Psi(U(t)) = L\left(c^{(0)} + 2\sum_{k\geq 1} c^{(k)} T_k(t)\right)$$

where

$$c^{(k)} = \begin{pmatrix} (c_1)_k \\ (c_2)_k \\ (c_3)_k \\ (c_4)_k \end{pmatrix} \stackrel{\text{def}}{=} \begin{pmatrix} (a_2)_k \\ -\frac{\gamma}{4}(a_1)_k - \frac{\sqrt{2}}{4}(a_3^2)_k + \frac{3}{8}(a_1^3)_k + 3(a_1a_3^2)_k \\ (a_4)_k \\ -\gamma(a_3)_k - \frac{\sqrt{2}}{2}(a_1a_3)_k + 9(a_3^3)_k + 3(a_1^2a_3)_k \end{pmatrix}. \tag{2.12}$$

Here $(a_ia_j)_k = (a_i * a_j)_k$ and $(a_ia_ja_\ell)_k = (a_i * a_j * a_\ell)_k$.

Denote by $x = (x_1, x_2, x_3, x_4, x_5, x_6, x_7) \stackrel{\text{def}}{=} (\psi, \phi_1, \phi_2, a_1, a_2, a_3, a_4)$ the variables that define the input (ψ, ϕ, U) of F in (2.7). By the standard properties of the Chebyshev polynomials (e.g. see [10]), we find that $F(\psi, \phi, U)(t) = 0$ can be reformulated in terms of Chebyshev coefficients as $f(x) = 0$, where $f = (f_i)_{i=1}^7$ is defined component-wise by

$$f_i(x) = \begin{cases} (a_1)_0 + 2\displaystyle\sum_{n\geq 1}(a_1)_n - P_1(\theta(\psi)), & i = 1, \\ (a_3)_0 + 2\displaystyle\sum_{n\geq 1}(a_3)_n - P_3(\theta(\psi)), & i = 2, \\ (a_4)_0 + 2\displaystyle\sum_{n\geq 1}(a_4)_n - P_4(\theta(\psi)), & i = 3, \\ \left((\tilde{f}_{i-3}(x))_k\right)_{k\geq 0}, & i = 4, 5, 6, 7, \end{cases} \tag{2.13}$$

with for $j = 1, 2, 3, 4$,

$$(\tilde{f}_j(x))_k = \begin{cases} (a_j)_0 + 2\displaystyle\sum_{n\geq 1}(-1)^n(a_j)_n - Q_j(\phi), & k = 0, \\ 2k(a_j)_k + L\left((c_j)_{k+1} - (c_j)_{k-1}\right), & k \geq 1. \end{cases}$$

The Banach space on which we study the zeroes of f is

$$X \stackrel{\text{def}}{=} \mathbb{R}^3 \times \left(\ell^1_\nu\right)^4, \tag{2.14}$$

endowed with the norm $\|x\|_X \stackrel{\text{def}}{=} \max\left(|x_1|, |x_2|, |x_3|, \|x_4\|_\nu, \|x_5\|_\nu, \|x_6\|_\nu, \|x_7\|_\nu\right)$. As in [10], it can be shown that $x \in X$ solves $f(x) = 0$ if and only if the corresponding (ψ, ϕ, U) is a solution of the integral operator (2.7). To find $x \in X$ such that $f(x) = 0$, we use the radii polynomial approach, which provides an efficient means of determining a set on which the contraction mapping theorem is applicable.

2.3 The radii polynomials

As already mentioned in Section 1, at the center of the method is an approximate solution $\bar{x} = (\bar{x}_1, \bar{x}_2, \bar{x}_3, \bar{x}_4, \bar{x}_5, \bar{x}_6, \bar{x}_7) = (\bar{\psi}, \bar{\phi}_1, \bar{\phi}_2, \bar{a}_1, \bar{a}_2, \bar{a}_3, \bar{a}_4) \in X$. This approximation is obtained by applying Newton's method on a finite dimensional projection of (2.13) (see Section 4.1 for details). Using the diagonal dominance of the Fréchet derivative $Df(\bar{x})$ of the map f at $\bar{x}$, we can define explicitly an approximate inverse A for $Df(\bar{x})$. The approximate inverse is, of course, chosen so that, given any $x \in X$, $Af(x) \in X$. We refer to (4.3) for the explicit definition of A. This choice allows defining a Newton-like operator $T : X \to X$ by

$$T(x) = x - Af(x).$$

Consider $B(r) \stackrel{\text{def}}{=} \{x : \|x\|_X \le r\} \subset X$ the closed ball of radius r centered at $0 \in X$. Our goal is to use the contraction mapping theorem to prove the existence of a unique fixed point of T within the set $B_{\bar{x}}(r) \stackrel{\text{def}}{=} \bar{x} + B(r)$. To achieve this goal, we need bounds on both the image and the contractivity of T. This is encapsulated in the concept of *radii polynomials*, which are defined in terms of bounds Y and Z. The bound $Y = (Y_1, \dots, Y_7)$ satisfies the inequalities

$$|[T(\bar{x}) - \bar{x}]_i| \le Y_i \quad \text{for} \quad i = 1, 2, 3, \quad \text{and} \quad \|[T(\bar{x}) - \bar{x}]_i\|_\nu \le Y_i \quad \text{for} \quad i = 4, \dots, 7, \tag{2.15}$$

and the *polynomial* bound $Z(r) = (Z_1(r), \dots, Z_7(r))$ satisfies the inequalities

$$\begin{aligned} \sup_{b,c \in B(r)} |[DT(\bar{x} + b)c]_i| &\le Z_i(r), \qquad \text{for } i = 1, 2, 3, \\ \sup_{b,c \in B(r)} \|[DT(\bar{x} + b)c]_i\|_\nu &\le Z_i(r), \qquad \text{for } i = 4, 5, 6, 7. \end{aligned} \tag{2.16}$$

Note that the bound Z can be expanded as a polynomial of finite degree in the variable radius r. More precisely, in this case, since Ψ defined in (2.4) is a vector field with cubic nonlinearities, each $Z_i(r)$ is a cubic polynomial.

Definition 2. *Consider the bounds Y and Z satisfying respectively* (2.15) *and* (2.16)*. The radii polynomials are given by*

$$p_i(r) \stackrel{\text{def}}{=} Y_i + Z_i(r) - r, \qquad i = 1, \dots, 7. \tag{2.17}$$

The construction of the radii polynomials requires some basic functional analytic tools (see Section 3.1) and computations using interval arithmetic [27, 28]. Also, since the functional equation (2.7) is defined in terms of the local parameterizations of the stable and unstable manifolds, we present in Section 3.2 some theory, based on the parameterization method [29, 30, 31], where we introduce explicit rigorous bounds used to enclose the local manifolds. The explicit construction of the radii polynomials is postponed to Section 4. Once the radii polynomials are defined, the following result provides a way of determining the radius r of the closed ball $B_{\bar{x}}(r) = \bar{x} + B(r) \subset X$ such that $T : B_{\bar{x}}(r) \to B_{\bar{x}}(r)$ is a contraction.

Proposition 4. *Define*

$$\mathcal{I} \stackrel{\text{def}}{=} \{r > 0 : p_i(r) < 0 \text{ for } i = 1, \dots, 7\}. \tag{2.18}$$

If $\mathcal{I} \neq \emptyset$, then for any $r \in \mathcal{I}$, there exists a unique fixed point of T, and hence a unique zero of f, within the set $B_{\bar{x}}(r) = \bar{x} + B(r)$.

Proof. The proof is presented in greater generality in [11, 14] and follows from an application of the contraction mapping theorem on the Banach space $B_{\bar{x}}(r) \subset X$. $\square$

3 Background

3.1 The dual space and linear operators

When studying nonlinear maps on ℓ^1_ν it is often necessary to estimate certain linear operators and functionals. The estimates are natural when viewed in the context of the Banach space dual of ℓ^1_ν. For an infinite sequence of real numbers $c = \{c_n\}_{n=0}^\infty$ define the ν-weighted supremum norm

$$\|c\|_\nu^\infty \stackrel{\text{def}}{=} \sup_{n \geq 0} \frac{|c_n|}{\nu^n},$$

and let

$$\ell_\nu^\infty \stackrel{\text{def}}{=} \left\{c = \{c_n\}_{n=0}^\infty : \|c\|_\nu^\infty < \infty\right\}.$$

The following result is classical in the elementary theory of Banach spaces.

Theorem 5. *For $\nu > 0$, the dual of ℓ^1_ν, denoted $(\ell^1_\nu)^*$, is isometrically isomorphic to ℓ^∞_ν.*

The proof is standard. For any $l \in (\ell^1_\nu)^*$, there is a unique $c \in \ell^\infty_\nu$, such that $l = \ell_c$, where for any $a \in \ell^1_\nu$,

$$\ell_c(a) = \sum_{n=0}^\infty c_n a_n \qquad \text{and} \qquad \|\ell_c\|_{(\ell^1_\nu)^*} = \|c\|^\infty_\nu.$$

Hence,

$$\sup_{\|a\|_\nu = 1} \left| \sum_{n=0}^\infty c_n a_n \right| = \|\ell_c\|_{(\ell^1_\nu)^*} = \|c\|^\infty_\nu = \sup_{n \geq 0} \frac{|c_n|}{\nu^n}. \tag{3.1}$$

This bound is used to estimate linear operators of the following type. Denote by $B(\ell^1_\nu, \ell^1_\nu)$ the space of bounded linear operators from ℓ^1_ν to ℓ^1_ν and by $\|\cdot\|_{B(\ell^1_\nu, \ell^1_\nu)}$ the operator norm.

Corollary 6. *Let A_F be an $m \times m$ matrix, $\{\mu_n\}_{n=m}^\infty$ be a sequence of numbers with*

$$|\mu_n| \leq |\mu_m|,$$

for all $n \geq m$, and $A\colon \ell^1_\nu \to \ell^1_\nu$ be the linear operator defined by

$$A(a) = \begin{pmatrix} A_F & & 0 & \\ & \mu_m & & \\ 0 & & \mu_{m+1} & \\ & & & \ddots \end{pmatrix} \begin{bmatrix} a_F \\ a_m \\ a_{m+1} \\ \vdots \end{bmatrix}.$$

Here $a_F = (a_0, a_1, \ldots, a_{m-1})^T \in \mathbb{R}^m$. Then $A \in B(\ell^1_\nu, \ell^1_\nu)$ is a bounded linear operator and

$$\|A\|_{B(\ell^1_\nu,\ell^1_\nu)} \le \max(K, \mu_m), \tag{3.2}$$

where

$$K \stackrel{\text{def}}{=} \max_{0\le n\le m-1} \frac{1}{\nu^n} \sum_{k=0}^{m-1} |A_{k,n}|\nu^k.$$

Proof. We have that

$$\begin{aligned}
\|A\|_{B(\ell^1_\nu,\ell^1_\nu)} &= \sup_{\|a\|_\nu=1} \|Aa\|_\nu \\
&= \sup_{\|a\|_\nu=1} \left(\sum_{n=0}^{m-1} \left| \sum_{k=0}^{m-1} A_{n,k} a_k \right| \nu^n + \sum_{n=m}^{\infty} |\mu_n a_n| \nu^n \right) \\
&\le \sup_{\|a\|_\nu=1} \left(\sum_{n=0}^{m-1} \left(\sum_{k=0}^{m-1} |A_{k,n}|\nu^k \right) |a_n| + \sum_{n=m}^{\infty} |\mu_n \nu^n||a_n| \right) \\
&= \sup_{\|a\|_\nu=1} \sum_{n=0}^{\infty} |a_n||c_n|,
\end{aligned}$$

where

$$c_n = \begin{cases} \displaystyle\sum_{k=0}^{m-1} |A_{k,n}|\nu^k, & \text{if} \quad 0 \le n \le m-1 \\ |\mu_n|\nu^n, & \text{if} \quad n \ge m. \end{cases}$$

Note that $c = \{c_n\}_{n=0}^\infty \in \ell^\infty_\nu$, since

$$\|c\|^\infty_\nu = \sup_{n\ge 0} \frac{|c_n|}{\nu^n} = \max(K, \mu_m),$$

with K and μ_m as given in the hypothesis of the corollary. We obtain the desired bound on $\|A\|_{B(\ell^1_\nu,\ell^1_\nu)}$ by applying (3.1). □

3.2 Parameterization method for stable/unstable manifolds

We review some computational aspects of the parameterization method for computing local stable/unstable manifolds of equilibria of vector fields. These computations and their validation are described in greater detail in [8]. The stable/unstable manifolds arising in the formulation of (2.7) are two dimensional and are associated with real distinct eigenvalues, hence we focus only on this case. We frame the discussion in terms of the stable manifold, as the unstable manifold is obtained by time reversal.

Let $\Psi : \mathbb{R}^4 \to \mathbb{R}^4$ be the vector field defined in (2.4). We choose $p \in \mathbb{R}^4$ such that $\Psi(p) = 0$, which means that $U = p$ is an equilibrium of $U' = \Psi(U)$. Moreover we assume that, after a change of variables if necessary, $D\Psi(p)$ is diagonalizable and hyperbolic with two stable and two unstable eigenvalues. Suppose that these eigenvalues are real and distinct and denote them by

$$\lambda_1 < \lambda_2 < 0 < \lambda_3 < \lambda_4.$$

Let

$$\Lambda \stackrel{\text{def}}{=} \begin{pmatrix} \lambda_1 & 0 \\ 0 & \lambda_2 \end{pmatrix} \quad \text{and} \quad \Sigma \stackrel{\text{def}}{=} \begin{pmatrix} \lambda_1 & \dots & 0 \\ \vdots & \ddots & \vdots \\ 0 & \dots & \lambda_4 \end{pmatrix}.$$

Furthermore, let $Q = [\xi_1|\dots|\xi_4]$ be the matrix whose columns are all of the associated eigenvectors.

The goal of the parameterization method is to find a map $P\colon \mathbb{R}^2 \to \mathbb{R}^4$ satisfying the invariance equation

$$\Psi[P(\theta)] = DP(\theta)\Lambda\theta, \tag{3.3}$$

for all $\theta \in [-\nu_s, \nu_s]^2$, with $\nu_s > 0$ to be determined explicitly later (see Remark 2), and having

$$P(0) = p, \qquad DP(0) = [\xi_1|\xi_2], \tag{3.4}$$

with ξ_1, ξ_2 the eigenvectors associated to the stable eigenvalues λ_1, λ_2. If P satisfies (3.3) and (3.4) then P parameterizes a local stable manifold for Ψ at p. Since Ψ is analytic we look for P in the form

$$P(\theta) = \sum_{m=0}^{\infty}\sum_{n=0}^{\infty} A_{mn}\theta_1^m\theta_2^n.$$

Fixing $A_{00} = p$, $A_{10} = \xi_1$, and $A_{01} = \xi_2$ imposes the linear constraints of Equation (3.4) on P. Inserting the power series for P in (3.3) and matching like powers of $\theta = (\theta_1, \theta_2)$ yields recurrence relations for the coefficients A_{mn} of the form

$$[D\Psi(p) - (m\lambda_1 + n\lambda_2)\mathrm{I}]\, A_{mn} = s_{mn}, \tag{3.5}$$

for all $m + n \geq 2$. Equation (3.5) is referred to as the *homological equation* for P. Here s_{mn} is a nonlinear function of the coefficients $A_{m'n'}$ with $m' + n' < m + n$, and the form of s_{mn} depends on the nonlinearity of Ψ (see also Remark 1 below).

Observe that (3.5) has unique solution A_{mn} as long as

$$m\lambda_1 + n\lambda_2 \neq \lambda_i, \tag{3.6}$$

for any $i = 1, 2, 3, 4$. Equation (3.6) is called a non-resonance condition for λ_1, λ_2, and we say that λ_1, λ_2 are non-resonant when (3.6) holds. In our specific case this reduces to the condition that λ_1 is not a multiple of λ_2.

Assume now that the stable eigenvalues of $D\Psi(p)$ are non-resonant. Then we can solve the homological equations to any desired finite order to obtain the polynomial approximation

$$P^{(N)}(\theta) = \sum_{m+n\leq N} A_{mn}\theta_1^m\theta_2^n. \tag{3.7}$$

Remark 1. A computation similar to the one illustrated in Section 5.1 of [8] shows that the right hand side s_{mn} of the homological equation associated with the vector field Ψ

of (2.4) is given by $s_{mn} = L(0, s^{(2)}_{mn}, 0, s^{(4)}_{mn})$ where

$$\begin{aligned}
s^{(2)}_{mn} &= -\frac{\sqrt{2}}{4}\sum_{j=0}^{n}\sum_{i=0}^{m}\tilde{A}^{(3)}_{(m-i)(n-j)}\tilde{A}^{(3)}_{ij} + \frac{3}{8}\sum_{j=0}^{n}\sum_{i=0}^{m}\sum_{k=0}^{j}\sum_{\ell=0}^{i}\tilde{A}^{(1)}_{(m-i)(n-j)}\tilde{A}^{(1)}_{(i-\ell)(n-j)}\tilde{A}^{(1)}_{\ell k} \\
&\quad +3\sum_{j=0}^{n}\sum_{i=0}^{m}\sum_{k=0}^{j}\sum_{\ell=0}^{i}\tilde{A}^{(1)}_{(m-i)(n-j)}\tilde{A}^{(3)}_{(i-\ell)(n-j)}\tilde{A}^{(3)}_{\ell k} \\
s^{(4)}_{mn} &= -\frac{\sqrt{2}}{2}\sum_{j=0}^{n}\sum_{i=0}^{m}\tilde{A}^{(1)}_{(m-i)(n-j)}\tilde{A}^{(3)}_{ij} + 9\sum_{j=0}^{n}\sum_{i=0}^{m}\sum_{k=0}^{j}\sum_{\ell=0}^{i}\tilde{A}^{(3)}_{(m-i)(n-j)}\tilde{A}^{(3)}_{(i-\ell)(n-j)}\tilde{A}^{(3)}_{\ell k} \\
&\quad +3\sum_{j=0}^{n}\sum_{i=0}^{m}\sum_{k=0}^{j}\sum_{\ell=0}^{i}\tilde{A}^{(1)}_{(m-i)(n-j)}\tilde{A}^{(1)}_{(i-\ell)(n-j)}\tilde{A}^{(3)}_{\ell k}
\end{aligned}$$

and

$$\tilde{A}^{(i)}_{k_1k_2} = \begin{cases} 0, & \text{if } k_1 = m \text{ and } k_2 = n \\ A^{(i)}_{k_1k_2}, & \text{otherwise} \end{cases}$$

with i either 1 or 3. These expressions are used in order to implement the (numerical) computation of the Taylor coefficients A_{mn} to any desired finite order.

Remark 2. Suppose that we have computed $P^{(N)}$ as discussed above, and that we choose $\nu_s > 0$ so that

$$\sup_{\theta\in[-\nu_s,\nu_s]^2} \|\Psi[P^{(N)}(\theta)] - DP^{(N)}(\theta)\Lambda\theta\| \leq \epsilon \ll 1.$$

The quantity ϵ is referred to as the a-posteriori error or defect associated with the approximate solution $P^{(N)}$ on the domain $[-\nu_s,\nu_s]^2$. In practice a good choice for ν_s is found by numerical experimentation. We would like to prove that there exists an analytic function $h : [-\nu_s,\nu_s]^2 \to \mathbb{R}^4$ such that $P^{(N)} + h$ is a true solution of (3.3), i.e. such that $P = P^{(N)} + h$ is a true parameterization of the local stable manifold. Indeed we would like to determine an explicit constant $\delta_s > 0$ such that

$$\sup_{\theta\in[-\nu_s,\nu_s]^2} \|h(\theta)\| \leq \delta_s. \tag{3.8}$$

This is accomplished using Theorem 4.2 of [8] (see also [32]).

Remark 3. Suppose, as discussed above, that we have obtained validated error bounds for the approximation with $P(\theta_1,\theta_2) = P^{(N)}(\theta_1,\theta_2)+h(\theta_1,\theta_2)$ for all $(\theta_1,\theta_2) \in [-\nu_s,\nu_s]^2$ such that (3.8) holds. In the applications to follow we will also require validated error bounds on the first derivative of $P = P^{(N)} + h$. Of course $DP^{(N)}$ can be computed explicitly so that we only need some bound on the derivative of the truncation error h. For this we employ the following estimate from complex analysis (the proof is found for example in [33]). The lemma gives us bounds for the derivatives if the truncation error h is considered on a domain strictly smaller than $[-\nu_s,\nu_s]^2$.

Lemma 7. *Let $\hat{\theta} \in [-\nu_s,\nu_s]^2$ with $\|\hat{\theta}\| = \max\left(|\hat{\theta}_1|, |\hat{\theta}_2|\right) \leq s < \nu_s$. Suppose that* (3.8) *holds. For $i \in \{1,2,3,4\}$ and $j \in \{1,2\}$, we have that*

$$\left|\frac{\partial h_i}{\partial \theta_j}(\hat{\theta})\right| \leq \frac{2\pi}{\nu_s \ln\left(\frac{\nu_s}{s}\right)}\delta_s.$$

4 Construction of the radii polynomials

As previously mentioned in Section 1, at the center of the radii polynomial approach is an approximate solution obtained through a numerical calculation. This approximation is obtained by applying Newton's method on a finite dimensional projection which we now introduce.

4.1 Finite dimensional projection

Let $m > 1$ and $x = (x_1, x_2, x_3, x_4, x_5, x_6, x_7) \in X = \mathbb{R}^3 \times (\ell^1_\nu)^4$, where $x_1, x_2, x_3 \in \mathbb{R}$ and $x_4, x_5, x_6, x_7 \in \ell^1_\nu$. Let $X_m \stackrel{\text{def}}{=} \mathbb{R}^{4m+3}$. Define the finite dimensional projection $\Pi_m : X \to X_m$ by

$$\begin{aligned}
\Pi_m x &= x_F \\
&= (x_1, x_2, x_3, (x_4)_F, (x_5)_F, (x_6)_F, (x_7)_F) \\
&\stackrel{\text{def}}{=} \left(x_1, x_2, x_3, \{(x_4)_k\}_{k=0}^{m-1}, \{(x_5)_k\}_{k=0}^{m-1}, \{(x_6)_k\}_{k=0}^{m-1}, \{(x_7)_k\}_{k=0}^{m-1}\right) \in X_m.
\end{aligned}$$

The Galerkin projection of $f = (f_1, \ldots, f_7)$ given in (2.13) is defined by

$$f^{(m)} : X_m \to X_m : x_F \mapsto \Pi_m f(x_F, 0_\infty),$$

where

$$(x_F, 0_\infty) \stackrel{\text{def}}{=} \left(x_1, x_2, x_3, \left(\{(x_4)_k\}_{k=0}^{m-1}, \{0\}_{k=m}^{\infty}\right), \ldots, \left(\{(x_7)_k\}_{k=0}^{m-1}, \{0\}_{k=m}^{\infty}\right)\right) \in X.$$

However, the boundary conditions depend on the local parameterizations P and Q of the stable and unstable manifolds, and these parameterizations are expressed in terms of infinite series expansions. For the purpose of computations, we can only work with a finite number of terms. We thus choose parameterization orders $N_s, N_u \in \mathbb{N}$ and, for $\alpha = (\alpha_1, \alpha_2) \in \mathbb{N}^2$, we define

$$P^{(N_s)}(\theta) = \sum_{|\alpha|=0}^{N_s} A_\alpha \theta^\alpha \quad \text{and} \quad Q^{(N_u)}(\phi) = \sum_{|\alpha|=0}^{N_u} B_\alpha \phi^\alpha,$$

as discussed in Section 3.2. Note that $|\alpha| = \alpha_1 + \alpha_2 \geq 0$. The finite dimensional projection $f^{(m,N_s,N_u)} : X_m \to X_m$ of f given in (2.13) is then defined by

$$f^{(m,N_s,N_u)}(x_F) = \begin{pmatrix} (a_1)_0 + 2\sum_{n=1}^{m-1}(a_1)_n - P_1^{(N_s)}(\theta(\psi)) \\ (a_3)_0 + 2\sum_{n=1}^{m-1}(a_3)_n - P_3^{(N_s)}(\theta(\psi)) \\ (a_4)_0 + 2\sum_{n=1}^{m-1}(a_4)_n - P_4^{(N_s)}(\theta(\psi)) \\ f_4^{(m,N_u)}(x_F) \\ f_5^{(m,N_u)}(x_F) \\ f_6^{(m,N_u)}(x_F) \\ f_7^{(m,N_u)}(x_F) \end{pmatrix} \in X_m, \tag{4.1}$$

where $f_i^{(m,N_u)}(x_F) = \left(\left(f_i^{(m,N_u)}(x_F)\right)_k\right)_{k=0}^{m-1} \in \mathbb{R}^m$ is given component-wise by

$$\left(f_i^{(m,N_u)}(x_F)\right)_k = \begin{cases} (a_i)_0 + 2\displaystyle\sum_{n=1}^{m-1}(-1)^n (a_i)_n - Q_i^{(N_u)}(\phi), & k = 0, \\ 2k(a_i)_k + L\left((c_i)_{k+1} - (c_i)_{k-1}\right), & k = 1, \ldots, m-1. \end{cases}$$

4.2 The Newton-like operator on $\boldsymbol{X}$

In order to define a fixed point problem equivalent to the problem $f = 0$, we assume the numerical calculations provide us with the following:

1. Suppose that we computed an approximate solution $\bar{x}$ of $f^{(m,N_s,N_u)}(x) = 0$ using Newton's method.

2. Assume that we computed the Jacobian matrix $Df^{(m,N_s,N_u)}(\bar{x})$.

3. Assume that we computed an approximate inverse $A^{(m)}$ of $Df^{(m,N_s,N_u)}(\bar{x})$.

4. Suppose that $A^{(m)}$ is injective. In practice, showing that $\|I - A^{(m)} Df^{(m,N_s,N_u)}(\bar{x})\| < 1$ is sufficient to prove that $A^{(m)}$ is injective.

Denote $A^{(m)}$ block-wise as

$$A^{(m)} = \begin{bmatrix} A_{11}^{(m)} & \dots & A_{13}^{(m)} & A_{14}^{(m)} & \dots & A_{17}^{(m)} \\ \vdots & \dots & \vdots & \vdots & \dots & \vdots \\ A_{31}^{(m)} & \dots & A_{33}^{(m)} & A_{34}^{(m)} & \dots & A_{37}^{(m)} \\ A_{41}^{(m)} & \dots & A_{43}^{(m)} & A_{44}^{(m)} & \dots & A_{47}^{(m)} \\ \vdots & \dots & \vdots & \vdots & \dots & \vdots \\ A_{71}^{(m)} & \dots & A_{73}^{(m)} & A_{74}^{(m)} & \dots & A_{77}^{(m)} \end{bmatrix} \in \mathbb{R}^{(4m+3)\times(4m+3)}, \tag{4.2}$$

with $A_{ij}^{(m)} \in \mathbb{R}$ for $1 \le i,j, \le 3$, $A_{ij}^{(m)} \in \mathbb{R}^{1\times m}$ for $1 \le i \le 3, 4 \le j \le 7$, $A_{ij}^{(m)} \in \mathbb{R}^{m\times 1}$ for $4 \le i \le 7, 1 \le j \le 3$ and $A_{ij}^{(m)} \in \mathbb{R}^{m\times m}$ for $4 \le i,j \le 7$. The operator A which acts as an approximate inverse for $Df(\bar{x})$ is given block-wise by

$$A = \begin{bmatrix} A_{11} & \dots & A_{13} & A_{14} & \dots & A_{17} \\ \vdots & \dots & \vdots & \vdots & \dots & \vdots \\ A_{31} & \dots & A_{33} & A_{34} & \dots & A_{37} \\ A_{41} & \dots & A_{43} & A_{44} & \dots & A_{47} \\ \vdots & \dots & \vdots & \vdots & \dots & \vdots \\ A_{71} & \dots & A_{73} & A_{74} & \dots & A_{77} \end{bmatrix}, \tag{4.3}$$

where

- $A_{ij} = A_{ij}^{(m)} \in \mathbb{R}$, for $1 \le i,j, \le 3$;
- $A_{ij} \in \left(\ell_\nu^1\right)^*$ for $1 \le i \le 3, 4 \le j \le 7$. For $x_j \in \ell_\nu^1$, $A_{ij}x_j = A_{ij}^{(m)} \cdot (x_j)_F \in \mathbb{R}$;
- $A_{ij} \in \ell_\nu^1$ for $4 \le i \le 7, 1 \le j \le 3$. For $x_j \in \mathbb{R}$, $A_{ij}x_j = (A_{ij}^{(m)}x_j, 0_\infty) \in \ell_\nu^1$;
- $A_{ij} \in B\left(\ell_\nu^1, \ell_\nu^1\right)$ for $4 \le i,j \le 7$. For $x_j \in \ell_\nu^1$,

$$(A_{ij}x_j)_k = \begin{cases} (A_{ij}^{(m)}(x_j)_F)_k, & k = 0,\dots,m-1, \\ \delta_{i,j}\frac{1}{2k}(x_j)_k, & k \ge m, \end{cases}$$

where $\delta_{i,j}$ equals 1 if $i = j$ and 0 otherwise.

Combining the above, A is a linear operator which acts on $x = (x_1, \dots, x_7) \in X$ component-wise as

$$(Ax)_i = \sum_{j=1}^{7} A_{ij} x_j,$$

with $(Ax)_i \in \mathbb{R}$ for $i = 1, 2, 3$ and $(Ax)_i \in \ell^1_\nu$, for $i = 4, 5, 6, 7$.

We are now ready to define the Newton-like operator and to show that it maps the Banach space X into itself.

Proposition 8. *Recalling the linear operator A in* (4.3)*, define*

$$T(x) = x - Af(x). \tag{4.4}$$

Then, $T : X \to X$.

Proof. Let $x = (x_1, x_2, x_3, x_4, x_5, x_6, x_7) \in X = \mathbb{R}^3 \times (\ell^1_\nu)^4$. For each fixed $i = 1, 2, 3$,

$$|(T(x))_i| = |x_i - (Af(x))_i| = \left| x_i - \sum_{j=1}^{3} A^{(m)}_{ij} f_j(x) - \sum_{j=4}^{7} A^{(m)}_{ij} \cdot (f_j(x))_F \right| < \infty,$$

since it consists of finite sums of finite quantities. Now for the case $i = 4, 5, 6, 7$,

$$(T(x))_i = x_i - \sum_{j=1}^{3} \left(A^{(m)}_{ij} f_j(x), 0_\infty \right) - \sum_{j=4}^{7} A_{ij} f_j(x).$$

Note that the first two terms of $(T(x))_i$ satisfy

$$\begin{aligned} \left\| x_i - \sum_{j=1}^{3} \left(A^{(m)}_{ij} f_j(x), 0_\infty \right) \right\|_\nu &\le \|x_i\|_\nu + \sum_{j=1}^{3} \left\| \left(A^{(m)}_{ij} f_j(x), 0_\infty \right) \right\|_\nu \\ &= \|x_i\|_\nu + \sum_{j=1}^{3} |f_j(x)| \sum_{k=0}^{m-1} \left| \left(A^{(m)}_{ij} \right)_k \right| \nu^k < \infty. \end{aligned}$$

We now show that $\| \sum_{j=4}^{7} A_{ij} f_j(x) \|_\nu < \infty$ for each $i = 4, \dots, 7$. Denote $(a_1, a_2, a_3, a_4) = (x_4, x_5, x_6, x_7) \in (\ell^1_\nu)^4$. Recall that for $k \ge 1$ and $j = 1, 2, 3, 4$,

$$\left(f_{j+3}(x) \right)_k = 2k(a_j)_k + L \left((c_j)_{k+1} - (c_j)_{k-1} \right),$$

with each $c_j = c_j(a_1, a_2, a_3, a_4)$ given component-wise by (2.12). Since ℓ^1_ν is a Banach algebra under discrete convolutions, $c_j \in \ell^1_\nu$ for each $j = 1, 2, 3, 4$. Finally, there exists a constant $C < \infty$ such that

$$\begin{aligned} \left\| \sum_{j=4}^{7} A_{ij} f_j(x) \right\|_\nu &\le \sum_{j=4}^{7} \sum_{k=0}^{m-1} \left| \left(A^{(m)}_{ij} (f_j(x))_F \right)_k \right| \nu^k + \sum_{k=m}^{\infty} \left| \left(\frac{1}{2k} (f_i(x))_k \right)_k \right| \nu^k \\ &\le \sum_{j=4}^{7} \sum_{k=0}^{m-1} \left| \left(A^{(m)}_{ij} (f_j(x))_F \right)_k \right| \nu^k + \|a_i\|_\nu \\ &\quad + L \sum_{k=m}^{\infty} \left| \left(\frac{1}{2k} ((c_i)_{k+1} - (c_i)_{k-1}) \right)_k \right| \nu^k \\ &\le \sum_{j=4}^{7} \sum_{k=0}^{m-1} \left| \left(A^{(m)}_{ij} (f_j(x))_F \right)_k \right| \nu^k + \|a_i\|_\nu + C\|c_i\|_\nu < \infty. \end{aligned}$$

We can conclude that

$$\|T(x)\|_X = \max\left(|T_1(x)|, |T_2(x)|, |T_3(x)|, \|T_4(x)\|_\nu, \ldots, \|T_7(x)\|_\nu\right) < \infty. \qquad \square$$

4.3 Explicit construction of the radii polynomials

In this section, we provide an explicit construction of the bound Y satisfying (2.15) and of the bound Z satisfying (2.16). The final computation of the bounds Y and Z is a combination of analytic estimates and rigorous computations using interval arithmetic.

To estimate the terms

$$P(\theta) = \sum_{|\alpha| \geq 0} A_\alpha \theta^\alpha \quad \text{and} \quad Q(\phi) = \sum_{|\alpha| \geq 0} B_\alpha \phi^\alpha,$$

which parameterize respectively the stable and unstable manifolds, we assume that we have computed a rigorous enclosure (using interval arithmetic) of the coefficients A_α for $0 \leq |\alpha| \leq N_s$ and of the coefficients B_α for $0 \leq |\alpha| \leq N_u$, forming the N_s-th and N_u-th order polynomial approximations

$$P^{(N_s)}(\theta) = \sum_{0 \leq |\alpha| \leq N_s} A_\alpha \theta^\alpha \quad \text{and} \quad Q^{(N_u)}(\phi) = \sum_{0 \leq |\alpha| \leq N_u} B_\alpha \phi^\alpha.$$

Furthermore, we assume that we have estimates of the forms

$$\sup_{\|\theta\| < \nu_s} \left| [P(\theta) - P^{(N_s)}(\theta)]_k \right| \leq \delta_s \quad (k = 1, 2, 3, 4) \tag{4.5}$$

and

$$\sup_{\|\phi\| < \nu_u} \left| [Q(\phi) - Q^{(N_u)}(\phi)]_k \right| \leq \delta_u \quad (k = 1, 2, 3, 4) \tag{4.6}$$

for some $\delta_s, \delta_u > 0$ and $\nu_s, \nu_u > 0$. This data is obtained using the methods discussed in Section 3.2. Finally, assume that $\rho < \nu_s$ and $\|\bar{\phi}\|_\nu = \max\left(|\bar{\phi}_1|, |\bar{\phi}_2|\right) < \nu_u$.

4.3.1 Construction of the bound Y

Let

$$y \stackrel{\text{def}}{=} T(\bar{x}) - \bar{x} = -Af(\bar{x}).$$

To compute $y_F \stackrel{\text{def}}{=} \Pi_m y$, we use the splitting

$$\Pi_m f(\bar{x}) = f^{(m,N_s,N_u)}(\bar{x}) + \begin{pmatrix} P_1^{(N_s)}(\bar{\theta}) - P_1(\bar{\theta}) \\ P_3^{(N_s)}(\bar{\theta}) - P_3(\bar{\theta}) \\ P_4^{(N_s)}(\bar{\theta}) - P_4(\bar{\theta}) \\ \left(Q_1^{(N_u)}(\bar{\phi}) - Q_1(\bar{\phi}), 0, 0, \ldots\right) \\ \left(Q_2^{(N_u)}(\bar{\phi}) - Q_2(\bar{\phi}), 0, 0, \ldots\right) \\ \left(Q_3^{(N_u)}(\bar{\phi}) - Q_3(\bar{\phi}), 0, 0, \ldots\right) \\ \left(Q_4^{(N_u)}(\bar{\phi}) - Q_4(\bar{\phi}), 0, 0, \ldots\right) \end{pmatrix}.$$

Using interval arithmetic, one can evaluate $f^{(m,N_s,N_u)}(\bar{x})$. Under the assumptions that $\|\theta\| < \nu_s$ and $\|\phi\| < \nu_u$, one can then use (4.5) and (4.6) to obtain the following component-wise upper bound for $|y_F|$

$$|y_F| \le \mathrm{v}_F \overset{\mathrm{def}}{=} |A^{(m)} f^{(m,N_s,N_u)}(\bar{x})| + \left|A^{(m)}\right| \begin{pmatrix} \delta_s \\ \delta_s \\ \delta_s \\ (\delta_u, 0, 0, \dots) \\ (\delta_u, 0, 0, \dots) \\ (\delta_u, 0, 0, \dots) \\ (\delta_u, 0, 0, \dots) \end{pmatrix}. \tag{4.7}$$

Since $(a_i)_k = 0$ for all $k \ge m$ and $(f_i(\bar{x}))_k$ involves the $(k-1)$th component of a cubic convolution for $i = 4,5,6,7$, we have that $(f_i(\bar{x}))_k = 0$ for all $k \ge 3m-1$. By definition of A, for $k = m, \dots, 3m-2$ and for $i = 4,5,6,7$,

$$|(y_i)_k| = \left| -\frac{1}{2k}(f_i(\bar{x}))_k \right| = \frac{1}{2k} |(f_i(\bar{x}))_k| .$$

More precisely,

$$\begin{aligned}
|(y_4)_k| &= \left|-\tfrac{1}{2k}(f_4(\bar{x}))_k\right| &=& \tfrac{L}{2k}\delta_{k,m}|(\bar{a}_2)_{k\pm1}|, \\
|(y_5)_k| &= \left|-\tfrac{1}{2k}(f_5(\bar{x}))_k\right| &=& \tfrac{L}{2k}\left|-\delta_{k,m}\tfrac{\gamma}{4}(\bar{a}_1)_{k\pm1} - \tfrac{\sqrt{2}}{4}(\bar{a}_3^2)_{k\pm1} + \tfrac{3}{8}(\bar{a}_1^3)_{k\pm1} + 3(\bar{a}_1\bar{a}_3^2)_{k\pm1}\right| \\
|(y_6)_k| &= \left|-\tfrac{1}{2k}(f_6(\bar{x}))_k\right| &=& \tfrac{L}{2k}\delta_{k,m}|(\bar{a}_4)_{k\pm1}|, \\
|(y_7)_k| &= \left|-\tfrac{1}{2k}(f_7(\bar{x}))_k\right| &=& \tfrac{L}{2k}\left|-\delta_{k,m}\gamma(\bar{a}_3)_{k\pm1} - \tfrac{\sqrt{2}}{2}(\bar{a}_1\bar{a}_3)_{k\pm1} + 9(\bar{a}_3^3)_{k\pm1} + 3(\bar{a}_1^2\bar{a}_3)_{k\pm1}\right|,
\end{aligned}$$

where we use the notation $a_{k\pm1} = a_{k+1} - a_{k-1}$.

Finally, for all $k \ge 3m-1$, we have that $(y_i)_k = 0$ for $i = 4,5,6,7$. Combining the previous equalities with (4.7), we define the bound $Y = (Y_1, \dots, Y_7)$ by

$$Y_i \overset{\mathrm{def}}{=} \begin{cases} |[\mathrm{v}_F]_i|, & i = 1,2,3, \\ \displaystyle\sum_{k=0}^{m-1} |([\mathrm{v}_F]_i)_k|\nu^k + \sum_{k=m}^{3m-2} \frac{1}{2k}|(f_i(\bar{x}))_k|\nu^k, & i = 4,5,6,7. \end{cases} \tag{4.8}$$

4.3.2 Construction of the bound Z

In order to simplify the computation of the bound Z, we introduce the bounded linear operator $A^\dagger$ defined component-wise by

$$A^\dagger = \begin{bmatrix} A^\dagger_{11} & \dots & A^\dagger_{13} & A^\dagger_{14} & \dots & A^\dagger_{17} \\ \vdots & \dots & \vdots & \vdots & \dots & \vdots \\ A^\dagger_{31} & \dots & A^\dagger_{33} & A^\dagger_{34} & \dots & A^\dagger_{37} \\ A^\dagger_{41} & \dots & A^\dagger_{43} & A^\dagger_{44} & \dots & A^\dagger_{47} \\ \vdots & \dots & \vdots & \vdots & \dots & \vdots \\ A^\dagger_{71} & \dots & A^\dagger_{73} & A^\dagger_{74} & \dots & A^\dagger_{77} \end{bmatrix}, \tag{4.9}$$

where

- $A^\dagger_{ij} = Df^{(m,N_s,N_u)}_{ij}(\bar{x}) \in \mathbb{R}$, for $1 \le i, j, \le 3$;
- $A^\dagger_{ij} \in \left(\ell^1_\nu\right)^*$ for $1 \le i \le 3, 4 \le j \le 7$.
  For $x_j \in \ell^1_\nu$, $A^\dagger_{ij} x_j = Df^{(m,N_s,N_u)}_{ij}(\bar{x}) \cdot (x_j)_F \in \mathbb{R}$;

- $A^\dagger_{ij} \in \ell^1_\nu$ for $4 \le i \le 7, 1 \le j \le 3$.
  For $x_j \in \mathbb{R}$, $A^\dagger_{ij} x_j = (Df_{ij}^{(m,N_s,N_u)}(\bar{x})x_j, 0_\infty) \in \ell^1_\nu$;

- $A^\dagger_{ij} \in B\left(\ell^1_\nu, \ell^1_{\nu'}\right)$ for $4 \le i, j \le 7$ and for any $\nu' < \nu$ (e.g. see [7]). For $x_j \in \ell^1_\nu$,

$$(A^\dagger_{ij} x_j)_k = \begin{cases} \left(Df_{ij}^{(m,N_s,N_u)}(\bar{x})(x_j)_F\right)_k, & k = 0, \dots, m-1, \\ \delta_{i,j} 2k (x_j)_k, & k \ge m, \end{cases}$$

  where $\delta_{i,j}$ equals 1 if $i = j$ and 0 otherwise.

Considering $b = (b_1, \dots, b_7)$, $c = (c_1, \dots, c_7) \in B(r)$ and recalling the definition of the Newton-like operator (4.4), notice that

$$DT(\bar{x} + b)c = [I - ADf(\bar{x} + b)]c = [I - AA^\dagger]c - A[Df(\bar{x} + b)c - A^\dagger c]. \tag{4.10}$$

The objective is to bound each component in the right-hand side of (4.10). Consider $u = (u_1, \dots, u_7)$, $v = (v_1, \dots, v_7) \in B(1)$ such that $b = ur$ and $c = vr$. Let $B \stackrel{\text{def}}{=} I - AA^\dagger$, which is denoted by

$$B = \begin{bmatrix} B_{11} & \dots & B_{13} & B_{14} & \dots & B_{17} \\ \vdots & \dots & \vdots & \vdots & \dots & \vdots \\ B_{31} & \dots & B_{33} & B_{34} & \dots & B_{37} \\ B_{41} & \dots & B_{43} & B_{44} & \dots & B_{47} \\ \vdots & \dots & \vdots & \vdots & \dots & \vdots \\ B_{71} & \dots & B_{73} & B_{74} & \dots & B_{77} \end{bmatrix}.$$

Note that by definition of the diagonal tails of A_{ij} and $A^\dagger_{ij}$, the tails of B_{ij} vanish, i.e., all B_{ij}, $4 \le i, j \le 7$ are represented by $m \times m$ matrices. For $i = 1, 2, 3$, let

$$Z_i^{(0)} \stackrel{\text{def}}{=} \begin{cases} \displaystyle\sum_{j=1}^{3} |B_{ij}| + \sum_{j=4}^{7} \left(\max_{0 \le k \le m-1} \frac{\left|(B_{ij})_k\right|}{\nu^k} \right), & i = 1, 2, 3 \\ \displaystyle\sum_{j=1}^{3} \left(\sum_{k=0}^{m-1} \left|(B_{ij})_k\right| \nu^k \right) + \sum_{j=4}^{7} \left(\max_{0 \le n \le m-1} \frac{1}{\nu^n} \sum_{k=0}^{m-1} \left|(B_{ij})_{k,n}\right| \nu^k \right), & i = 4, 5, 6, 7. \end{cases} \tag{4.11}$$

Using (3.1), one gets that for every $c \in B(r)$ and for $i = 1, 2, 3$,

$$\begin{aligned} \left|[(I - AA^\dagger)c]_i\right| &= \left|[(I - AA^\dagger)v]_i\right| r \\ &\le \sup_{\|v\|_X = 1} \left|[(I - AA^\dagger)v]_i\right| r \\ &\le \sum_{j=1}^{3} |B_{ij}| r + \sum_{j=4}^{7} \|B_{ij}\|^\infty_\nu r \\ &\le \left(\sum_{j=1}^{3} |B_{ij}| + \sum_{j=4}^{7} \left(\max_{0 \le k \le m-1} \frac{\left|(B_{ij})_k\right|}{\nu^k} \right) \right) r \\ &= Z_i^{(0)} r. \end{aligned} \tag{4.12}$$

Furthermore, using Corollary 6, one gets that for every $c \in B(r)$ and for $i = 4, 5, 6, 7$,

$$\begin{aligned}
\left\|[(I - AA^\dagger)c]_i\right\|_\nu &= \left\|[(I - AA^\dagger)v]_i\right\|_\nu r \\
&\leq \sup_{\|v\|_X = 1} \left\|[(I - AA^\dagger)v]_i\right\|_\nu r \\
&\leq \sum_{j=1}^{3} \|B_{ij}\|_\nu r + \sum_{j=4}^{7} \|B_{ij}\|_{B(\ell_\nu^1, \ell_\nu^1)} r \\
&\leq \left(\sum_{j=1}^{3} \left(\sum_{k=0}^{m-1} \left|(B_{ij})_k\right| \nu^k \right) + \sum_{j=4}^{7} \left(\max_{0 \leq n \leq m-1} \frac{1}{\nu^n} \sum_{k=0}^{m-1} \left|(B_{ij})_{k,n}\right| \nu^k \right) \right) r \\
&= Z_i^{(0)} r. \qquad (4.13)
\end{aligned}$$

The next step is to bound the components of the second term of (4.10), given by $-A[Df(\bar{x} + b)c - A^\dagger c]$. We consider separately the coefficients in front of r, r^2 and r^3. The coefficients in front of r needs to be smaller than 1 for the radii polynomials in (2.17) to have any prospect of being negative for some $r > 0$. We thus put extra effort in estimating these "linear" terms.

$|[\boldsymbol{Df(\bar{x}+b)c - A^\dagger c}]_{\boldsymbol{i}}|$**, for** $\boldsymbol{i = 1, 2, 3}$

We expand the first component of the parameterization of the stable manifold as $P_j = P_j^{(N_s)} + h_j^s$, $j = 1, 3, 4$ (corresponding to $i = 1, 2, 3$). We write out the estimates in detail for $i = 1$. By Lemma 7 (since we chose $\rho < \nu_s$) and by the mean value theorem, there exist $\sigma^{(j,s,1)} \in [\bar{\psi} - r, \bar{\psi} + r]$ for $j = 1, 2$ such that

$$\begin{aligned}
&\left|\left[Df(\bar{x} + b)c - A^\dagger c\right]_1\right| \\
&= \Bigg| \left[-\frac{\partial P_1}{\partial \theta_1}(\theta(\bar{\psi} + b_1))(-\rho \sin(\bar{\psi} + b_1))c_1 - \frac{\partial P_1}{\partial \theta_2}(\theta(\bar{\psi} + b_1))(\rho \cos(\bar{\psi} + b_1))c_1 + (c_4)_0 + 2\sum_{k=1}^{\infty}(c_4)_k \right] \\
&\quad - \left[-\frac{\partial P_1^{(N_s)}}{\partial \theta_1}(\theta(\bar{\psi}))(-\rho \sin(\bar{\psi}))c_1 - \frac{\partial P_1^{(N_s)}}{\partial \theta_2}(\theta(\bar{\psi}))(\rho \cos(\bar{\psi}))c_1 + (c_4)_0 + 2\sum_{k=1}^{m-1}(c_4)_k \right] \Bigg| \\
&\leq \left| \frac{\partial P_1^{(N_s)}}{\partial \theta_1}(\theta(\bar{\psi} + b_1))(-\rho \sin(\bar{\psi} + b_1)) - \frac{\partial P_1^{(N_s)}}{\partial \theta_1}(\theta(\bar{\psi}))(-\rho \sin(\bar{\psi})) \right| r \\
&\quad + \left| \frac{\partial P_1^{(N_s)}}{\partial \theta_2}(\theta(\bar{\psi} + b_1))(\rho \cos(\bar{\psi} + b_1)) - \frac{\partial P_1^{(N_s)}}{\partial \theta_2}(\theta(\bar{\psi}))(\rho \cos(\bar{\psi})) \right| r \\
&\quad + \left| \frac{\partial h_1^s}{\partial \theta_1}(\theta(\bar{\psi} + b_1))(-\rho \sin(\bar{\psi} + b_1)) + \frac{\partial h_1^s}{\partial \theta_2}(\theta(\bar{\psi} + b_1))(\rho \cos(\bar{\psi} + b_1)) \right| r + 2\sum_{k=m}^{\infty} |(v_4)_k| r. \\
&\leq \left(\left| \frac{\partial^2 P_1^{(N_s)}}{\partial \theta_1^2}(\theta(\sigma^{(1,s,1)})) \right| \rho^2 + \left| \frac{\partial^2 P_1^{(N_s)}}{\partial \theta_2 \partial \theta_1}(\theta(\sigma^{(1,s,1)})) \right| \rho^2 + \left| \frac{\partial P_1^{(N_s)}}{\partial \theta_1}(\theta(\sigma^{(1,s,1)})) \right| \rho \right) r^2 \\
&\quad + \left(\left| \frac{\partial P_1^{(N_s)}}{\partial \theta_2}(\theta(\sigma^{(2,s,1)})) \right| \rho + \left| \frac{\partial^2 P_1^{(N_s)}}{\partial \theta_1 \partial \theta_2}(\theta(\sigma^{(2,s,1)})) \right| \rho^2 + \left| \frac{\partial^2 P_1^{(N_s)}}{\partial \theta_2^2}(\theta(\sigma^{(2,s,1)})) \right| \rho^2 \right) r^2 \\
&\quad + \left(\frac{4\pi}{\nu_s \ln\left(\frac{\nu_s}{\rho}\right)} \delta_s \rho + \frac{2}{\nu^m} \right) r,
\end{aligned}$$

where the last inequality follows from the fact that (using (3.1))

$$\sup_{v\in B(1)}\sum_{k\geq m}|(v_4)_k| = \sup_{\|v_4\|_\nu=1}\sum_{k\geq m}|(v_4)_k| = \sup_{k\geq m}\frac{1}{\nu^k} = \frac{1}{\nu^m}.$$

To be able to choose $\sigma^{(j,s,1)}$ independent of r, we assume we have an a priori bound $r^* \geq r$ (this condition has to be checked for self-consistency after we determine r). Let $\boldsymbol{\sigma}^{(s)} = [\bar{\psi} - r^*, \bar{\psi} + r^*]$. Hence, $\sigma^{(1,s,1)}, \sigma^{(2,s,1)} \in \boldsymbol{\sigma}^{(s)}$. We define the intervals $\mathbf{\Psi}_1 = \rho\cos(\boldsymbol{\sigma}^{(s)})$ and $\mathbf{\Psi}_2 = \rho\sin(\boldsymbol{\sigma}^{(s)})$. Using interval arithmetic, we find $\mathbf{I}_{1,1}^{(s,1)}$, $\mathbf{I}_{2,1}^{(s,1)} = \mathbf{I}_{1,2}^{(s,1)}$, $\mathbf{I}_{2,2}^{(s,1)}$, $\mathbf{I}_{1}^{(s,1)}$ and $\mathbf{I}_{2}^{(s,1)}$ such that

$$\begin{aligned}
\frac{\partial^2 P_1^{(N_s)}}{\partial\theta_1^2}(\mathbf{\Psi}) &= \sum_{\alpha\in S_{1,1}^{(N_s)}} A_\alpha^{(1)}\alpha_1(\alpha_1-1)(\mathbf{\Psi}_1)^{\alpha_1-2}(\mathbf{\Psi}_2)^{\alpha_2} \subset \mathbf{I}_{1,1}^{(s,1)},\\
\frac{\partial^2 P_1^{(N_s)}}{\partial\theta_1\partial\theta_2}(\mathbf{\Psi}) &= \frac{\partial^2 P_1^{(N_s)}}{\partial\theta_2\partial\theta_1}(\mathbf{\Psi}) = \sum_{\alpha\in S_{2,1}^{(N_s)}} A_\alpha^{(1)}\alpha_1(\mathbf{\Psi}_1)^{\alpha_1-1}\alpha_2(\mathbf{\Psi}_2)^{\alpha_2-1} \subset \mathbf{I}_{2,1}^{(s,1)},\\
\frac{\partial^2 P_1^{(N_s)}}{\partial\theta_2^2}(\mathbf{\Psi}) &= \sum_{\alpha\in S_{2,2}^{(N_s)}} A_\alpha^{(1)}(\mathbf{\Psi}_1)^{\alpha_1}\alpha_2(\alpha_2-1)(\mathbf{\Psi}_2)^{\alpha_2-2} \subset \mathbf{I}_{2,2}^{(s,1)},\\
\frac{\partial P_1^{(N_s)}}{\partial\theta_1}(\mathbf{\Psi}) &= \sum_{\alpha\in S_{1}^{(N_s)}} A_\alpha^{(1)}\alpha_1(\mathbf{\Psi}_1)^{\alpha_1-1}(\mathbf{\Psi}_2)^{\alpha_2} \subset \mathbf{I}_{1}^{(s,1)},\\
\frac{\partial P_1^{(N_s)}}{\partial\theta_2}(\mathbf{\Psi}) &= \sum_{\alpha\in S_{2}^{(N_s)}} A_\alpha^{(1)}(\mathbf{\Psi}_1)^{\alpha_1}\alpha_2(\mathbf{\Psi}_2)^{\alpha_2-1} \subset \mathbf{I}_{2}^{(s,1)},
\end{aligned}$$

with

$$\begin{aligned}
S_{1,1}^{(N)} &\stackrel{\text{def}}{=} \{\alpha = (\alpha_1,\alpha_2)\in\mathbb{N}^2 : |\alpha|\leq N \text{ and } \alpha_1\geq 2\},\\
S_{2,1}^{(N)} &\stackrel{\text{def}}{=} \{\alpha = (\alpha_1,\alpha_2)\in\mathbb{N}^2 : |\alpha|\leq N \text{ and } \alpha_1,\alpha_2\geq 1\},\\
S_{2,2}^{(N)} &\stackrel{\text{def}}{=} \{\alpha = (\alpha_1,\alpha_2)\in\mathbb{N}^2 : |\alpha|\leq N \text{ and } \alpha_1\geq 2\},\\
S_{1}^{(N)} &\stackrel{\text{def}}{=} \{\alpha = (\alpha_1,\alpha_2)\in\mathbb{N}^2 : |\alpha|\leq N \text{ and } \alpha_1\geq 1\},\\
S_{2}^{(N)} &\stackrel{\text{def}}{=} \{\alpha = (\alpha_1,\alpha_2)\in\mathbb{N}^2 : |\alpha|\leq N \text{ and } \alpha_2\geq 1\}.
\end{aligned}$$

Using interval arithmetic, we can than find a bound $\Lambda^{(s,1)} \in \mathbb{R}^+$ satisfying

$$|\mathbf{I}_{1,1}^{(s,1)}|\rho^2 + 2|\mathbf{I}_{2,1}^{(s,1)}|\rho^2 + |\mathbf{I}_{2,2}^{(s,1)}|\rho^2 + |\mathbf{I}_{1}^{(s,1)}|\rho + |\mathbf{I}_{2}^{(s,1)}|\rho \leq \Lambda^{(s,1)}.$$

Hence, we get that

$$\left|\left[Df(\bar{x}+b)c - A^\dagger c\right]_1\right| \leq \Lambda^{(s,1)}r^2 + \left(\frac{4\pi}{\nu_s\ln\left(\frac{\nu_s}{\rho}\right)}\delta_s\rho + \frac{2}{\nu^m}\right)r. \tag{4.14}$$

Similarly, we can find $\Lambda^{(s,3)}, \Lambda^{(s,4)} \geq 0$ such that

$$\left|\left[Df(\bar{x}+b)c - A^{\dagger}c\right]_i\right| \leq \Lambda^{(s,i+1)}r^2 + \left(\frac{4\pi}{\nu_s \ln\left(\frac{\nu_s}{\rho}\right)}\delta_s\rho + \frac{2}{\nu^m}\right)r. \tag{4.15}$$

$\|[Df(\bar{x}+b)c - A^{\dagger}c]_i\|_\nu$, for $i = 4, 5, 6, 7$

We expand the parameterization of the unstable manifold as $Q_i = Q_i^{(N_u)} + h_i^u$ for $i = 1, 2, 3, 4$. We now assume that the a priori bound $r^* \geq r$ has been chosen to satisfy

$$r^* + \|\bar{\phi}\| = r^* + \max\left(|\bar{\phi}_1|, |\bar{\phi}_2|\right) < \nu_u. \tag{4.16}$$

By Lemma 7 (since $\|\bar{\phi}\| < \nu_u - r^* < \nu_u$) and by the mean value theorem, there exist $\sigma_k^{(j,u,i)} \in [\bar{\phi}_k - r, \bar{\phi}_k + r]$ for $j, k = 1, 2$ such that for $i = 1, 2, 3, 4$,

$$\begin{aligned}
&\left|\left(\left[Df(\bar{x}+b)c - A^{\dagger}c\right]_{i+3}\right)_0\right| \\
&= \Bigg|\left[-\frac{\partial Q_i}{\partial \phi_1}(\bar{\phi}_1 + b_2, \bar{\phi}_2 + b_3)c_2 - \frac{\partial Q_i}{\partial \phi_2}(\bar{\phi}_1 + b_2, \bar{\phi}_2 + b_3)c_3 + (c_{i+3})_0 + 2\sum_{k=1}^{\infty}(-1)^k (c_{i+3})_k\right] \\
&\quad - \left[-\frac{\partial Q_i^{(N_u)}}{\partial \phi_1}(\bar{\phi}_1, \bar{\phi}_2)c_2 - \frac{\partial Q_i^{(N_u)}}{\partial \phi_2}(\bar{\phi}_1, \bar{\phi}_2)c_3 + (c_{i+3})_0 + 2\sum_{k=1}^{m-1}(-1)^k (c_{i+3})_k\right]\Bigg| \\
&\leq \left|\frac{\partial Q_i^{(N_u)}}{\partial \phi_1}(\bar{\phi}_1 + b_2, \bar{\phi}_2 + b_3) - \frac{\partial Q_i^{(N_u)}}{\partial \phi_1}(\bar{\phi}_1, \bar{\phi}_2)\right| r + \left|\frac{\partial Q_i^{(N_u)}}{\partial \phi_2}(\bar{\phi}_1 + b_2, \bar{\phi}_2 + b_3) - \frac{\partial Q_i^{(N_u)}}{\partial \phi_2}(\bar{\phi}_1, \bar{\phi}_2)\right| r \\
&\quad + \left(\left|\frac{\partial h_i^u}{\partial \phi_1}(\bar{\phi}_1 + b_2, \bar{\phi}_1 + b_3)\right| + \left|\frac{\partial h_i^u}{\partial \phi_2}(\bar{\phi}_1 + b_2, \bar{\phi}_1 + b_3)\right| + 2\sum_{k=m}^{\infty}|(v_{i+3})_k|\right) r \\
&\leq \left|\frac{\partial^2 Q_i^{(N_u)}}{\partial \phi_1^2}(\sigma_1^{(1,u,i)}, \sigma_2^{(1,u,i)})\right| r^2 + \left|\frac{\partial^2 Q_i^{(N_u)}}{\partial \phi_2 \partial \phi_1}(\sigma_1^{(1,u,i)}, \sigma_2^{(1,u,i)})\right| r^2 + \left|\frac{\partial^2 Q_i^{(N_u)}}{\partial \phi_1 \partial \phi_2}(\sigma_1^{(2,u,i)}, \sigma_2^{(2,u,i)})\right| r^2 \\
&\quad + \left|\frac{\partial^2 Q_i^{(N_u)}}{\partial \phi_2^2}(\sigma_1^{(2,u,i)}, \sigma_2^{(2,u,i)})\right| r^2 + \left(\frac{4\pi}{\nu_u \ln\left(\frac{\nu_u}{\nu_u - r^*}\right)}\delta_u + \frac{2}{\nu^m}\right) r.
\end{aligned}$$

We notice that, for $i = 1, 2, 3, 4$ and $j, k = 1, 2$

$$\sigma_k^{(j,u,i)} \in [\bar{\phi}_k - r, \bar{\phi}_k + r] \subset [\bar{\phi}_k - r^*, \bar{\phi}_k + r^*].$$

Let $\boldsymbol{\sigma}_k^{(u)} \stackrel{\text{def}}{=} [\bar{\phi}_k - r^*, \bar{\phi}_k + r^*]$ for $k = 1, 2$. Given $i = 1, 2, 3, 4$, and using interval arithmetic, we define the intervals $\mathbf{I}_{1,1}^{(u,i)}$, $\mathbf{I}_{2,1}^{(u,i)} = \mathbf{I}_{1,2}^{(u,i)}$ and $\mathbf{I}_{2,2}^{(u,i)}$ such that

$$\begin{aligned}
\frac{\partial^2 Q_i^{(N_u)}}{\partial \phi_1^2}(\boldsymbol{\sigma}^{(u)}) &= \sum_{\alpha \in S_{1,1}^{(N_u)}} B_\alpha^{(i)} \alpha_1(\alpha_1 - 1)\left(\boldsymbol{\sigma}_1^{(u)}\right)^{\alpha_1 - 2}\left(\boldsymbol{\sigma}_2^{(u)}\right)^{\alpha_2} \subset \mathbf{I}_{1,1}^{(u,i)}, \\
\frac{\partial^2 Q_i^{(N_u)}}{\partial \phi_1 \partial \phi_2}(\boldsymbol{\sigma}^{(u)}) &= \frac{\partial^2 Q_i^{(N_u)}}{\partial \phi_2 \partial \phi_1}(\boldsymbol{\sigma}^{(u)}) = \sum_{\alpha \in S_{2,1}^{(N_u)}} B_\alpha^{(i)} \alpha_1\left(\boldsymbol{\sigma}_1^{(u)}\right)^{\alpha_1 - 1} \alpha_2\left(\boldsymbol{\sigma}_2^{(u)}\right)^{\alpha_2 - 1} \subset \mathbf{I}_{2,1}^{(u,i)}, \\
\frac{\partial^2 Q_i^{(N_u)}}{\partial \phi_2^2}(\boldsymbol{\sigma}^{(u)}) &= \sum_{\alpha \in S_{2,2}^{(N_u)}} B_\alpha^{(i)} \left(\boldsymbol{\sigma}_1^{(u)}\right)_1^{\alpha} \alpha_2(\alpha_2 - 1)\left(\boldsymbol{\sigma}_2^{(u)}\right)^{\alpha_2 - 2} \subset \mathbf{I}_{2,2}^{(u,i)},
\end{aligned}$$

Coefficients in front of r $(j = 1)$ and $k \geq 1$	
$z^{(1)}_{4,k}$	$\begin{cases} 0 & \text{for } 1 \leq k \leq m-1 \\ L(v_5)_{k\pm1} & \text{for } k \geq m \end{cases}$
$z^{(1)}_{5,k}$	$\begin{cases} L\left(\frac{9}{8}(\bar{a}_1^2 v_4^{(I)})_{k\pm1} + 3(\bar{a}_3^2 v_4^{(I)})_{k\pm1} - \frac{\sqrt{2}}{2}(\bar{a}_3 v_6^{(I)})_{k\pm1} + 6(\bar{a}_1\bar{a}_3 v_6^{(I)})_{k\pm1}\right) & \text{for } 1 \leq k \leq m-1 \\ L\left(\frac{9}{8}(\bar{a}_1^2 v_4)_{k\pm1} + 3(\bar{a}_3^2 v_4)_{k\pm1} - \frac{\sqrt{2}}{2}(\bar{a}_3 v_6)_{k\pm1} + 6(\bar{a}_1\bar{a}_3 v_6)_{k\pm1} - \frac{\gamma}{4}(v_4)_{k\pm1}\right) & \text{for } k \geq m \end{cases}$
$z^{(1)}_{6,k}$	$\begin{cases} 0 & \text{for } 1 \leq k \leq m-1 \\ L(v_7)_{k\pm1} & \text{for } k \geq m \end{cases}$
$z^{(1)}_{7,k}$	$\begin{cases} L\left(-\frac{\sqrt{2}}{2}(\bar{a}_3 v_4^{(I)})_{k\pm1} + 6(\bar{a}_1\bar{a}_3 v_4^{(I)})_{k\pm1} - \frac{\sqrt{2}}{2}(\bar{a}_1 v_6^{(I)})_{k\pm1} + 27(\bar{a}_3^2 v_6^{(I)})_{k\pm1} + 3(\bar{a}_1^2 v_6^{(I)})_{k\pm1}\right) & \text{for } 1 \leq k \leq m-1 \\ L\left(-\frac{\sqrt{2}}{2}(\bar{a}_3 v_4)_{k\pm1} + 6(\bar{a}_1\bar{a}_3 v_4)_{k\pm1} - \frac{\sqrt{2}}{2}(\bar{a}_1 v_6)_{k\pm1} + 27(\bar{a}_3^2 v_6)_{k\pm1} + 3(\bar{a}_1^2 v_6)_{k\pm1} - \gamma(v_6)_{k\pm1}\right) & \text{for } k \geq m \end{cases}$
Coefficients in front of r^2 $(j = 2)$ and $k \geq 1$	
$z^{(2)}_{5,k}$	$L\left(\frac{9}{4}(\bar{a}_1 u_4 v_4)_{k\pm1} + 6(\bar{a}_3 u_6 v_4)_{k\pm1} - \frac{\sqrt{2}}{2}(u_6 v_6)_{k\pm1} + 6(\bar{a}_1 u_6 v_6)_{k\pm1} + 6(\bar{a}_3 u_4 v_6)_{k\pm1}\right)$
$z^{(2)}_{7,k}$	$L\left(-\frac{\sqrt{2}}{2}(u_6 v_4)_{k\pm1} + 6(\bar{a}_1 u_6 v_4)_{k\pm1} + 6(\bar{a}_3 u_4 v_4)_{k\pm1} - \frac{\sqrt{2}}{2}(u_4 v_6)_{k\pm1} + 54(\bar{a}_3 u_6 v_6)_{k\pm1} + 6(\bar{a}_1 u_4 v_6)_{k\pm1}\right)$
Coefficients in front of r^3 $(j = 3)$ and $k \geq 1$	
$z^{(3)}_{5,k}$	$L\left(\frac{9}{8}(u_4^2 v_4)_{k\pm1} + 3(u_6^2 v_4)_{k\pm1} + 6(u_4 u_6 v_6)_{k\pm1}\right)$
$z^{(3)}_{7,k}$	$L\left(6(u_4 u_6 v_4)_{k\pm1} + 27(u_6^2 v_6)_{k\pm1} + 3(u_4^2 v_6)_{k\pm1}\right)$

Table 1: Coefficients in expansion (4.18) with $z^{(2)}_{4,k} = z^{(2)}_{6,k} = z^{(3)}_{4,k} = z^{(3)}_{6,k} = 0$ for all $k \geq 1$.

and then find a bound $\Lambda^{(u,i)} \in \mathbb{R}^+$ satisfying

$$|\mathbf{I}^{(u,i)}_{1,1}| + 2|\mathbf{I}^{(u,i)}_{2,1}| + |\mathbf{I}^{(u,i)}_{2,2}| \leq \Lambda^{(u,i)}.$$

Therefore, for $i = 4, 5, 6, 7$,

$$\left|\left(\left[Df(\bar{x}+b)c - A^\dagger c\right]_i\right)_0\right| \leq \Lambda^{(u,i-3)} r^2 + \left(\frac{4\pi}{\nu_u \ln\left(\frac{\nu_u}{\nu_u - r^*}\right)}\delta_u + \frac{2}{\nu^m}\right) r. \tag{4.17}$$

Recalling (2.12), we introduce the coefficients $z^{(1)}_{i,k}$, $z^{(2)}_{i,k}$ and $z^{(3)}_{i,k}$ (for $k \geq 1$ and $i = 4, 5, 6, 7$) such that

$$\left([Df(\bar{x}+b)c - A^\dagger c]_i\right)_k = z^{(1)}_{i,k} r + z^{(2)}_{i,k} r^2 + z^{(3)}_{i,k} r^3. \tag{4.18}$$

The coefficients are in Table 1, where we used the notation (for $i, j = 1, 3$ and $l = 4, 6$),

$$(\bar{a}_i v_l^{(I)})_k = \sum_{\substack{k_1+k_2=k \\ |k_2| \geq m}} (\bar{a}_i)_{k_1}(v_l)_{k_2} \quad \text{and} \quad (\bar{a}_i\bar{a}_j v_l^{(I)})_k = \sum_{\substack{k_1+k_2+k_3=k \\ |k_3| \geq m}} (\bar{a}_i)_{k_1}(\bar{a}_j)_{k_2}(v_l)_{k_3}.$$

Recalling (4.18) for $i = 4, 5, 6, 7$, define $z^{(1)}_i = \left\{z^{(1)}_{i,k}\right\}_{k\geq0}$, $z^{(2)}_i = \left\{z^{(2)}_{i,k}\right\}_{k\geq0}$ and $z^{(3)}_i = \left\{z^{(3)}_{i,k}\right\}_{k\geq0}$. As for $z^{(1)}_{i,0}$, $z^{(2)}_{i,0}$ and $z^{(3)}_{i,0}$, they can be defined using inequality (4.17) :

$$z_{i,0}^{(1)} = \frac{4\pi}{\nu_u \ln\left(\frac{\nu_u}{\nu_u - r^*}\right)}\delta_u + \frac{2}{\nu^m}, \quad z_{i,0}^{(2)} = \Lambda^{(u,i-3)}, \quad z_{i,0}^{(3)} = 0. \tag{4.19}$$

Recalling (4.14) and (4.15), for $\ell = 1,2,3$, we have that

$$\begin{aligned}
\left|\left(A[Df(\bar{x}+b)c - A^\dagger c]\right)_\ell\right| &\le \sum_{i=1}^{3}\left|A_{\ell i}[Df(\bar{x}+b)c - A^\dagger c]_i\right| + \sum_{i=4}^{7}\left|A_{\ell i}[Df(\bar{x}+b)c - A^\dagger c]_i\right| \\
&\le \sum_{i=1}^{3}|A_{\ell i}|\left(\frac{4\pi}{\nu_s \ln\left(\frac{\nu_s}{\rho}\right)}\delta_s\rho + \frac{2}{\nu^m}\right) r + \left(|A_{\ell 1}|\,\Lambda^{(s,1)} + |A_{\ell 2}|\,\Lambda^{(s,3)} + |A_{\ell 3}|\,\Lambda^{(s,4)}\right) r^2 \\
&\quad + \sum_{i=4}^{7}\left(\left|A_{\ell i} z_i^{(3)}\right| r^3 + \left|A_{\ell i} z_i^{(2)}\right| r^2 + \left|A_{\ell i} z_i^{(1)}\right| r\right) \\
&\le \sum_{i=1}^{3}|A_{\ell i}|\left(\frac{4\pi}{\nu_s \ln\left(\frac{\nu_s}{\rho}\right)}\delta_s\rho + \frac{2}{\nu^m}\right) r + \left(|A_{\ell 1}|\,\Lambda^{(s,1)} + |A_{\ell 2}|\,\Lambda^{(s,3)} + |A_{\ell 3}|\,\Lambda^{(s,4)}\right) r^2 \\
&\quad + \sum_{i=4}^{7}\left|A_{\ell i} z_i^{(1)}\right| r + \sum_{i=4}^{7}\left(\|A_{\ell i}\|_\nu^\infty\,\|z_i^{(3)}\|_\nu r^3 + \|A_{\ell i}\|_\nu^\infty\,\|z_i^{(2)}\|_\nu r^2\right),
\end{aligned} \tag{4.20}$$

and for $\ell = 4,5,6,7$, we have that

$$\begin{aligned}
\left\|\left(A[Df(\bar{x}+b)c - A^\dagger c]\right)_\ell\right\|_\nu &\le \sum_{i=1}^{3}\left\|A_{\ell i}[Df(\bar{x}+b)c - A^\dagger c]_i\right\|_\nu + \sum_{i=4}^{7}\left\|A_{\ell i}[Df(\bar{x}+b)c - A^\dagger c]_i\right\|_\nu \\
&\le \sum_{i=1}^{3}\|A_{\ell i}\|_\nu\left(\frac{4\pi}{\nu_s \ln\left(\frac{\nu_s}{\rho}\right)}\delta_s\rho + \frac{2}{\nu^m}\right) r + \left(\|A_{\ell 1}\|_\nu\,\Lambda^{(s,1)} + \|A_{\ell 2}\|_\nu\,\Lambda^{(s,3)} + \|A_{\ell 3}\|_\nu\,\Lambda^{(s,4)}\right) r^2 \\
&\quad + \sum_{i=4}^{7}\left(\left\|A_{\ell i} z_i^{(3)}\right\|_\nu r^3 + \left\|A_{\ell i} z_i^{(2)}\right\|_\nu r^2 + \left\|A_{\ell i} z_i^{(1)}\right\|_\nu r\right) \\
&\le \sum_{i=1}^{3}\|A_{\ell i}\|_\nu\left(\frac{4\pi}{\nu_s \ln\left(\frac{\nu_s}{\rho}\right)}\delta_s\rho + \frac{2}{\nu^m}\right) r + \left(\|A_{\ell 1}\|_\nu\,\Lambda^{(s,1)} + \|A_{\ell 2}\|_\nu\,\Lambda^{(s,3)} + \|A_{\ell 3}\|_\nu\,\Lambda^{(s,4)}\right) r^2 \\
&\quad + \sum_{i=4}^{7}\left\|A_{\ell i} z_i^{(1)}\right\|_\nu r + \sum_{i=4}^{7}\left(\|A_{\ell i}\|_{B(\ell_\nu^1,\ell_\nu^1)}\,\|z_i^{(3)}\|_\nu r^3 + \|A_{\ell i}\|_{B(\ell_\nu^1,\ell_\nu^1)}\,\|z_i^{(2)}\|_\nu r^2\right).
\end{aligned} \tag{4.21}$$

In order to bound the terms $\|z_i^{(j)}\|_\nu$ (for $i = 4,5,6,7$ and $j = 2,3$) in the above formulas, we use Lemma 3 to obtain that

$$\begin{aligned}
\sum_{k\geq 1} |z_{5,k}^{(2)}|\nu^k \quad &\leq \quad L\sum_{k\geq 1}\left|\frac{9}{4}(\bar{a}_1u_4v_4)_{k-1} + 6(\bar{a}_3u_6v_4)_{k-1} - \frac{\sqrt{2}}{2}(u_6v_6)_{k-1} + 6(\bar{a}_1u_6v_6)_{k-1} + 6(\bar{a}_3u_4v_6)_{k-1}\right|\nu^k \\
&\quad\; +L\sum_{k\geq 1}\left|\frac{9}{4}(\bar{a}_1u_4v_4)_{k+1} + 6(\bar{a}_3u_6v_4)_{k+1} - \frac{\sqrt{2}}{2}(u_6v_6)_{k+1} + 6(\bar{a}_1u_6v_6)_{k+1} + 6(\bar{a}_3u_4v_6)_{k+1}\right|\nu^k \\
&\leq \quad L\nu\sum_{k\geq 0}\left|\frac{9}{4}(\bar{a}_1u_4v_4)_{k} + 6(\bar{a}_3u_6v_4)_{k} - \frac{\sqrt{2}}{2}(u_6v_6)_{k} + 6(\bar{a}_1u_6v_6)_{k} + 6(\bar{a}_3u_4v_6)_{k}\right|\nu^k \\
&\quad\; +\frac{L}{\nu}\sum_{k\geq 2}\left|\frac{9}{4}(\bar{a}_1u_4v_4)_{k} + 6(\bar{a}_3u_6v_4)_{k} - \frac{\sqrt{2}}{2}(u_6v_6)_{k} + 6(\bar{a}_1u_6v_6)_{k} + 6(\bar{a}_3u_4v_6)_{k}\right|\nu^k \\
&\leq \quad L\left(\nu + \frac{1}{\nu}\right)\left(\frac{9}{4}\cdot 16\|\bar{a}_1\|_\nu + 6\cdot 16\|\bar{a}_3\|_\nu + \frac{\sqrt{2}}{2}\cdot 4 + 6\cdot 16\|\bar{a}_1\|_\nu + 6\cdot 16\|\bar{a}_3\|_\nu\right) \\
&= \quad L\left(\nu + \frac{1}{\nu}\right)\left(2\sqrt{2} + 132\|\bar{a}_1\|_\nu + 192\|\bar{a}_3\|_\nu\right),
\end{aligned}$$

and similarly

$$\begin{aligned}
&\sum_{k\geq 1} |z_{7,k}^{(2)}|\nu^k \leq L\left(\nu + \frac{1}{\nu}\right)\left(4\sqrt{2} + 192\|\bar{a}_1\|_\nu + 960\|\bar{a}_3\|_\nu\right), \\
&\sum_{k\geq 1} |z_{5,k}^{(3)}|\nu^k \leq 162L\left(\nu + \frac{1}{\nu}\right), \\
&\sum_{k\geq 1} |z_{7,k}^{(3)}|\nu^k \leq 576L\left(\nu + \frac{1}{\nu}\right).
\end{aligned}$$

Hence, using the definition of $z_{i,0}^{(2)}$ and $z_{i,0}^{(3)}$ given in (4.19), one gets that

$$\|z_4^{(2)}\|_\nu \leq \Lambda^{(u,1)}, \tag{4.22a}$$

$$\|z_6^{(2)}\|_\nu \leq \Lambda^{(u,3)}, \tag{4.22b}$$

$$\|z_5^{(2)}\|_\nu \leq \Lambda^{(u,2)} + L\left(\nu + \frac{1}{\nu}\right)\left(2\sqrt{2} + 132\|\bar{a}_1\|_\nu + 192\|\bar{a}_3\|_\nu\right), \tag{4.22c}$$

$$\|z_7^{(2)}\|_\nu \leq \Lambda^{(u,4)} + L\left(\nu + \frac{1}{\nu}\right)\left(4\sqrt{2} + 192\|\bar{a}_1\|_\nu + 960\|\bar{a}_3\|_\nu\right), \tag{4.22d}$$

$$\|z_5^{(3)}\|_\nu \leq 162L\left(\nu + \frac{1}{\nu}\right), \tag{4.22e}$$

$$\|z_7^{(3)}\|_\nu \leq 576L\left(\nu + \frac{1}{\nu}\right). \tag{4.22f}$$

For the analysis of the terms in (4.20) that are *linear* in r, we recall that $A_{\ell i} \in \left(\ell_\nu^1\right)^*$ for $4 \leq i \leq 7$ and that for $x_i \in \ell_\nu^1$, $A_{\ell i}x_i = A_{\ell i}^{(m)} \cdot (x_i)_F \in \mathbb{R}$. Since $u, v \in B(1)$, we have that for each $k \geq 0$ and for each $i = 4,5,6,7$, $|(u_i)_k|, |(v_i)_k| \leq \nu^{-k}$. Let $\omega_I \stackrel{\text{def}}{=}$

$(0,\ldots,0,\nu^{-m},\nu^{-(m+1)},\nu^{-(m+2)},\ldots)$. Recalling (4.17), the coefficients $z^{(1)}_{i,k}$ $(i=4,5,6,7)$ from Table 1 and equation (4.19), one has that (for $\ell=1,2,3$)

$$
\begin{aligned}
\sum_{i=4}^{7}\left|A_{\ell i}z_i^{(1)}\right| \quad &\le \quad \sum_{i=4}^{7}|(A_{\ell i})_0|\left(\frac{4\pi}{\nu_u\ln\left(\frac{\nu_u}{\nu_u-r^*}\right)}\delta_u+\frac{2}{\nu^m}\right)+\sum_{k=1}^{m-1}\left|(A_{\ell 5})_k z^{(1)}_{5,k}\right|+\sum_{k=1}^{m-1}\left|(A_{\ell 7})_k z^{(1)}_{7,k}\right| \\
&\le \sum_{i=4}^{7}|(A_{\ell i})_0|\left(\frac{4\pi}{\nu_u\ln\left(\frac{\nu_u}{\nu_u-r^*}\right)}\delta_u+\frac{2}{\nu^m}\right) \qquad (4.23)\\
&+L\sum_{k=1}^{m-1}|(A_{\ell 5})_k|\left(\frac{9}{8}(|\bar a_1|^2\omega_I)_{k\pm1}+3(|\bar a_3|^2\omega_I)_{k\pm1}+\frac{\sqrt{2}}{2}(|\bar a_3|\omega_I)_{k\pm1}+6(|\bar a_1||\bar a_3|\omega_I)_{k\pm1}\right)\\
&+L\sum_{k=1}^{m-1}|(A_{\ell 7})_k|\left(\frac{\sqrt{2}}{2}(|\bar a_3|\omega_I)_{k\pm1}+6(|\bar a_1||\bar a_3|\omega_I)_{k\pm1}+\frac{\sqrt{2}}{2}(|\bar a_1|\omega_I)_{k\pm1}+27(|\bar a_3|^2\omega_I)_{k\pm1}+3(|\bar a_1|^2\omega_I)_{k\pm1}\right).
\end{aligned}
$$

Given $\ell=1,2,3$, we use estimates (4.22) and (4.23) to bound the terms in (4.20), and finally get that

$$\left|\left(A[Df(\bar x+b)c-A^\dagger c]\right)_\ell\right|\le Z^{(1)}_\ell r+Z^{(2)}_\ell r^2+Z^{(3)}_\ell r^3, \qquad (4.24)$$

where

$$
\begin{aligned}
Z^{(1)}_\ell \quad &\stackrel{\text{def}}{=} \quad \sum_{i=1}^{3}|A_{\ell i}|\left(\frac{4\pi}{\nu_s\ln\left(\frac{\nu_s}{\rho}\right)}\delta_s\rho+\frac{2}{\nu^m}\right)+\sum_{i=4}^{7}|(A_{\ell i})_0|\left(\frac{4\pi}{\nu_u\ln\left(\frac{\nu_u}{\nu_u-r^*}\right)}\delta_u+\frac{2}{\nu^m}\right) \qquad (4.25)\\
&+L\sum_{k=1}^{m-1}|(A_{\ell 5})_k|\left(\frac{9}{8}(|\bar a_1|^2\omega_I)_{k\pm1}+3(|\bar a_3|^2\omega_I)_{k\pm1}+\frac{\sqrt{2}}{2}(|\bar a_3|\omega_I)_{k\pm1}+6(|\bar a_1||\bar a_3|\omega_I)_{k\pm1}\right)\\
&+L\sum_{k=1}^{m-1}|(A_{\ell 7})_k|\left(\frac{\sqrt{2}}{2}(|\bar a_3|\omega_I)_{k\pm1}+6(|\bar a_1||\bar a_3|\omega_I)_{k\pm1}+\frac{\sqrt{2}}{2}(|\bar a_1|\omega_I)_{k\pm1}+27(|\bar a_3|^2\omega_I)_{k\pm1}+3(|\bar a_1|^2\omega_I)_{k\pm1}\right),\\
Z^{(2)}_\ell \quad &\stackrel{\text{def}}{=} \quad |A_{\ell 1}|\,\Lambda^{(s,1)}+|A_{\ell 2}|\,\Lambda^{(s,3)}+|A_{\ell 3}|\,\Lambda^{(s,4)}+\|A_{\ell 4}\|^\infty_\nu\,\Lambda^{(u,1)}+\|A_{\ell 6}\|^\infty_\nu\,\Lambda^{(u,3)} \qquad (4.26)\\
&+\|A_{\ell 5}\|^\infty_\nu\left(\Lambda^{(u,2)}+L\left(\nu+\frac{1}{\nu}\right)\left(2\sqrt{2}+132\|\bar a_1\|_\nu+192\|\bar a_3\|_\nu\right)\right)\\
&+\|A_{\ell 7}\|^\infty_\nu\left(\Lambda^{(u,4)}+L\left(\nu+\frac{1}{\nu}\right)\left(4\sqrt{2}+192\|\bar a_1\|_\nu+960\|\bar a_3\|_\nu\right)\right),\\
Z^{(3)}_\ell \quad &\stackrel{\text{def}}{=} \quad \|A_{\ell 5}\|^\infty_\nu\,162L\left(\nu+\frac{1}{\nu}\right)+\|A_{\ell 7}\|^\infty_\nu\,576L\left(\nu+\frac{1}{\nu}\right). \qquad (4.27)
\end{aligned}
$$

Let us conclude by computing upper polynomial bounds for (4.21) where $\ell=4,5,6,7$. Once again, we need to put extra effort in the analysis of the terms that are *linear* in r.

Hence, we use (4.17) to get that

$$
\begin{aligned}
\sum_{i=4}^{7}\left\|A_{\ell i}z_i^{(1)}\right\|_\nu &\leq \sum_{i=4}^{7}\left(\left|\left(A_{\ell i}z_i^{(1)}\right)_0\right| + \sum_{j=1}^{m-1}\left|\left(A_{\ell i}z_i^{(1)}\right)_j\right|\nu^j + \sum_{j\geq m}\left|\left(A_{\ell i}z_i^{(1)}\right)_j\right|\nu^j\right)\\
&\leq \sum_{i=4}^{7}\left|(A_{\ell i})_{0,0}z_{i,0}^{(1)}\right| + \sum_{i=4}^{7}\sum_{k=1}^{m-1}\left|(A_{\ell i})_{0,k}z_{i,k}^{(1)}\right|\\
&\quad+\sum_{i=4}^{7}\left(\sum_{j=1}^{m-1}\left|\left(A_{\ell i}z_i^{(1)}\right)_j\right|\nu^j + \sum_{j\geq m}\left|\left(A_{\ell i}z_i^{(1)}\right)_j\right|\nu^j\right)\\
&\leq \left(\frac{4\pi}{\nu_u\ln\left(\frac{\nu_u}{\nu_u-r^*}\right)}\delta_u + \frac{2}{\nu^m}\right)\sum_{i=4}^{7}|(A_{\ell i})_{0,0}| + \sum_{k=1}^{m-1}\left|(A_{\ell 5})_{0,k}z_{5,k}^{(1)}\right| + \sum_{k=1}^{m-1}\left|(A_{\ell 7})_{0,k}z_{7,k}^{(1)}\right|\\
&\quad+\sum_{i=4}^{7}\left(\sum_{j=1}^{m-1}\left|\left(A_{\ell i}z_i^{(1)}\right)_j\right|\nu^j + \sum_{j\geq m}\left|\left(A_{\ell i}z_i^{(1)}\right)_j\right|\nu^j\right) \qquad (4.28)\\
&\leq \left(\frac{4\pi}{\nu_u\ln\left(\frac{\nu_u}{\nu_u-r^*}\right)}\delta_u + \frac{2}{\nu^m}\right)\sum_{i=4}^{7}|(A_{\ell i})_{0,0}|\\
&\quad+L\sum_{k=1}^{m-1}|(A_{\ell 5})_{0,k}|\left(\frac{9}{8}(|\bar a_1|^2\omega_I)_{k\pm1} + 3(|\bar a_3|^2\omega_I)_{k\pm1} + \frac{\sqrt{2}}{2}(|\bar a_3|\omega_I)_{k\pm1} + 6(|\bar a_1||\bar a_3|\omega_I)_{k\pm1}\right)\\
&\quad+L\sum_{k=1}^{m-1}|(A_{\ell 7})_{0,k}|\Bigg(\frac{\sqrt{2}}{2}(|\bar a_3|\omega_I)_{k\pm1} + 6(|\bar a_1||\bar a_3|\omega_I)_{k\pm1} + \frac{\sqrt{2}}{2}(|\bar a_1|\omega_I)_{k\pm1}\\
&\qquad\qquad+27(|\bar a_3|^2\omega_I)_{k\pm1} + 3(|\bar a_1|^2\omega_I)_{k\pm1}\Bigg)\\
&\quad+\sum_{i=4}^{7}\left(\sum_{j=1}^{m-1}\left|\left(A_{\ell i}^{(m)}(z_i^{(1)})_F\right)_j\right|\nu^j\right) + \sum_{j\geq m}\frac{1}{2j}\left|z_{\ell,j}^{(1)}\right|\nu^j,
\end{aligned}
$$

since

$$
\left(A_{\ell i}z_i^{(1)}\right)_j = \begin{cases} \left(A_{\ell i}^{(m)}(z_i^{(1)})_F\right)_j, & j=0,\dots,m-1,\\ \delta_{\ell,i}\frac{1}{2j}z_{i,j}^{(1)}, & j\geq m.\end{cases}
$$

We estimate the last two terms of the last inequality separately. For the first, note that

$$
\begin{aligned}
\sum_{i=4}^{7}\left(\sum_{j=1}^{m-1}\left|\left(A_{\ell i}^{(m)}(z_i^{(1)})_F\right)_j\right|\nu^j\right) &= \sum_{j=1}^{m-1}\left|\left(A_{\ell 5}^{(m)}(z_5^{(1)})_F\right)_j\right|\nu^j+\sum_{j=1}^{m-1}\left|\left(A_{\ell 7}^{(m)}(z_7^{(1)})_F\right)_j\right|\nu^j \\
\le \left(\frac{4\pi}{\nu_u\ln\left(\frac{\nu_u}{\nu_u-r^*}\right)}\delta_u+\frac{2}{\nu^m}\right)&\sum_{j=1}^{m-1}\left(\left|(A_{\ell 5}^{(m)})_{j,0}\right|+\left|(A_{\ell 7}^{(m)})_{j,0}\right|\right) \\
+L\sum_{j=1}^{m-1}\sum_{k=1}^{m-1}\left|(A_{\ell 5}^{(m)})_{j,k}\right|&\left(\frac{9}{8}(|\bar a_1|^2\omega_I)_{k\pm1}+3(|\bar a_3|^2\omega_I)_{k\pm1}+\frac{\sqrt2}{2}(|\bar a_3|\omega_I)_{k\pm1}+6(|\bar a_1||\bar a_3|\omega_I)_{k\pm1}\right)\nu^j \\
+L\sum_{j=1}^{m-1}\sum_{k=1}^{m-1}\left|(A_{\ell 7}^{(m)})_{j,k}\right|&\left(\frac{\sqrt2}{2}(|\bar a_3|\omega_I)_{k\pm1}+6(|\bar a_1||\bar a_3|\omega_I)_{k\pm1}+\frac{\sqrt2}{2}(|\bar a_1|\omega_I)_{k\pm1}+27(|\bar a_3|^2\omega_I)_{k\pm1}+3(|\bar a_1|^2\omega_I)_{k\pm1}\right)\nu^j
\end{aligned}
\tag{4.29}
$$

For the second, we use Lemma 3 to obtain that

$$
\begin{aligned}
\sum_{j\ge m}\frac{1}{2j}\left|z_{4,j}^{(1)}\right|\nu^j &= L\sum_{j\ge m}\frac{1}{2j}|(v_5)_{j\pm1}| \\
&\le z_4^{(1,\infty)} \overset{\text{def}}{=} \frac{L}{2m}\left(\nu+\frac{1}{\nu}\right), \qquad (4.30)\\
\sum_{j\ge m}\frac{1}{2j}\left|z_{5,j}^{(1)}\right|\nu^j &= L\sum_{j\ge m}\frac{1}{2j}\left|\frac{9}{8}(\bar a_1^2v_4)_{j\pm1}+3(\bar a_3^2v_4)_{j\pm1}-\frac{\sqrt2}{2}(\bar a_3v_6)_{j\pm1}+6(\bar a_1\bar a_3v_6)_{j\pm1}-\frac{\gamma}{4}(v_4)_{j\pm1}\right|\nu^j \\
&\le z_5^{(1,\infty)} \overset{\text{def}}{=} \frac{L}{2m}\left(\nu+\frac{1}{\nu}\right)\Big(18\|\bar a_1\|_\nu^2+48\|\bar a_3\|_\nu^2 \qquad (4.31)\\
&\qquad +2\sqrt2\|\bar a_3\|_\nu+96\|\bar a_1\|_\nu\|\bar a_3\|_\nu+\frac{\gamma}{4}\Big),\\
\sum_{j\ge m}\frac{1}{2j}\left|z_{6,j}^{(1)}\right|\nu^j &\le L\sum_{j\ge m}\frac{1}{2j}|(v_7)_{j\pm1}| \\
&\le z_6^{(1,\infty)} \overset{\text{def}}{=} \frac{L}{2m}\left(\nu+\frac{1}{\nu}\right), \qquad (4.32)\\
\sum_{j\ge m}\frac{1}{2j}\left|z_{7,j}^{(1)}\right|\nu^j &= L\sum_{j\ge m}\frac{1}{2j}\Big|-\frac{\sqrt2}{2}(\bar a_3v_4)_{j\pm1}+6(\bar a_1\bar a_3v_4)_{j\pm1}-\frac{\sqrt2}{2}(\bar a_1v_6)_{j\pm1}+27(\bar a_3^2v_6)_{j\pm1}\\
&\qquad +3(\bar a_1^2v_6)_{j\pm1}-\gamma(v_6)_{j\pm1}\Big|\nu^j\\
&\le z_7^{(1,\infty)} \overset{\text{def}}{=} \frac{L}{2m}\left(\nu+\frac{1}{\nu}\right)\Big(2\sqrt2\|\bar a_3\|_\nu+96\|\bar a_1\|_\nu\|\bar a_3\|_\nu \qquad (4.33)\\
&\qquad +2\sqrt2\|\bar a_1\|_\nu+432\|\bar a_3\|_\nu^2+48\|\bar a_1\|_\nu^2+\gamma\Big).
\end{aligned}
$$

Given $\ell=4,5,6,7$, we use estimates (4.22), (4.28) and (4.29) to bound the terms in (4.21), and finally get that

$$
\left\|\left(A[Df(\bar x+b)c-A^\dagger c]\right)_\ell\right\|_\nu \le Z_\ell^{(1)}r+Z_\ell^{(2)}r^2+Z_\ell^{(3)}r^3, \tag{4.34}
$$

where (recall the expressions for $z_\ell^{(1,\infty)}$ in (4.30), (4.31), (4.32) and (4.33)) we set

$$
\begin{aligned}
Z_\ell^{(1)} \quad &\stackrel{\text{def}}{=} \quad \sum_{i=1}^{3} \|A_{\ell i}\|_\nu \left(\frac{4\pi}{\nu_s \ln\left(\frac{\nu_s}{\rho}\right)} \delta_s \rho + \frac{2}{\nu^m} \right) + \sum_{i=4}^{7} |(A_{\ell i})_{0,0}| \left(\frac{4\pi}{\nu_u \ln\left(\frac{\nu_u}{\nu_u - r^*}\right)} \delta_u + \frac{2}{\nu^m} \right) \qquad (4.35)\\
&+ \left(\frac{4\pi}{\nu_u \ln\left(\frac{\nu_u}{\nu_u - r^*}\right)} \delta_u + \frac{2}{\nu^m} \right) \sum_{j=1}^{m-1} \left(\left|(A_{\ell 5}^{(m)})_{j,0}\right| + \left|(A_{\ell 7}^{(m)})_{j,0}\right| \right)\\
&+ L \sum_{j=0}^{m-1} \sum_{k=1}^{m-1} \left|(A_{\ell 5}^{(m)})_{j,k}\right| \left(\frac{9}{8}(|\bar a_1|^2 \omega_I)_{k\pm1} + 3(|\bar a_3|^2 \omega_I)_{k\pm1} + \frac{\sqrt{2}}{2}(|\bar a_3|\omega_I)_{k\pm1} + 6(|\bar a_1||\bar a_3|\omega_I)_{k\pm1} \right) \nu^j\\
&+ L \sum_{j=0}^{m-1} \sum_{k=1}^{m-1} \left|(A_{\ell 7}^{(m)})_{j,k}\right| \left(\frac{\sqrt{2}}{2}(|\bar a_3|\omega_I)_{k\pm1} + 6(|\bar a_1||\bar a_3|\omega_I)_{k\pm1} \right.\\
&\qquad\qquad \left. + \frac{\sqrt{2}}{2}(|\bar a_1|\omega_I)_{k\pm1} + 27(|\bar a_3|^2\omega_I)_{k\pm1} + 3(|\bar a_1|^2\omega_I)_{k\pm1} \right) \nu^j\\
&+ z_\ell^{(1,\infty)}\\
Z_\ell^{(2)} \quad &\stackrel{\text{def}}{=} \quad \|A_{\ell 1}\|_\nu \Lambda^{(s,1)} + \|A_{\ell 2}\|_\nu \Lambda^{(s,3)} + \|A_{\ell 3}\|_\nu \Lambda^{(s,4)} \qquad (4.36)\\
&+ \|A_{\ell 4}\|_{B(\ell_\nu^1,\ell_\nu^1)} \Lambda^{(u,1)} + \|A_{\ell 6}\|_{B(\ell_\nu^1,\ell_\nu^1)} \Lambda^{(u,3)}\\
&+ \|A_{\ell 5}\|_{B(\ell_\nu^1,\ell_\nu^1)} \left(\Lambda^{(u,2)} + L\left(\nu + \frac{1}{\nu}\right)\left(2\sqrt{2} + 132\|\bar a_1\|_\nu + 192\|\bar a_3\|_\nu\right) \right)\\
&+ \|A_{\ell 7}\|_{B(\ell_\nu^1,\ell_\nu^1)} \left(\Lambda^{(u,4)} + L\left(\nu + \frac{1}{\nu}\right)\left(4\sqrt{2} + 192\|\bar a_1\|_\nu + 960\|\bar a_3\|_\nu\right) \right),\\
Z_\ell^{(3)} \quad &\stackrel{\text{def}}{=} \quad \|A_{\ell 5}\|_{B(\ell_\nu^1,\ell_\nu^1)} 162L\left(\nu + \frac{1}{\nu}\right) + \|A_{\ell 7}\|_{B(\ell_\nu^1,\ell_\nu^1)} 576L\left(\nu + \frac{1}{\nu}\right). \qquad (4.37)
\end{aligned}
$$

We note that the matrix norms are bounded using Corollary 6.

Combining (4.11), (4.25), (4.26) and (4.27), (4.35), (4.36) and (4.37), we set

$$Z_\ell(r) \stackrel{\text{def}}{=} Z_\ell^{(3)} r^3 + Z_\ell^{(2)} r^2 + (Z_\ell^{(1)} + Z_\ell^{(0)}) r, \qquad \text{for } \ell = 1, \ldots, 7. \tag{4.38}$$

It follows from the above construction that

$$
\begin{aligned}
\sup_{b,c \in B(r)} |[DT(\bar x + b)c]_\ell| \quad &\le \quad Z_\ell(r), \qquad \text{for } \ell = 1, 2, 3,\\
\sup_{b,c \in B(r)} \|[DT(\bar x + b)c]_\ell\|_\nu \quad &\le \quad Z_\ell(r), \qquad \text{for } \ell = 4, 5, 6, 7.
\end{aligned}
$$

Combining (4.8) and (4.38), we have finished the explicit construction of the radii polynomials as defined in (2.17). We are now ready to present the proof of Theorem 1.

5 Proof of Theorem 1

Proof. Fix $\tilde\mu = \frac{7+3\sqrt{6}}{30}\tilde\beta^2$ and $\tilde c = 0$. Our goal is to prove the existence of a heteroclinic orbit of (1.2) between the hexagons and positive rolls and of a heteroclinic orbit between the hexagons and negative rolls, where all these equilibria are defined in (1.3). In Section 2.1 we showed that this problem is equivalent to proving the existence of heteroclinic orbits between the hexagons and positive or negative rolls for (2.1), where we fix the single parameter $\gamma = \frac{7+3\sqrt{6}}{30}$. We now choose the values for the following (computational) constants, where $+$ refers to the orbit with the positive rolls and $-$ refers to the orbit with the negative rolls:

$L_+ = L_- = 6$	—	time rescaling factor;
$(m_1)_+ = (m_1)_- = 50$	—	size of the non-zero part of $\bar{x}$;
$m_+ = m_- = 1000$	—	size of the projection;
$(N_u)_+ = 30$, $(N_u)_- = 20$	—	unstable manifold parameterization order;
$(N_s)_+ = 30$, $(N_s)_- = 20$	—	stable manifold parameterization order;
$(\nu_u)_+ = 0.35$, $(\nu_u)_- = 0.25$	—	domain radius of the parameterization of the unstable manifold;
$(\nu_s)_+ = 0.3$, $(\nu_s)_- = 0.25$	—	domain radius of the parameterization of the stable manifold;
$\rho_+ = 0.29$, $\rho_- = 0.24$	—	radius of the ball in the local parameterization of the stable manifold;
$(r^*)_+ = (r^*)_- = 1 \times 10^{-4}$	—	a priori upper bound satisfying (4.16);
$\nu_+ = \nu_- = 1.01$	—	decay rate in the definition of the Banach space.

All these were chosen after numerical experimentation.

The proof is similar for the two heteroclinic orbits, so we will only describe the one for the heteroclinic orbit between hexagons and negative rolls. To lighten the notation, we will drop the $-$ subscript. Before we start the rigorous proof, we need to compute the manifolds and an approximate solution.

First, we determine explicitly the coefficients A_α and B_α of the approximate parameterizations $P^{(N_s)}$ and $Q^{(N_u)}$. In the absence of resonance, we only need to fix the length of the eigenvectors in (3.4) so that the homological equation (3.5) has a unique solution. Based on numerical experimentation, we fix the length of the two stable eigenvectors to be 0.4 and 0.3 and the length of the two unstable eigenvectors to be 0.1 and 0.35. We then solve (3.5) up to order N_s for the stable manifold and N_u for the unstable manifold.

We also apply Newton's method to find a numerical approximation $\bar{x}$ of the zero of the finite dimensional reduction $f^{(m,N_s,N_u)}$ defined in (4.1). We truncate the solution so that the last Chebyshev coefficients are near the machine precision 10^{-16}. In this case, it is sufficient to keep the $4m_1+3$ first entries of $\bar{x}$, where $m_1 = 50$. We then add zeroes to $\bar{x}$ to obtain a vector of dimension $4m+3$ as needed.

The end of the proof requires success in the run of the Matlab computer program `proof_hex2neg_rolls.m`. This computer program uses the interval arithmetic package Intlab [28]. The program `proof_hex2neg_rolls.m` has four main parts.

Part I : We validate the approximate parameterizations $P^{(N_s)}$ and $Q^{(N_u)}$. This requires the computation of the validation values from Definition 4.1 in [8]. Those quantities are used to find δ_u and δ_s such that the hypotheses of Theorem 4.2 in [8] are satisfied. In this case, interval arithmetic gives us $\delta_u = 7.5468 \times 10^{-11}$ and $\delta_s = 7.2392 \times 10^{-13}$.

Part II : The assumptions stated at the beginning of Section 4.2 now have to be verified. Since we already applied Newton's method to find an approximate solution $\bar{x}$ of $f^{(m,N_s,N_u)}(x) = 0$, we know that assumption 1 is satisfied. In this part of the program, we compute $Df^{(m,N_s,N_u)}(\bar{x})$ as well as its approximate inverse $A^{(m)}$ using interval arithmetic. We then check that the matrix $A^{(m)}$ is injective by showing that $\|I_m - A^{(m)}Df^{(m,N_s,N_u)}(\bar{x})\|_\infty$ is less than one. In practice, this norm is tiny: 2.0953×10^{-7}.

Part III : We combine the computations from Parts I and II with the estimates in Section 4.3 to construct the radii polynomials. The computation of the bound Y is simplified using the parameter $m_1 = 50$. Indeed, $(\bar{a}_i)_k = 0$ for $i = 1,2,3,4$ and for $k \geq m_1$, so this implies that $(f_i(\bar{x}))_k = 0$ for $k \geq 3m_1 - 2 = 148$. In particular, $(f_i(\bar{x}))_k = 0$ for $k = m, \ldots, 3m-2$, since $m = 1000 \geq 3m_1 - 2 = 148$. Hence, in the definition of Y_i for $i = 4,5,6,7$ given in (4.8), the second sum is automatically zero.

While constructing the bound Λ, which is part of the definition of the bound Z, we verify that $\sup(\boldsymbol{\sigma}_k^{(u)}/\nu_u) < 1$ for $k = 1,2$ in order to make sure that we stay in the domain of definition of the parameterization of the unstable manifold. Using the radii polynomials, we find $r > 0$ satisfying the hypotheses of Proposition 4. In this case, we can choose $r = 9.8573 \times 10^{-6}$, which satisfies $r \leq r^*$. The set $B \stackrel{\text{def}}{=} B_{\bar{x}}(r)$ then contains a unique zero $\hat{x}$ of the operator f defined in (2.13).

Part IV : We verify that the boundary condition $U_2(1) = P_2(\theta)$, which we excluded to define the operator f, is also satisfied. We know from Part III that there exists $\hat{x} \in B$ such that $\hat{x}$ is a zero of f. By the energy argument in Lemma 2, we only need to show that $U_2(1)$ and $P_2(\hat{\theta})$ have the same sign. To prove it rigorously, we use analysis and interval arithmetics to enclose separately the value of $U_2(1)$ and the value of $P_2(\hat{\theta})$. In Section 5.1, we provide the details of how to perform this technical step. The interval enclosures that we obtain are $[-0.0300, -0.0259]$ for $U_2(1)$ and $[-0.0280, -0.0279]$ for $P_2(\theta)$, so they are both negative. Once this is done, we have a proof that the unique zero $\hat{x}$ of f corresponds to a heteroclinic orbit between hexagons and negative rolls for the system (1.2).

The program `proof_hex2pos_rolls.m` uses a similar method to prove the existence of a heteroclinic orbit between hexagons and positive rolls. However, in this case, we choose the length of the two stable eigenvectors to be 0.1 and 0.3 and the length of the two unstable eigenvectors to be 0.1 and 0.35. The other modified numerical values are

$$\begin{aligned}
&\delta_u = 1.0483 \times 10^{-10},\\
&\delta_s = 6.5042 \times 10^{-12},\\
&\|I_m - A^{(m)} Df^{(m,N_s,N_u)}(\bar{x})\|_\infty = 3.8353 \times 10^{-7},\\
&U_2(1) \in [0.0031, 0.0039],\\
&P_2(\theta) \in [0.0034, 0.0035].
\end{aligned}$$

The source codes of both programs are available at [35]. $\square$

5.1 Verification of the excluded boundary condition

In order to define the operator f in (2.13), we excluded the boundary condition

$$U_2(1) = P_2(\theta).$$

As seen in Lemma 2, if we show that $U_2(1)$ and $P_2(\theta)$ have the same sign, then we can conclude that $U_2(1) = P_2(\theta)$. We now show how to verify this in practice. Assume that the hypothesis of Proposition 4 is satisfied. Hence, there exist an $r > 0$ and a unique $\hat{x} \in B_{\bar{x}}(r)$ such that $f(\hat{x}) = 0$. Denote $\hat{x} = (\hat{\psi}, \hat{\phi}_1, \hat{\phi}_2, \hat{a}_1, \hat{a}_2, \hat{a}_3, \hat{a}_4)$. We now show how to separately compute a rigorous interval enclosure for $U_2(1)$ and for $P_2(\hat{\theta})$.

5.1.1 Rigorous interval enclosure for $U_2(1)$.

Note that the Chebyshev expansion of $U_2(1)$ is given by

$$U_2(1) = (\hat{a}_2)_0 + 2\sum_{k=1}^{\infty}(\hat{a}_2)_k.$$

Since $\hat{x} \in B_{\bar{x}}(r)$, we get that for each $k \geq 0$,

$$|(\bar{a}_2)_k - (\hat{a}_2)_k|\nu^k \leq \|\bar{a}_2 - \hat{a}_2\|_\nu = \sum_{k=0}^{\infty}|(\bar{a}_2)_k - (\hat{a}_2)_k|\nu^k \leq r.$$

This implies that $|(\bar{a}_2)_k - (\hat{a}_2)_k| \leq \frac{r}{\nu^k}$ and therefore $(\hat{a}_2)_k \in \left[(\bar{a}_2)_k - \frac{r}{\nu^k}, (\bar{a}_2)_k + \frac{r}{\nu^k}\right]$. Since $(\bar{a}_2)_k = 0$ for all $k \geq m$, one gets that

$$U_2(1) \in \left([(\bar{a}_2)_0 - r, (\bar{a}_2)_0 + r] + 2\sum_{k=1}^{m-1}\left(\left[(\bar{a}_2)_k - \frac{r}{\nu^k}, (\bar{a}_2)_k + \frac{r}{\nu^k}\right]\right) + 2\sum_{k\geq m}\left[-\frac{r}{\nu^k}, \frac{r}{\nu^k}\right]\right).$$

The first two terms can be evaluated using interval arithmetics while the last one respects the equality

$$2\sum_{k\geq m}\left[-\frac{r}{\nu^k}, \frac{r}{\nu^k}\right] = 2r[-1,1]\sum_{k\geq m}\frac{1}{\nu^k} = 2r[-1,1]\frac{1/\nu^m}{1-1/\nu} = \frac{2r}{\nu^{m-1}(\nu-1)}[-1,1].$$

Hence, a rigorous interval enclosure for the value of $U_2(1)$ is given by

$$U_2(1) \in \left(((\bar{a}_2)_0 + [-r,r]) + 2\sum_{k=1}^{m-1}\left((\bar{a}_2)_k + \left[-\frac{r}{\nu^k}, \frac{r}{\nu^k}\right]\right) + \frac{2r}{\nu^{m-1}(\nu-1)}[-1,1]\right). \tag{5.1}$$

5.1.2 Rigorous interval enclosure for $P_2(\hat{\theta})$.

Let $\hat{\theta} = \theta(\hat{\psi}) = (\rho\cos\hat{\psi}, \rho\sin\hat{\psi})$ and note that

$$P_2(\hat{\theta}) = \sum_{|\alpha|\geq 0} A_\alpha^{(2)}\hat{\theta}^\alpha = \sum_{0\leq|\alpha|\leq N_s} A_\alpha^{(2)}\hat{\theta}^\alpha + \sum_{|\alpha|>N_s} A_\alpha^{(2)}\hat{\theta}^\alpha.$$

Since $|\hat{\psi}-\bar{\psi}| \leq r$, one gets that $\hat{\psi} \in \boldsymbol{\psi} \stackrel{\text{def}}{=} [\bar{\psi}-r, \bar{\psi}+r]$ and then $\hat{\theta} \in \boldsymbol{\theta} \stackrel{\text{def}}{=} (\rho\cos\boldsymbol{\psi}, \rho\sin\boldsymbol{\psi})$. This allows us to compute the first term using interval arithmetics. For the second term, we apply a classical Cauchy estimate [34] to infer from (3.8) that

$$|A_\alpha^{(2)}| \leq \frac{\delta_s}{\nu_s^{|\alpha|}} \implies -\frac{\delta_s}{\nu_s^{|\alpha|}} \leq A_\alpha^{(2)} \leq \frac{\delta_s}{\nu_s^{|\alpha|}}.$$

Hence, we have that

$$\sum_{|\alpha|>N_s} A_\alpha^{(2)}\hat{\theta}^\alpha \in \sum_{|\alpha|>N_s}\left[-\frac{\delta_s}{\nu_s^{|\alpha|}}, \frac{\delta_s}{\nu_s^{|\alpha|}}\right]\boldsymbol{\theta}^\alpha = [-\delta_s, \delta_s]\sum_{|\alpha|>N_s}\left(\frac{\boldsymbol{\theta}_1}{\nu_s}\right)^{\alpha_1}\left(\frac{\boldsymbol{\theta}_2}{\nu_s}\right)^{\alpha_2}.$$

Let $\Theta_1 = \boldsymbol{\theta}_1/\nu_s$ and $\Theta_2 = \boldsymbol{\theta}_2/\nu_s$. By definition of ν_s, $\sup(\Theta_1) < 1$ and $\sup(\Theta_2) < 1$, so we deduce that

$$\begin{aligned}
\sum_{|\alpha|>N_s} \Theta_1^{\alpha_1}\Theta_2^{\alpha_2} &= \sum_{\alpha_2=0}^{\infty}\left(\sum_{\substack{\alpha_1=N_s+1-\alpha_2\\ \alpha_1\geq 0}}^{\infty} \Theta_1^{\alpha_1}\right)\Theta_2^{\alpha_2} \\
&= \sum_{\alpha_2=0}^{N_s} \Theta_2^{\alpha_2}\left(\frac{\Theta_1^{N_s+1-\alpha_2}}{1-\Theta_1}\right) + \sum_{\alpha_2=N_s+1}^{\infty} \Theta_2^{\alpha_2}\left(\frac{1}{1-\Theta_1}\right) \\
&= \frac{\Theta_1^{N_s+1}}{1-\Theta_1}\sum_{\alpha_2=0}^{N_s}\left(\frac{\Theta_2}{\Theta_1}\right)^{\alpha_2} + \left(\frac{1}{1-\Theta_1}\right)\left(\frac{\Theta_2^{N_s+1}}{1-\Theta_2}\right).
\end{aligned}$$

Thereby, we get that

$$P_2(\hat{\theta}) \in \left(\sum_{0\leq|\alpha|\leq N_s} A_\alpha^{(2)}\boldsymbol{\theta} + [-\delta_s,\delta_s]\left(\frac{\Theta_1^{N_s+1}}{1-\Theta_1}\sum_{\alpha_2=0}^{N_s}\left(\frac{\Theta_2}{\Theta_1}\right)^{\alpha_2} + \left(\frac{1}{1-\Theta_1}\right)\left(\frac{\Theta_2^{N_s+1}}{1-\Theta_2}\right)\right)\right). \tag{5.2}$$

Combining (5.1) and (5.2), we can obtain a rigorous interval enclosure for $U_2(1)$ and $P_2(\hat{\theta})$, and therefore (hopefully) conclude about their respective signs. Indeed the computer programs `proof_hex2pos_rolls.m` and `proof_hex2neg_rolls.m` explicitly check these conditions, and in both cases the checks agree and the proofs are complete.

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MATLAB codes to perform the proofs available at
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