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Existence of symmetric domain walls for the Bénard-Rayleigh convection problem

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Abstract

We prove the existence of domain walls for the B enard-Rayleigh convection problem. Our approach relies upon a spatial dynamics formulation of the hydrodynamic problem, a center manifold reduction, and a normal form analysis of a reduced system. Domain walls are constructed as heteroclinic orbits of this reduced system.

Running head: Domain walls for the B enard-Rayleigh convection problem

Keywords: B enard-Rayleigh convection, rolls, domain walls, bifurcations

1 Introduction

In fluid mechanics, the B enard-Rayleigh convection problem is concerned with the flow of a viscous fluid filling the region between two horizontal planes and heated from below. The governing equations are the Navier-Stokes equations in the Boussinesq approximation completed with an energy conservation equation (see the system (2.1)-(2.3)). Each of the two horizontal planar boundaries may be a rigid plane or a free boundary, hence leading to different possible types of boundary conditions: rigid-rigid, free-free, and free-rigid (see (2.5), (8.1), and (8.2)). Together with these boundary conditions, the equations are invariant under horizontal translations and rotations. In the cases of rigid-rigid and free-free boundary conditions, they have an additional vertical reflection symmetry. In dimensionless variables, the different physical parameters are reduced to two parameters which are the Rayleigh number \mathcal{R} and the Prandtl number \mathcal{P} (see (2.4)). We refer to [13, Vol. II] for a very complete discussion and bibliography on this problem, and in particular on the various geometries and boundary conditions.

The B enard-Rayleigh convection is one of the most studied, both analytically and experimentally, and perhaps best understood, pattern-forming system. In the hydrodynamic problem, the difference of temperature between the two horizontal planes modifies the fluid density, tending to place the lighter fluid below the heavier one. Having an opposite effect, gravity induces, through

the Archimedian force, an instability of the simple “conduction regime” leading to a “convective regime”. While the fluid is at rest and the temperature depends linearly on the vertical coordinate in the conduction regime, various steady regular patterns, such as rolls, hexagons, or squares, are formed in the convective regime. The fluid viscosity prevents this instability up to a certain level, and there is a critical value of the temperature difference, below which nothing happens and above which a steady convective regime bifurcates. In dimensionless variables, this bifurcation occurs at a critical value of the Rayleigh number \mathcal{R}_c . The numerical value of \mathcal{R}_c depends on the chosen boundary conditions and for the ones mentioned above it has already been computed in the forties by Pellew and Southwell [21]. Starting from the sixties, there has been extensive study of regular convective patterns and numerous mathematical existence results have been obtained. Without being exhaustive, we refer to the first works by Yudovich et al [26, 29, 30, 31], Rabinowitz [22], Görtler et al [7]; see also [15, 24], the monograph [16] for further references, and the recent work [2] on existence of quasipatterns.

The simplest, and perhaps most frequently observed, patterns are convective rolls aligned along a certain direction (see Figure 1.1 (a)-(b)). However, in many circumstances such a pattern is only experimentally observed in a part of the apparatus, while the rolls take another direction in another part of the apparatus. The connection between the two regimes is quite sharp, occurring along a plane, and the two regimes of rolls make a definite angle between them (see Figure 1.1 (c) and [11, 17, 4, 1] for experimental evidences not all on pure Bénard-Rayleigh convection). These line defects are referred to as domain walls or grain boundaries.

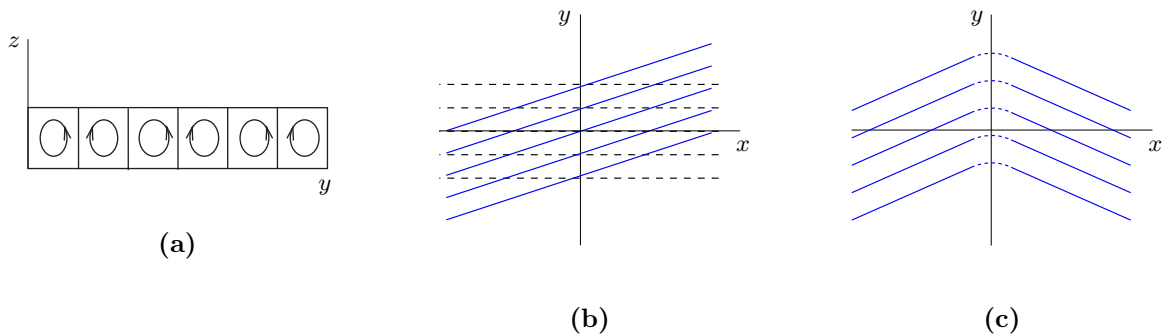


Figure 1.1: In cartesian coordinates (x, y, z) , schematic plots of two-dimensional rolls (periodic in y and constant in x), rotated rolls, and domain walls. **(a)** Level lines in the (y, z) -plane of two-dimensional rolls. **(b)** Level lines in the (x, y) -plane of two-dimensional rolls (dashed lines) and rolls rotated by an angle α (solid lines). **(c)** Level lines in the (x, y) -plane of symmetric domain walls constructed as heteroclinic connections between rolls rotated by opposite angles $\pm\alpha$.

The aim of this paper is to prove mathematically that domain walls are indeed solutions of the Navier-Stokes-Boussinesq equations (2.1)-(2.3). Despite constant interest over the years, there is so far no existence result for these fluid dynamics equations. Many works gave tentative justifications of the existence of such patterns using formally derived amplitude equations (see [20, 19, 6] and the references therein). Beyond amplitude equations, the only mathematical results have been obtained for the Swift-Hohenberg equation, a toy model which exhibits many

of the properties of the Bénard-Rayleigh convection problem [10, 25] (see also [18]). The domain walls constructed in [10] are symmetric, connecting rolls rotated by opposite angles $\pm\alpha$, for $\alpha \in (0, \pi/3)$. This result has been extended to arbitrary angles $\alpha \in (0, \pi/2)$ in [25]. We point out that there are no such results for domain walls which are not symmetric.

For the existence proof we use the same spatial dynamics approach as in [10]. The starting point of this analysis is a formulation of the steady problem as an infinite-dimensional dynamical system, in which one of the horizontal variables is taken as evolutionary variable. This idea goes back to the work of Kirchgässner [14], and since then it has been extensively used to prove the existence of nonlinear waves and patterns in many concrete problems arising in applied sciences, and in particular in fluid mechanics (see for instance [8] and the references therein). This infinite-dimensional dynamical system is typically ill-posed, but of interest are its small bounded solutions. An efficient way of finding these solutions is with the help of center-manifold techniques which reduce the infinite-dimensional system to a locally equivalent finite-dimensional dynamical system. An important property of this reduced system is that it preserves the symmetries of the original problem. Then normal forms and dynamical systems methods can be employed to construct bounded solutions of this reduced system.

We construct the domain walls as steady solutions of the Navier-Stokes-Boussinesq equations which are periodic in the horizontal coordinate y . In our spatial dynamics formulation, we take as evolutionary variable the horizontal coordinate x and the boundary conditions, including the periodicity in y , determine the choice of the associated phase space and domain of definition of operators. The rolls which are periodic in y and independent on x are then equilibria of the infinite-dimensional dynamical system, and through horizontal rotations we obtain a family of relative equilibria. Domain walls are found as heteroclinic orbits of the infinite-dimensional dynamical system connecting two symmetric relative equilibria.

We expect domain walls to bifurcate in the convective regime, at the same critical value \mathcal{R}_c of the Rayleigh number as the rolls. In the bifurcation problem, we take the Rayleigh number \mathcal{R} as bifurcation parameter, fix the Prandtl number \mathcal{P} and also fix the wavenumber k_y in y of the solutions. We choose $k_y = k_c \cos \alpha$, where k_c is the wavenumber of the rolls bifurcating at \mathcal{R}_c in the classical convection problem and α is a rotation angle. Then k_y represents the wavenumber in y of the bifurcating rolls rotated by the angle α .

The nature of the bifurcation is determined by the purely imaginary spectrum of the operator obtained by linearizing the dynamical system at the state of rest. Here, this operator has purely point spectrum and the number of its purely imaginary eigenvalues depends on the value of the rotation angle α . We restrict to the simplest situation in which $\alpha \in (0, \pi/3)$. Then the linear operator possesses two pairs of conjugated purely imaginary eigenvalues $\pm ik_c$, $\pm ik_x$, where $\pm ik_c$ are algebraically double and geometrically simple, and $\pm ik_x$ are algebraically quadruple and geometrically double. In addition, 0 is a simple eigenvalue due to an invariance of our spatial dynamics formulation. Except for this latter eigenvalue, the other purely imaginary eigenvalues are of the same type as those found for the Swift-Hohenberg equation in [10]. Upon increasing the angle α in the interval $(\pi/3, \pi/2)$, the number of purely imaginary eigenvalues increases, and there are infinitely many eigenvalues when $\alpha = \pi/2$. For the Swift-Hohenberg equation,

this case has been considered in [25].

The next step of our analysis is a center manifold reduction. The dimension of the reduced system being equal to the sum of the algebraic multiplicities of the purely imaginary above, we obtain here a reduced system of dimension 13. Due to the absence of the eigenvalue 0, the dimension of this reduced system was equal to 12 for the Swift-Hohenberg equation [10]. However, this additional dimension is easily eliminated, and then in the cases of rigid-rigid and free-free boundary conditions we use the reflection in the vertical coordinate to further eliminate 4 dimensions. This additional symmetry has not been used in [10]. The resulting system is 8-dimensional and the question of existence of domain walls consists now in the construction of a heteroclinic orbit for this system.

In contrast to the Swift-Hohenberg equation where the leading order terms of the reduced system have been computed explicitly, here the Navier-Stokes-Boussinesq equations are far too complicated to compute all these terms. We therefore need to replace the partial normal form analysis used in [10] by a full normal analysis for general 8-dimensional vector fields. To simplify this analysis, we restrict to terms of cubic order and take advantage of the symmetries of the original problem which are inherited by the reduced system, and then by the normal form.

The remaining part of the existence proof is based on the arguments from [10]. An appropriate change of variables allows us to identify a leading order system, for which the existence of a heteroclinic solution has been proved in [27]. Based on a variational method [23], this existence result requires that the quotient g of two coefficients in the cubic normal form is larger than 1. In [10] this quotient was equal to 2 and it was easily computed. Here, g depends on the angle α and the Prandtl number \mathcal{P} through complicated formulas. We prove that its value in the limit $\alpha \rightarrow 0$ is also equal to 2, but for arbitrary angles and Prandtl numbers, we can only determine its numerical values using the package Maple. It turns out that indeed the condition $g > 1$ holds for all angles $\alpha \in (0, \pi/3)$ and all positive Prandtl numbers \mathcal{P} , for both rigid-rigid and free-free boundary conditions. The final step consists in showing that this heteroclinic orbit found for the leading order system persists for the full system. We extend the persistence result in [10] from the case $g = 2$ to values $g \in (1, 4 + \sqrt{13})$, and use a Maple computation to determine the angles α and the Prandtl numbers \mathcal{P} for which this property holds (see Figures 6.1 and 8.1). The persistence of the heteroclinic orbit for $g \geq 4 + \sqrt{13}$ remains an open problem. We summarize our main result in the next theorem.

Theorem 1. *Consider the Navier-Stokes-Boussinesq system (2.1)-(2.3) with either rigid-rigid boundary conditions (2.5) or free-free boundary conditions (8.1). Denote by \mathcal{R}_c the critical Rayleigh number at which convective rolls with wavenumbers k_c bifurcate from the conduction state. For any angle $\alpha \in (0, \pi/3)$, there exists a nonnegative value $\mathcal{P}_*(\alpha)$ such that, for Prandtl numbers $\mathcal{P} > \mathcal{P}_*(\alpha)$ and Rayleigh numbers $\mathcal{R} = \mathcal{R}_c + \epsilon$, with $\epsilon > 0$ sufficiently small, the system possesses a symmetric domain wall connecting two rotated rolls which are the rotations by opposite angles $\pm(\alpha + O(\epsilon))$ of a roll with wavenumber $k_c + O(\epsilon)$.*

In our presentation we focus on the case of rigid-rigid boundary conditions, and then discuss the differences which occur in the cases of free-free and rigid-free boundary conditions in the last section of the paper. In Section 2 we present the hydrodynamic problem and recall the classical

bifurcation results for convective rolls. The spatial dynamics formulation is given in Section 3 and the bifurcation problem is analyzed in Section 4. The center manifold reduction is done in Section 5 and the normal form analysis in Section 6. The existence of the heteroclinic connection is proved in Section 7. Some technical results, including the lengthy computation of the two coefficients of the normal form needed in the existence proof, are given in Appendices A.1 and B.

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2 The classical Bénard-Rayleigh convection

The governing equations of the Bénard-Rayleigh convection consist of the Navier-Stokes system completed with an equation for energy conservation. We consider the Boussinesq approximation in which the dependency of the fluid density ρ on the temperature T is given by the relationship

$$\rho = \rho_0 (1 - \gamma(T - T_0)),$$

where γ is the (constant) volume expansion coefficient. In cartesian coordinates $(x, y, z) \in \mathbb{R}^3$, after rescaling variables, the fluid occupies the domain $\mathbb{R}^2 \times (0, 1)$ in which the particle velocity $\mathbf{V} = (V_x, V_y, V_z)$, the deviation of the temperature from the conduction profile θ , and the pressure p satisfy the system

$$\mathcal{R}^{-1/2} \Delta \mathbf{V} + \theta \mathbf{e}_z - \mathcal{P}^{-1} (\mathbf{V} \cdot \nabla) \mathbf{V} - \nabla p = 0, \quad (2.1)$$

$$\mathcal{R}^{-1/2} \Delta \theta + V_z - (\mathbf{V} \cdot \nabla) \theta = 0, \quad (2.2)$$

$$\nabla \cdot \mathbf{V} = 0. \quad (2.3)$$

Here $\mathbf{e}_z = (0, 0, 1)$, and the dimensionless constants \mathcal{R} and \mathcal{P} are the Rayleigh and the Prandtl numbers, respectively, defined as

$$\mathcal{R} = \frac{\gamma g d^3 (T_0 - T_1)}{\nu \kappa}, \quad \mathcal{P} = \frac{\nu}{\kappa}, \quad (2.4)$$

where ν is the kinematic viscosity, κ the thermal diffusivity, g the gravitational constant, and d the distance between the planes. For notational simplicity, we set

$$\mu = \mathcal{R}^{1/2}.$$

This system is a version of the formulation derived in [16] in which \mathbf{V} and θ are rescaled by $\mathcal{R}^{1/2}$ and \mathcal{R} , respectively. The equations (2.1)-(2.3) are completed by boundary conditions, and we consider here the case of “rigid-rigid” boundary conditions:

$$\mathbf{V}|_{z=0,1} = 0, \quad \theta|_{z=0,1} = 0. \quad (2.5)$$

With these boundary conditions, the equations (2.1)-(2.3) are invariant under horizontal translations and rotations, and have a reflection symmetry in each of the three coordinates (x, y, z) . These symmetries play an important role in our analysis.

In the classical approach, the system (2.1)-(2.3) is written in the form

$$\mathbf{L}_\mu \mathbf{u} + \mathbf{B}(\mathbf{u}, \mathbf{u}) = 0, \quad (2.6)$$

where $\mathbf{u} = (\mathbf{V}, \theta)$ lies in a suitable function space of divergence free velocity fields \mathbf{V} and the pressure term in (2.1) is eliminated via a projection on the divergence free vector field (see, for instance, [8, Chapter 5]). Then $\mathbf{L}_\mu \mathbf{u}$ is the linear part and $\mathbf{B}(\mathbf{u}, \mathbf{u})$ is the nonlinear part, quadratic in (\mathbf{V}, θ) , of the equations (2.1) and (2.2). The Prandtl number \mathcal{P} which only appears in the quadratic part is kept fixed, and the square root μ of the Rayleigh number is taken as bifurcation parameter. We recall below some of the basic results which are used later in the paper.

2.1 Two-dimensional convection

The simple classical convection problem restricts to velocity fields $\mathbf{V} = (0, V_y, V_z)$ which are two-dimensional and functions which are independent of x and periodic in y . The corresponding function space for the system (2.6) is

$$\mathcal{H} = \{\mathbf{u} \in \{0\} \times (L_{per}^2(\Omega))^3; \nabla \cdot \mathbf{V} = 0, V_z = 0 \text{ on } z = 0, 1\},$$

where $\Omega = \mathbb{R} \times (0, 1)$ and the subscript *per* means that the functions are $2\pi/k$ -periodic in y , for some fixed $k > 0$. The boundary conditions (2.5) are included in the domain \mathcal{D} of the linear operator \mathbf{L}_μ by taking

$$\mathcal{D} = \{\mathbf{u} \in \{0\} \times (H_{per}^2(\Omega))^3; \nabla \cdot \mathbf{V} = 0, V_y = V_z = \theta = 0 \text{ on } z = 0, 1\}.$$

In this setting, the linear operator \mathbf{L}_μ is selfadjoint with compact resolvent and the quadratic operator \mathbf{B} in (2.6) is symmetric and bounded from \mathcal{D} to \mathcal{H} .

As a consequence of the invariance of the equations (2.1)-(2.3) under horizontal translations and reflections, the system (2.6) is $O(2)$ -equivariant: both its linear and quadratic parts commute with the one-parameter family of linear maps $(\tau_a)_{a \in \mathbb{R}/2\pi\mathbb{Z}}$ and the discrete symmetry \mathbf{S}_2 defined through

$$\tau_a \mathbf{u}(y, z) = \mathbf{u}(y + a/k, z), \quad \mathbf{S}_2 \mathbf{u}(y, z) = (0, -V_y, V_z, \theta)(-y, z),$$

for any $\mathbf{u} \in \mathcal{H}$, and satisfying

$$\tau_a \mathbf{S}_2 = \mathbf{S}_2 \tau_{-a}, \quad \tau_0 = \tau_{2\pi} = \mathbb{I}.$$

An additional equivariance, under the action of the symmetry \mathbf{S}_3 defined through

$$\mathbf{S}_3 \mathbf{u}(y, z) = (0, V_y, -V_z, -\theta)(y, 1 - z),$$

which commutes with τ_a and \mathbf{S}_2 , is obtained from the invariance of the equations (2.1)-(2.3) under vertical reflections $z \mapsto 1 - z$.

Instabilities and bifurcations are determined by the kernel of \mathbf{L}_μ . Elements in the kernel of \mathbf{L}_μ are found by looking for solutions of the form $e^{iky} \widehat{\mathbf{u}}_k(z)$ for the linear equation

$$\mathbf{L}_\mu \mathbf{u} = 0, \quad (2.7)$$

and the boundary conditions $V_y = V_z = \theta = 0$ on $z = 0, 1$. A direct computation (see also [3]) gives

$$e^{iky} \widehat{\mathbf{u}}_k(z) = e^{iky} \begin{pmatrix} 0 \\ \frac{i}{k} DV \\ V \\ \theta \end{pmatrix}, \quad (2.8)$$

where $D = d/dz$ denotes the derivative with respect to z , and the functions $V = V(z)$ and $\theta = \theta(z)$ are real-valued solutions of the boundary value problem

$$(D^2 - k^2)^2 V = \mu k^2 \theta, \quad V = DV = 0 \text{ in } z = 0, 1, \quad (2.9)$$

$$(D^2 - k^2)\theta = -\mu V, \quad \theta = 0 \text{ in } z = 0, 1. \quad (2.10)$$

Yudovich [29] showed that, for any fixed $k > 0$, there is a countable sequence of parameter values $\mu_0(k) < \mu_1(k) < \mu_2(k) < \dots$ for which the boundary value problem (2.9)-(2.10) has a unique, up to a multiplicative constant, nontrivial solution (V, θ) , and that the function V is positive for $\mu = \mu_0(k)$. The functions $\mu_j(k)$ are analytic in k and in an analogous case Yudovich [28] showed that they tend to ∞ as k tends to 0 or ∞ . Of particular interest for the classical bifurcation problem, and also in our context, is the global minimum of $\mu_0(k)$. Combining analytical arguments and numerical calculations, Pellew and Southwell [21] computed a unique global minimum $\mu_c = \mu_0(k_c)$, for some $k = k_c$, but a complete analytical proof of this property is not available, so far. They also showed that the positive function V is symmetric with respect to $z = 1/2$. In Appendix B.5, we use the symbolic package Maple, to compute the numerical values

$$k_c \approx 3.116, \quad \mu_c \approx 41.325, \quad \mu_0''(k_c) \approx 6.265, \quad (2.11)$$

which are consistent with the ones found in [21], and the function V (see Figure B.1).

Going back to the kernel of \mathbf{L}_μ , as expected by the general theory of $O(2)$ -equivariant systems, for $\mu = \mu_0(k)$ and any $k > 0$ the kernel of $\mathbf{L}_{\mu_0(k)}$ is two-dimensional and spanned by the vectors

$$\boldsymbol{\xi}_0 = e^{iky} \widehat{\mathbf{u}}_k(z), \quad \overline{\boldsymbol{\xi}}_0 = e^{-iky} \overline{\widehat{\mathbf{u}}_k}(z),$$

satisfying

$$\tau_a \boldsymbol{\xi}_0 = e^{ia} \boldsymbol{\xi}_0, \quad \mathbf{S}_2 \boldsymbol{\xi}_0 = \overline{\boldsymbol{\xi}}_0, \quad \mathbf{S}_3 \boldsymbol{\xi}_0 = -\boldsymbol{\xi}_0.$$

Since the operator has compact resolvent, this shows that 0 is an isolated double semi-simple eigenvalue of $\mathbf{L}_{\mu_0(k)}$, and it turns out that all other eigenvalues are negative. This property is a key ingredient in the proof of existence of rolls, which bifurcate from the trivial solution at $\mu = \mu_0(k)$, for any fixed $k > 0$, in a steady bifurcation with $O(2)$ symmetry.

2.2 Existence of rolls

We briefly recall below the bifurcation analysis showing the existence of convective rolls. This type of proof was first made by Yudovich [30].

The $O(2)$ symmetry of the system (2.6) allows to restrict the existence proof to solutions \mathbf{u} which are invariant under the action of \mathbf{S}_2 , and then the one-parameter family of linear maps $(\tau_a)_{a \in \mathbb{R}/2\pi\mathbb{Z}}$ give the non-symmetric solutions. Using the Lyapunov-Schmidt method, symmetric rolls can be constructed as convergent series in \mathcal{D} ,

$$\mathbf{u} = \epsilon \mathbf{u}_1 + \epsilon^2 \mathbf{u}_2 + \epsilon^3 \mathbf{u}_3 + O(\epsilon^4),$$

for any fixed $k > 0$ and

$$\mu = \mu_0(k) + \epsilon \mu_1 + \epsilon^2 \mu_2 + O(\epsilon^3).$$

Inserting these expansions into (2.6), at orders ϵ , ϵ^2 and ϵ^3 we find the equalities

$$\mathbf{L}_0 \mathbf{u}_1 = 0, \tag{2.12}$$

$$\mathbf{L}_0 \mathbf{u}_2 + \mu_1 \mathbf{L}_1 \mathbf{u}_1 + \mathbf{B}(\mathbf{u}_1, \mathbf{u}_1) = 0, \tag{2.13}$$

$$\mathbf{L}_0 \mathbf{u}_3 + \mu_1 \mathbf{L}_1 \mathbf{u}_2 + (\mu_2 \mathbf{L}_1 + \mu_1 \mathbf{L}_2) \mathbf{u}_1 + 2\mathbf{B}(\mathbf{u}_1, \mathbf{u}_2) = 0, \tag{2.14}$$

in which

$$\mathbf{L}_0 = \mathbf{L}_{\mu_0(k)}, \quad \mathbf{L}_1 = \frac{d}{d\mu} \mathbf{L}_\mu \Big|_{\mu=\mu_0(k)}, \quad \mathbf{L}_2 = \frac{1}{2} \frac{d^2}{d\mu^2} \mathbf{L}_\mu \Big|_{\mu=\mu_0(k)}.$$

By successively solving these equations we can compute the leading order terms in the expansions of \mathbf{u} and μ .

First, the equality (2.12) implies that \mathbf{u}_1 belongs to the kernel of \mathbf{L}_0 . Due to the restriction to symmetric solutions, the kernel of \mathbf{L}_0 is now one-dimensional, and we take

$$\mathbf{u}_1 = \boldsymbol{\xi}_0 + \overline{\boldsymbol{\xi}_0}. \tag{2.15}$$

Next, by taking the L^2 -scalar product of the equality (2.13) with \mathbf{u}_1 , we find

$$\mu_1 \langle \mathbf{L}_1 \mathbf{u}_1, \mathbf{u}_1 \rangle = -\langle \mathbf{B}(\mathbf{u}_1, \mathbf{u}_1), \mathbf{u}_1 \rangle,$$

since \mathbf{L}_0 is selfadjoint and \mathbf{u}_1 belongs to its kernel. A direct computation gives

$$\langle \mathbf{L}_1 \mathbf{u}_1, \mathbf{u}_1 \rangle = 2 \operatorname{Re} \langle \mathbf{L}_1 \boldsymbol{\xi}_0, \boldsymbol{\xi}_0 \rangle = \frac{2}{k^2 \mu^2} \langle (D^2 - k^2)V, (D^2 - k^2)V \rangle + \frac{2}{\mu^2} (\|D\theta\|^2 + k^2 \|\theta\|^2) > 0, \tag{2.16}$$

and a remarkable property of the Navier-Stokes equations is that

$$\langle \mathbf{B}(\mathbf{u}, \mathbf{u}), \mathbf{u} \rangle = 0, \tag{2.17}$$

for any real-valued $\mathbf{u} \in \mathcal{D}$. Consequently, $\mu_1 = 0$ and then \mathbf{u}_2 is a symmetric solution of

$$\mathbf{L}_0 \mathbf{u}_2 = -\mathbf{B}(\mathbf{u}_1, \mathbf{u}_1).$$

Without loss of generality, \mathbf{u}_2 may be chosen orthogonal to \mathbf{u}_1 .

Finally, by taking the scalar product of the equality (2.14) with \mathbf{u}_1 , we find

$$\mu_2 \langle \mathbf{L}_1 \mathbf{u}_1, \mathbf{u}_1 \rangle = -\langle 2\mathbf{B}(\mathbf{u}_1, \mathbf{u}_2), \mathbf{u}_1 \rangle.$$

Writing the equality (2.17) for $\mathbf{u} = \mathbf{u}_1 + t\mathbf{u}_2$ and taking the term linear in t we find

$$\langle 2\mathbf{B}(\mathbf{u}_1, \mathbf{u}_2), \mathbf{u}_1 \rangle + \langle \mathbf{B}(\mathbf{u}_1, \mathbf{u}_1), \mathbf{u}_2 \rangle = 0,$$

hence

$$\mu_2 = \frac{\langle \mathbf{B}(\mathbf{u}_1, \mathbf{u}_1), \mathbf{u}_2 \rangle}{\langle \mathbf{L}_1 \mathbf{u}_1, \mathbf{u}_1 \rangle} = -\frac{\langle \mathbf{L}_0 \mathbf{u}_2, \mathbf{u}_2 \rangle}{\langle \mathbf{L}_1 \mathbf{u}_1, \mathbf{u}_1 \rangle}.$$

The sign of μ_2 determines the type of the bifurcation. We have $\langle \mathbf{L}_1 \mathbf{u}_1, \mathbf{u}_1 \rangle > 0$ by (2.16), and $\langle \mathbf{L}_0 \mathbf{u}_2, \mathbf{u}_2 \rangle < 0$, since \mathbf{L}_0 is a nonpositive selfadjoint operator, and \mathbf{u}_2 is orthogonal to its kernel. Consequently, $\mu_2 > 0$, implying that rolls bifurcate supercritically, for $\mu > \mu_0(k)$, and any fixed $k > 0$ (see Figure 2.1(a)). Fixing k , for any $\mu > \mu_0(k)$, sufficiently close to $\mu_0(k)$, we find a

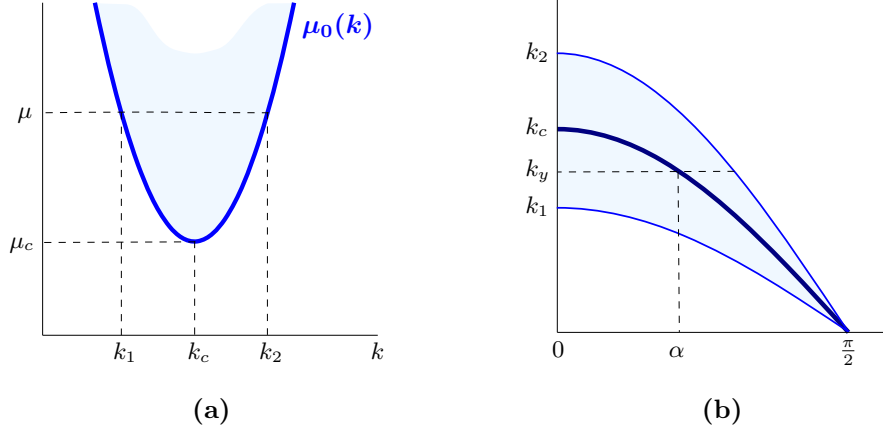


Figure 2.1: (a) Graph of $\mu_0(k)$. Two-dimensional rolls bifurcate in the shaded region situated above the curve $\mu_0(k)$. For $\mu > \mu_c$ sufficiently close to μ_c , two-dimensional rolls exist for wavenumbers $k \in (k_1, k_2)$ with $\mu = \mu_0(k_1) = \mu_0(k_2)$. (b) Plot of the wavenumbers $k_y = k \cos \alpha$ in y of the rolls rotated by angles $\alpha \in (0, \pi/2)$, for $k = k_1, k_c, k_2$. For $\mu > \mu_c$ sufficiently close to μ_c , rotated rolls exist in the shaded region. In the bifurcation analysis we fix $k_y = k_c \cos \alpha$, for some $\alpha \in (0, \pi/3)$.

circle of rolls $\tau_a(\mathbf{u}_{k,\mu})$, $a \in \mathbb{R}/2\pi\mathbb{Z}$, in which $\mathbf{u}_{k,\mu}$ and $\tau_\pi(\mathbf{u}_{k,\mu})$ are invariant under the action of \mathbf{S}_2 and exchanged by the action of \mathbf{S}_3 .

3 Spatial dynamics

The starting point of our analysis is a formulation of the system (2.1)-(2.3) as a dynamical system in which the evolutionary variable is the horizontal spatial coordinate x .

Set $\mathbf{V} = (V_x, V_\perp)$, where $V_\perp = (V_y, V_z)$, and consider the new variables

$$\mathbf{W} = \mu^{-1} \partial_x \mathbf{V} - p \mathbf{e}_x, \quad \phi = \partial_x \theta, \quad (3.1)$$

in which we write $\mathbf{W} = (W_x, W_\perp)$, and $W_\perp = (W_y, W_z)$. Using the equation (2.3) we obtain the formula for the pressure,

$$p = -\mu^{-1} \nabla_\perp \cdot V_\perp - W_x. \quad (3.2)$$

Then we write the system (2.1)-(2.3) in the form

$$\partial_x \mathbf{U} = \mathcal{L}_\mu \mathbf{U} + \mathcal{B}_\mu(\mathbf{U}, \mathbf{U}), \quad (3.3)$$

in which \mathbf{U} is the 8-components vector

$$\mathbf{U} = (V_x, V_\perp, W_x, W_\perp, \theta, \phi),$$

and the operators \mathcal{L}_μ and \mathcal{B}_μ are linear and quadratic, respectively, defined by

$$\mathcal{L}_\mu \mathbf{U} = \begin{pmatrix} -\nabla_\perp \cdot V_\perp \\ \mu W_\perp \\ -\mu^{-1} \Delta_\perp V_x \\ -\mu^{-1} \Delta_\perp V_\perp - \theta \mathbf{e}_z - \mu^{-1} \nabla_\perp (\nabla_\perp \cdot V_\perp) - \nabla_\perp W_x \\ \phi \\ -\Delta_\perp \theta - \mu V_z \end{pmatrix},$$

$$\mathcal{B}_\mu(\mathbf{U}, \mathbf{U}) = \begin{pmatrix} 0 \\ 0 \\ \mathcal{P}^{-1}((V_\perp \cdot \nabla_\perp) V_x - V_x (\nabla_\perp \cdot V_\perp)) \\ \mathcal{P}^{-1}((V_\perp \cdot \nabla_\perp) V_\perp + \mu V_x W_\perp) \\ 0 \\ \mu((V_\perp \cdot \nabla_\perp) \theta + V_x \phi) \end{pmatrix}.$$

We look for solutions of (3.3) which are periodic in y and satisfy the boundary conditions (2.5). For such solutions we have

$$\frac{d}{dx} \int_\Omega V_x dy dz = - \int_\Omega \nabla_\perp \cdot V_\perp dy dz = - \int_{\partial\Omega} n \cdot V_\perp ds = 0,$$

which implies that the flux

$$\mathcal{F}(x) = \int_\Omega V_x dy dz$$

is constant. Equivalently, this property implies that the dynamical system (3.3) leaves invariant the subspace orthogonal to the vector $\psi_0 = (1, 0, 0, 0, 0, 0, 0, 0)$. We restrict to this subspace, hence fixing the constant flux to 0. Including this property and the boundary conditions (2.5) in the definition of the phase space \mathcal{X} of the dynamical system (3.3), we take

$$\mathcal{X} = \{ \mathbf{U} \in (H_{per}^1(\Omega))^3 \times (L_{per}^2(\Omega))^3 \times H_{per}^1(\Omega) \times L_{per}^2(\Omega); \\ V_x = V_\perp = \theta = 0 \text{ on } z = 0, 1, \text{ and } \int_\Omega V_x dy dz = 0 \}.$$

As in Section 2, $\Omega = \mathbb{R} \times (0, 1)$ and the subscript *per* means that the functions are $2\pi/k_y$ -periodic in y , for some fixed $k_y > 0$. (In order to distinguish between periodicity in x and y , we add the

subscript y in the notation of the wavenumber k .) The phase space \mathcal{X} is a closed subspace of the Hilbert space

$$\tilde{\mathcal{X}} = (H_{per}^1(\Omega))^3 \times (L_{per}^2(\Omega))^3 \times H_{per}^1(\Omega) \times L_{per}^2(\Omega),$$

so that it is a Hilbert space endowed with the usual scalar product of $\tilde{\mathcal{X}}$. Accordingly, we define the domain of definition \mathcal{Z} of the linear operator \mathcal{L}_μ by

$$\begin{aligned} \mathcal{Z} = \{ \mathbf{U} \in \mathcal{X} \cap (H_{per}^2(\Omega))^3 \times (H_{per}^1(\Omega))^3 \times H_{per}^2(\Omega) \times H_{per}^1(\Omega) ; \\ \nabla_\perp \cdot V_\perp = W_\perp = \phi = 0 \text{ on } z = 0, 1 \}, \end{aligned}$$

so that \mathcal{L}_μ is closed and its domain \mathcal{Z} is dense and compactly embedded in \mathcal{X} . In particular, this latter property implies that \mathcal{L}_μ has purely point spectrum which consists of isolated eigenvalues with finite algebraic multiplicity.

The dynamical system (3.3) inherits the symmetries of the original system (2.1)-(2.5). As for the two-dimensional convection, horizontal translations $y \rightarrow y + a/k_y$ along the y direction give a one-parameter family of linear maps $(\tau_a)_{a \in \mathbb{R}/2\pi\mathbb{Z}}$ defined on \mathcal{X} through

$$\tau_a \mathbf{U}(y, z) = \mathbf{U}(y + a/k_y, z), \quad (3.4)$$

and which commute with \mathcal{L}_μ and \mathcal{B}_μ . The reflection $x \mapsto -x$ now gives a reversibility symmetry

$$\mathbf{S}_1 \mathbf{U}(y, z) = (-V_x, V_\perp, W_x, -W_\perp, \theta, -\phi)(y, z),$$

for $\mathbf{U} \in \mathcal{X}$, which anti-commutes with \mathcal{L}_μ and \mathcal{B}_μ , and the reflections $y \mapsto -y$ and $z \mapsto 1 - z$ give the symmetries

$$\begin{aligned} \mathbf{S}_2 \mathbf{U}(y, z) &= (V_x, -V_y, V_z, W_x, -W_y, W_z, \theta, \phi)(-y, z), \\ \mathbf{S}_3 \mathbf{U}(y, z) &= (V_x, V_y, -V_z, W_x, W_y, -W_z, -\theta, -\phi)(y, 1 - z), \end{aligned}$$

for $\mathbf{U} \in \mathcal{X}$, which both commute with \mathcal{L}_μ and \mathcal{B}_μ . Notice that

$$\tau_a \mathbf{S}_2 = \mathbf{S}_2 \tau_{-a}, \quad \tau_0 = \tau_{2\pi} = \mathbb{I},$$

so that the system (3.3) is $O(2)$ -equivariant, and that \mathbf{S}_3 commutes with τ_a .

In addition to these symmetries inherited from the original system (2.1)-(2.5), the dynamical system (3.3) has a specific invariance due to the new variable $\mathbf{W} = (W_x, W_\perp)$ in (3.1). While W_\perp satisfies the same boundary conditions as V_\perp , included in the domain of definition \mathcal{Z} of the linear operator, there are no such conditions for W_x because the pressure p in the definition of W_x is only defined up to a constant. As a consequence, the dynamical system is invariant upon adding any constant to W_x , i.e., the vector field is invariant under the action of the one-parameter family of maps $(\mathbf{T}_b)_{b \in \mathbb{R}}$, defined on \mathcal{X} through

$$\mathbf{T}_b \mathbf{U} = \mathbf{U} + b\boldsymbol{\varphi}_0, \quad \boldsymbol{\varphi}_0 = (0, 0, 0, 1, 0, 0, 0, 0)^t. \quad (3.5)$$

This invariance introduces the vector $\boldsymbol{\varphi}_0$ in the kernel of \mathcal{L}_μ (see Lemma 4.2).

4 The bifurcation problem

As for the two-dimensional convection, we fix the Prandtl number \mathcal{P} and take the square root μ of the Rayleigh number as bifurcation parameter.

4.1 Domain walls as heteroclinic orbits

The equilibria $\mathbf{U} \in \mathcal{Z}$ of the dynamical system (3.3) can be found as solutions $\mathbf{u} \in \mathcal{D}$ of the two-dimensional problem in Section 2, through the projection

$$\mathbf{u} = \Pi\mathbf{U} = (V_x, V_\perp, \theta). \quad (4.1)$$

In particular, for any $k_y = k > 0$ fixed, the rolls in Section 2 give a circle of equilibria $\tau_a(\mathbf{U}_{k,\mu}^*)$, for $a \in \mathbb{R}/2\pi\mathbb{Z}$, which bifurcate for $\mu > \mu_0(k)$ sufficiently close to $\mu_0(k)$, belong to \mathcal{D} , and satisfy

$$\mathbf{S}_1\mathbf{U}_{k,\mu}^* = \mathbf{S}_2\mathbf{U}_{k,\mu}^* = \mathbf{U}_{k,\mu}^*, \quad \mathbf{S}_3\mathbf{U}_{k,\mu}^* = \tau_\pi\mathbf{U}_{k,\mu}^*.$$

Due to the rotation invariance of the three-dimensional problem (2.6), horizontally rotated rolls are solutions of (2.6) and relative equilibria of the dynamical system (3.3). For any angle $\alpha \in \mathbb{R}/2\pi\mathbb{Z}$, we find the rotated rolls $\mathcal{R}_\alpha(\mathbf{U}_{k,\mu}^*)$, where the horizontal rotation \mathcal{R}_α acts on the 4-components vector $\mathbf{u} = \Pi\mathbf{U}$ through

$$\mathcal{R}_\alpha\mathbf{u}(x, y, z) = (\mathcal{R}_\alpha(V_x, V_y), V_z, \theta)(\mathcal{R}_{-\alpha}(x, y), z), \quad (4.2)$$

in which

$$\mathcal{R}_\alpha(x, y) = (x \cos \alpha - y \sin \alpha, x \sin \alpha + y \cos \alpha).$$

(We do not need here the more complicated representation formula for the 8-components vector \mathbf{U} .) For the dynamical system (3.3), a rotated roll $\mathcal{R}_\alpha(\mathbf{U}_{k,\mu}^*)$ is a $2\pi/k \sin \alpha$ -periodic solution in the phase-space \mathcal{X} with $k_y = k \cos \alpha$. While for the angles $\alpha = 0$ and $\alpha = \pi$ the rotated rolls are equilibria in the phase-space \mathcal{X} with $k_y = k$, for the orthogonal angles $\alpha = \pi/2$ and $\alpha = 3\pi/2$, they are $2\pi/k$ -periodic solutions, for any $k_y > 0$. Upon rotation, rolls lose their reversibility and the horizontal reflection invariance, the actions of \mathbf{S}_1 and \mathbf{S}_2 on a roll rotated by an angle α gives the same roll but rotated by a different angle,

$$\mathbf{S}_1\mathcal{R}_\alpha\mathbf{U}_{k,\mu}^* = \mathcal{R}_{-\alpha}\mathbf{U}_{k,\mu}^*, \quad \mathbf{S}_2\mathcal{R}_\alpha\mathbf{U}_{k,\mu}^* = \mathcal{R}_{\pi-\alpha}\mathbf{U}_{k,\mu}^*.$$

In particular, we can restrict to rotations with angles $\alpha \in [0, \pi/2]$.

We construct the domain walls as reversible heteroclinic solutions connecting two rotated rolls, $\mathcal{R}_\alpha\mathbf{U}_{k,\mu}^*$ at $x = -\infty$ and $\mathcal{R}_{-\alpha}\mathbf{U}_{k,\mu}^*$ at $x = \infty$. In contrast to rolls which bifurcate at $\mu = \mu_0(k)$, for any fixed $k > 0$, domain walls bifurcate at the minimum $\mu_c = \mu_0(k_c)$. For $\mu > \mu_c$ sufficiently close to μ_c , the dynamical system (3.3) has the two-parameter family of rotated rolls $\mathcal{R}_\alpha(\mathbf{U}_{k,\mu}^*)$ for angles $\alpha \in \mathbb{R}/2\pi\mathbb{Z}$ and wavenumbers $k_y \in (k_1 \cos \alpha, k_2 \cos \alpha)$ in y , where $\mu = \mu_0(k_1) = \mu_0(k_2)$ (see Figure 2.1). In the bifurcation problem, we will suitably fix k_y and take μ , close to μ_c , as bifurcation parameter. The next step of our analysis is to determine the purely imaginary eigenvalues of the linear operator \mathcal{L}_{μ_c} .

4.2 Connection with the classical linear problem

Solutions $\mathbf{U} = (V_x, V_\perp, W_x, W_\perp, \theta, \phi) \in \mathcal{Z}$ of the eigenvalue problem

$$\mathcal{L}_\mu \mathbf{U} = i\omega \mathbf{U}, \quad (4.3)$$

are linear combinations of vectors of the form $\mathbf{U}_{\omega,n}(y, z) = e^{ink_y y} \widehat{\mathbf{U}}_{\omega,n}(z)$, with $n \in \mathbb{Z}$, due to periodicity in y . Projecting with Π given by (4.1), we obtain a solution

$$\mathbf{u}_{\omega,n}(x, y, z) = e^{i(\omega x + nk_y y)} \Pi \widehat{\mathbf{U}}_{\omega,n}(z),$$

of the three-dimensional classical problem (2.6), and rotating by a suitable angle α we find a solution $e^{iky} \widehat{\mathbf{u}}_k(z)$ of the linear equation (2.7), with

$$k^2 = \omega^2 + n^2 k_y^2. \quad (4.4)$$

The angle α is determined by the equalities

$$\omega = k \sin \alpha, \quad nk_y = k \cos \alpha, \quad (4.5)$$

and we have the relationship

$$\Pi \widehat{\mathbf{U}}_{\omega,n}(z) = \mathcal{R}_{-\alpha} \widehat{\mathbf{u}}_k(z).$$

Consequently, for a given $k_y > 0$, the eigenvectors $\mathbf{U}_{\omega,n}$ associated with purely imaginary eigenvalues $\nu = i\omega$ of \mathcal{L}_μ are obtained by rotating with $\mathcal{R}_{-\alpha}$ the elements in the kernel of \mathbf{L}_μ given by (2.8), through the relationship (4.5) and

$$\Pi \mathbf{U}_{\omega,n}(y, z) = e^{ink_y y} \Pi \widehat{\mathbf{U}}_{\omega,n}(z) = e^{ink_y y} \mathcal{R}_{-\alpha} \widehat{\mathbf{u}}_k(z). \quad (4.6)$$

This holds for all eigenvectors $\mathbf{U}_{\omega,n}$ such that $\Pi \mathbf{U}_{\omega,n} \neq 0$. We obtain in this way all purely imaginary eigenvalues of \mathcal{L}_μ with associated eigenvectors \mathbf{U} such that $\Pi \mathbf{U} \neq 0$. Using the properties of the kernel of \mathcal{L}_μ in Section 2.1, we obtain the following result, for $\mu = \mu_0(k)$.

Lemma 4.1. *Assume that k_y and k are positive integers. Then the linear operator $\mathcal{L}_{\mu_0(k)}$ has the complex conjugated purely imaginary eigenvalues*

$$\pm i\omega_n(k), \quad \omega_n(k) = \sqrt{k^2 - n^2 k_y^2} > 0, \quad (4.7)$$

for any integer $0 \leq n < k/k_y$, and the following properties hold.¹

- (i) For $n = 0$, $\omega_0(k) = k$ and the complex conjugated eigenvalues $\pm ik$ are geometrically simple with associated eigenvector of the form

$$\mathbf{U}_{k,0}(y, z) = \widehat{\mathbf{U}}_{k,0}(z),$$

for the eigenvalue ik and the complex conjugated vector for the eigenvalue $-ik$.

¹If $k/k_y \in \mathbb{N}$, then the linear operator has an additional eigenvalue 0 which is geometrically triple. This situation is excluded from our bifurcation analysis.

(ii) For $0 < n < k/k_y$, the complex conjugated eigenvalues $\pm i\omega_n(k)$ are geometrically double with associated eigenvectors of the form

$$\mathbf{U}_{\omega_n(k), \pm n}(y, z) = e^{\pm ink_y y} \widehat{\mathbf{U}}_{\omega_n(k), \pm n}(z),$$

for the eigenvalue $i\omega_n(k)$ and the complex conjugated vectors for the eigenvalue $-i\omega_n(k)$.

(iii) The vectors $\widehat{\mathbf{U}}_{k,0}(z)$ and $\widehat{\mathbf{U}}_{\omega_1(k), \pm 1}(z)$ are given by ²

$$\widehat{\mathbf{U}}_{k,0}(z) = \begin{pmatrix} \frac{i}{k} DV_k \\ 0 \\ V_k \\ -\frac{1}{\mu_0(k)k^2} D^3 V_k \\ 0 \\ \frac{ik}{\mu_0(k)} V_k \\ \frac{1}{\mu_0(k)k^2} (D^2 - k^2)^2 V_k \\ \frac{i}{\mu_0(k)k} (D^2 - k^2)^2 V_k \end{pmatrix}, \quad \widehat{\mathbf{U}}_{\omega_1(k), \pm 1}(z) = \begin{pmatrix} \frac{i\omega_1(k)}{k^2} DV_k \\ \pm \frac{ik_y}{k^2} DV_k \\ V_k \\ -\frac{1}{\mu_0(k)k^2} (D^2 - k_y^2) DV_k \\ \mp \frac{k_y \omega_1(k)}{\mu_0(k)k^2} DV_k \\ \frac{i\omega_1(k)}{\mu_0(k)} V_k \\ \frac{1}{\mu_0(k)k^2} (D^2 - k^2)^2 V_k \\ \frac{i\omega_1(k)}{\mu_0(k)k^2} (D^2 - k^2)^2 V_k \end{pmatrix},$$

where the function V_k is a real-valued solution of the boundary value problem

$$(D^2 - k^2)^3 V_k + \mu_0(k)^2 k^2 V_k = 0, \quad V_k = DV_k = (D^2 - k^2)^2 V_k = 0 \text{ in } z = 0, 1. \quad (4.8)$$

Proof. First, notice that for eigenvectors \mathbf{U} with $\Pi\mathbf{U} = 0$, the eigenvalue problem (4.3) is reduced to the system

$$\begin{aligned} \mu W_\perp &= 0 \\ 0 &= i\omega W_x \\ -\nabla_\perp W_x &= 0 \\ \phi &= 0 \end{aligned}$$

for the variables (W_x, W_\perp, ϕ) . The only nontrivial solution of this system is $(W_x, 0, 0, 0)$, with W_x a constant function, when $\omega = 0$. This implies that 0 is an eigenvalue of \mathcal{L}_μ with associated eigenvector φ_0 given by (3.5), and that all other eigenvalues have associated eigenvectors \mathbf{U} with $\Pi\mathbf{U} \neq 0$. In particular, nonzero purely imaginary eigenvalues of \mathcal{L}_μ and their associated eigenvectors are all determined from the properties of the kernel of the operator \mathbf{L}_μ in Section 2.1 through the equalities (4.4), (4.5), and (4.6).

For $\mu = \mu_0(k)$, we obtain the eigenvalues given by (4.7). The uniqueness, up to a multiplicative constant, of the element in the kernel of $\mathbf{L}_{\mu_0(k)}$ given by (2.8), implies that the eigenvalues $\pm ik$, for $n = 0$, are geometrically simple, and since opposite numbers $\pm n$ give the same pair of eigenvalues $\pm i\omega_n(k)$, for $n \neq 0$, these eigenvalues are geometrically double. Finally, the equalities (4.6) and (2.8), allow to compute the projections $\Pi\mathbf{U}_{k,0}$ and $\Pi\mathbf{U}_{\omega_n(k), \pm n}$ of the eigenvectors and the remaining components (\mathbf{W}, ϕ) are found from (3.1) and (3.2). We obtain the formulas in (iii), which completes the proof of the lemma. \blacksquare

²For our purposes, we do not need the explicit formulas for $n > 1$.

4.3 The center spectrum of \mathcal{L}_{μ_c}

Lemma 4.1 shows that the linear operator \mathcal{L}_{μ_c} has the purely imaginary eigenvalues

$$\pm i\sqrt{k_c^2 - n^2 k_y^2},$$

for positive integers n such that $0 \leq n < k_c/k_y$. Upon decreasing k_y , the number of pairs of eigenvalues increases. Counted with geometric multiplicities, for $k_y > k_c$, there is one pair of purely imaginary eigenvalues with $n = 0$, for $k_c \geq k_y > k_c/2$ there are three pairs with $n = 0, \pm 1$, and more generally for $k_c/N \geq k_y > k_c/(N+1)$ there are $2N+1$ pairs with $n = 0, \pm 1, \dots, \pm N$. For the construction of domain walls we need at least one pair of purely imaginary eigenvalues with opposite Fourier modes $\pm n \neq 0$. We restrict here to the simplest situation when $k_c > k_y > k_c/2$ and \mathcal{L}_{μ_c} has six purely imaginary eigenvalues with Fourier modes $n = 0, \pm 1$.

For notational convenience, we set

$$k_y = k_c \cos \alpha, \quad k_x = k_c \sin \alpha$$

and take $\alpha \in (0, \pi/3)$. In the following lemma we give a complete description of the purely imaginary spectrum of the linear operator \mathcal{L}_{μ_c} .

Lemma 4.2. *Assume that $k_y = k_c \cos \alpha$ with $\alpha \in (0, \pi/3)$. Then the center spectrum $\sigma_c(\mathcal{L}_{\mu_c})$ of the linear operator \mathcal{L}_{μ_c} consists of five eigenvalues,*

$$\sigma_c(\mathcal{L}_{\mu_c}) = \{0, \pm ik_c, \pm ik_x\}, \quad k_x = k_c \sin \alpha, \quad (4.9)$$

with the following properties.

- (i) *The eigenvalue 0 is simple with associated eigenvector φ_0 given by (3.5), which is invariant under the actions of $\mathbf{S}_1, \mathbf{S}_2, \mathbf{S}_3$, and τ_a .*
- (ii) *The complex conjugated eigenvalues $\pm ik_c$ are algebraically double and geometrically simple with associated generalized eigenvectors of the form*

$$\zeta_0 = \widehat{\mathbf{U}}_0(z), \quad \Psi_0 = \widehat{\mathbf{\Psi}}_0(z),$$

for the eigenvalue ik_c and the complex conjugated vectors for the eigenvalue $-ik_c$, such that

$$(\mathcal{L}_{\mu_c} - ik_c)\zeta_0 = \mathbf{0}, \quad (\mathcal{L}_{\mu_c} - ik_c)\Psi_0 = \zeta_0,$$

and

$$\begin{aligned} \mathbf{S}_1 \zeta_0 &= \overline{\zeta_0}, & \mathbf{S}_2 \zeta_0 &= \zeta_0, & \mathbf{S}_3 \zeta_0 &= -\zeta_0, & \tau_a \zeta_0 &= \zeta_0, \\ \mathbf{S}_1 \Psi_0 &= -\overline{\Psi_0}, & \mathbf{S}_2 \Psi_0 &= \Psi_0, & \mathbf{S}_3 \Psi_0 &= -\Psi_0, & \tau_a \Psi_0 &= \Psi_0. \end{aligned}$$

(iii) The complex conjugated eigenvalues $\pm ik_x$ are algebraically quadruple and geometrically double with associated generalized eigenvectors of the form

$$\zeta_{\pm} = e^{\pm ik_y y} \widehat{\mathbf{U}}_{\pm}(z), \quad \Psi_{\pm} = e^{\pm ik_y y} \widehat{\mathbf{\Psi}}_{\pm}(z),$$

for the eigenvalue ik_x and the complex conjugated vectors for the eigenvalue $-ik_x$, such that

$$(\mathcal{L}_{\mu_c} - ik_x)\zeta_{\pm} = \mathbf{0}, \quad (\mathcal{L}_{\mu_c} - ik_x)\Psi_{\pm} = \zeta_{\pm},$$

and

$$\begin{aligned} \mathbf{S}_1 \zeta_+ &= \overline{\zeta_-}, & \mathbf{S}_2 \zeta_+ &= \zeta_-, & \mathbf{S}_3 \zeta_+ &= -\zeta_+, & \tau_a \zeta_+ &= e^{ia} \zeta_+, \\ \mathbf{S}_1 \zeta_- &= \overline{\zeta_+}, & \mathbf{S}_2 \zeta_- &= \zeta_+, & \mathbf{S}_3 \zeta_- &= -\zeta_-, & \tau_a \zeta_- &= e^{-ia} \zeta_-, \\ \mathbf{S}_1 \Psi_+ &= -\overline{\Psi_-}, & \mathbf{S}_2 \Psi_+ &= \Psi_-, & \mathbf{S}_3 \Psi_+ &= -\Psi_+, & \tau_a \Psi_+ &= e^{ia} \Psi_+, \\ \mathbf{S}_1 \Psi_- &= -\overline{\Psi_+}, & \mathbf{S}_2 \Psi_- &= \Psi_+, & \mathbf{S}_3 \Psi_- &= -\Psi_-, & \tau_a \Psi_- &= e^{-ia} \Psi_-. \end{aligned}$$

Proof. The result in Lemma 4.1 shows that $\pm ik_c$ and $\pm ik_x$ are purely imaginary eigenvalues of \mathcal{L}_{μ_c} and the first part of its proof implies that 0 is an eigenvalue of \mathcal{L}_{μ_c} . Since μ_c is the unique global minimum of $\mu_0(k)$, there are no other eigenvalues with zero real part. This proves the property (4.9). Furthermore, the eigenvalue 0 is geometrically simple, with associated eigenvector φ_0 given by (3.5), and the eigenvalues $\pm ik_c$ and $\pm ik_x$ have geometric multiplicities one and two, respectively. The associated eigenvectors ζ_0 and ζ_{\pm} are computed from the formulas in Lemma 4.1, by taking $n = 0$ and $n = \pm 1$, respectively, for $k = k_c$ and $k_y = k_c \cos \alpha$. We obtain

$$\zeta_0 = \widehat{\mathbf{U}}_0(z), \quad \zeta_{\pm} = e^{\pm ik_y y} \widehat{\mathbf{U}}_{\pm}(z),$$

where

$$\widehat{\mathbf{U}}_0(z) = \begin{pmatrix} \frac{i}{k_c} DV \\ 0 \\ V \\ -\frac{1}{\mu_c k_c^2} D^3 V \\ 0 \\ \frac{ik_c}{\mu_c} V \\ \frac{1}{\mu_c k_c^2} (D^2 - k_c^2)^2 V \\ \frac{i}{\mu_c k_c} (D^2 - k_c^2)^2 V \end{pmatrix}, \quad \widehat{\mathbf{U}}_{\pm}(z) = \begin{pmatrix} \frac{i \sin \alpha}{k_c} DV \\ \pm \frac{i \cos \alpha}{k_c} DV \\ V \\ -\frac{1}{k_c^2 \mu_c} (D^2 - k_c^2 \cos^2 \alpha) DV \\ \mp \frac{\sin \alpha \cos \alpha}{\mu_c} DV \\ \frac{ik_c \sin \alpha}{\mu_c} V \\ \frac{1}{\mu_c k_c^2} (D^2 - k_c^2)^2 V \\ \frac{i \sin \alpha}{\mu_c k_c} (D^2 - k_c^2)^2 V \end{pmatrix},$$

and the function V is a real-valued solution of the boundary value problem

$$(D^2 - k_c^2)^3 V + \mu_c^2 k_c^2 V = 0, \quad V = DV = (D^2 - k_c^2)^2 V = 0 \text{ in } z = 0, 1. \quad (4.10)$$

This boundary value problem being equivalent to (2.9)-(2.10) for $\mu = \mu_c$, the function V is positive and symmetric with respect to $z = 1/2$. The latter property and the explicit formulas above imply the symmetry properties of ζ_0 and ζ_{\pm} in (ii) and (iii).

Next, the algebraic multiplicity of the eigenvalue 0 is directly determined by solving the equation

$$\mathcal{L}_{\mu_c} \varphi_1 = \varphi_0.$$

Up to an element in the kernel of \mathcal{L}_{μ_c} , we find

$$\varphi_1 = \left(\frac{\mu_c}{2} z(1-z), 0, 0, 0, 0, 0, 0, 0 \right)^t.$$

Since $\varphi_1 \notin \mathcal{X}$, this proves that the eigenvalue 0 is algebraically simple. The invariance of φ_0 under the actions of \mathbf{S}_1 , \mathbf{S}_2 , \mathbf{S}_3 , and τ_a is easily checked, which completes the proof of part (i).

For the algebraic multiplicities of the nonzero eigenvalues $\pm ik_c$ and $\pm ik_x$, we use their continuation as eigenvalues of $\mathcal{L}_{\mu_0(k)}$, for k close to k_c . The latter eigenvalues are the geometrically simple eigenvalues $\pm ik$ and the geometrically double eigenvalues $\pm i\omega_1(k)$ in Lemma 4.1. In Appendix A.2 we prove that their algebraic multiplicities are equal to their geometric multiplicities. Then a standard continuation argument implies that the eigenvalues $\pm ik_c$ and $\pm ik_x$ of \mathcal{L}_{μ_c} are algebraically double and quadruple, respectively.

Finally, we compute the generalized eigenvectors Ψ_0 and Ψ_{\pm} associated with the eigenvalues ik_c and ik_x , respectively, from the eigenvectors associated with the eigenvalues ik and $i\omega_1(k)$ of $\mathcal{L}_{\mu_0(k)}$ given in Lemma 4.1. Differentiating the eigenvalue problems

$$\mathcal{L}_{\mu_0(k)} \mathbf{U}_{k,0} = ik \mathbf{U}_{k,0}, \quad \mathcal{L}_{\mu_0(k)} \mathbf{U}_{\omega_1(k),\pm 1} = i\omega_1(k) \mathbf{U}_{\omega_1(k),\pm 1},$$

with respect to k at $k = k_c$, and using the properties

$$\mu'_0(k_c) = 0, \quad \omega'_1(k_c) = \frac{k_c}{\sqrt{k_c^2 - k_y^2}} = \frac{1}{\sin \alpha},$$

we obtain the equalities

$$\begin{aligned} (\mathcal{L}_{\mu_c} - ik_c) \left(\frac{d}{dk} \mathbf{U}_{k,0} \Big|_{k=k_c} \right) &= i\zeta_0, \\ (\mathcal{L}_{\mu_c} - ik_x) \left(\frac{d}{dk} \mathbf{U}_{\omega_1(k),\pm 1} \Big|_{k=k_c} \right) &= \frac{i}{\sin \alpha} \zeta_{\pm}. \end{aligned}$$

Consequently, the generalized eigenvectors are given by

$$\Psi_0 = -i \left(\frac{d}{dk} \mathbf{U}_{k,0} \Big|_{k=k_c} \right), \quad \Psi_{\pm} = -i \sin \alpha \left(\frac{d}{dk} \mathbf{U}_{\omega_1(k),\pm 1} \Big|_{k=k_c} \right). \quad (4.11)$$

In particular, they have the same form

$$\Psi_0 = \widehat{\Psi}_0(z), \quad \Psi_{\pm} = e^{\pm ik_y y} \widehat{\Psi}_{\pm}(z),$$

as the eigenvectors $\mathbf{U}_{k,0}$ and $\mathbf{U}_{\omega_1(k),\pm 1}$ given in Lemma 4.1. Furthermore, since the function V_k in the expressions of $\widehat{\mathbf{U}}_{k,0}(z)$ and $\widehat{\mathbf{U}}_{\omega_1(k),\pm 1}(z)$ is symmetric with respect to $z = 1/2$, just as the function V in (4.10), the eigenvectors $\mathbf{U}_{k,0}$ and $\mathbf{U}_{\omega_1(k),\pm 1}$ have the same symmetry properties as the eigenvectors ζ_0 and ζ_{\pm} , respectively. Together with the formulas (4.11), this implies that Ψ_0 and Ψ_{\pm} have the symmetry properties given in (ii) and (iii), and completes the proof of the lemma. \blacksquare

5 Reduction of the nonlinear problem

The next step of our analysis is the center manifold reduction. Using the symmetries of the system (3.3), we identify an eight-dimensional invariant submanifold of the center manifold, which contains the heteroclinic orbits of (3.3) corresponding to domain walls.

5.1 Center manifold reduction

We set $\varepsilon = \mu - \mu_c$ and write the dynamical system (3.3) in the form

$$\partial_x \mathbf{U} = \mathcal{L}_{\mu_c} \mathbf{U} + \mathcal{R}(\mathbf{U}, \varepsilon), \quad (5.1)$$

where

$$\mathcal{R}(\mathbf{U}, \varepsilon) = (\mathcal{L}_\mu - \mathcal{L}_{\mu_c})\mathbf{U} + \mathcal{B}_\mu(\mathbf{U}, \mathbf{U}),$$

is a smooth map from $\mathcal{Z} \times (-\mu_c, \infty)$ into \mathcal{X} , and

$$\mathcal{R}(0, \varepsilon) = 0, \quad D_{\mathbf{U}}\mathcal{R}(0, 0) = 0.$$

In particular, \mathcal{R} satisfies the hypotheses of the center manifold theorem (see [8, Section 2.3.1]). We also have to check two hypotheses on the linear operator \mathcal{L}_{μ_c} . The first one requires that the center spectrum of \mathcal{L}_{μ_c} consists of finitely many purely imaginary eigenvalues with finite algebraic multiplicity and the result in Lemma 4.2 shows that this hypothesis holds. The second one is the estimate on the norm of resolvent of \mathcal{L}_{μ_c} obtained by taking $\mu = \mu_c$ in the lemma below.

Lemma 5.1. *For any $\mu > 0$, there exist positive constants C_μ and ω_μ such that*

$$\|(\mathcal{L}_\mu - i\omega)^{-1}\|_{\mathcal{L}(\mathcal{X})} \leq \frac{C_\mu}{|\omega|}, \quad (5.2)$$

for any real number ω , with $|\omega| > \omega_\mu$.

Proof. We write $\mathcal{L}_\mu = \mathcal{A}_\mu + \mathcal{B}_\mu$, where

$$\mathcal{A}_\mu \mathbf{U} = \begin{pmatrix} -\nabla_\perp \cdot V_\perp \\ \mu W_\perp \\ -\mu^{-1} \Delta_\perp V_x \\ -\mu^{-1} \Delta_\perp V_\perp - \mu^{-1} \nabla_\perp (\nabla_\perp \cdot V_\perp) - \nabla_\perp W_x \\ \phi \\ -\Delta_\perp \theta \end{pmatrix}, \quad \mathcal{B}_\mu \mathbf{U} = \begin{pmatrix} 0 \\ 0 \\ 0 \\ -\theta \mathbf{e}_z \\ 0 \\ -\mu V_z \end{pmatrix}.$$

Since the operator \mathcal{B}_μ is bounded in \mathcal{X} , the resolvent equality

$$(\mathcal{L}_\mu - i\omega)^{-1} = (\mathbb{I} + (\mathcal{A}_\mu - i\omega)^{-1} \mathcal{B}_\mu) (\mathcal{A}_\mu - i\omega)^{-1},$$

implies that it is enough to prove the result for \mathcal{A}_μ . The action of \mathcal{A}_μ on the components (\mathbf{V}, \mathbf{W}) and (θ, ϕ) of \mathbf{U} being decoupled, the operator is diagonal, $\mathcal{A}_\mu = \text{diag}(\mathcal{A}_\mu^{\text{St}}, \mathcal{A}_\mu^{\text{so}})$, where

$\mathcal{A}_\mu^{\text{St}}$ acting on (\mathbf{V}, \mathbf{W}) is a Stokes operator and $\mathcal{A}_\mu^{\text{so}}$ acting on (θ, ϕ) is a Laplace operator. The estimate (5.2) has been proved for the Stokes operator $\mathcal{A}_\mu^{\text{St}}$ in [12, Appendix 2], and it is easily obtained for the Laplace operator $\mathcal{A}_\mu^{\text{so}}$. This implies the result for \mathcal{A}_μ and completes the proof of the lemma. \blacksquare

Denote by \mathcal{X}_c the spectral subspace associated with the center spectrum of \mathcal{L}_{μ_c} , by \mathcal{P}_c the corresponding spectral projection, and set $\mathcal{Z}_h = (\mathbb{I} - \mathcal{P}_c)\mathcal{Z}$. Applying the center manifold theorem [8, Section 2.3.1], for any arbitrary, but fixed, $k \geq 3$, there exists a map $\Phi \in \mathcal{C}^k(\mathcal{X}_c \times \mathbb{R}, \mathcal{Z}_h)$, with

$$\Phi(0, \varepsilon) = 0, \quad D_{\mathbf{U}}\Phi(0, 0) = 0, \quad (5.3)$$

and a neighborhood $\mathcal{U}_1 \times \mathcal{U}_2$ of $(0, 0)$ in $\mathcal{Z} \times \mathbb{R}$ such that for any $\varepsilon \in \mathcal{U}_2$, the manifold

$$\mathcal{M}_c(\varepsilon) = \{\mathbf{U}_c + \Phi(\mathbf{U}_c, \varepsilon); \mathbf{U}_c \in \mathcal{X}_c\}, \quad (5.4)$$

has the following properties:

- (i) $\mathcal{M}_c(\varepsilon)$ is locally invariant, i.e., if \mathbf{U} is a solution of (5.1) satisfying $\mathbf{U}(0) \in \mathcal{M}_c(\varepsilon) \cap \mathcal{U}_1$ and $\mathbf{U}(x) \in \mathcal{U}_1$ for all $x \in [0, L]$, then $\mathbf{U}(x) \in \mathcal{M}_c(\varepsilon)$ for all $x \in [0, L]$;
- (ii) $\mathcal{M}_c(\varepsilon)$ contains the set of bounded solutions of (5.1) staying in \mathcal{U}_1 for all $x \in \mathbb{R}$, i.e., if \mathbf{U} is a solution of (5.1) satisfying $\mathbf{U}(x) \in \mathcal{U}_1$ for all $x \in \mathbb{R}$, then $\mathbf{U}(0) \in \mathcal{M}_c(\varepsilon)$;
- (iii) the invariant dynamics on the center manifold is determined by the reduced system

$$\frac{d\mathbf{U}_c}{dx} = \mathcal{L}_{\mu_c}|_{\mathcal{X}_c} \mathbf{U}_c + \mathcal{P}_c \mathcal{R}(\mathbf{U}_c + \Phi(\mathbf{U}_c, \varepsilon), \varepsilon) \stackrel{\text{def}}{=} f(\mathbf{U}_c, \varepsilon), \quad (5.5)$$

where

$$f(0, \varepsilon) = 0, \quad D_{\mathbf{U}_c} f(0, 0) = \mathcal{L}_{\mu_c}|_{\mathcal{X}_c};$$

- (iv) the reduced system (5.5) inherits the symmetries of (5.1), i.e., the reduced vector field $f(\cdot, \varepsilon)$ anti-commutes with \mathbf{S}_1 , commutes with \mathbf{S}_2 , \mathbf{S}_3 , and τ_a , and is invariant under the action of \mathbf{T}_b .

An immediate consequence of these properties is that the heteroclinic solutions of (5.1) representing domain walls belong to the center manifold $\mathcal{M}_c(\varepsilon)$, for sufficiently small ε , and can be constructed as solutions of the reduced system (5.5).

5.2 Reduced system

According to Lemma 4.2, the center space \mathcal{X}_c has dimension 13 and we can write

$$\begin{aligned} \mathbf{U}_c = & w\varphi_0 + A_0\zeta_0 + B_0\Psi_0 + A_+\zeta_+ + B_+\Psi_+ + A_-\zeta_- + B_-\Psi_- \\ & + \overline{A_0\zeta_0} + \overline{B_0\Psi_0} + \overline{A_+\zeta_+} + \overline{B_+\Psi_+} + \overline{A_-\zeta_-} + \overline{B_-\Psi_-}, \end{aligned} \quad (5.6)$$

where $w \in \mathbb{R}$ and $X = (A_0, B_0, A_+, B_+, A_-, B_-) \in \mathbb{C}^6$. Then the reduced system (5.5) takes the form

$$\frac{dw}{dx} = h(w, X, \bar{X}, \varepsilon), \quad (5.7)$$

$$\frac{dX}{dx} = F(w, X, \bar{X}, \varepsilon), \quad (5.8)$$

in which h is real-valued and $F = (f_0, g_0, f_+, g_+, f_-, g_-)$ has six complex-valued components. This system is completed by the complex conjugated equation of (5.8) for \bar{X} . Notice that the symmetries of the reduced system act on these variables through

$$\mathbf{S}_1(w, A_0, B_0, A_+, B_+, A_-, B_-) = (w, \bar{A}_0, -\bar{B}_0, \bar{A}_-, -\bar{B}_-, \bar{A}_+, -\bar{B}_+),$$

$$\mathbf{S}_2(w, A_0, B_0, A_+, B_+, A_-, B_-) = (w, A_0, B_0, A_-, B_-, A_+, B_+),$$

$$\mathbf{S}_3(w, A_0, B_0, A_+, B_+, A_-, B_-) = (w, -A_0, -B_0, -A_+, -B_+, -A_-, -B_-),$$

$$\tau_a(w, A_0, B_0, A_+, B_+, A_-, B_-) = (w, A_0, B_0, e^{ia} A_+, e^{ia} B_+, e^{-ia} A_-, e^{-ia} B_-),$$

$$\mathbf{T}_b(w, A_0, B_0, A_+, B_+, A_-, B_-) = (w + b, A_0, B_0, A_+, B_+, A_-, B_-).$$

Using the last three symmetries above, we obtain the following result.

Lemma 5.2. *For any ε sufficiently small, the reduced system (5.7)-(5.8) has the following properties:*

- (i) *the reduced vector field (h, F) does not depend on w ;*
- (ii) *the components (f_0, g_0) of F are odd functions in the variables $(A_0, B_0, \bar{A}_0, \bar{B}_0)$ and even functions in the variables $(A_+, B_+, \bar{A}_+, \bar{B}_+, A_-, B_-, \bar{A}_-, \bar{B}_-)$;*
- (iii) *the components (f_+, g_+, f_-, g_-) of F are even functions in the variables $(A_0, B_0, \bar{A}_0, \bar{B}_0)$ and odd functions in the variables $(A_+, B_+, \bar{A}_+, \bar{B}_+, A_-, B_-, \bar{A}_-, \bar{B}_-)$.*

Proof. Due to the invariance of the reduced system (5.7)- (5.8) under the action of \mathbf{T}_b , the vector field (h, F) satisfies

$$(h, F)(w + b, X, \bar{X}, \varepsilon) = (h, F)(w, X, \bar{X}, \varepsilon),$$

for any real number b . This implies that (h, F) does not depend on w and proves (i).

Next, the vector field F , which only depends on X and \bar{X} , commutes with the symmetries τ_π and $\mathbf{S}_3\tau_\pi$ acting on these components through

$$\tau_\pi(A_0, B_0, A_+, B_+, A_-, B_-) = (A_0, B_0, -A_+, -B_+, -A_-, -B_-),$$

$$\mathbf{S}_3\tau_\pi(A_0, B_0, A_+, B_+, A_-, B_-) = (-A_0, -B_0, A_+, B_+, A_-, B_-).$$

The first equality implies the parity properties of the components $(f_0, g_0, f_+, g_+, f_-, g_-)$ of F in the variables $(A_+, B_+, \bar{A}_+, \bar{B}_+, A_-, B_-, \bar{A}_-, \bar{B}_-)$ and the second one implies the parity properties in the variables $(A_0, B_0, \bar{A}_0, \bar{B}_0)$. This proves the properties (ii) and (iii). \blacksquare

An immediate consequence of the first property in the lemma above being that the two equations (5.7) and (5.8) are decoupled, we can first solve (5.8) for X , and then integrate (5.7) to determine w . We therefore restrict our existence analysis to the equation

$$\frac{dX}{dx} = F(X, \bar{X}, \varepsilon), \quad (5.9)$$

which together with the complex conjugate equation for \bar{X} form a 12-dimensional system. For this system, the parity properties of the vector field F in Lemma 5.2, imply that there exist two invariant subspaces:

$$E_0 = \{(X, \bar{X}), X \in \mathbb{C}^6; (A_+, B_+, A_-, B_-) = 0\},$$

which is 4-dimensional, and

$$E_{\pm} = \{(X, \bar{X}), X \in \mathbb{C}^6; (A_0, B_0) = 0\},$$

which is 8-dimensional. Each of these subspaces give an invariant submanifold of the center manifold. Solutions in the submanifold associated with E_0 are invariant under the action of τ_{π} and solutions in the submanifold associated with E_{\pm} are invariant under the action of $\mathbf{S}_3\tau_{\pi}$. It is not difficult to check that by restricting to E_0 we obtain solutions of the full dynamical system (3.3) which do not depend on y , whereas by restricting to E_{\pm} we find truly three-dimensional solutions. For the construction of domain walls we restrict to the subspace E_{\pm} .

6 Normal form analysis

We write the reduced system (5.9) restricted to the invariant 8-dimensional subspace E_{\pm} in the form

$$\frac{dY}{dx} = G(Y, \bar{Y}, \varepsilon), \quad (6.1)$$

in which $Y = (A_+, B_+, A_-, B_-) \in \mathbb{C}^4$. Taking into account the properties of the reduced system (5.5), the formula (5.6), and the choice for the generalized eigenvectors in Lemma 4.2, we find

$$G(0, 0, \varepsilon) = 0, \quad D_Y G(0, 0, 0) = L_0, \quad D_{\bar{Y}} G(0, 0, 0) = 0,$$

where L_0 is a Jordan matrix acting on Y through

$$L_0 = \begin{pmatrix} ik_x & 1 & 0 & 0 \\ 0 & ik_x & 0 & 0 \\ 0 & 0 & ik_x & 1 \\ 0 & 0 & 0 & ik_x \end{pmatrix}. \quad (6.2)$$

Using a general normal form theorem for parameter-dependent vector fields in the presence of symmetries (e.g., see [8, Chapter 3]), we determine a normal form of the system (6.1) up to cubic order.

6.1 Cubic normal form of the reduced system

The following result is valid for any system of the form (6.1) which has a linear part as in (6.2) and the symmetries \mathbf{S}_1 , \mathbf{S}_2 , \mathbf{S}_3 , and τ_a given in Section 5.2.

Lemma 6.1. *For any $k \geq 3$, there exist neighborhoods \mathcal{V}_1 and \mathcal{V}_2 of 0 in \mathbb{C}^4 and \mathbb{R} , respectively, such that for any $\varepsilon \in \mathcal{V}_2$, there is a polynomial $\mathbf{P}_\varepsilon : \mathbb{C}^4 \times \overline{\mathbb{C}^4} \rightarrow \mathbb{C}^4$ of degree 3 in the variables (Y, \overline{Y}) , such that for $Y \in \mathcal{V}_1$, the polynomial change of variable*

$$Y = Z + \mathbf{P}_\varepsilon(Z, \overline{Z}), \quad (6.3)$$

transforms the equation (6.1) into the normal form

$$\frac{dZ}{dx} = L_0 Z + N(Z, \overline{Z}, \varepsilon) + \rho(Z, \overline{Z}, \varepsilon), \quad (6.4)$$

with the following properties:

(i) *the map ρ belongs to $\mathcal{C}^k(\mathcal{V}_1 \times \overline{\mathcal{V}_1} \times \mathcal{V}_2, \mathbb{C}^4)$, and*

$$\rho(Z, \overline{Z}, \varepsilon) = O(|\varepsilon|^2 \|Z\| + \varepsilon \|Z\|^3 + \|Z\|^5);$$

(ii) *both $N(\cdot, \cdot, \varepsilon)$ and $\rho(\cdot, \cdot, \varepsilon)$ anti-commute with \mathbf{S}_1 and commute with \mathbf{S}_2 , \mathbf{S}_3 , and τ_a , for any $\varepsilon \in \mathcal{V}_2$;*

(iii) *the four components (N_+, M_+, N_-, M_-) of N are of the form*

$$\begin{aligned} N_+ &= iA_+ P_+ + A_- R_+ \\ M_+ &= iB_+ P_+ + B_- R_+ + A_+ Q_+ + iA_- S_+ \\ N_- &= iA_- P_- - A_+ \overline{R_+} \\ M_- &= iB_- P_- - B_+ \overline{R_+} + A_- Q_- - iA_+ \overline{S_+} \end{aligned}$$

in which

$$\begin{aligned} P_+ &= \beta_0 \varepsilon + \beta_1 A_+ \overline{A_+} + i\beta_2 (A_+ \overline{B_+} - \overline{A_+} B_+) + \beta_3 A_- \overline{A_-} + i\beta_4 (A_- \overline{B_-} - \overline{A_-} B_-) \\ P_- &= \beta_0 \varepsilon + \beta_3 A_+ \overline{A_+} + i\beta_4 (A_+ \overline{B_+} - \overline{A_+} B_+) + \beta_1 A_- \overline{A_-} + i\beta_2 (A_- \overline{B_-} - \overline{A_-} B_-) \\ Q_+ &= b_0 \varepsilon + b_1 A_+ \overline{A_+} + ib_2 (A_+ \overline{B_+} - \overline{A_+} B_+) + b_3 A_- \overline{A_-} + ib_4 (A_- \overline{B_-} - \overline{A_-} B_-) \\ Q_- &= b_0 \varepsilon + b_3 A_+ \overline{A_+} + ib_4 (A_+ \overline{B_+} - \overline{A_+} B_+) + b_1 A_- \overline{A_-} + ib_2 (A_- \overline{B_-} - \overline{A_-} B_-) \\ R_+ &= \gamma_5 (A_+ \overline{B_-} - \overline{A_-} B_+), \quad S_+ = c_5 (A_+ \overline{B_-} - \overline{A_-} B_+), \end{aligned}$$

where (A_+, B_+, A_-, B_-) are the four components of Z and the coefficients β_j , b_j , γ_5 and c_5 are all real.

Proof. The existence of the polynomial \mathbf{P}_ε and the first two properties in Lemma 6.1 follow from the general normal form theorems in [8, Sections 3.2.1, 3.3.1, and 3.3.2]. In addition, $N(\cdot, \cdot, \varepsilon)$ is an odd polynomial of degree 3 such that $N(0, 0, \varepsilon) = 0$ and the identity

$$D_Z N(Z, \bar{Z}, \varepsilon) L_0^* Z + D_{\bar{Z}} N(Z, \bar{Z}, \varepsilon) \bar{L}_0^* \bar{Z} = L_0^* N(Z, \bar{Z}, \varepsilon), \quad (6.5)$$

in which L_0^* is the adjoint of L_0 , holds for any $Z \in \mathbb{C}^4$ and $\varepsilon \in \mathcal{V}_2$. We write

$$N(Z, \bar{Z}, \varepsilon) = N_1(Z, \bar{Z})\varepsilon + N_3(Z, \bar{Z}),$$

where N_1 and N_3 denote the linear and cubic terms, respectively, of N . It is now straightforward to check that the linear part N_1 has the form in Lemma 6.1 (iii), and it remains to check the cubic terms N_3 .

We set $N_3 = (N_+, M_+, N_-, M_-)$. Then the identity (6.5) becomes

$$\begin{aligned} (\mathcal{D}^* + ik_x)N_+ &= 0, & (\mathcal{D}^* + ik_x)M_+ &= N_+, \\ (\mathcal{D}^* + ik_x)N_- &= 0, & (\mathcal{D}^* + ik_x)M_- &= N_-, \end{aligned}$$

in which

$$\begin{aligned} \mathcal{D}^* &= -ik_x A_+ \frac{\partial}{\partial A_+} + (A_+ - ik_x B_+) \frac{\partial}{\partial B_+} - ik_x A_- \frac{\partial}{\partial A_-} + (A_- - ik_x B_-) \frac{\partial}{\partial B_-} \\ &\quad + ik_x \bar{A}_+ \frac{\partial}{\partial \bar{A}_+} + (\bar{A}_+ + ik_x \bar{B}_+) \frac{\partial}{\partial \bar{B}_+} + ik_x \bar{A}_- \frac{\partial}{\partial \bar{A}_-} + (\bar{A}_- + ik_x \bar{B}_-) \frac{\partial}{\partial \bar{B}_-}. \end{aligned}$$

Due to the equivariance of the normal form under the action of the symmetry \mathbf{S}_2 , it is enough to determine (N_+, M_+) , the components (N_-, M_-) being obtained by switching the indices $+$ and $-$ in the expressions of (N_+, M_+) .

Cubic monomials are of the form

$$A_+^{p_+} \bar{A}_+^{q_+} B_+^{r_+} \bar{B}_+^{s_+} A_-^{p_-} \bar{A}_-^{q_-} B_-^{r_-} \bar{B}_-^{s_-},$$

with nonnegative exponents such that

$$p_+ + q_+ + r_+ + s_+ + p_- + q_- + r_- + s_- = 3. \quad (6.6)$$

We claim that the cubic monomials in N_+ and M_+ also satisfy

$$p_+ - q_+ + r_+ - s_+ + p_- - q_- + r_- - s_- = 1. \quad (6.7)$$

Indeed, for any monomial as above we have

$$\begin{aligned} \mathcal{D}^* \left(A_+^{p_+} \bar{A}_+^{q_+} B_+^{r_+} \bar{B}_+^{s_+} A_-^{p_-} \bar{A}_-^{q_-} B_-^{r_-} \bar{B}_-^{s_-} \right) &= \\ & -ik_x (p_+ - q_+ + r_+ - s_+ + p_- - q_- + r_- - s_-) A_+^{p_+} \bar{A}_+^{q_+} B_+^{r_+} \bar{B}_+^{s_+} A_-^{p_-} \bar{A}_-^{q_-} B_-^{r_-} \bar{B}_-^{s_-} \\ & + r_+ A_+^{p_+ + 1} \bar{A}_+^{q_+} B_+^{r_+ - 1} \bar{B}_+^{s_+} A_-^{p_-} \bar{A}_-^{q_-} B_-^{r_-} \bar{B}_-^{s_-} \\ & + s_+ A_+^{p_+} \bar{A}_+^{q_+ + 1} B_+^{r_+} \bar{B}_+^{s_+ - 1} A_-^{p_-} \bar{A}_-^{q_-} B_-^{r_-} \bar{B}_-^{s_-} \\ & + r_- A_+^{p_+} \bar{A}_+^{q_+} B_+^{r_+} \bar{B}_+^{s_+} A_-^{p_- + 1} \bar{A}_-^{q_-} B_-^{r_- - 1} \bar{B}_-^{s_-} \\ & + s_- A_+^{p_+} \bar{A}_+^{q_+} B_+^{r_+} \bar{B}_+^{s_+} A_-^{p_-} \bar{A}_-^{q_- + 1} B_-^{r_-} \bar{B}_-^{s_- - 1}, \end{aligned}$$

implying that the subspace of monomials for which the sum in the left hand side of (6.7) is constant is invariant under the action of \mathcal{D}^* . Ordering the monomials by decreasing exponents p_+ , q_+ , r_+ , s_+ , p_- , q_- , r_- , and s_- , this action is represented by a lower triangular matrix with equal elements on the diagonal given by

$$-ik_x(p_+ - q_+ + r_+ - s_+ + p_- - q_- + r_- - s_-).$$

Consequently, the polynomials N_+ and M_+ , which belong to the kernel and generalized kernel of $\mathcal{D}_* + ik_x$, respectively, belong to the subspace for which (6.7) holds. This proves the claim. Furthermore, the commutativity of N_3 and τ_a , implies that monomials in (N_+, M_+) also satisfy

$$p_+ - q_+ + r_+ - s_+ - p_- + q_- - r_- + s_- = 1. \quad (6.8)$$

Collecting all possible monomials in (N_+, M_+) for which the conditions (6.6)-(6.8) hold, we compute:

$$\begin{aligned} (\mathcal{D}^* + ik_x)(A_+^2 \overline{A_+}) &= 0, \\ (\mathcal{D}^* + ik_x)(A_+^2 \overline{B_+}) &= (\mathcal{D}^* + ik_x)(A_+ \overline{A_+} B_+) = A_+^2 \overline{A_+}, \\ (\mathcal{D}^* + ik_x)(A_+ B_+ \overline{B_+}) &= A_+^2 \overline{B_+} + A_+ \overline{A_+} B_+, \quad (\mathcal{D}^* + ik_x)(\overline{A_+} B_+^2) = 2A_+ \overline{A_+} B_+, \\ (\mathcal{D}^* + ik_x)(B_+^2 \overline{B_+}) &= 2A_+ B_+ \overline{B_+} + \overline{A_+} B_+^2, \end{aligned}$$

and

$$\begin{aligned} (\mathcal{D}^* + ik_x)(A_+ A_- \overline{A_-}) &= 0, \\ (\mathcal{D}^* + ik_x)(A_+ A_- \overline{B_-}) &= (\mathcal{D}^* + ik_x)(A_+ \overline{A_-} B_-) = (\mathcal{D}^* + ik_x)(B_+ A_- \overline{A_-}) = A_+ A_- \overline{A_-} \\ (\mathcal{D}^* + ik_x)(A_+ B_- \overline{B_-}) &= A_+ A_- \overline{B_-} + A_+ \overline{A_-} B_-, \\ (\mathcal{D}^* + ik_x)(B_+ A_- \overline{B_-}) &= A_+ A_- \overline{B_-} + B_+ A_- \overline{A_-}, \\ (\mathcal{D}^* + ik_x)(B_+ \overline{A_-} B_-) &= A_+ \overline{A_-} B_- + B_+ A_- \overline{A_-}, \\ (\mathcal{D}^* + ik_x)(B_+ B_- \overline{B_-}) &= A_+ B_- \overline{B_-} + B_+ A_- \overline{B_-} + B_+ \overline{A_-} B_-. \end{aligned}$$

Since N_+ and M_+ are necessarily linear combinations of these 14 monomials, the equalities above imply that they are of the form

$$\begin{aligned} N_+ &= A_+ \tilde{P}_+(u_1, u_2, u_3, u_4) + A_- \tilde{R}_+(u_5), \\ M_+ &= B_+ \tilde{P}_+(u_1, u_2, u_3, u_4) + B_- \tilde{R}_+(u_5) + A_+ \tilde{Q}_+(u_1, u_2, u_3, u_4) + A_- \tilde{S}_+(u_5), \end{aligned}$$

with \tilde{P}_+ , \tilde{R}_+ , \tilde{Q}_+ , \tilde{S}_+ linear in their arguments, which are the quadratic expressions

$$\begin{aligned} u_1 &= A_+ \overline{A_+}, \quad u_2 = i(A_+ \overline{B_+} - \overline{A_+} B_+), \quad u_3 = A_- \overline{A_-}, \\ u_4 &= i(A_- \overline{B_-} - \overline{A_-} B_-), \quad u_5 = (A_+ \overline{B_-} - \overline{A_-} B_+). \end{aligned}$$

This proves the expressions of N_+ and M_+ in (iii). Finally, taking into account the action of the reversibility \mathbf{S}_1 , it is straightforward to check that the coefficients β_j , b_j , γ_5 , and c_5 are real. \blacksquare

6.2 Leading order system

We further transform the normal form (6.4) by taking new variables

$$\hat{x} = |\varepsilon|^{1/2}x, \quad A_{\pm}(x) = e^{ik_x x}|\varepsilon|^{1/2}C_{\pm}(\hat{x}), \quad B_{\pm}(x) = e^{ik_x x}|\varepsilon|D_{\pm}(\hat{x}). \quad (6.9)$$

We obtain the first order system,

$$\begin{aligned} C'_+ &= D_+ + \hat{f}_+(C_{\pm}, D_{\pm}, \overline{C_{\pm}}, \overline{D_{\pm}}, e^{\pm ik_x \hat{x}/|\varepsilon|^{1/2}}, |\varepsilon|^{1/2}, \varepsilon), \\ D'_+ &= (b_0 \text{sign}(\varepsilon) + b_1|C_+|^2 + b_3|C_-|^2) C_+ + \hat{g}_+(C_{\pm}, D_{\pm}, \overline{C_{\pm}}, \overline{D_{\pm}}, e^{\pm ik_x \hat{x}/|\varepsilon|^{1/2}}, |\varepsilon|^{1/2}, \varepsilon), \\ C'_- &= D_- + \hat{f}_-(C_{\pm}, D_{\pm}, \overline{C_{\pm}}, \overline{D_{\pm}}, e^{\pm ik_x \hat{x}/|\varepsilon|^{1/2}}, |\varepsilon|^{1/2}, \varepsilon), \\ D'_- &= (b_0 \text{sign}(\varepsilon) + b_3|C_+|^2 + b_1|C_-|^2) C_- + \hat{g}_-(C_{\pm}, D_{\pm}, \overline{C_{\pm}}, \overline{D_{\pm}}, e^{\pm ik_x \hat{x}/|\varepsilon|^{1/2}}, |\varepsilon|^{1/2}, \varepsilon), \end{aligned}$$

where \hat{f}_+ , \hat{g}_+ , \hat{f}_- , \hat{g}_- are of order $O(|\varepsilon|^{1/2}(|C_{\pm}| + |D_{\pm}|))$ and C^k -functions in their arguments. Solving the first and the third equations for (D_+, D_-) , we rewrite this system as a second order system

$$C''_+ = (b_0 \text{sign}(\varepsilon) + b_1|C_+|^2 + b_3|C_-|^2) C_+ + \hat{h}_+(C_{\pm}, C'__{\pm}, \overline{C_{\pm}}, \overline{C'__{\pm}}, e^{\pm ik_x \hat{x}/|\varepsilon|^{1/2}}, |\varepsilon|^{1/2}, \varepsilon), \quad (6.10)$$

$$C''_- = (b_0 \text{sign}(\varepsilon) + b_3|C_+|^2 + b_1|C_-|^2) C_- + \hat{h}_-(C_{\pm}, C'__{\pm}, \overline{C_{\pm}}, \overline{C'__{\pm}}, e^{\pm ik_x \hat{x}/|\varepsilon|^{1/2}}, |\varepsilon|^{1/2}, \varepsilon), \quad (6.11)$$

in which \hat{h}_+ and \hat{h}_- are of order $O(|\varepsilon|^{1/2}(|C_{\pm}| + |C'_{\pm}|))$ and C^k -functions in their arguments. Notice that both systems inherit the symmetries of the normal form (6.4).

Lemma 6.2. *The coefficients b_0 , b_1 , and b_3 in the system (6.10)-(6.11) have the following properties:*

- (i) $b_0 < 0$ and $b_1 > 0$, for any Prandtl number \mathcal{P} and any angle $\alpha \in (0, \pi/3)$;
- (ii) for any Prandtl number \mathcal{P} , there exists an angle $\alpha_*(\mathcal{P}) \in (0, \pi/3]$ such that $b_1 < b_3 < 3b_1$, for any $\alpha \in (0, \alpha_*(\mathcal{P}))$.

Proof. We compute the coefficient b_0 from the eigenvalues of the matrix obtained by linearizing the normal form (6.4) at $Z = 0$. The eigenvalues of this matrix are the continuation of the eigenvalues $\pm ik_x$ of \mathcal{L}_{μ_c} as eigenvalues of \mathcal{L}_{μ} for $\mu = \mu_c + \varepsilon$ and sufficiently small ε . Since $\mu_c = \mu_0(k_c)$ is a minimum of $\mu_0(k)$, for $\varepsilon > 0$, there exist $k_1 < k_c < k_2$ such that $\mu = \mu_0(k_1) = \mu_0(k_2)$ and the operator \mathcal{L}_{μ} has the purely imaginary eigenvalues $\pm i\omega_1(k_1)$ and $\pm i\omega_1(k_2)$ in Lemma 4.1. Computing the eigenvalues of the normal form (6.4) we obtain the relationship

$$i\omega_1(k_1) = i \left(k_x - \sqrt{-b_0\varepsilon} + O(\varepsilon) \right). \quad (6.12)$$

Since the eigenvalues are purely imaginary, this proves that $b_0 < 0$.

As a consequence of the existence of rolls we have that $b_0 b_1 < 0$. Indeed, for any $\mu > \mu_c$ sufficiently close to μ_c , the rotated roll $\mathcal{R}_{-\alpha}(\mathbf{U}_{k_c, \mu}^*)$ in Section 4.1 is a solution of the dynamical

system (3.3) and belongs to the center submanifold associated with the subspace E_{\pm} . From the classical result in Section 2.2, we obtain that

$$\mathcal{R}_{-\alpha}(\mathbf{U}_{k_c, \mu}^*)(x, y, z) = \varepsilon^{1/2} e^{i(k_x x + k_y y)} \widehat{\mathbf{u}}^*(z) + \varepsilon^{1/2} e^{-i(k_x x + k_y y)} \overline{\widehat{\mathbf{u}}^*(z)} + O(\varepsilon),$$

with $\varepsilon = \mu - \mu_c > 0$ and some complex-valued function $\widehat{\mathbf{u}}^*(z)$ which can be determined from the expression of $\boldsymbol{\xi}_0$ in Section 2.1. Taking into account the center manifold reduction, the normal transformation, and the change of variables (6.9), we conclude that the system (6.10)-(6.11) has a nontrivial equilibrium $(c_+^*, 0)$ when $\varepsilon = 0$. Since $\text{sign}(\varepsilon) > 0$, this implies that $b_0 b_1 < 0$. Consequently, we have that $b_1 > 0$.

Finally, the result in the second part of the lemma is an immediate consequence of the property (B.12) proved in Appendix B.4, which shows that the limit as α tends to 0 of the quotient b_3/b_1 is equal to 2. \blacksquare

The existence proof in the next section requires that the quotient

$$g = \frac{b_3}{b_1} \tag{6.13}$$

takes values in the interval $(1, 4 + \sqrt{13})$. The lemma above shows that this property holds at least for small angles $\alpha \in (0, \alpha_*(\mathcal{P}))$, for some $\alpha_*(\mathcal{P}) \in (0, \pi/3]$, and any positive Prandtl number \mathcal{P} . In Appendix B.5 we use the package Maple to compute symbolically the quotient g . It turns out that the inequality $g > 1$ holds for any Prandtl number $\mathcal{P} > 0$ and any angle $\alpha \in (0, \pi/3)$, and that the inequality $g < 4 + \sqrt{13}$ holds in a region of the (α, \mathcal{P}) -plane which includes all positive values of the Prandtl number \mathcal{P} , for sufficiently small angles $\alpha \leq \alpha_*$, with $\alpha_* \approx \pi/9.112$, and all angles $\alpha \in (0, \pi/3)$, for sufficiently large Prandtl numbers $\mathcal{P} \geq \mathcal{P}_*$, with $\mathcal{P}_* \approx 0.126$ (see Figure 6.1).

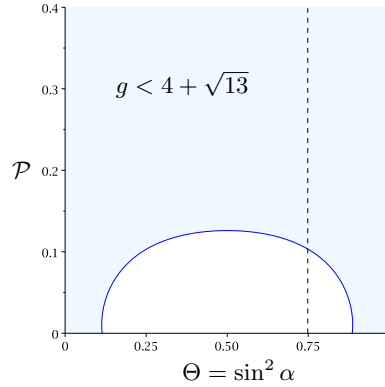


Figure 6.1: In the (Θ, \mathcal{P}) -plane, with $\Theta = \sin^2 \alpha$, Maple plot of the curve along which $g = 4 + \sqrt{13}$, for $\Theta \in (0, 1)$. The inequality $g < 4 + \sqrt{13}$ holds in the shaded regions, whereas the inequality $g > 1$ holds everywhere. Domain walls are constructed in the shaded region situated to the left of the vertical line $\Theta = \sin^2(\pi/3) = 0.75$.

Remark 6.3. Replacing the formula for $\omega_1(k_1)$ in Lemma 4.1 and the equality $\varepsilon = \mu_0(k_1) - \mu_c$ into (6.12), we obtain

$$k_x - \omega_1(k_1) = k_c \sin \alpha - \sqrt{k_1^2 - k_c^2 \cos^2 \alpha} = \sqrt{-b_0} \sqrt{\mu_0(k_1) - \mu_c} + O(\mu_0(k_1) - \mu_c),$$

from which we can determine the value of b_0 ,

$$b_0 = -\frac{2}{\mu_0''(k_c) \sin^2 \alpha} \approx -\frac{0.319}{\sin^2 \alpha} < 0.$$

7 Existence of domain walls

Following the approach developed in [10] for the reduced system obtained in the case of the Swift-Hohenberg equation, we construct a reversible heteroclinic solution for the system (6.10)-(6.11), which then corresponds to a symmetric domain wall for the Bénard-Rayleigh problem. We start by constructing a heteroclinic solution for the leading order system ($\varepsilon = 0$) and then using the implicit function theorem we show that it persists for the full system. In contrast to the reduced system in [10] which was 12-dimensional, we only have to consider here the 8-dimensional subsystem (6.10)-(6.11). This simplifies parts of the proofs. A second difference is that here the quotient g may take different values depending on the Prandtl number \mathcal{P} and the angle α (see Figure 6.1), whereas $g = 2$ in [10]. It turns out that the property of the leading order heteroclinic in Lemma 7.1 below, which was easily checked in [10], is enough to make the arguments work. However, this property requires that the quotient g belongs to the interval $(1, 4 + \sqrt{13})$, which restricts our existence result to the values of the Prandtl number \mathcal{P} and the angle α indicated in Figure 6.1. We recall below the main steps and refer to [10] for the details of proofs.

We assume $\varepsilon > 0$, so that rolls exist. For convenience, we rescale variables and coordinates by taking

$$\tilde{x} = |b_0|^{1/2} \hat{x}, \quad C_{\pm}(\hat{x}) = \left| \frac{b_0}{b_1} \right|^{1/2} \tilde{C}_{\pm}(\tilde{x}),$$

and, after dropping the tilde, we obtain the system

$$C_+'' = (-1 + |C_+|^2 + g|C_-|^2) C_+ + h_+(C_{\pm}, C_{\pm}', \overline{C_{\pm}}, \overline{C_{\pm}'}, e^{\pm i k_x x / |b_0 \varepsilon|^{1/2}}, |\varepsilon|^{1/2}), \quad (7.1)$$

$$C_-'' = (-1 + g|C_+|^2 + |C_-|^2) C_- + h_-(C_{\pm}, C_{\pm}', \overline{C_{\pm}}, \overline{C_{\pm}'}, e^{\pm i k_x x / |b_0 \varepsilon|^{1/2}}, |\varepsilon|^{1/2}), \quad (7.2)$$

with g given by (6.13). The nonautonomous terms h_+ and h_- are of order $O(|\varepsilon|^{1/2}(|C_{\pm}| + |C_{\pm}'|))$ and C^k -functions in their arguments, due to the assumption $\varepsilon > 0$.

7.1 Leading order heteroclinic

Consider the leading order system

$$C_+'' = (-1 + |C_+|^2 + g|C_-|^2) C_+, \quad (7.3)$$

$$C_-'' = (-1 + g|C_+|^2 + |C_-|^2) C_-, \quad (7.4)$$

obtained by setting $\varepsilon = 0$ in (7.1)-(7.2). Under the assumption that $g > 1$ ³, it has been shown in [27] that the system (7.3)-(7.4) possesses a heteroclinic orbit (C_+^*, C_-^*) . The two components C_+^* and C_-^* are smooth real-valued functions defined on \mathbb{R} and have the following properties:

- (i) $\lim_{x \rightarrow -\infty} (C_+^*(x), C_-^*(x)) = (1, 0)$ and $\lim_{x \rightarrow \infty} (C_+^*(x), C_-^*(x)) = (0, 1)$;
- (ii) $C_+^*(x) = C_-^*(-x), \quad \forall x \in \mathbb{R}$;
- (iii) $C_+^*(x)^2 + C_-^*(x)^2 \leq 1$ and $C_+^*(x) + C_-^*(x) \geq \min(1, 2/\sqrt{g+1}), \quad \forall x \in \mathbb{R}$;
- (iv) $(C_+^{*'}(x))^2 + (C_-^{*'}(x))^2 = \frac{1}{2} (C_+^*(x)^2 + C_-^*(x)^2 - 1)^2 + (g-1)C_+^*(x)^2 C_-^*(x)^2, \quad \forall x \in \mathbb{R}$.

The latter property is a consequence of the Hamiltonian structure of the system (7.3)-(7.4), which was one of the key ingredients in the existence proof in [27]. In addition to these properties, we need the following result.

Lemma 7.1. *Assume that $g \in (1, 4 + \sqrt{13})$. Then the heteroclinic solution (C_+^*, C_-^*) of the system (7.3)-(7.4) satisfies the inequality*

$$3C_+^{*2}(x) + gC_-^{*2}(x) > 1, \quad \forall x \in \mathbb{R}. \quad (7.5)$$

Proof. For $g \in (3/2, 4 + \sqrt{13})$ the property (7.5) is an immediate consequence of the second inequality in the property (iii) above. We set

$$f_g(x) = 3C_+^{*2}(x) + gC_-^{*2}(x) - 1,$$

so that f_g is a smooth function defined on \mathbb{R} and f_g is positive for any $g \in (3/2, 4 + \sqrt{13})$. Assuming that there exists $g \in (1, 3/2]$ such that (7.5) does not hold, since f_g has positive limits at $x = \pm\infty$,

$$\lim_{x \rightarrow -\infty} f_g(x) = 2, \quad \lim_{x \rightarrow \infty} f_g(x) = g - 1 > 0,$$

and since the property holds for any $g \in (3/2, 4 + \sqrt{13})$, there exists $g \in (1, 3/2]$ and $x_* \in \mathbb{R}$ such that

$$f_g(x_*) = 0, \quad f_g'(x_*) = 0, \quad f_g''(x_*) \geq 0, \quad (7.6)$$

i.e., f_g vanishes at a local minimum x_* .

For notational simplicity, we set

$$U = C_+^{*2}(x_*), \quad V = C_-^{*2}(x_*), \quad X = (C_+'(x_*))^2, \quad Y = (C_-'(x_*))^2.$$

Then the two equalities in (7.6) imply,

$$3U + gV = 1, \quad 9UX = g^2VY,$$

and from the property (iv) above we find that

$$X + Y = \frac{1}{2}(U + V - 1)^2 + (g-1)UV.$$

³It turns out that this condition is necessary and sufficient.

Consequently, we can write V, X, Y as functions of U ,

$$\begin{aligned} V &= \frac{1}{g}(1 - 3U), \\ X &= \frac{1}{2} \frac{(1 - 3U)((5g^2 - 9)U^2 + 6(1 - g)U - (g - 1)^2)}{g(3(g - 3)U - g)}, \\ Y &= \frac{9}{2} \frac{U((5g^2 - 9)U^2 + 6(1 - g)U - (g - 1)^2)}{g^2(3(g - 3)U - g)}, \end{aligned}$$

and then compute

$$\begin{aligned} f_g''(x_*) &= 2(3X + gY + 3U(-1 + U + gV) + gV(-1 + gU + V)) \\ &= (18(g - 1)(g^2 - 9)U^3 + (12g(9 - g^2) - 27(3 + g^2))U^2 \\ &\quad + 2g(g^2 + 6g - 9)U + (g - 1)(g - 3)) / (g(g - 3(g - 3)U)). \end{aligned}$$

For $g \in (1, 3/2)$ and $U \in (0, 1)$ we find that $f_g''(x_*) < 0$, which proves the result. \blacksquare

This result allows us to transfer the arguments used in [10] in the case $g = 2$ to more general values $g \in (1, 4 + \sqrt{13})$. In particular, we find that C_+^* and C_-^* have the asymptotic behavior

$$C_+^*(x) = 1 - \beta_* e^{\sqrt{2}x} + O(e^{(\sqrt{2}+\delta)x}), \quad C_-^*(x) = \alpha_* e^{\sqrt{g-1}x} + O(e^{(\sqrt{g-1}+\delta)x}), \quad \alpha_* > 0, \beta_* > 0,$$

as $x \rightarrow -\infty$, for some $\delta > 0$, and

$$C_+^*(x) = \alpha_* e^{-\sqrt{g-1}x} + O(e^{-(\sqrt{g-1}+\delta)x}), \quad C_-^*(x) = 1 - \beta_* e^{-\sqrt{2}x} + O(e^{-(\sqrt{2}+\delta)x}), \quad (7.7)$$

as $x \rightarrow \infty$.

7.2 Persistence of the heteroclinic

A key step of the persistence proof is the analysis of the operator obtained by linearizing the system (7.3)-(7.4), together with the complex conjugated equations, at (C_+^*, C_-^*) , i.e., the linear operator \mathcal{L}_* acting on C_+, C_- through

$$\mathcal{L}_* \begin{pmatrix} C_+ \\ C_- \end{pmatrix} = \begin{pmatrix} C_+'' - (-1 + 2C_+^{*2} + gC_-^{*2}) C_+ - C_+^{*2} \overline{C_+} - gC_+^* C_-^* (C_- + \overline{C_-}) \\ C_-'' - (-1 + gC_+^{*2} + 2C_-^{*2}) C_- - C_-^{*2} \overline{C_-} - gC_+^* C_-^* (C_+ + \overline{C_+}) \end{pmatrix}.$$

In the space of exponentially decaying functions

$$\mathcal{X}_\eta = \{(C_+, C_-, \overline{C_+}, \overline{C_-}) \in (L_\eta^2)^4\}, \quad L_\eta^2 = \left\{ f : \mathbb{R} \rightarrow \mathbb{C} ; \int_{\mathbb{R}} e^{2\eta|x|} |f(x)|^2 < \infty \right\},$$

for some $\eta > 0$, \mathcal{L}_* is a closed operator with dense domain

$$\mathcal{Y}_\eta = \{(C_+, C_-, \overline{C_+}, \overline{C_-}) \in (H_\eta^2)^4\}, \quad H_\eta^2 = \{f : \mathbb{R} \rightarrow \mathbb{C} ; f, f', f'' \in L_\eta^2\}.$$

We are interested in the properties of its restriction to the invariant subspace of reversible functions

$$\mathcal{X}_\eta^r = \{(C_+, C_-, \overline{C_+}, \overline{C_-}) \in \mathcal{X}_\eta ; C_+(x) = \overline{C_-}(-x), x \in \mathbb{R}\}.$$

Due to Lemma 7.1, the properties found in [10, Lemma 4.1] remain valid for $g \in (1, 4 + \sqrt{13})$. We have the following result.

Lemma 7.2. *Assume that $g \in (1, 4 + \sqrt{13})$. For any $\eta > 0$ sufficiently small, the operator \mathcal{L}_* acting in \mathcal{X}_η^r is Fredholm with index -1 . The kernel of \mathcal{L}_* is trivial, and the one-dimensional kernel of its L^2 -adjoint is spanned by $(iC_+^*, -iC_-^*, -iC_+^*, iC_-^*)$.*

The remaining arguments, which rely upon the implicit function theorem, are the same as in the proof of [10, Theorem 2]. Since the operator \mathcal{L}_* in Lemma 7.2 is injective with index -1 , and not bijective, we need an additional parameter to conclude. We introduce this parameter by considering the periodic solutions $((1 - \theta^2)^{1/2} e^{i\theta x}, 0)$, for small θ , of the leading order normal form. Their orbits surround the equilibrium $(1, 0)$, and persist as periodic orbits

$$\mathbf{P}_{\varepsilon, \theta}(x) = \left((1 - \theta^2)^{1/2} e^{i\theta x}, 0 \right) + O(\varepsilon^{1/2}), \quad (7.8)$$

of the full system (7.1)-(7.2). While the equilibrium $(1, 0)$ corresponds to the rotated rolls $\mathcal{R}_\alpha(\mathbf{U}_{k, \mu}^*)$ in Section 4.1 with wavenumbers $k = k_c$, these periodic orbits correspond to the rolls with wavenumbers k close to k_c . These solutions are not reversible, so that the reversibility symmetry \mathbf{S}_1 generates a second family of periodic orbits

$$\mathbf{Q}_{\varepsilon, \theta}(x) = (\mathbf{S}_1 \mathbf{P}_{\varepsilon, \theta})(-x) = \left(0, (1 - \theta^2)^{1/2} e^{i\theta x} \right) + O(\varepsilon^{1/2}).$$

From [10, Theorem 2] we obtain the following result, which completes the persistence proof and implies the result in Theorem 1.

Theorem 2. *Assume that $g \in (1, 4 + \sqrt{13})$. For any ε sufficiently small, there exists $\theta = \theta(\sqrt{\varepsilon})$, $\theta(0) = 0$, such that the system (7.1)-(7.2) possesses a heteroclinic orbit \mathbf{C}_ε connecting the periodic orbit $\mathbf{P}_{\varepsilon, \theta}$, as $x \rightarrow \infty$, to $\mathbf{Q}_{\varepsilon, \theta}$, as $x \rightarrow -\infty$.*

8 Discussion

This approach can also be used for other boundary conditions, when one, or both, of the rigid boundaries is replaced by a free boundary. It turns out that the arguments remain the same when both boundaries are free, but a major difference occurs in the case of one rigid and one free boundaries. We briefly discuss these two cases below.

8.1 Free-free boundary conditions

In the case of two free boundaries, the rigid-rigid boundary conditions (2.5) are replaced by the “free-free” boundary conditions

$$\partial_z V_x|_{z=0,1} = \partial_z V_y|_{z=0,1} = 0, \quad V_z|_{z=0,1} = \theta|_{z=0,1} = 0, \quad (8.1)$$

the horizontal components (V_x, V_y) of the velocity field \mathbf{V} satisfying now Neumann boundary conditions along the vertical axis z , instead of Dirichlet boundary conditions. The equations in the system (2.1)-(2.3) are the same, and with these boundary conditions the system has exactly the same symmetries as in the case of rigid-rigid boundary conditions.

In the classical two-dimensional convection, the existence of rolls is shown as in Section 2.2. The sequence of parameter values $\mu_0(k) < \mu_1(k) < \mu_2(k) < \dots$ has the same properties as in Section 2.1, the difference being that in the boundary value problem (2.9)-(2.10) the equality $DV = 0$ is replaced by $D^2V = 0$. This changes the formula for $\mu_0(k)$, which is now explicit (see [21]),

$$\mu_0(k) = \frac{1}{|k|} (k^2 + \pi^2)^{3/2},$$

from which we easily obtain the numerical values

$$k_c = \frac{\pi}{\sqrt{2}}, \quad \mu_c = \frac{3\sqrt{3}}{2}\pi^2.$$

Furthermore, the solution V of the boundary value problem (2.9)-(2.10) is now explicit,

$$V(z) = \sin(\pi z).$$

In our approach, we replace the spaces \mathcal{X} and \mathcal{Z} in the spatial dynamics formulation (3.3) by

$$\begin{aligned} \mathcal{X} = \{ & \mathbf{U} \in (H_{per}^1(\Omega))^3 \times (L_{per}^2(\Omega))^3 \times H_{per}^1(\Omega) \times L_{per}^2(\Omega) ; \\ & V_z = \theta = 0 \text{ on } z = 0, 1, \text{ and } \int_{\Omega} V_x dy dz = 0 \}, \end{aligned}$$

and

$$\begin{aligned} \mathcal{Z} = \{ & \mathbf{U} \in \mathcal{X} \cap (H_{per}^2(\Omega))^3 \times (H_{per}^1(\Omega))^3 \times H_{per}^2(\Omega) \times H_{per}^1(\Omega) ; \\ & \partial_z V_x = \partial_z V_y = W_z = \phi = 0 \text{ on } z = 0, 1 \}. \end{aligned}$$

The equations in (3.3) and the symmetries τ_a , \mathbf{S}_1 , \mathbf{S}_2 , \mathbf{S}_3 , and \mathbf{T}_b in Section 3 do not change, and the results and arguments in Sections 4-7, including the existence result in Theorem 2, remain valid. The only differences are at the computational level, in the different boundary value problems involving the component V_z of the velocity field, the equality $DV_z = 0$ being replaced by $D^2V_z = 0$ (these are the boundary value problems for V and v in the proof of Lemma 4.2 and the boundary value problems for V_{ijkl} in the computation of the coefficients b_1 and b_3 in Appendix B).

The explicit formulas for $\mu_0(k)$ and for the solution V of the boundary value problem (2.9)-(2.10) given above, make the computation of the quotient g in Section B.5 much simpler in this case. From (B.24) and (B.20) we compute

$$\phi(z) = -\frac{2}{3\pi^2} \sin(2\pi z), \quad R_1(z) = -\frac{2}{3\pi} (1 - \Theta) \sin(2\pi z), \quad R_2(z) = -3\pi^3 (1 - \Theta) \sin(2\pi z),$$

where $\Theta = \sin^2 \alpha$, and by solving the boundary values problems (B.21) and (B.22), in which the boundary conditions are changed as explained above, we find

$$V_j(z) = \frac{1}{\ell_\Theta} R_j(z), \quad \ell_\Theta = \pi^6 \left(\frac{27}{2} \Theta - 8(2 + \Theta)^3 \right), \quad j = 1, 2.$$

Finally, using (B.17)-(B.19) and (B.16) we obtain that

$$b_{31}(\Theta) = \frac{18\sqrt{3}\pi^8(1 - \Theta)^2}{\ell_\Theta} \left((\Theta + 2)^2 + \frac{9}{2}\Theta \mathcal{P}^{-1} + 3\Theta(\Theta + 2)\mathcal{P}^{-2} \right).$$

In particular,

$$b_{31}(1) = 0, \quad b_{31}(0) = -\frac{9\sqrt{3}\pi^2}{8},$$

so that the denominator of g in (B.15) does not depend on \mathcal{P}^{-1} . This implies that the quotient g is a quadratic polynomial in \mathcal{P}^{-1} , whereas it was a bounded rational function in the case of rigid-rigid boundary conditions, hence taking arbitrarily large values for sufficiently small Prandtl numbers \mathcal{P} , for any fixed angle α . Consequently, the inequality $g < 4 + \sqrt{13}$ can only hold in this case for not too small Prandtl numbers $\mathcal{P} > \mathcal{P}_*(\alpha) > 0$, for any fixed angle α . Since the result in Lemma 6.2 remains valid, we necessarily have $\mathcal{P}_*(0) = 0$. A Maple computation of the quotient g gives the plot of the curve $\mathcal{P}_*(\alpha)$ in Figure 8.1, and also shows that the inequality $g > 1$ holds for any Prandtl number $\mathcal{P} > 0$ and any angle $\alpha \in (0, \pi/3)$, just as in the case of rigid-rigid boundary conditions. Whether the persistence proof in Section 7.2 can be extended

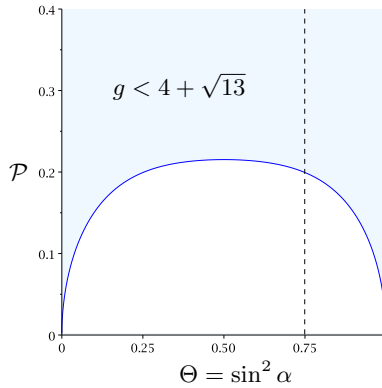


Figure 8.1: In the (Θ, \mathcal{P}) -plane, with $\Theta = \sin^2 \alpha \in (0, 1)$, Maple plot of the curve along which $g = 4 + \sqrt{13}$, in the case of free-free boundary conditions. The inequality $g < 4 + \sqrt{13}$ holds in the shaded regions, whereas the inequality $g > 1$ holds everywhere. Domain walls are constructed in the shaded region situated to the left of the vertical line $\Theta = \sin^2(\pi/3) = 0.75$.

to values $g \geq 4 + \sqrt{13}$ remains an open question.

8.2 Rigid-free boundary conditions

In the case of one rigid and one free boundaries, the boundary conditions (2.5) are replaced by the “rigid-free” boundary conditions

$$V_x|_{z=0} = V_y|_{z=0} = 0, \quad \partial_z V_x|_{z=1} = \partial_z V_y|_{z=1} = 0, \quad V_z|_{z=0,1} = \theta|_{z=0,1} = 0, \quad (8.2)$$

and, as in the previous case, the equations (2.1)-(2.3) remain the same. In contrast to the rigid-rigid and free-free boundary conditions, these rigid-free boundary conditions are asymmetric and the system loses its reflection symmetry in the vertical coordinate z . As an immediate consequence, in the spatial dynamics formulation, the system (3.3) is not equivariant under the action of the symmetry \mathbf{S}_3 anymore. While the spectral properties of the linear operator \mathcal{L}_{μ_c} in Section 4 and the center manifold reduction in Section 5 remain valid, the parity properties of the reduced vector field in Lemma 5.2 do not hold. Consequently, in this case we do not have an invariant 8-dimensional center submanifold, and we have to treat the full 12-dimensional reduced system. This leads to two additional difficulties.

First, the normal form analysis in Section 6 becomes more complicated since it has to be done for 12-dimensional vector fields instead of 8-dimensional vector fields. As a result, we expect that the system replacing (6.10)-(6.11) will be a system of three second order ODEs, and that to leading order it will be of the form:

$$C_0''' = (a_0 \text{sign}(\varepsilon) + a_1 |C_0|^2 + a_2 (|C_+|^2 + |C_-|^2)) C_0, \quad (8.3)$$

$$C_+''' = (b_0 \text{sign}(\varepsilon) + a_3 |C_0|^2 + b_1 |C_+|^2 + b_3 |C_-|^2) C_+, \quad (8.4)$$

$$C_-''' = (b_0 \text{sign}(\varepsilon) + a_3 |C_0|^2 + b_3 |C_+|^2 + b_1 |C_-|^2) C_-. \quad (8.5)$$

This system is similar to the one found in [10] for the Swift-Hohenberg equation, and assuming that $b_0 \text{sign}(\varepsilon) < 0$ and $b_3/b_1 > 1$, it has the heteroclinic solution $(0, C_+^*, C_-^*)$, where (C_+^*, C_-^*) is the leading order heteroclinic in Section 7.1.

Next, the persistence proof from [10], which has been done for particular values of the coefficients in the leading order system, has to be extended to more general systems of the form (8.3)-(8.5). We expect that this will lead to additional conditions, to be determined, on the coefficients in the system (8.3)-(8.5). Checking these conditions will require a computation similar to the one in Appendix B, but longer. This case will make the object of future work.

A Some properties of linear operators

A.1 Adjoint operator

Denote by $\langle \cdot, \cdot \rangle$ the scalar product in $(L_{per}^2(\Omega))^8$ and consider the closed subspace

$$\mathcal{H}_0 = \left\{ \mathbf{U} = (V_x, V_\perp, W_x, W_\perp, \theta, \phi) \in (L_{per}^2(\Omega))^8 ; \int_\Omega V_x dy dz = 0 \right\} \subset (L_{per}^2(\Omega))^8,$$

which is the closure in $(L_{per}^2(\Omega))^8$ of both \mathcal{X} and the domain of definition \mathcal{Z} of the operator \mathcal{L}_μ . We compute the adjoint \mathcal{L}_μ^* of \mathcal{L}_μ from the scalar product $\langle \mathcal{L}_\mu \mathbf{U}, \mathbf{U}' \rangle$, for $\mathbf{U} \in \mathcal{Z}$, and choose

$\mathbf{U}' \in \mathcal{H}_0$ such that $\mathbf{U} \mapsto \langle \mathcal{L}_\mu \mathbf{U}, \mathbf{U}' \rangle$ is a linear continuous form on \mathcal{H}_0 . We obtain the linear operator

$$\mathcal{L}_\mu^* \mathbf{U} = \begin{pmatrix} -\mu^{-1} (\Delta_\perp W_x - \langle \Delta_\perp W_x \rangle) \\ \nabla_\perp V_x - \mu^{-1} \Delta_\perp W_\perp - \mu^{-1} \nabla_\perp (\nabla_\perp \cdot W_\perp) - \mu \phi \mathbf{e}_z \\ \nabla_\perp \cdot W_\perp \\ \mu V_\perp \\ -W_z - \Delta_\perp \phi \\ \theta \end{pmatrix},$$

where

$$\langle \Delta_\perp W_x \rangle = \int_\Omega \Delta_\perp W_x(y, z) dy dz.$$

The operator \mathcal{L}_μ^* is closed in the space \mathcal{X}^* defined by

$$\mathcal{X}^* = \{ \mathbf{U} \in (L_{per}^2(\Omega))^3 \times (H_{per}^1(\Omega))^3 \times L_{per}^2(\Omega) \times H_{per}^1(\Omega) ; \\ W_x = W_\perp = \phi = 0 \text{ on } z = 0, 1, \text{ and } \int_\Omega V_x dy dz = 0 \},$$

with domain

$$\mathcal{Z}^* = \{ \mathbf{U} \in \mathcal{X}^* \cap (H_{per}^1(\Omega))^3 \times (H_{per}^2(\Omega))^3 \times H_{per}^1(\Omega) \times H_{per}^2(\Omega) ; \\ V_\perp = \nabla_\perp \cdot W_\perp = \theta = 0 \text{ on } z = 0, 1 \}.$$

The adjoint operator \mathcal{L}_μ^* has the same center spectrum as the operator \mathcal{L}_μ . For our purposes we need to compute its kernel, an eigenvector associated with the eigenvalue $-ik$ of $\mathcal{L}_{\mu_0(k)}^*$, and one of the eigenvectors associated with the eigenvalue $-ik_x$ of $\mathcal{L}_{\mu_c}^*$.

The kernel of \mathcal{L}_μ^* is easily computed by solving the equation $\mathcal{L}_\mu^* \mathbf{U} = 0$, and we find that it is spanned by the vector

$$\varphi_0^* = (0, 0, 0, z(1-z), 0, 0, 0, 0)^t.$$

We use this vector in the computation of the coefficients of the cubic normal form in Appendix B.

Next, for $\mu = \mu_0(k)$, the operator $\mathcal{L}_{\mu_0(k)}^*$ has the geometrically simple eigenvalues $\pm ik$, just as the operator $\mathcal{L}_{\mu_0(k)}$. In Appendix A.2 we need the expression of an eigenvector $\Psi_{k,0}^*$ associated with the eigenvalue $-ik$. A direct calculation gives

$$\Psi_{k,0}^*(y, z) = \widehat{\Psi}_{k,0}^*(z), \quad \widehat{\Psi}_{k,0}^*(z) = \begin{pmatrix} -\frac{1}{\mu_0(k)k^2} (D^3 V_k - \langle D^3 V_k \rangle) \\ 0 \\ \frac{ik}{\mu_0(k)} V_k \\ -\frac{i}{k} D V_k \\ 0 \\ -V_k \\ -ik \phi_k \\ \phi_k \end{pmatrix}, \quad (\text{A.1})$$

where

$$\langle D^3 V_k \rangle = \int_{\Omega} D^3 V_k(z) dy dz,$$

V_k is the solution of the boundary value problem (4.8), and ϕ_k is the unique solution of the boundary value problem

$$(D^2 - k^2)\phi_k = V_k, \quad \phi_k|_{z=0,1} = 0.$$

Finally, in the computations in Appendix B we also need an eigenvector associated with the eigenvalue $-ik_x$ of $\mathcal{L}_{\mu_c}^*$ which is of the form

$$\Psi_+^* = \widehat{\Psi}_+^*(z)e^{ik_y y}.$$

We obtain that

$$\widehat{\Psi}_+^*(z) = \begin{pmatrix} -\frac{1}{\mu_c k_c^2} (D^2 - k_c^2 \cos^2 \alpha) DV \\ -\frac{\sin \alpha \cos \alpha}{\mu_c} DV \\ \frac{ik_c \sin \alpha}{\mu_c} V \\ -\frac{i \sin \alpha}{k_c} DV \\ -\frac{i \cos \alpha}{k_c} DV \\ -V \\ -ik_c (\sin \alpha) \phi \\ \phi \end{pmatrix},$$

where V is the solution of the boundary value problem (4.10), and ϕ is the unique solution of the boundary value problem

$$(D^2 - k_c^2)\phi = V, \quad \phi|_{z=0,1} = 0.$$

Notice that the function ϕ is related to the function θ in the boundary value problem (2.9)-(2.10), taken at $k = k_c$, through the equality $\theta = -\mu_c \phi$.

A.2 Algebraic multiplicities of $\pm ik$ and $\pm i\omega_1(k)$

For $k_y = k_c \cos \alpha$ with $\alpha \in (0, \pi/3)$ and $k \neq k_c$, sufficiently close to k_c , consider the geometrically simple eigenvalues $\pm ik$ and the geometrically double eigenvalues $\pm i\omega_1(k)$ of the operator $\mathcal{L}_{\mu_0(k)}$ found in Lemma 4.1. We show that their algebraic multiplicities are equal to their geometric multiplicities, or equivalently, that their index is equal to 1. We prove the result for the eigenvalue ik , the arguments being the same for the eigenvalue $i\omega_1(k)$.

Assuming that the index of the eigenvalue ik is larger than 1, there exists a vector $\Psi_{k,0}$ such that

$$(\mathcal{L}_{\mu_0(k)} - ik)\Psi_{k,0} = \mathbf{U}_{k,0}. \tag{A.2}$$

Differentiating the eigenvalue problem

$$\mathcal{L}_{\mu_0(k)} \mathbf{U}_{k,0} = ik \mathbf{U}_{k,0},$$

with respect to k leads to the equality

$$(\mathcal{L}_{\mu_0(k)} - ik) \left(\frac{d}{dk} \mathbf{U}_{k,0} \right) = \left(i - \mu'_0(k) \frac{\partial}{\partial \mu} \mathcal{L}_\mu \Big|_{\mu=\mu_0(k)} \right) \mathbf{U}_{k,0}.$$

Since $\mu'_0(k) \neq 0$ for $k \neq k_c$, this identity and (A.2) imply that there is a solution $\Phi_{k,0}$ of the linear equation

$$(\mathcal{L}_{\mu_0(k)} - ik) \Phi_{k,0} = \frac{\partial}{\partial \mu} \mathcal{L}_\mu \Big|_{\mu=\mu_0(k)} \mathbf{U}_{k,0}. \quad (\text{A.3})$$

As a consequence, the vector in the right hand side of the above equation is orthogonal to the kernel of the adjoint operator $(\mathcal{L}_{\mu_0(k)}^* + ik)$. In particular, it is orthogonal to the eigenvector $\Psi_{k,0}^*$ computed in Appendix A.1 and given by (A.1). A direct computation gives the term in the right hand side of (A.3),

$$\frac{\partial}{\partial \mu} \mathcal{L}_\mu \Big|_{\mu=\mu_0(k)} \widehat{\mathbf{U}}_{k,0} = \begin{pmatrix} 0 \\ 0 \\ \frac{ik}{\mu_0(k)} V_k \\ \frac{i}{\mu_0^2(k)k} D^3 V_k \\ 0 \\ \frac{2}{\mu_0^2(k)} D^2 V_k \\ 0 \\ -V_k \end{pmatrix},$$

and taking its L^2 -scalar product with the vector $\Psi_{k,0}^*$ given by (A.1) we obtain

$$\frac{1}{\mu_0^2(k)k^2} (\|D^2 V_k\|^2 + 2k^2 \|DV_k\|^2 + k^4 \|V_k\|^2) + \|D\phi_k\|^2 + k^2 \|\phi_k\|^2 > 0.$$

The positivity of the scalar product contradicts the solvability condition for the equation (A.3), and proves that the index of the eigenvalue ik is equal to 1.

B Coefficients of the cubic normal form

B.1 General formulas

For the computation of the coefficients b_1 and b_3 , we follow the method in [8, Section 3.4.1]. We restrict to the 8-dimensional center manifold

$$\mathcal{M}_\pm(\varepsilon) = \{\mathbf{U}_c + \Phi(\mathbf{U}_c, \varepsilon) ; \mathbf{U}_c \in E_\pm\}.$$

Recall that solutions on this submanifold are invariant under the action of $\mathbf{S}_3 \tau_\pi$. Combining the transformations from the center manifold reduction in Section 5.1 and the normal form in Lemma 6.1, we write

$$\begin{aligned} \mathbf{U} &= A_+ \zeta_+ + B_+ \Psi_+ + A_- \zeta_- + B_- \Psi_- + \overline{A_+ \zeta_+} + \overline{B_+ \Psi_+} + \overline{A_- \zeta_-} + \overline{B_- \Psi_-} \\ &\quad + \widetilde{\Phi}(A_+, B_+, A_-, B_-, \overline{A_+}, \overline{B_+}, \overline{A_-}, \overline{B_-}, \varepsilon), \end{aligned}$$

in which $Z = (A_+, B_+, A_-, B_-)$ satisfies the normal form (6.4). Substituting \mathbf{U} given by this formula in the dynamical system (3.3), and using the expressions of the derivatives of A_+ , B_+ , A_- , B_- given by the normal form in Lemma 6.1, we obtain an equality for the variables A_+ , B_+ , A_- , B_- and their complex conjugates. We find the coefficients of the normal form, and in particular b_1 and b_3 , by identifying the coefficients of suitably chosen monomials in this equality.

We denote by Φ_{rstu} the coefficient of the monomial $A_+^r \overline{A_+}^s A_-^t \overline{A_-}^u$ in the expansion of $\tilde{\Phi}$. Identifying successively the coefficients of the monomials $A_+^2 \overline{A_+}$, $A_+ A_- \overline{A_-}$, and then A_+^2 , $A_+ \overline{A_+}$, $A_+ A_-$, $A_+ \overline{A_-}$, $A_- \overline{A_-}$, we find the equalities

$$i\beta_1 \zeta_+ + b_1 \Psi_+ = (\mathcal{L}_{\mu_c} - ik_x) \Phi_{2100} + 2\mathcal{B}_{\mu_c}(\Phi_{2000}, \overline{\zeta_+}) + 2\mathcal{B}_{\mu_c}(\Phi_{1100}, \zeta_+),$$

$$i\beta_3 \zeta_+ + b_3 \Psi_+ = (\mathcal{L}_{\mu_c} - ik_x) \Phi_{1011} + 2\mathcal{B}_{\mu_c}(\Phi_{1010}, \overline{\zeta_-}) + 2\mathcal{B}_{\mu_c}(\Phi_{1001}, \zeta_-) + 2\mathcal{B}_{\mu_c}(\Phi_{0011}, \zeta_+),$$

and

$$(\mathcal{L}_{\mu_c} - 2ik_x) \Phi_{2000} = -\mathcal{B}_{\mu_c}(\zeta_+, \zeta_+), \quad (\text{B.1})$$

$$\mathcal{L}_{\mu_c} \Phi_{1100} = -2\mathcal{B}_{\mu_c}(\zeta_+, \overline{\zeta_+}), \quad (\text{B.2})$$

$$(\mathcal{L}_{\mu_c} - 2ik_x) \Phi_{1010} = -2\mathcal{B}_{\mu_c}(\zeta_+, \zeta_-), \quad (\text{B.3})$$

$$\mathcal{L}_{\mu_c} \Phi_{1001} = -2\mathcal{B}_{\mu_c}(\zeta_+, \overline{\zeta_-}), \quad (\text{B.4})$$

$$\mathcal{L}_{\mu_c} \Phi_{0011} = -2\mathcal{B}_{\mu_c}(\zeta_-, \overline{\zeta_-}). \quad (\text{B.5})$$

We determine the coefficients b_1 and b_3 by taking the scalar product of the first two equalities above with the vector Ψ_+^* in the kernel of the adjoint operator $(\mathcal{L}_{\mu_c} - ik_x)^*$ computed in Appendix A.1,

$$b_1 \langle \Psi_+, \Psi_+^* \rangle = \langle 2\mathcal{B}_{\mu_c}(\Phi_{2000}, \overline{\zeta_+}) + 2\mathcal{B}_{\mu_c}(\Phi_{1100}, \zeta_+), \Psi_+^* \rangle, \quad (\text{B.6})$$

$$b_3 \langle \Psi_+, \Psi_+^* \rangle = \langle 2\mathcal{B}_{\mu_c}(\Phi_{1010}, \overline{\zeta_-}) + 2\mathcal{B}_{\mu_c}(\Phi_{1001}, \zeta_-) + 2\mathcal{B}_{\mu_c}(\Phi_{0011}, \zeta_+), \Psi_+^* \rangle, \quad (\text{B.7})$$

where Φ_{2000} , Φ_{1100} , Φ_{1010} , Φ_{1001} , and Φ_{0011} are solutions of the linear equations (B.1)-(B.5).

In the equations (B.1) and (B.3), the linear operator $(\mathcal{L}_{\mu_c} - 2ik_x)$ is invertible, except in the case $\alpha = \pi/6$ when $2k_x = k_c$. Nevertheless, we only have to solve the equations in the subspace of vectors which are invariant under the action of $\mathbf{S}_3 \tau_\pi$ and the restriction of $(\mathcal{L}_{\mu_c} - ik_c)$ to this subspace is invertible, since its two-dimensional kernel is spanned by ζ_0 and $\overline{\zeta_0}$ which do not belong to this subspace. Consequently, Φ_{2000} and Φ_{1010} are uniquely determined. In the equations (B.2), (B.4) and (B.5), the linear operator \mathcal{L}_{μ_c} has a one-dimensional kernel spanned by the vector φ_0 in Lemma 4.2 (i), and the kernel of its adjoint is spanned by the vector φ_0^* in Appendix A.1. The solvability condition is easily checked in all cases, so that we can solve these equations up to an element in the kernel of \mathcal{L}_μ . The choice of this element in the kernel does not influence the result from (B.6)-(B.7), since \mathcal{B}_μ is invariant upon adding a multiple of φ_0 .

Without going into the detailed computations, in the next two sections we give the results for the different quantities in the right hand sides of (B.6) and (B.7). For the vectors Φ_{rstu} we do not compute explicitly the component W_x , because it is not needed in the computation of \mathcal{B}_{μ_c} .

Remark B.1. In this way we can also compute the coefficient b_0 . By identifying the coefficients of the terms εA_+ , and then taking the scalar product with Ψ_+^* we obtain

$$b_0 \langle \Psi_+, \Psi_+^* \rangle = \langle \mathcal{L}^{(1)} \zeta_+, \Psi_+^* \rangle,$$

in which $\mathcal{L}^{(1)}$ is the derivative with respect to μ of the operator \mathcal{L}_μ in (A.3) taken at $\mu = \mu_c$. A direct computation gives

$$b_0 \langle \Psi_+, \Psi_+^* \rangle = \frac{1}{\mu_c^2 k_c^2} (\|D^2 V\|^2 + 2k_c^2 \|DV\|^2 + k_c^4 \|V\|^2) + \|D\phi\|^2 + k_c^2 \|\phi\|^2 > 0, \quad (\text{B.8})$$

and implies that $\langle \Psi_+, \Psi_+^* \rangle < 0$, since $b_0 < 0$. We point out that it is not obvious to determine the sign of this scalar product directly from the explicit formulas of Ψ_+ and Ψ_+^* .

B.2 Computation of b_1

For the first term in the right hand side of (B.6) we obtain, successively,⁴

$$\mathcal{B}_{\mu_c}(\zeta_+, \zeta_+) = \begin{pmatrix} \mathbf{0}_3 \\ \frac{i \sin \alpha}{k_c} \mathcal{P}^{-1} (VD^2 V - (DV)^2) \\ \frac{i \cos \alpha}{k_c} \mathcal{P}^{-1} (VD^2 V - (DV)^2) \\ \mathbf{0}_2 \\ \frac{1}{k_c^2} (V(D^2 - k_c^2)^2 DV - DV(D^2 - k_c^2)^2 V) \end{pmatrix} e^{2ik_y y},$$

$$\Phi_{2000} = \begin{pmatrix} \frac{i \sin \alpha}{2k_c} DV_{2000} \\ \frac{i \cos \alpha}{2k_c} DV_{2000} \\ V_{2000} \\ W_{2000} \\ -\frac{\sin \alpha \cos \alpha}{\mu_c} DV_{2000} \\ \frac{2ik_c \sin \alpha}{\mu_c} V_{2000} \\ \theta_{2000} \\ 2ik_c (\sin \alpha) \theta_{2000} \end{pmatrix} e^{2ik_y y},$$

in which

$$\theta_{2000} = \frac{1}{4\mu_c k_c^2} (D^2 - 4k_c^2)^2 V_{2000} - \frac{1}{2k_c^2} \mathcal{P}^{-1} D (VD^2 V - (DV)^2),$$

$$(D^2 - 4k_c^2)^3 V_{2000} + 4\mu_c^2 k_c^2 V_{2000} = 2\mu_c \mathcal{P}^{-1} D (D^2 - 4k_c^2) (VD^2 V - (DV)^2) \\ + 4\mu_c (V(D^2 - k_c^2)^2 DV - DV(D^2 - k_c^2)^2 V),$$

and V_{2000} satisfies the boundary conditions

$$V_{2000} = DV_{2000} = (D^2 - 4k_c^2)^2 V_{2000} = 0 \text{ in } z = 0, 1,$$

⁴In a column vector, the notation $\mathbf{0}_k$ means that 0 appears on k consecutive rows.

$$2\mathcal{B}_{\mu_c}(\Phi_{2000}, \overline{\zeta}_+) = \begin{pmatrix} \mathbf{0}_3 \\ \frac{i \sin \alpha}{2k_c} \mathcal{P}^{-1} (D(VDV_{2000}) - 2(D^2V)V_{2000}) \\ \frac{i \cos \alpha}{2k_c} \mathcal{P}^{-1} (D(VDV_{2000}) - 2(D^2V)V_{2000}) \\ \frac{3}{2} \mathcal{P}^{-1} (VDV_{2000} + 2(DV)V_{2000}) \\ 0 \\ \phi^{(B_{02})} \end{pmatrix} e^{iky},$$

with

$$\phi^{(B_{02})} = \frac{1}{2k_c^2} (DV_{2000}(D^2 - k_c^2)^2V + 2V_{2000}(D^2 - k_c^2)^2DV) + \mu_c (2\theta_{2000}DV + VD\theta_{2000}),$$

and the scalar product

$$\begin{aligned} \langle 2\mathcal{B}_{\mu_c}(\Phi_{2000}, \overline{\zeta}_+), \Psi_+^* \rangle &= \frac{1}{2k_c^2} \mathcal{P}^{-1} \langle V_{2000}, D((DV)^2 - VD^2V) \rangle + \mu_c \langle \theta_{2000}, \phi DV - VD\phi \rangle \\ &+ \frac{1}{2k_c^2} \langle V_{2000}, \phi(D^2 - k_c^2)^2DV - (D\phi)(D^2 - k_c^2)^2V \rangle. \end{aligned}$$

Using the equation for ϕ , we find

$$\phi(D^2 - k_c^2)^2DV - (D\phi)(D^2 - k_c^2)^2V = 0,$$

so that the last term in the right hand side of this scalar product vanishes.

For the second term the calculations are simpler. Here we find

$$2\mathcal{B}_{\mu_c}(\zeta_+, \overline{\zeta}_+) = \begin{pmatrix} \mathbf{0}_5 \\ 4\mathcal{P}^{-1}VDV \\ 0 \\ \frac{2}{k_c^2} D(V(D^2 - k_c^2)^2V) \end{pmatrix},$$

$$\Phi_{1100} = \begin{pmatrix} \mathbf{0}_3 \\ W_{1100} \\ \mathbf{0}_2 \\ \theta_{1100} \\ 0 \end{pmatrix}, \quad D^2\theta_{1100} = \frac{2}{k_c^2} D(V(D^2 - k_c^2)^2V),$$

$$2\mathcal{B}_{\mu_c}(\Phi_{1100}, \zeta_+) = \begin{pmatrix} \mathbf{0}_7 \\ \mu_c VD\theta_{1100} \end{pmatrix} e^{iky},$$

and the scalar product

$$\langle 2\mathcal{B}_{\mu_c}(\Phi_{1100}, \zeta_+), \Psi_+^* \rangle = \mu_c \langle D\theta_{1100}, V\phi \rangle.$$

Summing up, we obtain

$$\begin{aligned} b_1 \langle \Psi_+, \Psi_+^* \rangle &= \frac{1}{2k_c^2} \mathcal{P}^{-1} \langle V_{2000}, D((DV)^2 - VD^2V) \rangle \\ &+ \mu_c (\langle \theta_{2000}, \phi DV - VD\phi \rangle + \langle D\theta_{1100}, V\phi \rangle). \end{aligned}$$

Notice that the right hand side in this equality does not depend on the angle α . For our purposes we do not need to compute the scalar product $\langle \Psi_+, \Psi_+^* \rangle$.

B.3 Computation of \mathbf{b}_3

Similarly, for the first term in the right hand side of (B.7) we find

$$2\mathcal{B}_{\mu_c}(\zeta_+, \zeta_-) = \begin{pmatrix} \mathbf{0}_3 \\ \frac{2i \sin \alpha}{k_c} \mathcal{P}^{-1} (\cos(2\alpha)(DV)^2 + VD^2V) \\ 0 \\ 4\mathcal{P}^{-1}(\cos^2 \alpha)VDV \\ 0 \\ \frac{2}{k_c^2} (V(D^2 - k_c^2)^2DV + \cos(2\alpha)DV(D^2 - k_c^2)^2V) \end{pmatrix},$$

$$\Phi_{1010} = \begin{pmatrix} \frac{i}{2k_c \sin \alpha} DV_{1010} \\ 0 \\ V_{1010} \\ W_{1010} \\ 0 \\ \frac{2ik_c \sin \alpha}{\mu_c} V_{1010} \\ \theta_{1010} \\ 2ik_c(\sin \alpha)\theta_{1010} \end{pmatrix},$$

in which

$$(D^2 - 4k_c^2 \sin^2 \alpha)\theta_{1010} = -\mu_c V_{1010} + \frac{2}{k_c^2} (V(D^2 - k_c^2)^2DV + \cos(2\alpha)DV(D^2 - k_c^2)^2V), \quad (\text{B.9})$$

$$\begin{aligned} \theta_{1010} &= -\frac{1}{k_c^2} \mathcal{P}^{-1} D (\cos(2\alpha)(DV)^2 + VD^2V) + 4\mathcal{P}^{-1} \cos^2 \alpha (VDV) \\ &\quad + \frac{1}{4k_c^2 \mu_c \sin^2 \alpha} (D^2 - 4k_c^2 \sin^2 \alpha)^2 V_{1010}, \end{aligned}$$

$$(D^2 - 4k_c^2 \sin^2 \alpha)^3 V_{1010} + 4k_c^2 \mu_c^2 (\sin^2 \alpha) V_{1010} = (\sin^2 \alpha) G_{1010},$$

where

$$\begin{aligned} G_{1010} &= 8\mu_c (V(D^2 - k_c^2)^2DV + \cos(2\alpha)DV(D^2 - k_c^2)^2V) \\ &\quad + 4\mu_c \mathcal{P}^{-1} (D^2 - 4k_c^2 \sin^2 \alpha) D (\cos(2\alpha)(DV)^2 + VD^2V) \\ &\quad - 16k_c^2 \mu_c \mathcal{P}^{-1} \cos^2 \alpha (D^2 - 4k_c^2 \sin^2 \alpha) (VDV), \end{aligned}$$

and V_{1010} satisfies the boundary conditions

$$V_{1010} = DV_{1010} = (D^2 - 4k_c^2 \sin^2 \alpha)^2 V_{1010} = 0 \text{ in } z = 0, 1.$$

Next, we write

$$2\mathcal{B}_{\mu_c}(\Phi_{1010}, \bar{\zeta}_-) = \begin{pmatrix} \mathbf{0}_3 \\ W_x^{(1)} \\ W_y^{(1)} \\ W_z^{(1)} \\ 0 \\ \phi^{(1)} \end{pmatrix} e^{ik_y y},$$

where we find

$$\begin{aligned} W_x^{(1)} &= \frac{i \sin \alpha}{2k_c} \mathcal{P}^{-1} (DV DV_{1010} - 2(D^2 V) V_{1010}) + \frac{i}{2k_c \sin \alpha} \mathcal{P}^{-1} V D^2 V_{1010}, \\ W_y^{(1)} &= \frac{i \cos \alpha}{2k_c} \mathcal{P}^{-1} (2(D^2 V) V_{1010} + (DV) DV_{1010}), \\ W_z^{(1)} &= \frac{1}{2} \mathcal{P}^{-1} (3V DV_{1010} + 2(1 + 2 \sin^2 \alpha)(DV) V_{1010}), \\ \phi^{(1)} &= \frac{1}{k_c^2} V_{1010} (D^2 - k_c^2)^2 DV + \frac{1}{2k_c^2} (DV_{1010}) (D^2 - k_c^2)^2 V + \\ &\quad + \mu_c (VD \theta_{1010} + 2 \sin^2 \alpha (DV) \theta_{1010}), \end{aligned}$$

and we have the formula for the scalar product

$$\langle 2\mathcal{B}_{\mu_c}(\Phi_{1010}, \bar{\zeta}_-), \Psi_+^* \rangle = \frac{i}{k_c} \langle (\sin \alpha) W_x^{(1)} + (\cos \alpha) W_y^{(1)}, DV \rangle - \langle W_z^{(1)}, V \rangle + \langle \phi^{(1)}, \phi \rangle.$$

Notice that the dependence on α of the right hand side in this equality is through $\sin^2 \alpha$, only, so that we can write the scalar product as a function of $\sin^2 \alpha$,

$$\langle 2\mathcal{B}_{\mu_c}(\Phi_{1010}, \bar{\zeta}_-), \Psi_+^* \rangle = b_{31}(\sin^2 \alpha), \quad (\text{B.10})$$

and the function $b_{31}(\cdot)$, which does not depend on α , can be determined from the above formulas.

For the second term in the right hand side of (B.7) we obtain successively,

$$2\mathcal{B}_{\mu_c}(\zeta_+, \bar{\zeta}_-) = \begin{pmatrix} \mathbf{0}_4 \\ \frac{2i \cos \alpha}{k_c} \mathcal{P}^{-1} (V D^2 V - \cos(2\alpha)(DV)^2) \\ 4\mathcal{P}^{-1}(\sin^2 \alpha) V DV \\ 0 \\ \frac{2}{k_c^2} (V(D^2 - k_c^2)^2 DV - \cos(2\alpha) DV(D^2 - k_c^2)^2 V) \end{pmatrix} e^{2ik_y y},$$

$$\Phi_{1001} = \begin{pmatrix} 0 \\ \frac{i}{2k_c \cos \alpha} DV_{1001} \\ V_{1001} \\ W_{1001} \\ \mathbf{0}_2 \\ \theta_{1001} \\ 0 \end{pmatrix} e^{2ik_y y},$$

with

$$\begin{aligned}\theta_{1001} &= -\frac{1}{k_c^2} \mathcal{P}^{-1} D (VD^2V - \cos(2\alpha)(DV)^2) + 4\mathcal{P}^{-1} \sin^2 \alpha (VDV) \\ &\quad + \frac{1}{4\mu_c k_c^2 \cos^2 \alpha} (D^2 - 4k_c^2 \cos^2 \alpha)^2 V_{1001}, \\ (D^2 - 4k_c^2 \cos^2 \alpha)^3 V_{1001} + 4k_c^2 \mu_c^2 \cos^2 \alpha V_{1001} &= (\cos^2 \alpha) G_{1001},\end{aligned}$$

where

$$\begin{aligned}G_{1001} &= 8\mu_c (V(D^2 - k_c^2)^2 DV - \cos(2\alpha)DV(D^2 - k_c^2)^2 V) \\ &\quad + 4\mu_c \mathcal{P}^{-1} (D^2 - 4k_c^2 \cos^2 \alpha) D (VD^2V - \cos(2\alpha)(DV)^2) \\ &\quad - 16k_c^2 \mu_c \mathcal{P}^{-1} (\sin^2 \alpha) (D^2 - 4k_c^2 \cos^2 \alpha) (VDV),\end{aligned}$$

and V_{1001} satisfies the boundary conditions

$$V_{1001} = DV_{1001} = (D^2 - 4k_c^2 \cos^2 \alpha)^2 V_{1001} = 0 \text{ in } z = 0, 1.$$

As for the previous term, we write

$$2\mathcal{B}_{\mu_c}(\Phi_{1001}, \zeta_-) = \begin{pmatrix} \mathbf{0}_3 \\ W_x^{(2)} \\ W_y^{(2)} \\ W_z^{(2)} \\ 0 \\ \phi^{(2)} \end{pmatrix} e^{ik_y y},$$

where

$$\begin{aligned}W_x^{(2)} &= \frac{i \sin \alpha}{2k_c} \mathcal{P}^{-1} (D V D V_{1001} + 2(D^2 V) V_{1001}), \\ W_y^{(2)} &= \frac{i \cos \alpha}{2k_c} \mathcal{P}^{-1} ((D V) D V_{1001} - 2(D^2 V) V_{1001}) + \frac{i}{2k_c \cos \alpha} \mathcal{P}^{-1} V D^2 V_{1001}, \\ W_z^{(2)} &= \frac{1}{2} \mathcal{P}^{-1} (3V D V_{1001} + 2(1 + 2 \cos^2 \alpha) (D V) V_{1001}), \\ \phi^{(2)} &= \frac{1}{k_c^2} V_{1001} (D^2 - k_c^2)^2 D V + \frac{1}{2k_c^2} (D V_{1001}) (D^2 - k_c^2)^2 V \\ &\quad + \mu_c (V D \theta_{1001} + 2 \cos^2 \alpha (D V) \theta_{1001}),\end{aligned}$$

and obtain the formula for the scalar product

$$\langle 2\mathcal{B}_{\mu_c}(\Phi_{1001}, \zeta_-), \Psi_+^* \rangle = \frac{i}{k_c} \langle (\sin \alpha) W_x^{(2)} + (\cos \alpha) W_y^{(2)}, D V \rangle - \langle W_z^{(2)}, V \rangle + \langle \phi^{(2)}, \phi \rangle.$$

Comparing this formula with the one obtained for $\langle 2\mathcal{B}_{\mu_c}(\Phi_{1010}, \overline{\zeta_-}), \Psi_+^* \rangle$, we find that

$$\langle 2\mathcal{B}_{\mu_c}(\Phi_{1001}, \zeta_-), \Psi_+^* \rangle = b_{31}(\cos^2 \alpha), \quad (\text{B.11})$$

where b_{31} is the function defined in (B.10).

Finally, for the last term we obtain

$$2\mathcal{B}_{\mu_c}(\zeta_-, \overline{\zeta_-}) = 2\mathcal{B}_{\mu_c}(\zeta_+, \overline{\zeta_+}),$$

which implies that Φ_{0011} is equal to the vector Φ_{1100} computed in the previous section, so that

$$\langle 2\mathcal{B}_{\mu_c}(\Phi_{0011}, \zeta_+), \Psi_+^* \rangle = \langle 2\mathcal{B}_{\mu_c}(\Phi_{1100}, \zeta_+), \Psi_+^* \rangle = \mu_c \langle D\theta_{1100}, V\phi \rangle.$$

Summing up, we have

$$b_3 \langle \Psi_+, \Psi_+^* \rangle = b_{31}(\sin^2 \alpha) + b_{31}(\cos^2 \alpha) + \mu_c \langle D\theta_{1100}, V\phi \rangle,$$

with b_{31} determined by (B.10).

B.4 The limit $\alpha \rightarrow 0$

We show that

$$\lim_{\alpha \rightarrow 0} \left(\frac{b_3}{b_1} \right) = 2. \quad (\text{B.12})$$

Taking the limit $\alpha \rightarrow 0$ in the computation of the scalar product in (B.10), and using the equality (B.9), we find

$$\lim_{\alpha \rightarrow 0} V_{1010} = 0, \quad \lim_{\alpha \rightarrow 0} \theta_{1010} = \theta_{1100},$$

and then

$$\lim_{\alpha \rightarrow 0} \langle 2\mathcal{B}_{\mu_c}(\Phi_{1010}, \overline{\zeta_-}), \Psi_+^* \rangle = \mu_c \langle D\theta_{1100}, V\phi \rangle,$$

or, equivalently

$$b_{31}(0) = \langle 2\mathcal{B}_{\mu_c}(\Phi_{1100}, \zeta_+), \Psi_+^* \rangle.$$

Similarly, we take the limit $\alpha \rightarrow 0$ in the computation of the scalar product in (B.11) and find

$$\lim_{\alpha \rightarrow 0} V_{1001} = 2V_{2000}, \quad \lim_{\alpha \rightarrow 0} \theta_{1001} = 2\theta_{2000}.$$

Then

$$\lim_{\alpha \rightarrow 0} \langle 2\mathcal{B}_{\mu_c}(\Phi_{1001}, \zeta_-), \Psi_+^* \rangle = 2 \langle 2\mathcal{B}_{\mu_c}(\Phi_{2000}, \overline{\zeta_+}), \Psi_+^* \rangle,$$

or, equivalently

$$b_{31}(1) = 2 \langle 2\mathcal{B}_{\mu_c}(\Phi_{2000}, \overline{\zeta_+}), \Psi_+^* \rangle.$$

Summarizing, we have

$$b_3 \langle \Psi_+, \Psi_+^* \rangle = b_{31}(\sin^2 \alpha) + b_{31}(\cos^2 \alpha) + b_{31}(0), \quad (\text{B.13})$$

$$b_1 \langle \Psi_+, \Psi_+^* \rangle = \frac{1}{2} b_{31}(1) + b_{31}(0), \quad (\text{B.14})$$

which proves (B.12).

B.5 Symbolic computation of the quotient b_3/b_1

According to (B.13)-(B.14), we have

$$\frac{b_3}{b_1} = \frac{b_{31}(\sin^2 \alpha) + b_{31}(\cos^2 \alpha) + b_{31}(0)}{\frac{1}{2}b_{31}(1) + b_{31}(0)}, \quad (\text{B.15})$$

with b_{31} determined by (B.10). We set $\Theta = \sin^2 \alpha$. Using the formulas leading to (B.10), we write

$$b_{31}(\Theta) = A_{31}(\Theta) + B_{31}(\Theta)\mathcal{P}^{-1} + C_{31}(\Theta)\mathcal{P}^{-2}, \quad (\text{B.16})$$

in which we obtain

$$A_{31}(\Theta) = 2\mu_c^3 \langle (D^2 - 4k_c^2\Theta)^2 V_1, R_1 \rangle, \quad (\text{B.17})$$

$$B_{31}(\Theta) = 4\mu_c^3 \Theta (\langle V_1, R_2 \rangle + \langle V_2, R_1 \rangle), \quad (\text{B.18})$$

$$C_{31}(\Theta) = -\frac{2\mu_c\Theta}{k_c^2} \langle (D^2 - 4k_c^2\Theta)V_2, R_2 \rangle, \quad (\text{B.19})$$

where

$$R_1 = VD\phi + (1 - 2\Theta)\phi DV, \quad R_2 = (D^2 - 4k_c^2(1 - \Theta))(VDV) - 4\Theta(DV)(D^2V), \quad (\text{B.20})$$

and V_1, V_2 are the unique solutions of the boundary value problems

$$\begin{aligned} (D^2 - 4k_c^2\Theta)^3 V_1 + 4k_c^2\mu_c^2\Theta V_1 &= R_1, \\ V_1 = DV_1 = (D^2 - 4k_c^2\Theta)^2 V_1 &= 0 \text{ in } z = 0, 1, \end{aligned} \quad (\text{B.21})$$

and

$$\begin{aligned} (D^2 - 4k_c^2\Theta)^3 V_2 + 4k_c^2\mu_c^2\Theta V_2 &= R_2, \\ V_2 = (D^2 - 4k_c^2\Theta)V_2 = (D^2 - 4k_c^2\Theta)DV_2 &= 0 \text{ in } z = 0, 1, \end{aligned} \quad (\text{B.22})$$

respectively. With the help of the symbolic package Maple we compute, successively,

- (i) the numerical values of k_c and μ_c ;
- (ii) the functions V and ϕ defined for $z \in [0, 1]$;
- (iii) the functions R_1, R_2, V_1, V_2 defined for $z \in [0, 1]$ and $\Theta \in [0, 1]$;
- (iv) $A_{31}(\Theta), B_{31}(\Theta), C_{31}(\Theta), b_{31}(\Theta)$, and finally g , for $\Theta \in [0, 1]$ and $\mathcal{P} > 0$;

The main result of our Maple computation is the plot in Figure 6.1, showing the region in the (Θ, \mathcal{P}) -plane where $g = b_3/b_1$ belongs to the interval $(1, 4 + \sqrt{13})$.

(i) We obtain the numerical values of k_c and μ_c from the plot of the graph of $\mu_0(k)$ in the (k, μ) -plane. The function $\mu_0(k)$ is determined from the boundary value problem (2.9)-(2.10), by looking for nontrivial solutions (V, θ) , with V a real-valued, symmetric with respect to $z = 1/2$, and positive function. Substituting θ given by (2.9) into (2.10), we obtain a boundary value problem written for V alone,

$$(D^2 - k^2)^3 V + \mu^2 k^2 V = 0, \quad V = DV = (D^2 - k)^2 V = 0 \text{ in } z = 0, 1.$$

For $k = k_c$ and $\mu = \mu_c$ this is precisely the boundary value problem (4.10).

Real-valued and symmetric with respect to $z = 1/2$ solutions of this 6th-order ordinary differential equations are of the form

$$V(z) = A_1 \cosh(2l_1 \zeta) + A_2 \cosh(2l_2 \zeta) + A_3 \cosh(2l_3 \zeta),$$

in which A_1, A_2 , and A_3 are real numbers, we set $\zeta = z - 1/2$, so that the function V is an even function in ζ , and $\pm l_1, \pm l_2, \pm l_3$ are the six solutions, perhaps complex, of the algebraic equation

$$((2l)^2 - k^2)^3 + \mu^2 k^2 = 0.$$

Consequently,

$$l_j = \frac{1}{2} \left(k^2 - \omega_j (\mu^2 k^2)^{1/3} \right)^{1/2}, \quad j = 1, 2, 3,$$

where

$$\omega_1 = 1, \quad \omega_2 = -\frac{1}{2} + i\frac{\sqrt{3}}{2}, \quad \omega_3 = -\frac{1}{2} - i\frac{\sqrt{3}}{2},$$

are the three complex roots of $\omega^3 = 1$. Due to the symmetry in z , it is enough to check the boundary conditions in $z = 1$, or equivalently, $\zeta = 1/2$. We obtain a system of three homogeneous linear equations for $\mathbf{A} = (A_1, A_2, A_3)$,

$$\mathcal{M}\mathbf{A} = 0, \tag{B.23}$$

in which the 3×3 matrix \mathcal{M} is given by

$$\mathcal{M} = \begin{pmatrix} \cosh(l_1) & \cosh(l_2) & \cosh(l_3) \\ l_1 \sinh(l_1) & l_2 \sinh(l_2) & l_3 \sinh(l_3) \\ ((2l_1)^2 - k^2)^2 \cosh(l_1) & ((2l_2)^2 - k^2)^2 \cosh(l_2) & ((2l_3)^2 - k^2)^2 \cosh(l_3) \end{pmatrix}.$$

The condition that the determinant of the matrix \mathcal{M} vanishes,

$$\det(\mathcal{M}) = l_1 \tanh(l_1) + \omega_3 l_2 \tanh(l_2) + \omega_3 l_2 \tanh(l_2) = 0,$$

insures the existence of a nontrivial solution V of the boundary value problem and implicitly relates μ and k . Then $\mu_0(k)$ is the smallest μ for which this equality holds, and an implicit Maple plot gives the result in Figure B.1 (left plot), from which we deduce the values of k_c and μ_c in (2.11). This type of calculation has been done in [21] where the authors obtained similar values (without any help from a numerical software, just by using numerical tables for trigonometric functions).

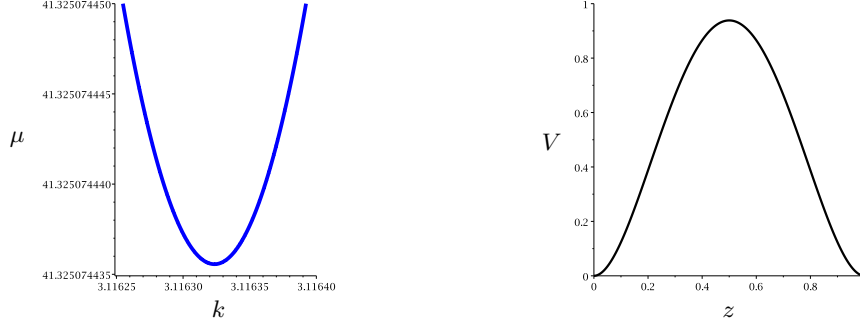


Figure B.1: Maple plots of the graphs of $\mu_0(k)$ (left plot) and the function V with $A_1 = 1$ (right plot).

(ii) For the function V , we take $k = k_c$ and $\mu = \mu_c$ and choose the solution of linear system (B.23) with $A_1 = 1$. We determine the values of A_2 and A_3 by solving the first two equations (see Figure B.1 for a plot of V).

Next, we compute ϕ from the boundary value problem

$$(D^2 - k^2)\phi = V, \quad \phi = 0 \text{ in } z = 0, 1. \quad (\text{B.24})$$

The right hand side of the differential equation being a trigonometric polynomial, we look for a particular solution of the same form and find

$$\phi(z) = -\frac{1}{(k_c^2 \mu_c^2)^{1/3}} (\cosh(2l_1\zeta) + \omega_3 A_2 \cosh(2l_2\zeta) + \omega_2 A_3 \cosh(2l_3\zeta)).$$

The boundary conditions being satisfied by this particular solution, the function ϕ above is the unique solution of the boundary value problem (B.24).

(iii) Inserting the formulas for V and ϕ into (B.20), we obtain that R_1 and R_2 are trigonometric polynomials of the form

$$R_j(x) = \sum_{pq\pm} [R_j]_{pq\pm} \sinh(2\Lambda_{pq\pm}\zeta), \quad j = 1, 2,$$

in which $\Lambda_{pq\pm} = l_p \pm l_q$ and $1 \leq p \leq q \leq 3$. Then we compute V_1 and V_2 by solving the boundary value problems (B.21)-(B.22),

$$V_j = V_j^{(p)} + V_j^{(h)}, \quad j = 1, 2,$$

in which $V_j^{(p)}$ is a particular solution of the non homogeneous differential equation and $V_j^{(h)}$ is a solution of the homogeneous differential equation chosen such that the boundary conditions hold. While $V_j^{(p)}$, $j = 1, 2$, are trigonometric polynomial of the same form as R_j ,

$$V_j^{(p)}(x) = \sum_{pq\pm} [V_j^{(p)}]_{pq\pm} \sinh(2\Lambda_{pq\pm}\zeta), \quad j = 1, 2,$$

in which

$$[V_j^{(p)}]_{pq\pm} = \frac{[R_j]_{pq\pm}}{64 (\Lambda_{pq\pm}^2 - k_c^2 \Theta)^3 + 4k_c^2 \mu_c^2 \Theta}, \quad j = 1, 2,$$

the solutions $V_j^{(h)}$, $j = 1, 2$, of the homogeneous equation are trigonometric polynomials of the form

$$V_j^{(h)}(x) = \sum_{r=1}^3 [V_j^{(h)}]_r \sinh(2h_r \zeta), \quad j = 1, 2,$$

where

$$h_r = \frac{1}{2} \left(4k_c^2 \Theta - \omega_r (4k_c^2 \mu_c^2 \Theta)^{1/3} \right)^{1/2}, \quad r = 1, 2, 3.$$

From the boundary conditions for V_1 and V_2 , we obtain two nonhomogeneous linear systems of three equations for the coefficients $[V_1^{(h)}]_r$, $r = 1, 2, 3$, and $[V_2^{(h)}]_r$, $r = 1, 2, 3$, respectively. We obtain the values of these coefficients by solving these linear systems.

(iv) Inserting the formulas for V_1 , V_2 , R_1 , and R_2 , obtained as above, into (B.17)-(B.19) we compute $A_{31}(\Theta)$, $B_{31}(\Theta)$, $C_{31}(\Theta)$, and then from (B.16) and (B.15) we obtain $b_{31}(\Theta)$ and b_3/b_1 , respectively, which are functions of $\Theta \in [0, 1]$ and $\mathcal{P} > 0$.

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