

Nonlinear dynamics of surfactant–laden multilayer shear flows and related systems

A thesis submitted for the Imperial College London degree of

Doctor of Philosophy in Mathematics

by

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I certify that this thesis, and the research to which it refers, are the product of my own work, and that any ideas or quotations from the work of other people, published or otherwise, are fully acknowledged in accordance with the standard referencing practices of the discipline.

Signed: Anna Kalogirou

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“Πάντα ρεῖ καὶ οὐδὲν μένει.”

Ἡράκλειτος, 535–475 π.Χ.

“Everything flows and nothing stands still.”

Heraclitus, 535–475 B.C.

To my family and friends.

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Abstract

The nonlinear stability of two-fluid shear flows in the presence of inertia and/or an insoluble surfactant at the interface is studied in this thesis. Asymptotic analysis in the limit of a thin lower layer is performed and a system of coupled weakly nonlinear evolution equations is derived. The system describes the spatiotemporal evolution of the interface and its local surfactant concentration. It contains a nonlocal term which arises by appropriately matching solutions of the linearised Navier–Stokes equations in the thicker layer to the thin layer solution. The problem corresponding to two-dimensional flows is first solved numerically, by implementing highly accurate linearly implicit schemes in time with spectral discretisations in space. Numerical experiments for asymptotically small and finite Reynolds numbers indicate that the solutions are mostly nonlinear travelling waves or time-periodic waves. As the length of the system increases, the dynamics become more complex and include quasi-periodic and chaotic fluctuations. The stability in three-dimensions of the nonlinear travelling waves observed in two-dimensional flows is also examined. The model derived is also shown to be appropriate in describing interfacial wave structures arising in two-fluid Couette flow experiments.

A related two-dimensional dissipative–dispersive partial differential equation is considered in the second part of the thesis. The PDE is similar to the surfactant-free version of the interfacial evolution equation derived in the previous part. A generalisation of that equation with a nonlinearity written in a gradient form provides the well-known two-dimensional Kuramoto–Sivashinsky equation (2D KSE). The 2D KSE has received attention with respect to its mathematical analysis, but numerical solutions are obtained for the first time here. For relatively small domain sizes the

solutions are steady states or travelling waves and as the domain becomes increasingly larger, solutions are trapped into a chaotic attractor which is characterised by energy equipartition and symmetry of the energy spectrum.

List of Publications

The material presented in this thesis is the outcome of a collaboration between the author, Anna Kalogirou, and her supervisor, Professor Demetrios T. Papageorgiou. Parts of the thesis resulted from further collaborations with Dr Eric E. Keaveny, Professor Yiorgos–Sokratis Smyrlis and Professor Georgios Akrivis. The following publications and articles in preparation are the result of this work:

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- Kalogirou, A. & Papageorgiou, D. T. Nonlinear dynamics of surfactant–laden two–fluid Couette flows at order one Reynolds numbers. *In preparation.*
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List of Symbols

ρ	Density of the two fluids
μ_1, μ_2	Viscosity of lower fluid 1 or upper fluid 2
d	Channel depth
U	Upper plate horizontal speed
γ	Surface tension
Γ	Local surfactant concentration
m	Viscosity ratio
$Re_{1,2}$	Reynolds number in fluid 1 or 2
Pe	Peclet number
Ma	Marangoni number
Ca	Capillary number
We	Weber number
J	Non-dimensional number measuring surface tension effects
β	Sensitivity of the surface tension on the surfactant concentration
Γ_0	Initial surfactant concentration
Re_e	Reynolds number in the upper fluid (equal to Re_2)

Λ	Parameter depending on the viscosity ratio
η	Parameter representing surfactant diffusivity
$\nu, \nu_{1,2}$	Bifurcation parameters proportional to the inverse of the domain lengths squared
$\mathcal{F}$	Fourier transform
$\Re$	Real part of a complex function
$\Im$	Imaginary part of a complex function
$\mathcal{H}_{per}^s$	Periodic Sobolev space of order s

Part I

Two-fluid shear flows with surfactants

1 Introduction

In this chapter, an overview of the subject of two-fluid channel flows in the presence of surfactants is provided, together with a source of motivation based on related scientific or technological applications. A review of relevant studies found in the literature is also given, summarising the techniques used and outlining their main findings. The novel features used to tackle the problem in the present study and an outline of the main objectives are then described. Finally, the structure of the first part of the thesis is given, with a short description of the content of every chapter.

1.1 Overview of the subject

A two-fluid channel flow is a parallel flow consisting of two immiscible and superposed layers of viscous fluids confined between two horizontal infinite plates. When one of the plates is moving and/or a pressure gradient is present (and gravity is negligible), a shear-driven flow is created which can be found exactly; this is the standard two-fluid Couette or Poiseuille flow (Figure 1). The supported shear is constant (Couette flow) or linear (Poiseuille flow), but also different in each fluid region due to viscosity stratification. In this case, the interface between the two fluids is flat and parallel to the channel walls. The exact parallel flow is susceptible to interfacial instabilities at finite but non-vanishing values of the Reynolds number (Yih [1]) and can produce complex spatiotemporal dynamics of the interface.

The presence of insoluble surfactants in two-fluid shear flows leads to reduction of the local interfacial tension and the action of surface tension gradients (Bassom et al. [2], Oron et al. [3], Otis et al. [4]). Such surface tension gradients arise due to the dependence of surface tension on the local surfactant concentration and give rise to the so-called *Marangoni effect*. The Marangoni stresses are driving the spread of surfactant molecules away from regions of high surfactant concentration (Matar & Craster [5]) and the surface tension gradients cause the fluid to flow away from regions of low surface tension. Therefore the film height disturbances resulting from Marangoni forces can generate instabilities (Afsar-Siddiqui et al. [6], Wei [7]), not present in problems with clean interfaces. The effect of surfactants on flow stability can be assessed by deriving a coupled system of nonlinear evolution equations that control the dynamics of the flow in the asymptotic limit of a thin lower layer (Bassom et al. [2], Kas-Danouche et al. [8]). When the interface is not populated with surfactants, the interfacial surface tension is constant and the flow is unstable only in the presence of inertia. In this case, the system reduces to the well-known dispersively modified Kuramoto-Sivashinsky equation (for extensive numerical experiments of the Kuramoto-Sivashinsky, see Papageorgiou & Smyrlis [9] and Smyrlis & Papageorgiou [10, 11]).

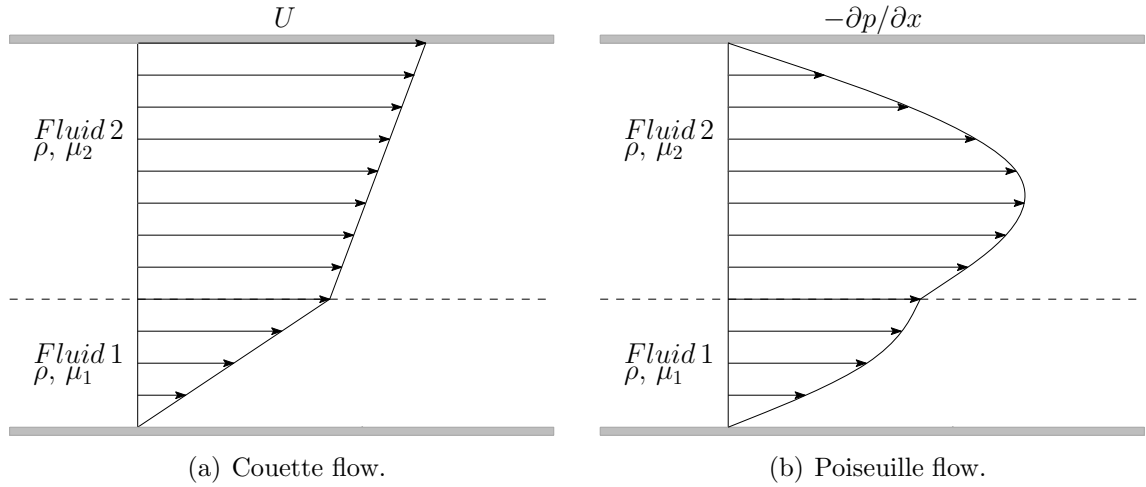


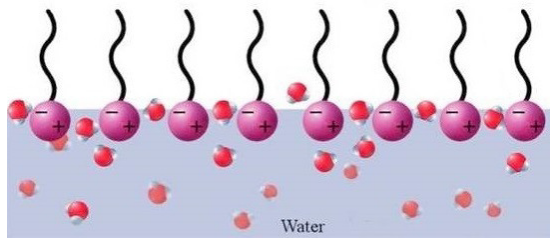
Figure 1: Base state two-layer flows in a horizontal channel, consisting of two fluids with the same density ρ and different viscosities μ_1, μ_2 . (a) Plane Couette flow caused by the upper plate motion with a velocity U . (b) Plane Poiseuille flow caused by a constant pressure gradient $-\partial p/\partial x$ parallel to the plates.

1.2 Motivation & applications

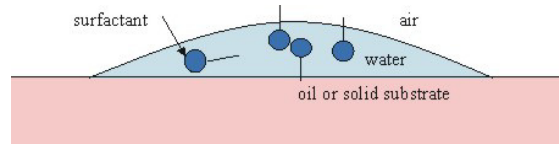
Thin film flows have attracted scientists over the past years. Such flows have become of interest in connection with numerous applications in various fields, such as coating flows (Weinstein & Ruschak [12]) and the recently developed areas of microfluidics and nanofluidics (Craster & Matar [13]). Thin film flows also appear in engineering in the area of nanotechnology (Eijkel & van den Berg [14]) and in geophysics, for example, in gravity currents (Huppert [15]). Theories involving thin films can be also found in biological and biophysical applications, for instance in studies regarding oxygen flow and transport in lung airways (Grotberg [16]).

The presence of surface tension reducing agents, i.e. surfactants, on thin film flows leads to dynamically more complex flows. The importance of surfactant spreading on thin films can be seen when looking at some of their several industrial and biomedical applications; these include rupture of soap films (Figure 2(a)¹) and surfactant

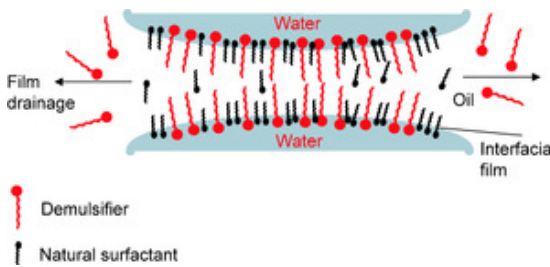
¹New Directions Australia (2010) *Adding essential oils to surfactant solutions*. [Online] Available from: <http://www.newdirections.com.au/articles/article.php?aid=62> [Accessed: 11 June 2014].



(a) Surface tension reduction in oil–water mixtures.



(b) Spreading on a solid substrate.



(c) Film drainage in foams.



(d) Airplane de-icing.

Figure 2: Applications of thin film flows with surfactants. (a) Surfactant molecules in a soap mixture, acting as a stabiliser by reducing the surface tension at the interface between oil and water (Online source: New Directions Australia, 2010). (b) Water and surfactant solution spreading on oil or a solid substrate (Online source: Research Radke Lab, 2000). (c) Film drainage with demulsifiers and surfactants present on the interface of a thin film (Online source: Society of Petroleum Engineers, 2013). (d) Anti-icing of an aircraft to delay the reformation of ice (Online source: Wright & Wellman, 2013).

spreading on films on a solid substrate (Figure 2(b)²) (De Wit et al. [17]). Addition of surfactant is also necessary to foam fabrication in order to preserve film drainage (Braun et al. [18]), as shown schematically in Figure 2(c)³. Moreover, surfactants are included in the composition of anti-icing sprays used on aircraft bodies before takeoff to remove ice and snow and to delay the reformation of ice (Afsar-Siddiqui et

²Research Radke Lab (2000) *Where oil and water mix*. [Online] Available from: http://www.cchem.berkeley.edu/cjrgrp/res/research_summary_2000.html [Accessed: 11 June 2014].

³Society of Petroleum Engineers (2013) *Oil demulsification*. [Online] Available from: http://petrowiki.org/index.php?title=Oil_demulsification [Accessed: 11 June 2014].

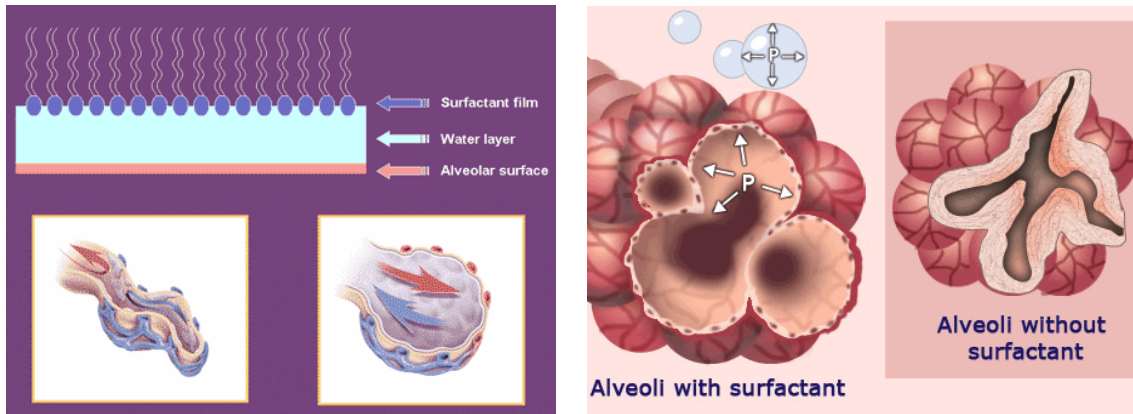


Figure 3: Respiratory distress syndrome: insufficient production of surfactant by the lungs causes collapse of alveoli, resulting in inadequate oxygen exchange. In normal conditions, surfactant lines alveoli on top of the water layer and allows the alveoli to expand by lowering the surface tension (Online sources: Weiss, 2004 (left) and Curoservice, 2014 (right)).

al. [6]), as seen for example in Figure 2(d)⁴. One of the most important applications of film flows with surfactants is surfactant replacement therapy (SRT) for neonates (Afsar-Siddiqui et al. [6], Craster & Matar [13], Jensen & Grotberg [19]). SRT was developed as a method of treatment for respiratory distress syndrome (RDS) and is now a widely used therapy. The respiratory distress syndrome is caused by incapability of the lungs of neonates to regulate their surface tension (Grotberg [16]). The disease usually affects prematurely born infants, whose lungs may not be sufficiently developed to produce sufficient amount of pulmonary surfactant, resulting in alveoli collapse (Figure 3^{5,6}). As a consequence, until the 1990s when SRT was established, the RDS was responsible for a large fatality rate in neonates (Craster & Matar [13]).

⁴Wright, S. & Wellman, A. (2013) *Hundreds stranded in snow and there's more chaos on the way*. [Online] Available from: <http://www.mirror.co.uk/news/uk-news/uk-snow-more-snow-set-1546162> [Accessed: 11 June 2014].

⁵Weiss, K. S. (2004) *Respiratory disease in the neonate: What are the best approaches?* [Online] Available from: <http://www.medscape.org/viewarticle/494960> [Accessed: 11 June 2014].

⁶Curoservice (2014) *Surfactant composition and action*. [Online] Available from: http://www.curoservice.com/parents_visitors/surfactant/surfactant_composition_action.asp [Accessed: 11 June 2014].

1.3 Literature review

The stability of Couette–Poiseuille flows of two superposed fluid layers between two parallel plates was first investigated in 1967 by Yih [1]. Yih’s calculations reveal that the flow can be linearly unstable to long wavelength perturbations however small the Reynolds number is, but not at zero Reynolds number. This instability can only arise if there is a viscosity jump across the interface, and depends on the viscosity and thickness ratios of the two fluid layers (density ratio and surface tension were held fixed in Yih’s study).

Interestingly, the channel walls play a crucial role in determining the instability type. In 1983, Hooper & Boyd [20] examined the stability of unbounded two–fluid flows and showed that in the absence of surface tension the flow is always unstable to short wavelength perturbations. Therefore they arrived at the conclusion that surface tension has a stabilising influence on the flow. A physical explanation of the mechanism of the short wave instability was provided one year later by Hinch [21], in terms of advection of the vorticity disturbances developed at the sheared interface by velocity disturbances. In a related study in 1985, Hooper [22] considered the semi–infinite problem (the upper wall of the channel was moved to infinity) and studied the stability of the interface with surface tension, by assuming a thinner lower fluid layer compared to the upper layer. The results reveal that the flow is always linearly unstable if the thin lower fluid is more viscous than the upper fluid. This effect is called the “thin layer effect” and is often found in multilayer flows (Craster & Matar [13]). Furthermore, Hooper proved that the presence of one wall causes long wave instabilities. The larger growth rate found by Hooper suggests a stronger instability than the one calculated by Yih, confirming that the presence of a second wall has a stabilising effect on the flow. The long wave assumption was removed by Renardy [23, 24] in 1985 & 1987, who solved the linear problem numerically and determined the spectrum for arbitrary flow parameters and wavenumbers.

Based on the same flow configuration used by Hooper in 1985, Hooper & Boyd [25] demonstrated two years later that the semi–bounded problem can be destabilised by three types of instability. Firstly, the long wave instability found by Yih [1], which

disappears if the less viscous fluid is in a relatively thin undisturbed layer. Secondly, the short wave instability found by Hooper & Boyd [20], which can be removed by a sufficient amount of surface tension (Joseph & Renardy [26]). In addition to these, Hooper & Boyd [25] discovered a new instability confined to the lower bounded layer, leaving the upper unbounded fluid relatively undisturbed. This new instability is typical for shear flows; it arises at large Reynolds numbers and only if the viscosity of the lower fluid is less than the viscosity of the upper fluid (unlike the thin layer effect which holds for small Reynolds numbers).

A “phase–diagram” of interfacial instabilities in two–layer Couette flows was provided in 2000 by Charru & Hinch [27]. They explained that the long wave instability found by Yih [1] and Hooper [22] is typical of the shallow viscous flow regime and is related to the presence of the wall close to the interface. Moreover, the short wave instability reported by Hooper & Boyd [20] is associated with the deep viscous regime, i.e. it arises when one fluid layer is much thicker than the other. The third type of instability, namely the shear flow instability found by Hooper & Boyd [25], corresponds to strong shear rates and arises in the inviscid flow regime. Charru & Hinch [27] also proposed a physical explanation of the “thin layer effect” arising in two–layer Couette flows. The initiating mechanism is that in order to satisfy continuity, out–of–phase velocity disturbances develop at the sheared interface due to advection of the basic flow. These disturbances then create a pressure gradient (in order to satisfy the no net flow requirement), effective only in the thick layer where inertial effects are much greater. The out–of–phase flow in the thick layer then induces a shear stress on the thin layer, producing a linear flow there. Thus the sign of the velocity disturbance in the thick layer, which depends on the viscosity ratio, is responsible for the growth or decay of interfacial perturbations.

In a long wave weakly nonlinear study in 1985, Hooper & Grimshaw [28] derived a Kuramoto–Sivashinsky equation for the interface by using the method of multiple scales. They showed that even when including weakly nonlinear effects in the analysis, surface tension still stabilises the linear long wave instability. Three years later, the same authors presented travelling wave solutions of the KSE (Hooper & Grimshaw [29]). They solved the problem numerically for a wide range of param-

ters and their results indicated the existence of complicated families of solutions (of periodic or quasi-periodic nature). For weaker surface tension effects, higher order nonlinear and dispersive terms need to be included in the KSE in order to break the reflectional symmetry of the equation, according to Charru & Fabre [30]. These terms are necessary because the basic flow does not possess such symmetry, so the KSE is expected to fail in describing the interfacial waves.

The linear stability of two-fluid shear flows in the presence of an insoluble surfactant at the interface was first investigated by Frenkel & Halpern [31] and Halpern & Frenkel [32], in 2002 and 2003 respectively. The authors carried out a long wavelength expansion in the former paper and in the latter paper considered arbitrary perturbations in the Stokes flow limit. Then they discussed that the addition of surfactant in the flow considered by Yih [1], induces a Marangoni instability even for zero Reynolds number. This non-inertial instability, in contrast to Yih's instability, does not require the jump of viscosity at the interface (it actually persists for equal fluid viscosities) and disappears in the absence of shearing motion or interfacial surfactant. A recent study of Marangoni effects in two-layer semi-infinite flows can be found in Pozrikidis & Hill [33]. Interestingly, the presence of a wall appears to be a necessary but not sufficient condition for the Marangoni instability, according to the results of the latter paper.

The effect of inertia on the Marangoni instability of the interface was studied numerically by Pozrikidis [34] and by a linear stability analysis for arbitrary wavelength perturbations by Blyth & Pozrikidis [35], both in 2004. The role of inertia was further investigated by Frenkel & Halpern [36] one year later, for perturbations of long wavelength. The outcomes of these papers suggest that increased inertia acts to widen the range of unstable wavenumbers, making the flow more susceptible to linear instability. In addition, if one fluid layer is much thicker than the other, inertial effects in the thick fluid (measured by the Reynolds number in the fluid) are considerably greater than in the thin fluid layer (Charru & Hinch [27]).

The first to perform nonlinear numerical calculations were Blyth & Pozrikidis [37] in 2004, who confirmed Frenkel and Halpern's [31, 32] findings and also generalised the linear stability analysis for arbitrary wavenumbers to include the effect of gravity

and surfactant surface diffusivity. Due to the difficulty of performing direct simulations on large domains, Blyth and Pozrikidis presented numerical simulations on relatively small sized periodic domains that revealed saturated travelling wave solutions. Two years later, Frenkel & Halpern [38] carried out tests for many wave periods and indicated that the saturated travelling waves predicted by Blyth and Pozrikidis vanish when the period of the domain becomes larger. Frenkel and Halpern used a dimensionally reduced model by assuming that one of the fluids is thin compared to other. Letting the upper fluid layer become semi-infinite and assuming small amplitude perturbations, they derived a system of weakly nonlinear equations coupling the film thickness and the surfactant concentration. Their numerical results of solving the evolution equations demonstrate that as the domain size is increased, the solutions become unstable to small wavenumber perturbations.

Along with studies on channel flows, studies on core-annular flows have also been developed. In 1987, Frenkel et al. [39] analysed core-annular flows in the limit of a thin annular fluid layer and performed an asymptotic analysis planned to retain nonlinearity in the leading order evolution equation for the film thickness. The authors examined the simplified case in which the core fluid and the film have equal viscosities and derived a Kuramoto-Sivashinsky equation describing the film dynamics. Three years later, Papageorgiou, Maldarelli & Rumschitzki [40] derived a nonlinear evolution equation for the general case of different-viscosity fluids. In their evolution equation, the film dynamics are coupled to the core region motion through a nonlocal integral term.

The effect of insoluble surfactants on the stability of core-annular flows was first investigated in 2005 by Wei [7] and Wei & Rumschitzki [41], and also by Blyth, Luo & Pozrikidis [42] a year later. The authors performed a linear stability analysis to discover an increase on the long wave instability due to Marangoni forces. In 2009, Kas-Danouche, Papageorgiou & Siegel [8] followed the instability in the nonlinear regime by extending the analysis by Papageorgiou et al. [40] to include an insoluble surfactant. They retained Marangoni effects in the leading order dynamics by assuming small initial surfactant concentration. The nonlinear evolution equation in Kas-Danouche et al. [8] is a generalisation of the modified Kuramoto-Sivashinsky

equation derived by Papageorgiou et al. [40]. The resulting system, consisting of a weakly nonlinear evolution equation for the film thickness coupled with a convection–diffusion equation for the surfactant concentration, was tackled numerically. More recently in 2012, Bassom, Blyth & Papageorgiou [43] studied a different problem of a rod–annular flow with a surfactant–laden interface, consisting of two coaxial fluids in a circular pipe with a solid rod mounted on the axis of the pipe. The problem was solved numerically in the limits of thin outer or inner fluid layer; in the case of thin outer layer and for vanishing rod radius, their results reduced to the ones by Kas–Danouche et al. [8]. The authors also investigated the stability of the flow for different viscosity ratios, layer thicknesses and Reynolds numbers.

Based on the analysis by Kas–Danouche et al. [8] for core–annular flows, in 2010 Bassom, Blyth & Papageorgiou [2] have considered the problem of the two–layer flow in a horizontal channel when the lower layer is thin compared to the upper layer. The authors have derived a pair of coupled weakly nonlinear equations describing the interfacial and surfactant dynamics. In the evolution equation for the film thickness, there is a nonlocal integral term (a pseudo–differential operator) coupling the dynamics in the film to those in the upper layer fluid. Numerical calculations have been carried out for the cases of asymptotically small (of the order of the film thickness) and order one Reynolds number in the upper layer. In the case of asymptotically small Reynolds number, finite–amplitude travelling wave solutions have been observed to arise from the simulations. Periodic travelling waves, chaotic solutions and generally more complex dynamics result if the Reynolds number is of order one. In a more recent study in 2013, Samanta [44] has considered the linear problem governed by an Orr–Sommerfeld system, along with model equations derived using depth–averaging methods; Bassom et al.’s [2] study is quite distinct from this since it considers the nonlocal coupling between thin and finite–thickness fluid layers.

1.4 Objectives of this thesis

In this thesis, the problem of a two–layer flow in a channel in the presence of surfactants is revisited. The evolution equations are derived again under the assumption

of a thin lower layer in comparison to the thickness of the overlying fluid. However, for the first time the channel considered is *three-dimensional* and hence the evolution equations derived here are more general than the ones derived in Bassom et al. [2].

The authors of the aforementioned paper have derived the two-dimensional evolution equation but actually solved numerically a localisation of that equation. Specifically, they approximated the nonlocal term by a small wavenumber expansion (Smyrlis & Papageorgiou [45]). The aim of this study is to solve *the full nonlocal system* and compare solutions between local and nonlocal systems to identify where deviations may occur. Calculations are performed for both asymptotically small and finite Reynolds number in the upper layer. The innovation of this work also lies in the study of the stability of the three-dimensional flow via investigation of validity of a Squire's type theorem. The stability in three-dimensions of the nonlinear travelling wave solutions observed in the two-dimensional flow is also examined.

The asymptotic theory described here retains the effect of inertia in the thicker layer in order to generate dynamics that extend beyond the reach of usual lubrication theories. Inertial effects are included in the nonlocal term which incorporates the effect of the upper layer dynamics to the evolution of the film thickness. The resulting evolution equation for the film thickness is also solved in the case of absence of surfactants and used to compare interfacial shapes observed in experiments (Barthelet et al. [46]), for relatively high Reynolds number values (up to approximately 500). Similar nonlocal equations are found in various physical contexts; their importance can be seen by considering their connections with turbulent shear flows in riverbed dynamics (Fowler [47]), the dynamics of electrified falling films (Tseluiko & Papageorgiou [48]) or the dynamics of falling films below turbulent gas flows (an empirical nonlocal KS-type model was derived in Tseluiko & Kalliadasis [49]).

The structure of this part of the thesis is as follows: Chapter 2 describes the mathematical model, governing equations and details of the surface gradient operator required in the analysis. It also introduces the asymptotic expansions and details about the derivation of evolution equations, including a careful explanation of the scalings involved in producing the weakly nonlinear model. Chapter 3 presents relevant asymptotic properties of the nonlocal term that appears in the interfacial

evolution equation. Chapter 4 describes the numerical methods used to solve the system as a periodic initial value problem. Chapter 5 contains the main results obtained for the simplified case of a two-dimensional flow, including a comparison of numerical solutions to experimental results for two-fluid Couette flows without surfactants. Chapter 6 that follows provides stability properties of three-dimensional flows and some numerical results. Finally, Chapter 7 summarises the outcomes of this study, pointing out novel results and possible future extensions.

2 Derivation of Evolution Equations

The aim of this chapter is to provide the mathematical formulation of a three-dimensional two-layer Couette flow with insoluble surfactants. The governing equations and boundary conditions are given, together with a convection–diffusion equation describing the variation of surfactant concentration at the interface. A detailed formulation of the surface gradient operator and the vectors that appear in the equations is then provided, followed by the non-dimensionalisation of the governing equations and boundary conditions. In addition, the base state two-layer Couette flow is obtained, which is then perturbed and a detailed scaling analysis follows to determine the size of the perturbations. Asymptotic theory based on the assumption of a thin lower layer is performed, leading to the final evolution equations. These consist of a system of two equations describing the spatiotemporal evolution of the interface and its local surfactant concentration.

2.1 Mathematical model

Consider the flow of two superposed viscous and immiscible fluid layers in a channel. Usual cartesian coordinates (x, y, z) are used, with the x - and z -axis being perpendicular to one another and drawn along the surface of the lower plate, and the y -axis drawn perpendicular to the plates (see also Figure 4). The channel consists of two impermeable parallel flat plates, situated at $y = 0$ and $y = d$. The flow is driven by the motion of the upper plate with longitudinal velocity U . Moreover, the fluid densities are the same and equal to ρ and their viscosities are in general different and assumed to be μ_1 for the lower fluid and μ_2 for the upper fluid. The interface between the two fluids is flat in the undisturbed state and is located at $y = \ell d$, with $0 < \ell < 1$. When the basic flow is perturbed, it is assumed to take the shape $y = S(x, z, t)$ which is in general a function of space and time. Lastly, an insoluble surfactant is also present, which is only allowed to move on the interface and whose local concentration is denoted by $\Gamma(x, z, t)$.

The flow velocity in each region is written in a vector form as $\mathbf{u}_i(x, y, z, t)$, $i = 1, 2$, where subscripts 1 and 2 refer to the lower and upper fluids, respectively, and the velocity components are $\mathbf{u}_i = (u_i, v_i, w_i)$. Gravitational effects do not affect the flow of two same-density fluids in a horizontal channel, so gravity is neglected in the analysis that follows. The flow in each fluid region $i = 1, 2$ is described by the Navier–Stokes equations and the continuity equation, given by

$$\rho \left(\frac{\partial \mathbf{u}_i}{\partial t} + \mathbf{u}_i \cdot \nabla \mathbf{u}_i \right) = -\nabla p_i + \mu_i \nabla^2 \mathbf{u}_i, \quad (2.1a)$$

$$\nabla \cdot \mathbf{u}_i = 0. \quad (2.1b)$$

The above equations are subject to boundary conditions of no-slip and no-penetration on the walls and continuity of fluid velocities at the interface, namely

$$\begin{aligned} \mathbf{u}_1 &= (0, 0, 0) \quad \text{at} \quad y = 0, \\ \mathbf{u}_2 &= (U, 0, 0) \quad \text{at} \quad y = d, \\ \mathbf{u}_1 &= \mathbf{u}_2 \quad \text{at} \quad y = S(x, z, t). \end{aligned} \quad (2.2)$$

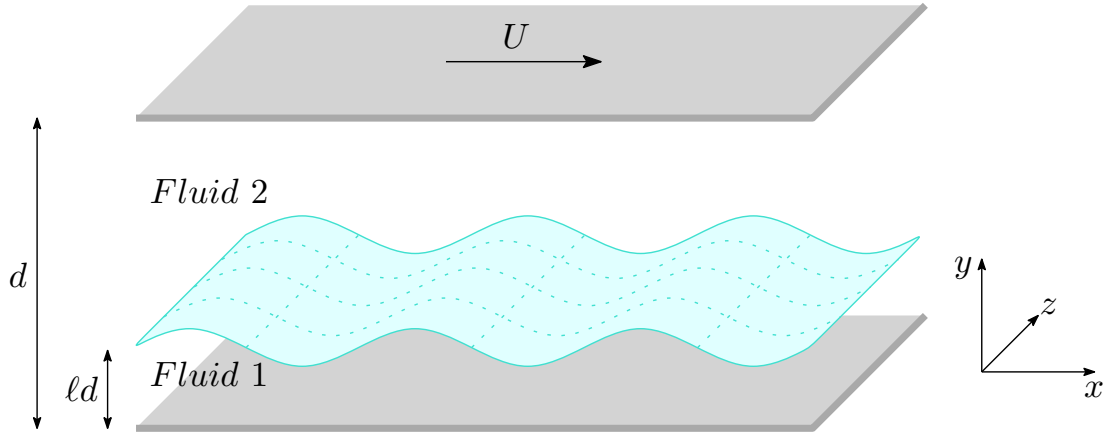


Figure 4: Geometry of the three-dimensional problem: two superposed fluid layers in a channel of depth d . The flow is driven by the upper wall motion with horizontal speed U . The blue surface corresponds to the perturbed interface, which in the undisturbed state is flat and located at a distance ℓd from the lower plate, $0 < \ell < 1$. The interface is populated with an insoluble surfactant.

In addition to these boundary conditions, the following kinematic condition is imposed at the interface

$$(\partial_t + \mathbf{u}_i \cdot \nabla)(y - S(x, z, t)) = 0, \quad i = 1, 2. \quad (2.3)$$

The interest is to study the development of the flow when it is perturbed from the basic state. The perturbation leads to an alteration in the basic (undisturbed) constant surfactant concentration on the interface. This modification is described by the convection–diffusion equation (Wong et al. [50], Pereira & Kalliadasis [51])

$$\frac{\partial \Gamma}{\partial t} - \frac{\partial \mathbf{r}}{\partial t} \cdot \nabla_s \Gamma + \nabla_s \cdot (\Gamma \mathbf{u}_s) + \Gamma \kappa (\mathbf{u}_1 \cdot \mathbf{n}) - \mathcal{D}_s (\nabla_s^2 \Gamma) = 0. \quad (2.4)$$

The derivation of this equation is based on the argument that the rate of change of the total amount of surfactant on an interfacial area is equal to the net amount which enters through the perimeter of the interface by convection or diffusion. It is also based on the assumption that the surface flux is given by Fick’s law of diffusion (Li & Pozrikidis [52]). The first three terms in the above equation correspond to convection of surfactant molecules moving with interfacial fluid particles; in particular, the second term originates from the displacement of fluid particles in three-dimensional space

(in a Lagrangian description of the flow kinematics). The fourth and fifth terms represent the effects of interfacial curvature and diffusion on the variation of surfactant concentration, respectively. The variables that appear in the surfactant transport equation are the following: $\mathbf{r}$ is the position vector of the interface, ∇_s is the surface gradient operator (discussed in Section 2.2), $\mathbf{u}_I$ is the velocity vector at the interface given by either $\mathbf{u}_1(x, S, z)$ or $\mathbf{u}_2(x, S, z)$ (they are both equal due to velocity continuity at the interface, see condition (2.2)), $\mathbf{u}_s$ is the velocity tangent to the interface, $\mathcal{D}_s$ is the constant surfactant diffusivity, κ is the mean curvature of the interface and $\mathbf{n}$ is the unit normal vector (pointing into fluid 1 – for definition see Section 2.2).

The change in the surfactant concentration at the interface results in variation in the interfacial surface tension γ (Levich [53]). The dependence of surface tension on Γ is described by an equation of state of the form $\gamma = \gamma(\Gamma)$ (Edwards et al. [54], Frumkin & Levich [55]) and is taken to be (Kas-Danouche [56], Pozrikidis [57])

$$\gamma = \gamma_c + \mathcal{R}T\Gamma_\infty \ln \left(1 - \frac{\Gamma}{\Gamma_\infty} \right), \quad (2.5)$$

where γ_c is the value of the surface tension established in the absence of surfactant (namely when the interface is clean of surfactant), Γ_∞ is the maximum packing concentration of surfactant (exists in the absence of any flow), $\mathcal{R}$ is the universal gas constant and T is the absolute temperature. Assuming that the surfactant is present only in dilute concentration (this case is frequently encountered in applications), the logarithm can be expanded in Taylor series and a linear relation can be used instead. The final equation of state is called the linear Gibbs' isotherm (Blyth & Pozrikidis [37], Li & Pozrikidis [52]) and is given by

$$\gamma = \gamma_c - \mathcal{R}T\Gamma. \quad (2.6)$$

In addition, the dynamic condition requires the stress to be continuous across the interface. In the problem studied here, there exists a capillary pressure jump in the normal stress due to interfacial curvature jump and the variability of surface tension causes a jump in the tangential stress. Taking these into account, the stress jump at

the interface is given by (Milliken et al. [58], Stone [59] – see also Batchelor [60] for the case of constant surface tension)

$$\mathbf{n} \cdot (\boldsymbol{\sigma}_1 - \boldsymbol{\sigma}_2) = \kappa \gamma \mathbf{n} - \nabla_s \gamma, \quad (2.7)$$

where $\boldsymbol{\sigma}_i$ is the stress tensor in fluid i (defined in the following section). The normal stress balance is provided by taking the dot product of (2.7) with the unit normal $\mathbf{n}$, and is equal to

$$[\mathbf{n} \cdot (\mathbf{n} \cdot \boldsymbol{\sigma}_i)]_2^1 = \kappa \gamma, \quad (2.8a)$$

where the jump notation $[f_i]_2^1 = f_1 - f_2$ is used. To find the tangential stress balance, it is first noted that there is a tangent plane passing through any point on the interface and therefore there are two vectors that form the contravariant basis of the tangent plane. Hence there exist two tangential stress balances, obtained by taking the dot product of (2.7) with the unit tangents $\mathbf{t}_1, \mathbf{t}_2$ (in x - and z -direction, respectively) and are given by

$$[\mathbf{t}_1 \cdot (\mathbf{n} \cdot \boldsymbol{\sigma}_i)]_2^1 = -\mathbf{t}_1 \cdot \nabla_s \gamma, \quad (2.8b)$$

$$[\mathbf{t}_2 \cdot (\mathbf{n} \cdot \boldsymbol{\sigma}_i)]_2^1 = -\mathbf{t}_2 \cdot \nabla_s \gamma. \quad (2.8c)$$

So far, many quantities have been introduced without being defined. These include the unit normal vector $\mathbf{n}$, the contravariant basis of the tangent plane consisting of the unit vectors $\mathbf{t}_1, \mathbf{t}_2$ and the surface gradient operator ∇_s . All of the above and all the terms in the surfactant convection–diffusion equation (2.4) are defined explicitly in the following section.

2.2 Explicit forms of governing equations

Considering the perturbed interfacial shape to be given by $y = S(x, z, t)$, then any point on the interface has position vector

$$\mathbf{r} = (x, S(x, z, t), z). \quad (2.9)$$

The contravariant base vectors $\mathbf{t}_1$, $\mathbf{t}_2$ of the tangent plane to the interface can be found by taking partial derivatives of the position vector $\mathbf{r}$ with respect to x and z respectively (Kas–Danouche [56], Papageorgiou [61], Stone & Leal [62]), i.e. at any point on the interface

$$\mathbf{t}_1 = \frac{\partial \mathbf{r}}{\partial x} = (1, S_x, 0), \quad \mathbf{t}_2 = \frac{\partial \mathbf{r}}{\partial z} = (0, S_z, 1). \quad (2.10a)$$

In addition, the unit normal vector is defined by

$$\mathbf{n} = \frac{\mathbf{t}_1 \times \mathbf{t}_2}{\sqrt{h}} = \frac{(S_x, -1, S_z)}{\sqrt{1 + S_x^2 + S_z^2}}, \quad (2.10b)$$

where $\times$ here symbolizes the standard cross product and h is the metric tensor determinant. Defining the covariant components of the surface metric tensor by

$$\begin{aligned} h_{11} &= \mathbf{t}_1 \cdot \mathbf{t}_1 = 1 + S_x^2, & h_{12} &= \mathbf{t}_1 \cdot \mathbf{t}_2 = S_x S_z, \\ h_{21} &= h_{12} = \mathbf{t}_2 \cdot \mathbf{t}_1 = S_x S_z, & h_{22} &= \mathbf{t}_2 \cdot \mathbf{t}_2 = 1 + S_z^2, \end{aligned} \quad (2.11)$$

then the metric tensor determinant is equal to (Aris [63])

$$h = h_{11}h_{22} - h_{12}^2 = 1 + S_x^2 + S_z^2. \quad (2.12)$$

To find the surface gradient operator, the covariant base vectors are introduced by the following formulae (Wheeler & McFadden [64])

$$\mathbf{t}^1 = -\frac{\mathbf{n} \times \mathbf{t}_2}{\sqrt{h}} = \frac{(1 + S_z^2, S_x, -S_x S_z)}{\sqrt{1 + S_x^2 + S_z^2}}, \quad (2.13a)$$

$$\mathbf{t}^2 = \frac{\mathbf{n} \times \mathbf{t}_1}{\sqrt{h}} = \frac{(-S_x S_z, S_z, 1 + S_x^2)}{\sqrt{1 + S_x^2 + S_z^2}}. \quad (2.13b)$$

These vectors are reciprocal to the contravariant base vectors and have the properties

$$\mathbf{t}^1 \cdot \mathbf{t}_1 = 1, \quad \mathbf{t}^2 \cdot \mathbf{t}_2 = 1, \quad \mathbf{t}^1 \cdot \mathbf{t}_2 = \mathbf{t}^2 \cdot \mathbf{t}_1 = 0. \quad (2.14)$$

The surface gradient operator is defined as

$$\nabla_s = \mathbf{t}^1 \frac{\partial}{\partial x} + \mathbf{t}^2 \frac{\partial}{\partial z}. \quad (2.15)$$

The divergence of any vector field $\mathbf{V}$ written in its contravariant form as $\mathbf{V} = V_1 \mathbf{t}_1 + V_2 \mathbf{t}_2 + V_3 \mathbf{n}$ is then given by (Papageorgiou [61])

$$\nabla_s \cdot \mathbf{V} = \frac{1}{\sqrt{h}} \left[\frac{\partial}{\partial x} (\sqrt{h} V_1) + \frac{\partial}{\partial z} (\sqrt{h} V_2) \right] + V_3 \kappa, \quad (2.16)$$

where $\kappa = 2H$ and $H = \frac{1}{2} (\nabla_s \cdot \mathbf{n})$ is the mean curvature of the interface; κ is equal to (Spivak [65])

$$\kappa = \frac{(1 + S_x^2) S_{zz} - 2S_x S_z S_{xz} + (1 + S_z^2) S_{xx}}{(1 + S_x^2 + S_z^2)^{3/2}}. \quad (2.17)$$

The surfactant surface gradient is easily obtained by applying (2.15) on the scalar Γ and is given by

$$\nabla_s \Gamma = \mathbf{t}^1 \Gamma_x + \mathbf{t}^2 \Gamma_z. \quad (2.18)$$

The surface gradient of the surfactant can be also written as $\nabla_s \Gamma = \Gamma_1 \mathbf{t}_1 + \Gamma_2 \mathbf{t}_2 + \Gamma_n \mathbf{n}$, and by taking dot product of this expression and (2.18) with the unit normal and contravariant tangent vectors, the following equations are obtained

$$\begin{aligned} \mathbf{t}_1 \cdot (\nabla_s \Gamma) &= (1 + S_x^2) \Gamma_1 + S_x S_z \Gamma_2 = \Gamma_x, \\ \mathbf{t}_2 \cdot (\nabla_s \Gamma) &= S_x S_z \Gamma_1 + (1 + S_z^2) \Gamma_2 = \Gamma_z, \\ \mathbf{n} \cdot (\nabla_s \Gamma) &= \Gamma_n = 0. \end{aligned} \quad (2.19)$$

Solving for Γ_1 and Γ_2 leads to

$$\Gamma_1 = \frac{\Gamma_x (1 + S_z^2) - \Gamma_z S_x S_z}{1 + S_x^2 + S_z^2}, \quad \Gamma_2 = \frac{\Gamma_z (1 + S_x^2) - \Gamma_x S_x S_z}{1 + S_x^2 + S_z^2}. \quad (2.20)$$

Hence the surfactant surface Laplacian can be calculated by using (2.16) and (2.20), and reads

$$\begin{aligned}\nabla_s^2 \Gamma &= \nabla_s \cdot (\nabla_s \Gamma) \\ &= \frac{1}{\sqrt{1 + S_x^2 + S_z^2}} \left[\frac{\partial}{\partial x} \left(\sqrt{1 + S_x^2 + S_z^2} \Gamma_1 \right) + \frac{\partial}{\partial z} \left(\sqrt{1 + S_x^2 + S_z^2} \Gamma_2 \right) \right].\end{aligned}\quad (2.21)$$

Furthermore, the velocity vector $\mathbf{u}_I = (u_I, v_I, w_I)$ at the interface can be written in its contravariant form as

$$\mathbf{u}_I = u^{(1)} \mathbf{t}_1 + u^{(2)} \mathbf{t}_2 + u_n \mathbf{n} = \mathbf{u}_s + u_n \mathbf{n}, \quad (2.22)$$

where $\mathbf{u}_s$ is the vector component of the velocity that lies on the tangent plane (Stone & Leal [62]). Taking the dot product of the velocity vector with the unit normal and tangent vectors, yields

$$\mathbf{t}_1 \cdot \mathbf{u}_I = (1 + S_x^2) u^{(1)} + S_x S_z u^{(2)} = u_I + v_I S_x, \quad (2.23a)$$

$$\mathbf{t}_2 \cdot \mathbf{u}_I = S_x S_z u^{(1)} + (1 + S_z^2) u^{(2)} = v_I S_z + w_I, \quad (2.23b)$$

$$\mathbf{n} \cdot \mathbf{u}_I = u_n = \frac{u_I S_x - v_I + w_I S_z}{\sqrt{1 + S_x^2 + S_z^2}}, \quad (2.23c)$$

leading to

$$u^{(1)} = \frac{(u_I + v_I S_x)(1 + S_z^2) - (v_I S_z + w_I) S_x S_z}{1 + S_x^2 + S_z^2}, \quad (2.24a)$$

$$u^{(2)} = \frac{(v_I S_z + w_I)(1 + S_x^2) - (u_I + v_I S_x) S_x S_z}{1 + S_x^2 + S_z^2}, \quad (2.24b)$$

and eventually to the following result

$$\nabla_s \cdot (\Gamma \mathbf{u}_s) = \frac{1}{\sqrt{1 + S_x^2 + S_z^2}} \left[\frac{\partial}{\partial x} \left(\sqrt{1 + S_x^2 + S_z^2} u^{(1)} \Gamma_1 \right) + \frac{\partial}{\partial z} \left(\sqrt{1 + S_x^2 + S_z^2} u^{(2)} \Gamma_2 \right) \right]. \quad (2.25)$$

Additionally,

$$\frac{\partial \mathbf{r}}{\partial t} = (0, S_t, 0) \quad (2.26)$$

and

$$\frac{\partial \mathbf{r}}{\partial t} \cdot (\nabla_s \Gamma) = \frac{S_t}{1 + S_x^2 + S_z^2} (\Gamma_x S_x + \Gamma_z S_z). \quad (2.27)$$

Based on the above analysis, the full system (2.1)–(2.8) can be now given in explicit form. The Navier–Stokes equations (2.1) become

$$\rho \left(\frac{\partial u_i}{\partial t} + u_i \frac{\partial u_i}{\partial x} + v_i \frac{\partial u_i}{\partial y} + w_i \frac{\partial u_i}{\partial z} \right) = -\frac{\partial p_i}{\partial x} + \mu_i \left(\frac{\partial^2 u_i}{\partial x^2} + \frac{\partial^2 u_i}{\partial y^2} + \frac{\partial^2 u_i}{\partial z^2} \right), \quad (2.28a)$$

$$\rho \left(\frac{\partial v_i}{\partial t} + u_i \frac{\partial v_i}{\partial x} + v_i \frac{\partial v_i}{\partial y} + w_i \frac{\partial v_i}{\partial z} \right) = -\frac{\partial p_i}{\partial y} + \mu_i \left(\frac{\partial^2 v_i}{\partial x^2} + \frac{\partial^2 v_i}{\partial y^2} + \frac{\partial^2 v_i}{\partial z^2} \right), \quad (2.28b)$$

$$\rho \left(\frac{\partial w_i}{\partial t} + u_i \frac{\partial w_i}{\partial x} + v_i \frac{\partial w_i}{\partial y} + w_i \frac{\partial w_i}{\partial z} \right) = -\frac{\partial p_i}{\partial z} + \mu_i \left(\frac{\partial^2 w_i}{\partial x^2} + \frac{\partial^2 w_i}{\partial y^2} + \frac{\partial^2 w_i}{\partial z^2} \right), \quad (2.28c)$$

$$\frac{\partial u_i}{\partial x} + \frac{\partial v_i}{\partial y} + \frac{\partial w_i}{\partial z} = 0. \quad (2.28d)$$

The boundary conditions (2.2) are written explicitly as

$$\begin{aligned} u_1 = v_1 = w_1 = 0 & \quad \text{at } y = 0, \\ u_2 = U, v_2 = w_2 = 0 & \quad \text{at } y = d, \\ u_1 = u_2, v_1 = v_2, w_1 = w_2 & \quad \text{at } y = S(x, z, t). \end{aligned} \quad (2.29)$$

At the interface, the kinematic condition (2.3) is given by

$$v_i - S_t - u_i S_x - w_i S_z = 0, \quad i = 1, 2. \quad (2.30)$$

Collecting terms (2.17), (2.21), (2.23c), (2.25), (2.27) and substituting them into the surfactant transport equation (2.4), results in

$$\begin{aligned} & \frac{\partial \Gamma}{\partial t} - \frac{S_t}{(1 + S_x^2 + S_z^2)} \left(\Gamma_x S_x + \Gamma_z S_z \right) \\ & + \frac{1}{\sqrt{1 + S_x^2 + S_z^2}} \left[\frac{\partial}{\partial x} \left(\sqrt{1 + S_x^2 + S_z^2} u^{(1)} \Gamma \right) + \frac{\partial}{\partial z} \left(\sqrt{1 + S_x^2 + S_z^2} u^{(2)} \Gamma \right) \right] \\ & + \frac{\Gamma (u_I S_x - v_I + w_I S_z)}{\sqrt{1 + S_x^2 + S_z^2}} \left(\frac{(1 + S_x^2) S_{zz} - 2 S_x S_z S_{xz} + (1 + S_z^2) S_{xx}}{\sqrt{1 + S_x^2 + S_z^2}} \right) \\ & - \frac{\mathcal{D}_s}{\sqrt{1 + S_x^2 + S_z^2}} \left[\frac{\partial}{\partial x} \left(\frac{\Gamma_x (1 + S_z^2) - \Gamma_z S_x S_z}{\sqrt{1 + S_x^2 + S_z^2}} \right) + \frac{\partial}{\partial z} \left(\frac{\Gamma_z (1 + S_x^2) - \Gamma_x S_x S_z}{\sqrt{1 + S_x^2 + S_z^2}} \right) \right] \\ & = 0. \end{aligned} \quad (2.31)$$

Finally, to write the vector equations for the stress balances at the interface explicitly, the following definition of the stress tensor is used (Batchelor [60])

$$(\boldsymbol{\sigma}_i)_{k\ell} = -p\delta_{k\ell} + \mu_i \left(\frac{\partial u_k}{\partial x_\ell} + \frac{\partial u_\ell}{\partial x_k} \right), \quad k, \ell = 1, 2, 3, \quad (2.32)$$

where $\delta_{k\ell}$ is the Kronecker delta function. Inserting the contravariant unit tangent vectors (2.10a) and the unit normal vector (2.10b) into the stress jump equations (2.8), the following expressions for the normal and tangential stress balances at the interface are obtained, respectively

$$\left[-p_i + \frac{2\mu_i}{1 + S_x^2 + S_z^2} \left(S_x^2 \frac{\partial u_i}{\partial x} + S_z^2 \frac{\partial w_i}{\partial z} + \frac{\partial v_i}{\partial y} - S_x \left(\frac{\partial u_i}{\partial y} + \frac{\partial v_i}{\partial x} \right) - S_z \left(\frac{\partial v_i}{\partial z} + \frac{\partial w_i}{\partial y} \right) + S_x S_z \left(\frac{\partial u_i}{\partial z} + \frac{\partial w_i}{\partial x} \right) \right) \right]_2^1 = \kappa \gamma, \quad (2.33a)$$

$$\frac{1}{\sqrt{1 + S_x^2 + S_z^2}} \left[\mu_i \left(2S_x \left(\frac{\partial u_i}{\partial x} - \frac{\partial v_i}{\partial y} \right) + S_z \left(\frac{\partial u_i}{\partial z} + \frac{\partial w_i}{\partial x} \right) + S_x S_z \left(\frac{\partial v_i}{\partial z} + \frac{\partial w_i}{\partial y} \right) + (S_x^2 - 1) \left(\frac{\partial u_i}{\partial y} + \frac{\partial v_i}{\partial x} \right) \right) \right]_2^1 = -\frac{\partial \gamma}{\partial x}, \quad (2.33b)$$

$$\frac{1}{\sqrt{1 + S_x^2 + S_z^2}} \left[\mu_i \left(2S_z \left(\frac{\partial w_i}{\partial z} - \frac{\partial v_i}{\partial y} \right) + S_x \left(\frac{\partial u_i}{\partial z} + \frac{\partial w_i}{\partial x} \right) + S_x S_z \left(\frac{\partial u_i}{\partial y} + \frac{\partial v_i}{\partial x} \right) + (S_z^2 - 1) \left(\frac{\partial v_i}{\partial z} + \frac{\partial w_i}{\partial y} \right) \right) \right]_2^1 = -\frac{\partial \gamma}{\partial z}. \quad (2.33c)$$

The right hand side derivative terms $\frac{\partial \gamma}{\partial x}$ and $\frac{\partial \gamma}{\partial z}$ in (2.33b), (2.33c) respectively, are the Marangoni stresses arising from variations in the surface tension, and play an important role in the dynamics of the flow.

2.3 Non-dimensional variables

In order to express the problem in non-dimensional form, the channel depth d is used to scale lengths, the upper plate velocity U to scale velocities, fluid pressures are scaled by ρU^2 and time by $\frac{d}{U}$. Also, surface tension is scaled by the clean surface tension γ_c and the surfactant concentration by the maximum packing surfactant concentration Γ_∞ . In summary, the following transformation of variables is performed

$$\begin{aligned} x \rightarrow dx, \quad y \rightarrow dy, \quad z \rightarrow dz, \quad u_i \rightarrow Uu_i, \quad v_i \rightarrow Uv_i, \quad w_i \rightarrow Uw_i, \\ t \rightarrow \frac{d}{U}t, \quad p \rightarrow \rho U^2 p, \quad \gamma \rightarrow \gamma_c \gamma, \quad \Gamma \rightarrow \Gamma_\infty \Gamma. \end{aligned} \quad (2.34)$$

The momentum and continuity equations written in terms of the non-dimensional variables are

$$\frac{\partial u_i}{\partial t} + u_i \frac{\partial u_i}{\partial x} + v_i \frac{\partial u_i}{\partial y} + w_i \frac{\partial u_i}{\partial z} = -\frac{\partial p_i}{\partial x} + \frac{1}{Re_i} \left(\frac{\partial^2 u_i}{\partial x^2} + \frac{\partial^2 u_i}{\partial y^2} + \frac{\partial^2 u_i}{\partial z^2} \right), \quad (2.35a)$$

$$\frac{\partial v_i}{\partial t} + u_i \frac{\partial v_i}{\partial x} + v_i \frac{\partial v_i}{\partial y} + w_i \frac{\partial v_i}{\partial z} = -\frac{\partial p_i}{\partial y} + \frac{1}{Re_i} \left(\frac{\partial^2 v_i}{\partial x^2} + \frac{\partial^2 v_i}{\partial y^2} + \frac{\partial^2 v_i}{\partial z^2} \right), \quad (2.35b)$$

$$\frac{\partial w_i}{\partial t} + u_i \frac{\partial w_i}{\partial x} + v_i \frac{\partial w_i}{\partial y} + w_i \frac{\partial w_i}{\partial z} = -\frac{\partial p_i}{\partial z} + \frac{1}{Re_i} \left(\frac{\partial^2 w_i}{\partial x^2} + \frac{\partial^2 w_i}{\partial y^2} + \frac{\partial^2 w_i}{\partial z^2} \right), \quad (2.35c)$$

$$\frac{\partial u_i}{\partial x} + \frac{\partial v_i}{\partial y} + \frac{\partial w_i}{\partial z} = 0. \quad (2.35d)$$

The non-dimensional numbers $Re_{1,2}$ denote the *Reynolds number* in each fluid and are equal to

$$Re_1 = \frac{\rho U d}{\mu_1}, \quad Re_2 = \frac{\rho U d}{\mu_2} = \frac{Re_1}{m}, \quad (2.36)$$

where $m = \mu_2/\mu_1$ is the viscosity ratio. The no-slip and no-penetration conditions become

$$\begin{aligned} u_1 = v_1 = w_1 = 0 \quad \text{at} \quad y = 0, \\ u_2 = 1, \quad v_2 = w_2 = 0 \quad \text{at} \quad y = 1, \end{aligned} \quad (2.37)$$

and the velocity continuity condition at the interface remains the same as in (2.29);

the kinematic condition reads

$$v_i = S_t + u_i S_x + w_i S_z, \quad i = 1, 2. \quad (2.38)$$

Moreover, the surfactant transport equation (2.31) takes the following dimensionless form

$$\begin{aligned} & \frac{\partial \Gamma}{\partial t} - \frac{S_t}{(1 + S_x^2 + S_z^2)} (\Gamma_x S_x + \Gamma_z S_z) \\ & + \frac{1}{\sqrt{1 + S_x^2 + S_z^2}} \left[\frac{\partial}{\partial x} \left(\sqrt{1 + S_x^2 + S_z^2} u^{(1)} \Gamma \right) + \frac{\partial}{\partial z} \left(\sqrt{1 + S_x^2 + S_z^2} u^{(2)} \Gamma \right) \right] \\ & + \frac{\Gamma (u_I S_x - v_I + w_I S_z)}{\sqrt{1 + S_x^2 + S_z^2}} \left(\frac{(1 + S_x^2) S_{zz} - 2 S_x S_z S_{xz} + (1 + S_z^2) S_{xx}}{\sqrt{1 + S_x^2 + S_z^2}} \right) \\ & - \frac{1}{Pe} \frac{1}{\sqrt{1 + S_x^2 + S_z^2}} \left[\frac{\partial}{\partial x} \left(\frac{\Gamma_x (1 + S_z^2) - \Gamma_z S_x S_z}{\sqrt{1 + S_x^2 + S_z^2}} \right) + \frac{\partial}{\partial z} \left(\frac{\Gamma_z (1 + S_x^2) - \Gamma_x S_x S_z}{\sqrt{1 + S_x^2 + S_z^2}} \right) \right] \\ & = 0, \end{aligned} \quad (2.39)$$

where $u^{(1)}, u^{(2)}$ are defined in (2.24) and $Pe = \frac{Ud}{\mathcal{D}_s}$ is the *Peclet number*. The linear equation of state (2.6) written in non-dimensional variables is

$$\gamma = 1 - \beta \Gamma, \quad (2.40)$$

where $\beta = \frac{\mathcal{RT}\Gamma_\infty}{\gamma_c}$ is an elasticity parameter that measures the sensitivity of interfacial tension to changes in the surfactant concentration (Wei [7]). Using this result, the dimensionless normal and tangential stress jumps at the interface are respectively given by

$$\begin{aligned} & \left[-p_i (1 + S_x^2 + S_z^2) + \frac{2}{Re_i} \left(S_x^2 \frac{\partial u_i}{\partial x} + S_z^2 \frac{\partial w_i}{\partial z} + \frac{\partial v_i}{\partial y} - S_x \left(\frac{\partial u_i}{\partial y} + \frac{\partial v_i}{\partial x} \right) - S_z \left(\frac{\partial v_i}{\partial z} + \frac{\partial w_i}{\partial y} \right) \right. \right. \\ & \left. \left. + S_x S_z \left(\frac{\partial u_i}{\partial z} + \frac{\partial w_i}{\partial x} \right) \right) \right]_2^1 = \frac{(1 - \beta \Gamma)}{We} \left(\frac{(1 + S_x^2) S_{zz} - 2 S_x S_z S_{xz} + (1 + S_z^2) S_{xx}}{\sqrt{1 + S_x^2 + S_z^2}} \right), \end{aligned} \quad (2.41a)$$

$$\left[m_i \left(2S_x \left(\frac{\partial u_i}{\partial x} - \frac{\partial v_i}{\partial y} \right) + S_z \left(\frac{\partial u_i}{\partial z} + \frac{\partial w_i}{\partial x} \right) + S_x S_z \left(\frac{\partial v_i}{\partial z} + \frac{\partial w_i}{\partial y} \right) + (S_x^2 - 1) \left(\frac{\partial u_i}{\partial y} + \frac{\partial v_i}{\partial x} \right) \right) \right]_2^1 = Ma \Gamma_x \sqrt{1 + S_x^2 + S_z^2}, \quad (2.41b)$$

$$\left[m_i \left(2S_z \left(\frac{\partial w_i}{\partial z} - \frac{\partial v_i}{\partial y} \right) + S_x \left(\frac{\partial u_i}{\partial z} + \frac{\partial w_i}{\partial x} \right) + S_x S_z \left(\frac{\partial u_i}{\partial y} + \frac{\partial v_i}{\partial x} \right) + (S_z^2 - 1) \left(\frac{\partial v_i}{\partial z} + \frac{\partial w_i}{\partial y} \right) \right) \right]_2^1 = Ma \Gamma_z \sqrt{1 + S_x^2 + S_z^2}, \quad (2.41c)$$

where $m_1 = 1$, $m_2 = m$. The dimensionless numbers appearing above include the *Marangoni number* $Ma = \frac{\beta}{Ca}$ (Wei [7], Kas–Danouche et al. [8], Wei & Rumschitzki [41]), where $Ca = \frac{\mu_1 U}{\gamma_c}$ is the *Capillary number*, and the *Weber number* $We = \frac{\rho U^2 d}{\gamma_c} = Ca Re_1$. Note that the coefficient $\frac{1}{We}$ in (2.41a) also appears in the literature as $\frac{J}{Re_1^2}$, where $J = \frac{\rho \gamma_c d}{\mu_1^2} = \frac{Re_1}{Ca}$ is a number measuring surface tension effects (Chandrasekhar [66]), also known as *Suratman number* Su (Jensen [67]).

The full system (2.35)–(2.41) is intractable analytically and in general needs to be addressed numerically using direct numerical simulations (DNS). The interest of this study is in making analytical progress to obtain reduced dimensional models that can be used to probe the flow dynamics efficiently and for a large range of parameters. This is taken up in Section 2.4 onwards.

2.4 Basic flow

To complete the description of the mathematical model, it is useful (and necessary in the analysis that follows) to find the basic flow. In the unperturbed state, the interface between the fluids is planar. Based on the assumptions of infinite plates ($\partial_x = \partial_z = 0$), unidirectional ($v_i = w_i = 0$) and steady ($\partial_t = 0$) flow, constant pressure and zero gravity, the Navier–Stokes equations reduce to

$$\frac{\partial^2 u_i}{\partial y^2} = 0, \quad i = 1, 2. \quad (2.42)$$

The exact steady solution can be then obtained by solving the above equation in both fluids and applying the boundary conditions (2.37), together with continuity of velocities at the interface

$$u_1(\ell) = u_2(\ell), \quad (2.43a)$$

and the requirement of continuous shear stress at the interface

$$\mu_1 \frac{\partial u_1}{\partial y}(\ell) = \mu_2 \frac{\partial u_2}{\partial y}(\ell). \quad (2.43b)$$

The basic flow is the standard two-fluid Couette flow and in this case it is found to be

$$\begin{aligned} \bar{U}_1 &= a_1 y, \quad \bar{U}_2 = a_2 y + b_2, \\ \bar{V}_1 &= \bar{V}_2 = 0, \quad \bar{W}_1 = \bar{W}_2 = 0, \quad \bar{P}_1 = \bar{P}_2 = 0, \end{aligned} \quad (2.44)$$

where the coefficients a_1, a_2, b_2 are defined by

$$a_1 = \frac{m}{\ell(m-1)+1}, \quad a_2 = \frac{a_1}{m}, \quad b_2 = \frac{\ell(m-1)}{\ell(m-1)+1}. \quad (2.45)$$

2.5 Scalings for thin lower layers

In what follows, the lower layer is assumed to be very thin in comparison to the upper layer, i.e. $\ell = \epsilon$, $\epsilon \ll 1$. The objective is to derive a weakly nonlinear evolution equation for the film thickness (lower fluid) and this is achieved by introducing small perturbations to the interface and the surfactant concentration

$$\begin{aligned} S(x, z, t) &= \epsilon + \delta_1(\epsilon)H(x, z, t), \\ \Gamma(x, z, t) &= \Gamma_0 + \delta_2(\epsilon)\tilde{\Gamma}(x, z, t), \end{aligned} \quad (2.46)$$

with $H, \tilde{\Gamma}$ being $\mathcal{O}(1)$ and $\delta_1(\epsilon), \delta_2(\epsilon) \ll 1$. The aim is to conveniently choose δ_1, δ_2 to ensure that the nonlinear evolution equation for the film thickness perturbation $H(x, z, t)$ is coupled to the fluid dynamics of the upper layer at leading order in the limit $\epsilon \rightarrow 0$. It is important to note that the basic surfactant concentration Γ_0

has to be in a dilute level to retain Marangoni forces in the leading order governing equations. Moreover, the ensuing analysis is based on the assumption of $m = \mathcal{O}(1)$.

The basic flow velocities and pressures are perturbed away from the basic state (2.44) by

$$u_i = \overline{U}_i + \tilde{u}_i, \quad v_i = \tilde{v}_i, \quad w_i = \tilde{w}_i, \quad p_i = \tilde{p}_i, \quad i = 1, 2, \quad (2.47)$$

where overbars denote basic flows and tildes denote small perturbations. In fluid 1, the new order one independent variable $\xi = y/\epsilon$ is introduced. The continuity equation in both fluids at leading order becomes, respectively

$$\frac{\partial \tilde{u}_1}{\partial x} + \frac{1}{\epsilon} \frac{\partial \tilde{v}_1}{\partial \xi} + \frac{\partial \tilde{w}_1}{\partial z} = 0, \quad (2.48a)$$

$$\frac{\partial \tilde{u}_2}{\partial x} + \frac{\partial \tilde{v}_2}{\partial y} + \frac{\partial \tilde{w}_2}{\partial z} = 0, \quad (2.48b)$$

leading to the following orders of magnitude

$$\tilde{u}_1 \sim \tilde{w}_1, \quad \tilde{v}_1 \sim \epsilon \tilde{u}_1 \sim \epsilon \tilde{w}_1, \quad \tilde{u}_2 \sim \tilde{v}_2 \sim \tilde{w}_2. \quad (2.49)$$

The Navier–Stokes equations in fluid 1 at leading order result in the lubrication equations

$$0 = -\frac{\partial \tilde{p}_1}{\partial x} + \frac{1}{Re_1} \frac{1}{\epsilon^2} \frac{\partial^2 \tilde{u}_1}{\partial \xi^2}, \quad (2.50a)$$

$$0 = \frac{1}{\epsilon} \frac{\partial \tilde{p}_1}{\partial \xi}, \quad (2.50b)$$

$$0 = -\frac{\partial \tilde{p}_1}{\partial z} + \frac{1}{Re_1} \frac{1}{\epsilon^2} \frac{\partial^2 \tilde{w}_1}{\partial \xi^2}, \quad (2.50c)$$

and in fluid 2 in the linearised Navier–Stokes equations, to leading order,

$$\overline{U}_2 \frac{\partial \tilde{u}_2}{\partial x} + \tilde{v}_2 \overline{U}_2' = -\frac{\partial \tilde{p}_2}{\partial x} + \frac{1}{Re_2} \left(\frac{\partial^2 \tilde{u}_2}{\partial x^2} + \frac{\partial^2 \tilde{u}_2}{\partial y^2} + \frac{\partial^2 \tilde{u}_2}{\partial z^2} \right), \quad (2.51a)$$

$$\overline{U}_2 \frac{\partial \tilde{v}_2}{\partial x} = -\frac{\partial \tilde{p}_2}{\partial y} + \frac{1}{Re_2} \left(\frac{\partial^2 \tilde{v}_2}{\partial x^2} + \frac{\partial^2 \tilde{v}_2}{\partial y^2} + \frac{\partial^2 \tilde{v}_2}{\partial z^2} \right), \quad (2.51b)$$

$$\overline{U}_2 \frac{\partial \tilde{w}_2}{\partial x} = -\frac{\partial \tilde{p}_2}{\partial z} + \frac{1}{Re_2} \left(\frac{\partial^2 \tilde{w}_2}{\partial x^2} + \frac{\partial^2 \tilde{w}_2}{\partial y^2} + \frac{\partial^2 \tilde{w}_2}{\partial z^2} \right), \quad (2.51c)$$

where a slow time scale is anticipated (see also (2.63)). From equations (2.50)–(2.51) it is easily concluded that

$$\tilde{u}_1 \sim \tilde{w}_1 \sim \epsilon^2 Re_1 \tilde{p}_1, \quad (2.52a)$$

$$\tilde{u}_2 \sim \tilde{v}_2 \sim \tilde{w}_2 \sim Re_2 \tilde{p}_2. \quad (2.52b)$$

The leading order interfacial normal stress balance becomes

$$\begin{aligned} -\tilde{p}_1 + \frac{2}{Re_1} \left(\frac{1}{\epsilon} \frac{\partial \tilde{v}_1}{\partial \xi} - \delta_1 H_x \left(\frac{1}{\epsilon} \frac{\partial \tilde{u}_1}{\partial \xi} + \frac{\partial \tilde{v}_1}{\partial x} \right) - \delta_1 H_z \left(\frac{\partial \tilde{v}_1}{\partial z} + \frac{1}{\epsilon} \frac{\partial \tilde{w}_1}{\partial \xi} \right) \right) \\ + \tilde{p}_2 - \frac{2}{Re_2} \left(\frac{\partial \tilde{v}_2}{\partial y} - \delta_1 H_x \left(\frac{\partial \tilde{u}_2}{\partial y} + \frac{\partial \tilde{v}_2}{\partial x} \right) - \delta_1 H_z \left(\frac{\partial \tilde{v}_2}{\partial z} + \frac{\partial \tilde{w}_2}{\partial y} \right) \right) \\ = \frac{\delta_1}{We} \left(1 - \beta \delta_2 \tilde{\Gamma} \right) (H_{xx} + H_{zz}). \end{aligned} \quad (2.53)$$

Having in mind scalings (2.52) and (2.49), the pressure jump perturbation at the interface dominates the left hand side of equation (2.53) and hence the following pressure perturbations scaling

$$\tilde{p}_1 - \tilde{p}_2 \sim \frac{\delta_1}{We} = \frac{\delta_1}{Ca Re_1} \quad (2.54)$$

is required to retain surface tension effects ($\beta \delta_2 \ll 1$ by assumption).

At this point, the velocity jump at the interface must be obtained. The base flow velocities at the interface are found to be

$$\begin{aligned} \overline{U}_1|_{y=\epsilon+\delta_1 H} &= m\epsilon + m\delta_1 H = \overline{U}_1(\epsilon) + m\delta_1 H, \\ \overline{U}_2|_{y=\epsilon+\delta_1 H} &= \epsilon + \delta_1 H = \overline{U}_2(\epsilon) + \delta_1 H. \end{aligned} \quad (2.55)$$

Since the basic flow satisfies the condition of velocity continuity at the interface $\overline{U}_1(\epsilon) = \overline{U}_2(\epsilon)$, it is observed that there is a velocity jump at the deformed interface, given by

$$\tilde{u}_1 - \tilde{u}_2 \sim (m - 1)\delta_1 H. \quad (2.56)$$

This velocity jump arises physically from the presence of viscosity stratification and sets the size of perturbation velocities in the upper layer.

The pressure perturbations jump (2.54) and velocity perturbations jump (2.56) at the interface can be combined together with scalings (2.52) to obtain that $\tilde{p}_2 \ll \tilde{p}_1$. Using the scaling (2.54) in (2.52a) and (2.49), provides the following film velocity perturbation estimates

$$\tilde{u}_1, \tilde{w}_1 \sim \frac{\epsilon^2 \delta_1}{Ca}, \quad \tilde{v}_1 \sim \frac{\epsilon^3 \delta_1}{Ca}. \quad (2.57)$$

The estimates (2.57) show that the size of the horizontal velocity perturbation in the film is much smaller than δ_1 (the order of magnitude of (2.56)) as long as $Ca \gg \epsilon^2$ (i.e. anticipating (2.60b)). The following magnitudes for the upper fluid perturbed velocities and pressure result from (2.52b) and (2.56)

$$\tilde{u}_2, \tilde{v}_2, \tilde{w}_2, Re_2 \tilde{p}_2 \sim \delta_1. \quad (2.58)$$

Furthermore, both the two tangential stress balances reduce to the same scalings. Particularly, the longitudinal tangential stress balance reduces at leading order to

$$\begin{aligned} & 2\delta_1 H_x \left(\frac{\partial \tilde{u}_1}{\partial x} - \frac{1}{\epsilon} \frac{\partial \tilde{v}_1}{\partial \xi} \right) + \delta_1 H_z \left(\frac{\partial \tilde{u}_1}{\partial z} + \frac{\partial \tilde{w}_1}{\partial x} \right) - \left(\frac{1}{\epsilon} \frac{\partial \tilde{u}_1}{\partial \xi} + \frac{\partial \tilde{v}_1}{\partial x} \right) \\ & - m \left(2\delta_1 H_x \left(\frac{\partial \tilde{u}_2}{\partial x} - \frac{\partial \tilde{v}_2}{\partial y} \right) + \delta_1 H_z \left(\frac{\partial \tilde{u}_2}{\partial z} + \frac{\partial \tilde{w}_2}{\partial x} \right) - \left(\frac{\partial \tilde{u}_2}{\partial y} + \frac{\partial \tilde{v}_2}{\partial x} \right) \right) = Ma \delta_2 \tilde{\Gamma}_x. \end{aligned} \quad (2.59)$$

Here, the largest upper fluid contribution comes from the term $m\tilde{u}_{2y}$, the largest film contribution comes from $\frac{1}{\epsilon}\tilde{u}_{1\xi}$ and the largest Marangoni contribution is of order of $Ma\delta_2$. Having in mind the estimates in (2.57) and (2.58), a balance between the term contributing the most in each fluid and the right hand side Marangoni force results in the following scalings

$$m\delta_1 \sim Ma\delta_2 \quad \Rightarrow \quad Ma \sim m\delta_1\delta_2^{-1}, \quad (2.60a)$$

$$\frac{\epsilon\delta_1}{Ca} \sim Ma\delta_2 \quad \Rightarrow \quad Ca \sim \frac{\epsilon}{m}. \quad (2.60b)$$

This is done to ensure coupling between the dynamics of the film and the upper layer fluid.

Turning to the kinematic condition and using (2.57) and (2.60b), new order-one variables U_1 , V_1 , W_1 are introduced and are defined by

$$\tilde{u}_1 = m\epsilon\delta_1 U_1, \quad \tilde{v}_1 = m\epsilon^2\delta_1 V_1, \quad \tilde{w}_1 = m\epsilon\delta_1 W_1. \quad (2.61)$$

Substituting these into (2.38), results in

$$m\epsilon^2\delta_1 V_1 = \delta_1 H_t + (\bar{U}_1(\epsilon) + m\delta_1 H + m\epsilon\delta_1 U_1) \delta_1 H_x + m\epsilon\delta_1^2 W_1 H_z. \quad (2.62)$$

The dominant terms in this equation are the first two on the right hand side, which are of order δ_1 . The linear term can be removed by an appropriate Galilean transformation and the unsteady term is retained in the final evolution equation by a transformation in time leading to a slower time scale. For example, the following transformation can be performed

$$\partial_t \rightarrow \delta_1 \partial_t - \bar{U}_1(\epsilon) \partial_x. \quad (2.63)$$

Consequently, a balance is possible between the left hand side term and the third term on the right hand side in order to retain nonlinearity. As $m = \mathcal{O}(1)$, the balance yields

$$m\epsilon^2\delta_1 \sim m\delta_1^2 \quad \Rightarrow \quad \delta_1 \sim \epsilon^2. \quad (2.64)$$

Finally, it remains to insert the perturbations (2.47) in the surfactant transport equation at the interface, resulting in

$$\begin{aligned} & \delta_2 \tilde{\Gamma}_t - \delta_1^2 \delta_2 H_t (\tilde{\Gamma}_x H_x + \tilde{\Gamma}_z H_z) \\ & + \left[\frac{\partial}{\partial x} \left((u + v\delta_1 H_x) (\Gamma_0 + \delta_2 \tilde{\Gamma}) \right) + \frac{\partial}{\partial z} \left((v\delta_1 H_z + w) (\Gamma_0 + \delta_2 \tilde{\Gamma}) \right) \right] \\ & + \delta_1 \delta_2 (\Gamma_0 + \delta_2 \tilde{\Gamma}) (u\delta_1 H_x - v + w\delta_1 H_z) (H_{xx} + H_{zz}) - \frac{\delta_2}{Pe} (\tilde{\Gamma}_{xx} + \tilde{\Gamma}_{zz}) = 0, \end{aligned} \quad (2.65)$$

where $u = \overline{U}_1(\epsilon) + m\delta_1 H + m\epsilon\delta_1 U_1$, $v = m\epsilon^2\delta_1 V_1$, $w = m\epsilon\delta_1 W_1$. At leading order, equation (2.65) reduces to

$$\delta_2 \tilde{\Gamma}_t + m\delta_1 \Gamma_0 H_x + m\epsilon\delta_1 \Gamma_0 U_{1x} + \delta_2 \overline{U}_1(\epsilon) \tilde{\Gamma}_x + m\delta_1 \delta_2 \left(H \tilde{\Gamma} \right)_x + m\epsilon\delta_1 W_{1z} \Gamma_0 - \frac{\delta_2}{Pe} \left(\tilde{\Gamma}_{xx} + \tilde{\Gamma}_{zz} \right) = 0. \quad (2.66)$$

To get a nonlinear equation, the linear term $\delta_2 \tilde{\Gamma}_t + \delta_2 \overline{U}_1(\epsilon) \tilde{\Gamma}_x$ must dominate to the leading order so that it can be removed by the same Galilean transformation (2.63) that is used in the kinematic condition. Producing nonlinear dynamics at leading order is only possible if the assumption of small base surfactant concentration Γ_0 holds. The third and sixth terms are higher order terms and are ignored in the leading order analysis. Balancing the second term with the nonlinear fifth term, implies

$$\Gamma_0 \sim \delta_2, \quad (2.67)$$

so the two balanced terms now can be written as $m\delta_1 \left(H(\Gamma_0 + \delta_2 \tilde{\Gamma}) \right)_x$. Balance between the nonlinear and diffusive terms gives

$$Pe \sim \delta_1^{-1}. \quad (2.68)$$

To sum everything up, when applying (2.60), (2.64), (2.67) and (2.68), the following scalings are adopted

$$\delta_1 = \epsilon^2, \quad \Gamma_0 = \delta_2 \tilde{\Gamma}_0, \quad Ca = \epsilon Ca_0, \quad Ma = \epsilon^2 \delta_2^{-1} Ma_0, \quad Pe = \epsilon^{-2} Pe_0, \quad (2.69)$$

where $\tilde{\Gamma}_0$, Ca_0 , Ma_0 , Pe_0 are all of $\mathcal{O}(1)$. The perturbations to the flow velocities and pressures can be obtained by using the above scalings in (2.54), (2.57), (2.58) and assuming $Re_1 = mRe_2 = \mathcal{O}(1)$; they are given by

$$\begin{aligned} \tilde{u}_1 &= \epsilon^3 U_1, & \tilde{v}_1 &= \epsilon^4 V_1, & \tilde{w}_1 &= \epsilon^3 W_1, & \tilde{p}_1 &= \epsilon P_1, \\ \tilde{u}_2 &= \epsilon^2 U_2, & \tilde{v}_2 &= \epsilon^2 V_2, & \tilde{w}_2 &= \epsilon^2 W_2, & \tilde{p}_2 &= \epsilon^2 P_2, \end{aligned} \quad (2.70)$$

for $U_{1,2}$, $V_{1,2}$, $W_{1,2}$, $P_{1,2} = \mathcal{O}(1)$. Finally, setting $\Gamma' = \tilde{\Gamma}_0 + \tilde{\Gamma}$, the perturbations to the interface and the surfactant concentration become

$$\begin{aligned} S(x, z, t) &= \epsilon + \epsilon^2 H(x, z, t), \\ \Gamma(x, z, t) &= \delta_2 \Gamma'(x, z, t). \end{aligned} \quad (2.71)$$

2.6 Asymptotic expansions

In fluid 1, the flow is perturbed away from the basic state by

$$\begin{aligned} u_1 &= \overline{U}_1(\xi; \epsilon) + \epsilon^3 U_1(x, \xi, z, t) + \mathcal{O}(\epsilon^4), \quad v_1 = \epsilon^4 V_1(x, \xi, z, t) + \mathcal{O}(\epsilon^5), \\ w_1 &= \epsilon^3 W_1(x, \xi, z, t) + \mathcal{O}(\epsilon^4), \quad p_1 = \epsilon P_1(x, \xi, z, t) + \mathcal{O}(\epsilon^2). \end{aligned} \quad (2.72)$$

Note that $\overline{U}_1(\xi; \epsilon) = \epsilon a_1 \xi$ from (2.44). In fluid 2 the flow expands as follows

$$\begin{aligned} u_2 &= \overline{U}_2(y) + \epsilon^2 U_2(x, y, z, t) + \mathcal{O}(\epsilon^3), \quad v_2 = \epsilon^2 V_2(x, y, z, t) + \mathcal{O}(\epsilon^3), \\ w_2 &= \epsilon^2 W_2(x, y, z, t) + \mathcal{O}(\epsilon^3), \quad p_2 = \epsilon^2 P_2(x, y, z, t) + \mathcal{O}(\epsilon^3). \end{aligned} \quad (2.73)$$

Substituting expansions (2.72) in the non-dimensional Navier–Stokes equations (2.35) and working with leading terms only, results in

$$0 = -\frac{\partial P_1}{\partial x} + \frac{1}{Re_1} \frac{\partial^2 U_1}{\partial \xi^2}, \quad (2.74a)$$

$$0 = \frac{\partial P_1}{\partial \xi}, \quad (2.74b)$$

$$0 = -\frac{\partial P_1}{\partial z} + \frac{1}{Re_1} \frac{\partial^2 W_1}{\partial \xi^2}, \quad (2.74c)$$

$$\frac{\partial U_1}{\partial x} + \frac{\partial V_1}{\partial \xi} + \frac{\partial W_1}{\partial z} = 0. \quad (2.74d)$$

Equation (2.74b) yields that P_1 is independent of ξ , thus $P_1 = P_1(x, z, t)$. Inserting the same expansions into the normal stress balance at the interface (2.41a), at leading order it converts into

$$P_1 = -\frac{(H_{xx} + H_{zz})}{Re_1 Ca_0}. \quad (2.75)$$

Similarly, the tangential stress balances (2.41b), (2.41c) at leading order become

$$-\frac{\partial U_1}{\partial \xi} \Big|_{\xi=1} + m \left(\frac{\partial U_2}{\partial y} + \frac{\partial V_2}{\partial x} \right) \Big|_{y=0} = Ma_0 \Gamma'_x, \quad (2.76a)$$

$$-\frac{\partial W_1}{\partial \xi} \Big|_{\xi=1} + m \left(\frac{\partial V_2}{\partial z} + \frac{\partial W_2}{\partial y} \right) \Big|_{y=0} = Ma_0 \Gamma'_z. \quad (2.76b)$$

Inserting (2.75) into (2.74a) and (2.74c), integrating across the film and using conditions (2.76) at $\xi = 1$ to specify the constants of integration, gives

$$\frac{\partial U_1}{\partial \xi} = \frac{(H_{xxx} + H_{xzz})}{Ca_0} (1 - \xi) + \left[m \left(\frac{\partial U_2}{\partial y} + \frac{\partial V_2}{\partial x} \right) \Big|_{y=0} - Ma_0 \Gamma'_x \right], \quad (2.77a)$$

$$\frac{\partial W_1}{\partial \xi} = \frac{(H_{xxz} + H_{zzz})}{Ca_0} (1 - \xi) + \left[m \left(\frac{\partial V_2}{\partial z} + \frac{\partial W_2}{\partial y} \right) \Big|_{y=0} - Ma_0 \Gamma'_z \right]. \quad (2.77b)$$

Equations (2.77) are integrated again and the no-slip condition for the perturbed velocities is used to determine the constants of integration, i.e. $U_1 = W_1 = 0$ at $\xi = 0$. The final result is the horizontal and spanwise velocity perturbations in the film, given by

$$U_1 = \frac{(H_{xxx} + H_{xzz})}{Ca_0} \left(\xi - \frac{\xi^2}{2} \right) + \left[m \left(\frac{\partial U_2}{\partial y} + \frac{\partial V_2}{\partial x} \right) \Big|_{y=0} - Ma_0 \Gamma'_x \right] \xi, \quad (2.78a)$$

$$W_1 = \frac{(H_{xxz} + H_{zzz})}{Ca_0} \left(\xi - \frac{\xi^2}{2} \right) + \left[m \left(\frac{\partial V_2}{\partial z} + \frac{\partial W_2}{\partial y} \right) \Big|_{y=0} - Ma_0 \Gamma'_z \right] \xi. \quad (2.78b)$$

Substituting these into the leading order continuity equation (2.74d) and integrating across the film once more, yields the lateral velocity perturbation V_1 . This perturbation will be required in the kinematic condition (2.38) and thus it needs to be evaluated at the interface. When calculated at $\xi = 1$, it becomes

$$V_1 \Big|_{\xi=1} = -\frac{1}{3Ca_0} (H_{xxxx} + 2H_{xxzz} + H_{zzzz}) + \frac{Ma_0}{2} (\Gamma'_{xx} + \Gamma'_{zz}) - \frac{m}{2} T \Big|_{y=0}, \quad (2.79)$$

where $T(x, y, z) = U_{2xy} + V_{2xx} + V_{2zz} + W_{2zy}$ is found by solving the problem in the upper layer.

Now moving on to the kinematic condition (2.38) and introducing the Galilean transformation

$$x' = x - \overline{U}_1(\epsilon)t \quad (2.80a)$$

and the slow time scale

$$t' = \epsilon^2 t, \quad (2.80b)$$

at leading order it converts into

$$H_{t'} + mHH_{x'} = V_1|_{\xi=1}. \quad (2.81)$$

Note that the term on the right hand side of equation (2.81) (see also (2.79)) provides coupling between upper and lower layers and is the source of nonlocality in the final evolution system.

Lastly, substituting expansions (2.72) into the surfactant transport equation (2.39) and making use of the transformations (2.80), implies at leading order

$$\Gamma'_{t'} + m(H\Gamma')_{x'} = \frac{1}{Pe_0} (\Gamma'_{x'x'} + \Gamma'_{zz}). \quad (2.82)$$

What remains in order to obtain the desired weakly nonlinear evolution equation for the film thickness, is to solve the problem in the upper layer. The nonlocal term $T|_{y=0}$ ensures coupling of the film dynamics to the dynamics in the upper layer fluid. The dynamics in the upper layer depend on the size of the Reynolds number Re_2 , so two different regimes can be considered for Re_2 . When the Reynolds number Re_2 is small and of the order of the film thickness ϵ (or smaller), the upper layer dynamics are governed to leading order by the Stokes equations. Physically, this corresponds to a slow moving upper layer fluid and moderate surface tension ($J = \frac{mRe_2}{Ca} = \mathcal{O}(1)$). A Reynolds number of order one leads to different evolution equations coming from linearised Navier–Stokes equations in the upper layer, and is associated with strong surface tension ($J = \mathcal{O}(\frac{1}{\epsilon})$).

The scaling analysis presented in Section 2.5 was based on the assumption of $Re_1 = \mathcal{O}(1)$, $m = \mathcal{O}(1)$ and since $Re_1 = mRe_2$, then $Re_2 = \mathcal{O}(1)$. Hence the

ensuing analysis is also performed for a general $Re_2 = \mathcal{O}(1)$, but simplifications of the evolution equation in the limit $Re_2 \rightarrow 0$ will be considered later. In the case where $Re_2 = \mathcal{O}(\epsilon)$, a similar scaling analysis should be carried out but it is omitted here since it is a subcase and straightforward. The only difference from the analysis in Section 2.5 is that the pressure perturbations scale differently, with $\tilde{p}_1 = \mathcal{O}(1)$ and $\tilde{p}_2 = \mathcal{O}(\epsilon)$. From now on, the subscript from Re_2 is omitted and Re is used instead.

To find the solution in the upper layer, expansions (2.73) are substituted into the non-dimensional momentum equations (2.35), yielding the steady linearised Navier–Stokes equations

$$y \frac{\partial U_2}{\partial x} + V_2 = -\frac{\partial P_2}{\partial x} + \frac{1}{Re} \left(\frac{\partial^2 U_2}{\partial x^2} + \frac{\partial U_2^2}{\partial y^2} + \frac{\partial U_2^2}{\partial z^2} \right), \quad (2.83a)$$

$$y \frac{\partial V_2}{\partial x} = -\frac{\partial P_2}{\partial y} + \frac{1}{Re} \left(\frac{\partial^2 V_2}{\partial x^2} + \frac{\partial V_2^2}{\partial y^2} + \frac{\partial V_2^2}{\partial z^2} \right), \quad (2.83b)$$

$$y \frac{\partial W_2}{\partial x} = -\frac{\partial P_2}{\partial z} + \frac{1}{Re} \left(\frac{\partial^2 W_2}{\partial x^2} + \frac{\partial W_2^2}{\partial y^2} + \frac{\partial W_2^2}{\partial z^2} \right), \quad (2.83c)$$

$$\frac{\partial U_2}{\partial x} + \frac{\partial V_2}{\partial y} + \frac{\partial W_2}{\partial z} = 0. \quad (2.83d)$$

Taking Fourier transforms gives

$$ik_1 y \hat{U}_2 + \hat{V}_2 = -ik_1 \hat{P}_2 + \frac{1}{Re} \left(\frac{\partial^2 \hat{U}_2}{\partial y^2} - (k_1^2 + k_2^2) \hat{U}_2 \right), \quad (2.84a)$$

$$ik_1 y \hat{V}_2 = -\frac{\partial \hat{P}_2}{\partial y} + \frac{1}{Re} \left(\frac{\partial^2 \hat{V}_2}{\partial y^2} - (k_1^2 + k_2^2) \hat{V}_2 \right), \quad (2.84b)$$

$$ik_1 y \hat{W}_2 = -ik_2 \hat{P}_2 + \frac{1}{Re} \left(\frac{\partial^2 \hat{W}_2}{\partial y^2} - (k_1^2 + k_2^2) \hat{W}_2 \right), \quad (2.84c)$$

$$ik_1 \hat{U}_2 + \frac{\partial \hat{V}_2}{\partial y} + ik_2 \hat{W}_2 = 0, \quad (2.84d)$$

where hats will symbolise Fourier transforms from now on and the Fourier transform of $U_2(x, z, t)$ is defined as

$$\hat{U}_2(k_1, k_2) = \int_{-\infty}^{+\infty} \int_{-\infty}^{+\infty} U_2(x, z, t) e^{-i(k_1 x + k_2 z)} dx dz. \quad (2.85)$$

From the continuity equation (2.84d) a new function f is introduced and the following result is obtained

$$f = ik_1 \hat{U}_2 + ik_2 \hat{W}_2 \quad \Rightarrow \quad f = -\frac{\partial \hat{V}_2}{\partial y}. \quad (2.86)$$

Multiplying (2.84a) by ik_1 , (2.84c) by ik_2 and adding them together, results in

$$ik_1 y f + ik_1 \hat{V}_2 = (k_1^2 + k_2^2) \hat{P}_2 + \frac{1}{R_e} \left(\frac{\partial^2 f}{\partial y^2} - (k_1^2 + k_2^2) f \right). \quad (2.87)$$

Inserting the last part of (2.86) into (2.87) and differentiating with respect to y , yields

$$-ik_1 y \frac{\partial^2 \hat{V}_2}{\partial y^2} = (k_1^2 + k_2^2) \frac{\partial \hat{P}_2}{\partial y} - \frac{1}{R_e} \left(\frac{\partial^4 \hat{V}_2}{\partial y^4} - (k_1^2 + k_2^2) \frac{\partial^2 \hat{V}_2}{\partial y^2} \right). \quad (2.88)$$

What is left is to multiply (2.84b) by $(k_1^2 + k_2^2)$ and add the result to (2.88) to eliminate the pressure, obtaining

$$\left(\frac{\partial^4 \hat{V}_2}{\partial y^4} - 2(k_1^2 + k_2^2) \frac{\partial^2 \hat{V}_2}{\partial y^2} + (k_1^2 + k_2^2)^2 \hat{V}_2 \right) - ik_1 R_e y \left(\frac{\partial^2 \hat{V}_2}{\partial y^2} - (k_1^2 + k_2^2) \hat{V}_2 \right) = 0. \quad (2.89)$$

The no-slip condition at the upper wall and the requirement for velocity continuity at the interface provide four boundary conditions, namely

$$\hat{V}_2 = \frac{\partial \hat{V}_2}{\partial y} = 0 \quad \text{at} \quad y = 1, \quad (2.90a)$$

$$\hat{V}_2 = 0, \quad \frac{\partial \hat{V}_2}{\partial y} = -ik_1(m-1)\hat{H} \quad \text{at} \quad y = 0. \quad (2.90b)$$

If $\hat{V}_2 = -ik_1(m-1)\hat{H}F(y)$, then $F(y)$ satisfies the boundary value problem

$$(F^{(iv)} - 2k^2 F'' + k^4 F) - ik_1 R_e y (F'' - k^2 F) = 0, \quad (2.91a)$$

$$F(0) = 0, \quad F'(0) = 1, \quad F(1) = 0, \quad F'(1) = 0, \quad (2.91b)$$

where $k = \sqrt{k_1^2 + k_2^2}$. This is an Orr–Sommerfeld type problem and it describes

the y -dependent amplitude of a Fourier mode of wavenumbers (k_1, k_2) and zero wavespeed.

The leading order upper layer solution U_2, V_2, W_2 is provided by obtaining the nonlocal term $T(x, y, z) = U_{2xy} + V_{2xx} + V_{2zz} + W_{2zy}$. In particular, it is first calculated in Fourier space

$$\begin{aligned}\hat{T} &= ik_1 \hat{U}_{2y} + ik_2 \hat{W}_{2y} - (k_1^2 + k_2^2) \hat{V}_2 \\ &= -\hat{V}_{2yy} - k^2 \hat{V}_2 \\ &= ik_1(m-1) \hat{H} (F''(y) + k^2 F(y)),\end{aligned}\tag{2.92}$$

where equation (2.84d) and the definition $\hat{V}_2 = -ik_1(m-1)\hat{H}F(y)$ have been used. Therefore, from (2.91b),

$$\hat{T}|_{y=0} = ik_1(m-1)\hat{H}F''(0).\tag{2.93}$$

Applying inverse Fourier transform results in

$$T|_{y=0} = 2i(1-m)\frac{1}{4\pi^2} \int_{-\infty}^{+\infty} \int_{-\infty}^{+\infty} \mathcal{N}(k_1, k_2) \hat{H}(k_1, k_2) e^{i(k_1 x + k_2 z)} dk_1 dk_2,\tag{2.94}$$

with $\mathcal{N}(k_1, k_2)$ given by

$$\mathcal{N}(k_1, k_2) = -\frac{k_1}{2} F''(0).\tag{2.95}$$

Note that for simplicity the nonlocal term was developed using Fourier transforms, but will be later specialised to Fourier series on $2\pi \times 2\pi$ -periodic domains (used in the numerical analysis in Chapter 4).

Finally, substituting (2.94) into (2.79) and the result into equation (2.81), yields the following weakly nonlinear equation for the film thickness

$$H_{\eta'} + mHH_{x'} + \frac{1}{3Ca_0} (H_{x'x'x'x'} + 2H_{x'x'zz} + H_{zzzz}) + \frac{m}{2} T|_{y=0} - \frac{Ma_0}{2} (\Gamma'_{x'x'} + \Gamma'_{zz}) = 0.\tag{2.96}$$

2.7 Evolution equations

The derivation of the evolution equations is complete, but as a final step the dashes are dropped from all terms and the following canonical rescaling is applied

$$H \rightarrow \frac{1}{3m Ca_0} H, \quad \Gamma \rightarrow \frac{2}{9m Ca_0^2 Ma_0} \Gamma, \quad t \rightarrow 3Ca_0 t. \quad (2.97)$$

The evolution equation for the film thickness and the leading order surfactant transport equation form the system

$$H_t + HH_x + \nabla^4 H + \frac{i\Lambda}{4\pi^2} \int_{-\infty}^{+\infty} \int_{-\infty}^{+\infty} \mathcal{N}(k_1, k_2) \hat{H}(k_1, k_2) e^{i(k_1 x + k_2 z)} dk_1 dk_2 - \nabla^2 \Gamma = 0, \quad (2.98)$$

$$\Gamma_t + (H\Gamma)_x - \eta \nabla^2 \Gamma = 0, \quad (2.99)$$

where $\nabla^2 = \partial_x^2 + \partial_z^2$ is the Laplacian operator and $\nabla^4 = \partial_x^4 + 2\partial_x^2 \partial_z^2 + \partial_z^4$ the bi-Laplacian operator. The parameters Λ and η that appear in the above equations are defined by

$$\Lambda = 3Ca_0 m(1 - m), \quad \eta = \frac{3Ca_0}{Pe_0}. \quad (2.100)$$

The parameter Λ is positive if $m < 1$, i.e. when the film is more viscous than the upper layer fluid, and negative otherwise. Parameter η represents the surfactant diffusivity and is always positive.

3 Asymptotic Properties

This chapter presents asymptotic properties of the nonlocal term that are of intrinsic interest and of relevance to the construction of accurate and stable numerical schemes. The asymptotic results lead to simplifications of the evolution equations, and this is achieved by considering different limits in equation (2.91) and finding simpler expressions for the function $\mathcal{N}(k_1, k_2)$ from (2.95). The limits considered include: small wavenumber limit which corresponds to long waves and will be very useful in the linear stability analysis performed later in Chapters 5–6, large wavenumber limit used in the numerical analysis in Chapter 4, zero Reynolds number limit corresponding to the Stokes flow, large Reynolds number limit, and large wavenumber together with large Reynolds number limit.

Numerical solutions for the boundary value problem (2.91) are obtained via finite difference methods and details can be found in Appendix A. All the results that follow were verified graphically by comparing numerical solutions with asymptotic solutions, but only the comparisons for the case of a two-dimensional flow (this corresponds to $k_2 = 0$) are presented here because the interesting features can be visualised better in this case. For completeness, the real and imaginary part of $F''(0)$ as a function of both k_1, k_2 are given in Figure 5.

3.1 Long-wave limit

According to Smyrlis & Papageorgiou [45], a localisation of the evolution equation can be considered instead of the full nonlocal equation. They have demonstrated numerically that global and local solutions are almost identical for a range of dynamical behaviours. The localisation of the evolution equation is achieved by considering the long wave limit of the nonlocal term in the evolution equation (this is the limit $k_{1,2} \rightarrow 0$ in $\mathcal{N}(k_1, k_2)$). Particularly, a Taylor expansion of $F(y)$ for small k_1, k_2 is substituted in (2.91a), i.e.

$$F(y) = F_0(y) + k_1 F_1(y) + k_2 F_2(y) + k_1^2 F_3(y) + k_1 k_2 F_4(y) + k_2^2 F_5(y) + \dots \quad (3.1)$$

The coefficients are then obtained by matching same-order terms and are given by

$$\begin{aligned} F_0(y) &= y^3 - 2y^2 + y, \\ F_1(y) &= \frac{iR_e}{60} (y^6 - 2y^5 + 2y^3 - y^2), \\ F_2(y) &= 0, \\ F_3(y) &= \frac{1}{30} \left[3y^5 - 10y^4 + 11y^3 - 4y^2 \right. \\ &\quad \left. + \frac{R_e^2}{120} \left(\frac{25}{42}y^9 - \frac{10}{7}y^8 + 2y^6 - y^5 + \frac{25}{42}y^3 - \frac{15}{35}y^2 \right) \right], \\ F_4(y) &= 0, \\ F_5(y) &= \frac{1}{30} (3y^5 - 10y^4 + 11y^3 - 4y^2), \end{aligned} \quad (3.2)$$

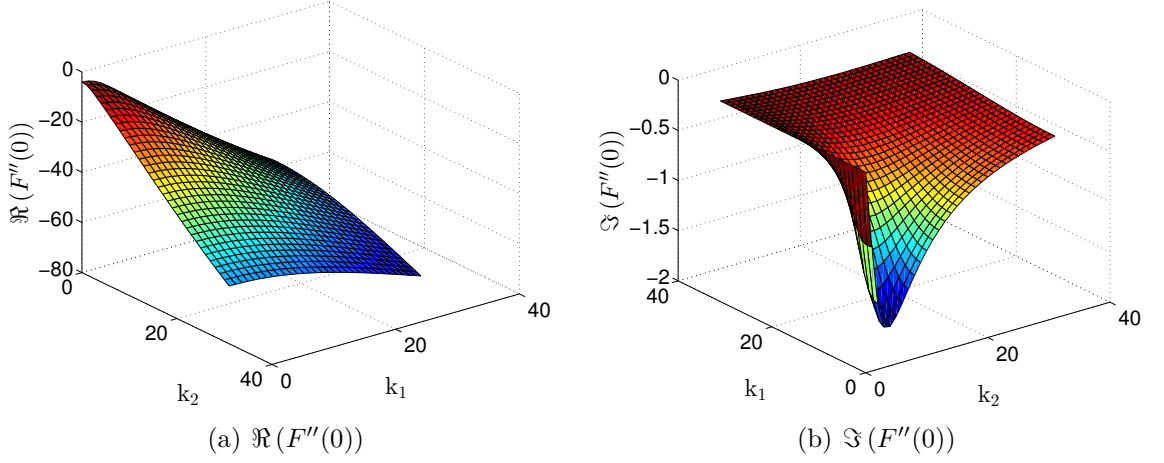


Figure 5: Real and imaginary parts of the two-dimensional function $F''(0)$, plotted against k_1, k_2 for $R_e = 25$.

and therefore

$$F''(0) = -4 - \frac{iR_e}{30}k_1 - \left(\frac{4}{15} + \frac{R_e^2}{4200}\right)k_1^2 - \frac{4}{15}k_2^2 + \dots \quad (3.3)$$

Disregarding terms of order higher than three in (3.3) and inserting the result in (2.95), yields the localised form of $\mathcal{N}(k_1, k_2)$, given by

$$\mathcal{N}(k_1, k_2) \approx 2k_1 + \frac{iR_e}{60}k_1^2 + \left(\frac{2}{15} + \frac{R_e^2}{8400}\right)k_1^3 + \frac{2}{15}k_1k_2^2. \quad (3.4)$$

A comparison between the real and imaginary parts of $F''(0)$ as found in (3.3) and the ones computed numerically can be seen in Figures 6(a) and 6(b) respectively, in the case of $k_2 = 0$ (which implies $k_1 = k$) and for $R_e = 25$. The black solid lines correspond to the numerical solutions and the red dashed lines to the asymptotic solutions. It is clear from the graphs that the two curves are identical for small wavenumbers.

3.2 Short-wave limit

Short waves correspond to large wavenumbers $k_1, k_2 \gg 1$ and in this case the asymptotic solution for $F(y)$ can be found using boundary layer theory. The implementation

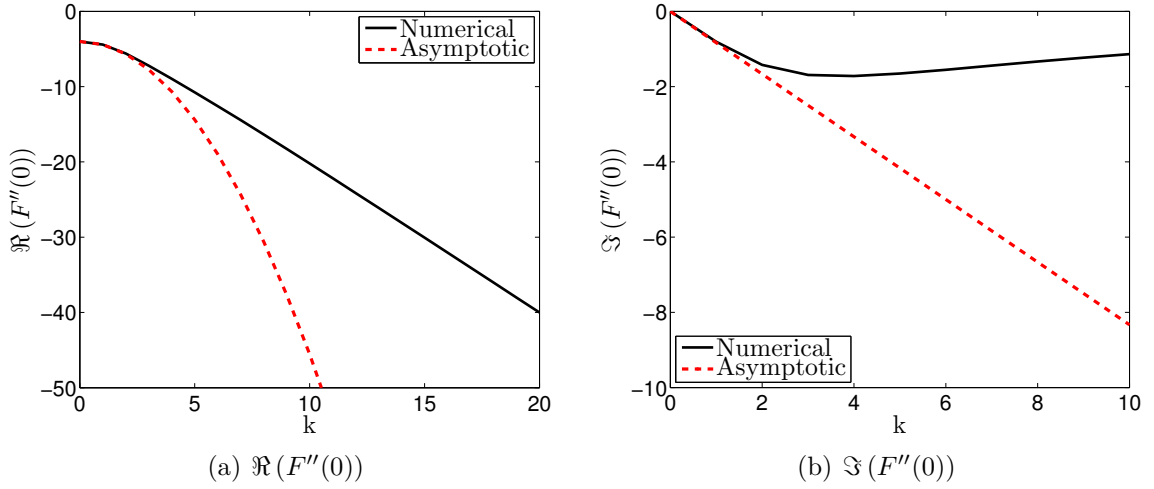


Figure 6: Real and imaginary parts of $F''(0)$ as functions of k , for $R_e = 25$. Solid lines represent the numerical solution and dashed lines represent the asymptotic solution (3.3) obtained for small wavenumbers k .

of this is to set

$$k_1 = \frac{\kappa_1}{\delta}, \quad k_2 = \frac{\kappa_2}{\delta} \quad \text{and} \quad k = \frac{\sqrt{\kappa_1^2 + \kappa_2^2}}{\delta} = \frac{\kappa}{\delta} \quad (3.5)$$

in (2.91), where $\kappa_{1,2}$, κ are order one parameters and δ is arbitrarily small, and then consider the limit as $\delta \rightarrow 0$. To that end, (2.91a) is written as

$$(\delta^4 F^{(iv)} - 2\delta^2 \kappa^2 F'' + \kappa^4 F) - i\delta \kappa_1 R_e y (\delta^2 F'' - \kappa^2 F) = 0. \quad (3.6)$$

This is a singular perturbation problem and therefore the method of matched asymptotic expansions must be used to determine the asymptotic expansion of $F(y)$. A boundary layer exists near $y = 0$ but not near $y = 1$, so an *outer solution* $F_{out}(y)$ is defined to satisfy the boundary conditions at $y = 1$ and it is found to be $F_{out}(y) = 0$.

In the boundary layer at $y = 0$ the inner variable $\xi = \delta^{-1}y$, $\xi = \mathcal{O}(1)$ is introduced and the solution of the following boundary value problem

$$\left(\frac{d^4 F}{d\xi^4} - 2\kappa^2 \frac{d^2 F}{d\xi^2} + \kappa^4 F \right) - i\delta^2 \kappa_1 R_e \xi \left(\frac{d^2 F}{d\xi^2} - \kappa^2 F \right) = 0, \quad (3.7a)$$

$$F(0) = 0, \quad \frac{dF}{d\xi}(0) = \delta, \quad (3.7b)$$

defines the *inner solution* $F_{in}(\xi)$. This is then written as

$$F_{in}(\xi) = F_0(\xi) + \delta^2 F_1(\xi) + \delta^4 F_2(\xi) + \dots . \quad (3.8)$$

An additional condition to the boundary conditions (3.7b) is provided by matching the inner solution with the outer solution in an “intermediate” region, namely by satisfying the matching condition

$$\lim_{\xi \rightarrow \infty} F_{in}(\xi) = \lim_{y \rightarrow 0} F_{out}(y). \quad (3.9)$$

The final inner solution is found to be

$$F_{in}(\xi) = \delta \xi e^{-\kappa \xi} - \delta^3 \frac{\kappa_1}{\kappa} \frac{i R_e}{12} \left(\xi^3 + \frac{3}{\kappa} \xi^2 \right) e^{-\kappa \xi} + \dots . \quad (3.10)$$

Consequently, the leading order asymptotic form of $\mathcal{N}(k_1, k_2)$ as $k_{1,2} \rightarrow \infty$ is found by first obtaining

$$F''(0) = \frac{\partial^2 F}{\partial y^2}(0) = \frac{1}{\delta^2} \frac{\partial^2 F_{in}}{\partial \xi^2}(0) = -2k - \frac{i R_e}{2} \frac{k_1}{k^2} + \dots \quad (3.11)$$

and then inserting this into (2.95) (after omitting the dots which include higher order terms), and it is given by

$$\mathcal{N}(k_1, k_2) \sim k_1 k + \frac{i R_e}{4} \frac{k_1^2}{k^2}, \quad k_1, k_2 \gg 1. \quad (3.12)$$

The asymptotic expression (3.11) for $F''(0)$ is compared to the numerical solution (for $k_2 = 0$) and the outcome is illustrated in Figure 7 for $R_e = 25$. Panel (a) shows the real part of $F''(0)$ and panel (b) the imaginary part. Numerical solutions are plotted with solid lines and asymptotic solutions with dashed lines, and obviously they have negligible difference for large k .

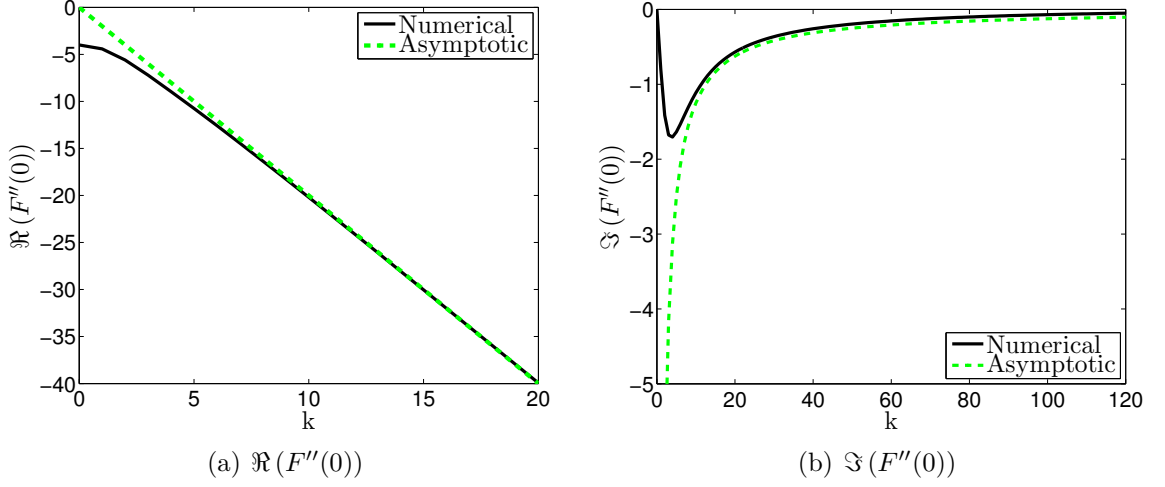


Figure 7: Real and imaginary parts of $F''(0)$ as functions of k , for $R_e = 25$. The numerical solution is plotted with solid lines and the asymptotic solution for large wavenumbers k (3.11) is plotted with dashed lines.

3.3 Stokes flow limit: small R_e

Assuming a small Reynolds number in the upper layer, i.e. taking the limit $R_e \rightarrow 0$, then (2.91a) converts into

$$F^{(iv)} - 2k^2 F'' + k^4 F = 0. \quad (3.13)$$

Equation (3.13) has an analytic solution, which after imposing boundary conditions (2.91b) takes the following form

$$F(y) = \frac{k \sinh(ky) - \sinh^2 k y \cosh(ky) - (k - \cosh k \sinh k) y \sinh(ky)}{1 + k^2 - \cosh^2 k}. \quad (3.14)$$

Therefore in the limit $R_e \rightarrow 0$, the function $\mathcal{N}(k_1, k_2)$ is found to be

$$\mathcal{N}(k_1, k_2) = \frac{k_1 k (k - \cosh k \sinh k)}{1 + k^2 - \cosh^2 k}. \quad (3.15)$$

The function $F(y)$ is purely real in this case, and $\mathcal{N}(k_1, k_2)$ is an odd function of k_1, k_2 , i.e. $\mathcal{N}(-k_1, -k_2) = -\mathcal{N}(k_1, k_2)$. This asymptotic limit was studied in detail for the two-dimensional flow (i.e. for $k_2 = 0, k = k_1$) by Bassom et al. [2]. The plot

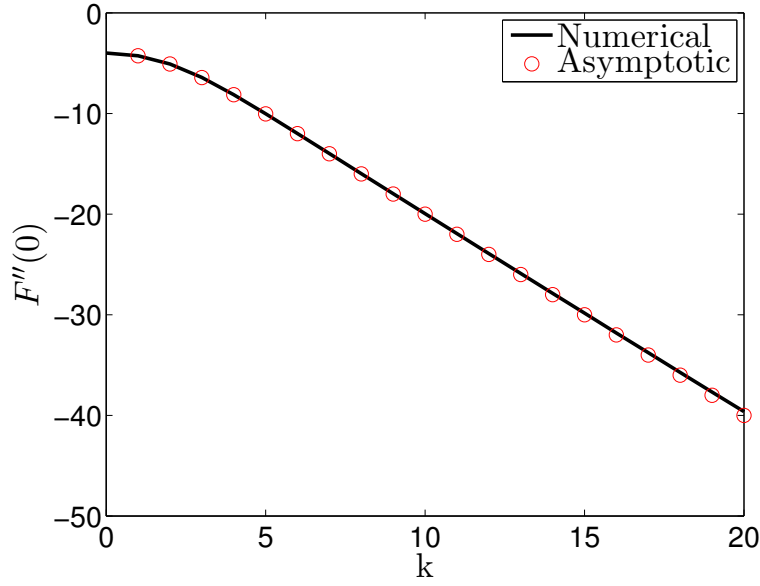


Figure 8: Real part of $F''(0)$ against k for $R_e = 0$. The solid line corresponds to the numerical solution and the circles to the asymptotic solution.

of $F''(0)$ against k for $R_e = 0$ can be seen in Figure 8. The numerical (solid) and asymptotic solutions (circles) in this case are identical, as expected.

Note that taking the limits $k_{1,2} \rightarrow 0$ and $k_{1,2} \rightarrow \infty$ in (3.15), gives $\mathcal{N}(k_1, k_2) \approx 2k_1 + \frac{2}{15}k_1k^2$ and $\mathcal{N}(k_1, k_2) \sim k_1k$ respectively. These are equivalent to taking the limit $R_e \rightarrow 0$ in (3.4) and (3.12).

3.4 Large Reynolds numbers

The next asymptotic limit to be considered is the case of large Reynolds numbers $R_e \gg 1$. The asymptotic solution for $F''(0)$ can be obtained by introducing matched asymptotic expansions about the small parameter $\delta = \frac{1}{R_e}$ and using the asymptotic theory described by Drazin & Reid [68] (this method was actually used by Fowler [47], who found the same asymptotic solution as the one derived in this section). Nevertheless, a different approach to solving Orr–Sommerfeld type equations like (2.91), leading to an exact solution of $F(y)$ in terms of Airy functions, was suggested by Hooper & Boyd [20] and will be followed here.

To be more specific, by setting $G = F'' - k^2 F$ equation (2.91a) becomes

$$G'' - ik_1 R_e \left(y - i \frac{k^2}{k_1} R_e^{-1} \right) G = 0, \quad (3.16)$$

with solution $G(y) = b_1 A(y) + b_2 B(y)$; b_1, b_2 are constants and

$$\begin{aligned} A(y) &= Ai \left(k_1^{\frac{1}{3}} R_e^{\frac{1}{3}} e^{\frac{i\pi}{6}} \left(y - i \frac{k^2}{k_1} R_e^{-1} \right) \right), \\ B(y) &= Bi \left(k_1^{\frac{1}{3}} R_e^{\frac{1}{3}} e^{\frac{i\pi}{6}} \left(y - i \frac{k^2}{k_1} R_e^{-1} \right) \right), \end{aligned} \quad (3.17)$$

are the Airy functions of the first and second kind, respectively. Therefore, $F(y)$ is now the solution of the non-homogeneous ordinary differential equation

$$F''(y) - k^2 F(y) = b_1 A(y) + b_2 B(y), \quad (3.18)$$

which can be solved by use of the method of variation of parameters, giving

$$\begin{aligned} F(y) &= a_1 e^{ky} + a_2 e^{-ky} - \frac{b_1}{2k} \left(e^{-ky} \int_0^y e^{ks} A(s) ds + e^{ky} \int_y^1 e^{-ks} A(s) ds \right) \\ &\quad - \frac{b_2}{2k} \left(e^{-ky} \int_0^y e^{ks} B(s) ds + e^{ky} \int_y^1 e^{-ks} B(s) ds \right). \end{aligned} \quad (3.19)$$

Boundary conditions (2.91b) help to determine the four constants a_1, a_2, b_1, b_2 . In particular, imposing the boundary conditions in (3.19) implies the following four equations

$$\begin{aligned} a_1 + a_2 - b_1 \mathcal{J}_1 - b_2 \mathcal{J}_2 &= 0, \\ a_1 - a_2 - b_1 \mathcal{J}_1 - b_2 \mathcal{J}_2 &= 1/k, \\ a_1 e^k + a_2 e^{-k} - (b_1 \mathcal{L}_1 + b_2 \mathcal{L}_2) e^{-k} &= 0, \\ a_1 e^k - a_2 e^{-k} + (b_1 \mathcal{L}_1 + b_2 \mathcal{L}_2) e^{-k} &= 0, \end{aligned} \quad (3.20)$$

with

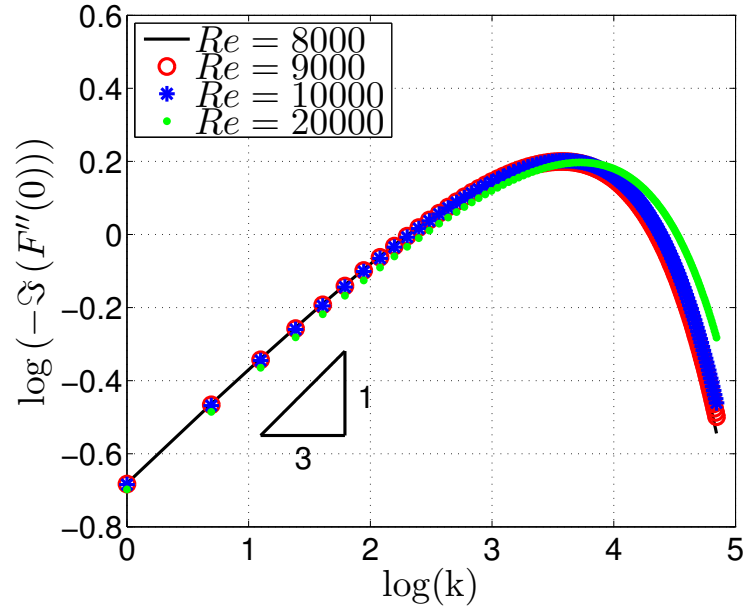


Figure 9: Logarithm of the imaginary part of $F''(0)$ plotted against the logarithm of k , for large $Re = 8000, 9000, 10000, 20000$. The slope for moderate values of k is approximately $1/3$.

$$\begin{aligned}\mathcal{J}_1 &= \frac{1}{2k} \int_0^1 e^{-ks} A(s) ds, & \mathcal{J}_2 &= \frac{1}{2k} \int_0^1 e^{-ks} B(s) ds, \\ \mathcal{L}_1 &= \frac{1}{2k} \int_0^1 e^{ks} A(s) ds, & \mathcal{L}_2 &= \frac{1}{2k} \int_0^1 e^{ks} B(s) ds.\end{aligned}\tag{3.21}$$

The solution of the linear system (3.20) is

$$a_1 = 0, \quad a_2 = -\frac{1}{2k}, \quad b_1 = -\frac{1}{2k} \frac{1}{\mathcal{J}_1} \frac{\left(1 - \frac{\mathcal{J}_2}{\mathcal{L}_2}\right)}{\left(1 - \frac{\mathcal{J}_2 \mathcal{L}_1}{\mathcal{L}_2 \mathcal{J}_1}\right)}, \quad b_2 = -\frac{1}{2k} \frac{1}{\mathcal{J}_2} \frac{\left(1 - \frac{\mathcal{J}_1}{\mathcal{L}_1}\right)}{\left(1 - \frac{\mathcal{J}_1 \mathcal{L}_2}{\mathcal{L}_1 \mathcal{J}_2}\right)}.\tag{3.22}$$

Finally, $F''(0) = b_1 A(0) + b_2 B(0)$. The asymptotic behaviour of $A(0)$ and $B(0)$ for large Reynolds numbers is

$$\begin{aligned}A(0) &= Ai\left(-ik^2 k_1^{-\frac{2}{3}} Re^{-\frac{2}{3}} e^{\frac{i\pi}{6}}\right) \sim Ai(0), \\ B(0) &= Bi\left(-ik^2 k_1^{-\frac{2}{3}} Re^{-\frac{2}{3}} e^{\frac{i\pi}{6}}\right) \sim Bi(0) = \sqrt{3} Ai(0).\end{aligned}\tag{3.23}$$

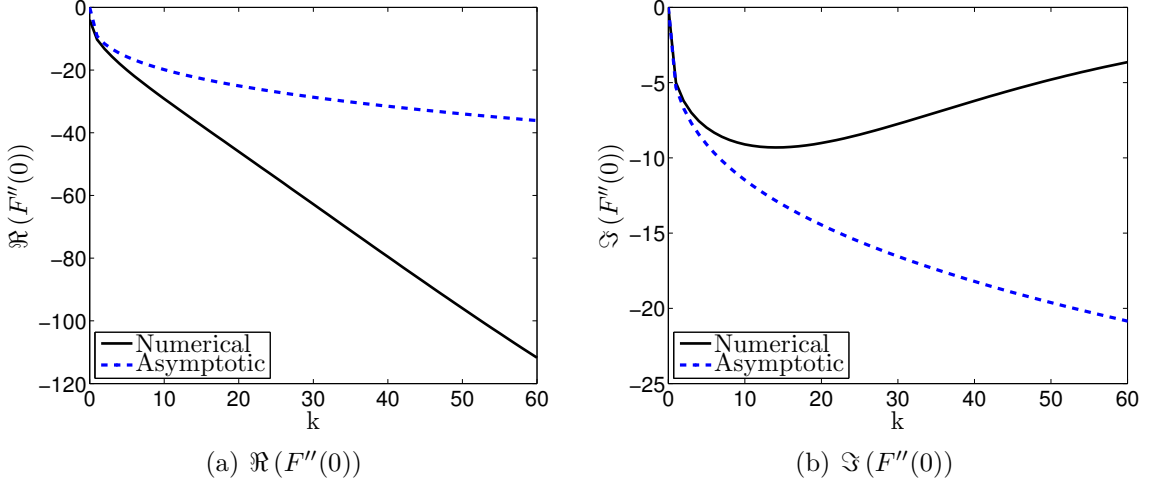


Figure 10: Real and imaginary parts of $F''(0)$ as functions of k , for large $R_e = 1000$. Solid lines represent the numerical solution and dashed lines represent the asymptotic solution (3.24) obtained for large Reynolds numbers.

Additionally, $b_2 \sim 0$ and $b_1 \sim -\frac{1}{2k} \frac{1}{\mathcal{J}_1}$, where $\mathcal{J}_1 \sim \frac{1}{6} k^{-1} k_1^{-\frac{1}{3}} R_e^{-\frac{1}{3}} e^{\frac{i\pi}{6}}$ and $\mathcal{J}_2 = o\left(e^{R_e^{1/2}}\right)$ as $R_e \rightarrow \infty$ (for a derivation of these asymptotic results see Appendix B). Consequently, the asymptotic form at leading order for $F''(0)$ as $R_e \rightarrow \infty$ is given by

$$F''(0) \sim -3Ai(0)k_1^{\frac{1}{3}}R_e^{\frac{1}{3}}e^{\frac{i\pi}{6}}, \quad (3.24)$$

and the corresponding leading order asymptotic result for $N(k_1, k_2)$ is

$$\mathcal{N}(k_1, k_2) \sim \frac{3}{2}Ai(0)k_1^{\frac{4}{3}}R_e^{\frac{1}{3}}e^{\frac{i\pi}{6}}. \quad (3.25)$$

A graphical confirmation of the result that $F''(0)$ is a function of $k^{\frac{1}{3}}$ in the case of large Reynolds numbers (and $k_2 = 0$) is provided in Figure 9, only for the imaginary part of $F''(0)$ and for $R_e = 8000, 9000, 10000, 20000$. The figure shows that the logarithm of $-\Im(F''(0))$ grows linearly with $\log(k)$ (for moderate values of k) with slope approximately equal to $1/3$, confirming the theory. Once again, a comparison between the numerical and asymptotic solutions for $F''(0)$ is performed and is demonstrated in Figure 10, for $R_e = 1000$. In panel (a) the real part $\Re(F''(0))$ is shown and similarly in panel (b) the imaginary part $\Im(F''(0))$, where the solid lines

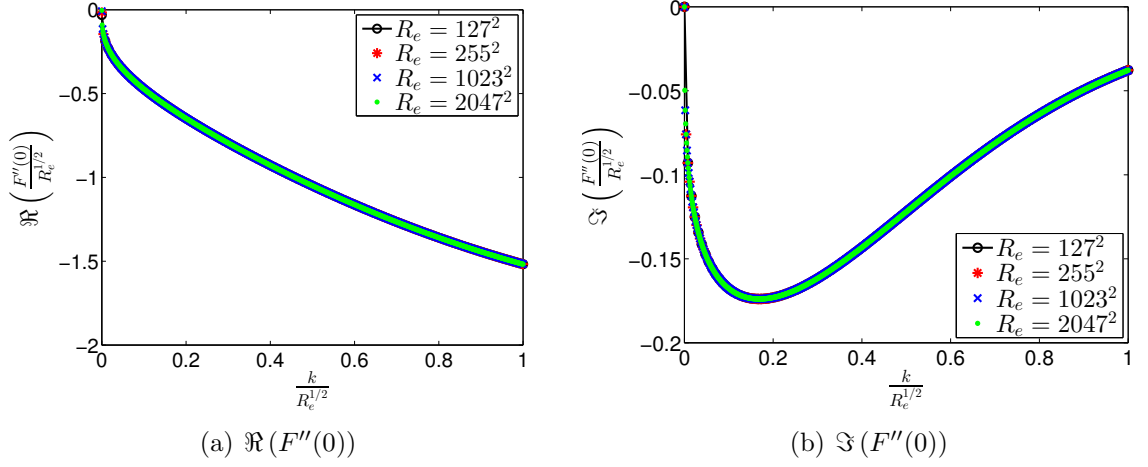


Figure 11: Real and imaginary parts of $F''(0)/R_e^{1/2}$ plotted against $k/R_e^{1/2}$, for large $R_e = 127^2, 255^2, 1023^2, 2047^2$. Different symbols correspond to different values of the Reynolds number.

correspond to the numerical solution and the dashed lines to the asymptotic solution in both panels. It can be seen that the curves have indistinguishable differences only for small values of the wavenumber k , suggesting a narrow range of validity of the approximation.

3.5 Short-wave limit and large Reynolds numbers

When $k_1, k_2 \gg 1$, $R_e \gg 1$, a solution is only possible if all terms balance in the boundary layer equation. A general procedure is to set $k_{1,2} = R_e^a n_{1,2}$ (and $k = R_e^a n$, with $n^2 = n_1^2 + n_2^2$) and define the inner variable to be $y = R_e^{-b} \xi$. Substituting these into equation (2.91a), gives the following boundary layer equation

$$R_e^{4b} \frac{d^4 F}{d\xi^4} - (2n^2 R_e^{2(a+b)} + in_1 R_e^{1+a+b} \xi) \frac{d^2 F}{d\xi^2} + (in_1 n^2 R_e^{1+3a-b} \xi + n^4 R_e^{4a}) F = 0. \quad (3.26)$$

Balance of all terms is possible if $a = b = \frac{1}{2}$, in which case the above equation converts into

$$(F^{(iv)} - 2n^2 F'' + n^4 F) - in_1 \xi (F'' - n^2 F) = 0, \quad (3.27)$$

where derivatives are with respect to ξ . A similar solution as in Section 3.4 may be obtained for equation (3.27), which is found to be

$$F''(0) \sim C R_e^{\frac{1}{2}} \text{Ai} \left(k_1^{-\frac{2}{3}} k^2 R_e^{-\frac{2}{3}} e^{-\frac{i\pi}{3}} \right), \quad C = - \left(\int_0^\infty e^{-(R_e^{-1/2} k)s} A(s) ds \right)^{-1}. \quad (3.28)$$

An accurate and efficient algorithm for the evaluation of complex Airy functions is described in Schulten et al. [69]. In addition, Coreless et al. [70] performed computations for the numerical evaluation of Airy functions with complex arguments. Their results can be applied here, but this was not attempted.

Lastly, the solution obtained numerically is first divided by $R_e^{1/2}$ and plotted against $k/R_e^{1/2}$ in Figure 11, for four values of $R_e = 127^2, 255^2, 1023^2, 2047^2$. Panel (a) shows the real part of $F''(0)$ and panel (b) the imaginary part of $F''(0)$. In both panels the curves for all Reynolds numbers collapse to a universal curve thus confirming the asymptotic theory for $R_e \gg 1$, namely that $F''(0) \sim R_e^{1/2}$ and $k \sim R_e^{1/2}$.

4 Numerical Methods

This chapter describes the methods used to perform the numerical computations which will be presented in Chapters 5–6. More specifically, the evolution equations are rescaled so that solutions are periodic in the domain $[0, 2\pi] \times [0, 2\pi]$. Spectral methods used for spatial discretisation are described first and then stable implicit–explicit BDF time–stepping schemes are presented and analysed. Lastly, some properties of the linear and nonlinear operators of the system are proved which are necessary conditions for the stability of the numerical schemes.

4.1 Governing equations on periodic domains

The system describing the evolution of the flow is solved numerically on $2L_x \times 2L_z$ -periodic domains. Firstly, it is useful to rescale the evolution equations onto the canonical square domain $[0, 2\pi] \times [0, 2\pi]$ using the following transformations

$$x \rightarrow \frac{L_x}{\pi}x, \quad z \rightarrow \frac{L_z}{\pi}z, \quad t \rightarrow \left(\frac{L_x}{\pi}\right)^2 t, \quad H \rightarrow \frac{\pi}{L_x}H, \quad \Gamma \rightarrow \frac{\pi}{L_x}\Gamma. \quad (4.1)$$

On $2\pi \times 2\pi$ -periodic domains, the nonlocal term in (2.98), which from now on will be symbolised by the linear pseudo-differential operator $\mathcal{P}H$, has the following Fourier series representation

$$\mathcal{P}H = i\Lambda\nu_1^{-1} \sum_{k_1=-\infty}^{+\infty} \sum_{k_2=-\infty}^{+\infty} \mathcal{N}(k_1\sqrt{\nu_1}, k_2\sqrt{\nu_2}) \hat{H}(k_1, k_2) e^{i(k_1x+k_2z)}, \quad (4.2)$$

where

$$\hat{H}(k_1, k_2) = \frac{1}{(2\pi)^2} \int_0^{2\pi} \int_0^{2\pi} H(\bar{x}, \bar{z}, t) e^{-i(k_1\bar{x}+k_2\bar{z})} d\bar{x}d\bar{z}, \quad (4.3)$$

are the Fourier coefficients of $H(x, z, t)$ and $\nu_1, \nu_2 > 0$ are new bifurcation parameters defined by

$$\nu_1 = \left(\frac{\pi}{L_x}\right)^2, \quad \nu_2 = \left(\frac{\pi}{L_z}\right)^2. \quad (4.4)$$

The parameters ν_1, ν_2 play an important role in the dynamics of the flow. Their value reduces as the lengths L_x, L_z increase, resulting in more unstable modes entering into the dynamics (see Section 5.4). The transformed evolution equations are

$$H_t + HH_x + \left(\nu_1 H_{xxxx} + 2\nu_2 H_{xxzz} + \frac{\nu_2^2}{\nu_1} H_{zzzz}\right) + \mathcal{P}H - \left(\Gamma_{xx} + \frac{\nu_2}{\nu_1}\Gamma_{zz}\right) = 0, \quad (4.5)$$

$$\Gamma_t + (H\Gamma)_x - \eta \left(\Gamma_{xx} + \frac{\nu_2}{\nu_1}\Gamma_{zz}\right) = 0. \quad (4.6)$$

The above system is solved numerically with initial conditions

$$H(x, z, 0) = H_0(x, z), \quad \Gamma(x, z, 0) = G_0(x, z), \quad (4.7)$$

where $H_0(x, z)$ is a function of zero spatial mean (i.e. $\int_0^{2\pi} \int_0^{2\pi} H_0(x, z) dx dz = 0$) and $G_0(x, z) = \bar{\Gamma}$ is constant and equal to the average of the initial surfactant concentration. Integrating the system (4.5)–(4.6) over the spatial domain and invoking periodicity of solutions, proves that the following quantities in brackets are conserved

$$\frac{d}{dt} \left(\int_0^{2\pi} \int_0^{2\pi} H(x, z, t) dx dz \right) = 0 \quad \text{and} \quad \frac{d}{dt} \left(\int_0^{2\pi} \int_0^{2\pi} \Gamma(x, z, t) dx dz \right) = 0. \quad (4.8)$$

The set of equations (4.5)–(4.6) is solved using a pseudospectral numerical method. Specifically, a second-order accurate method is used for discretisation in time, and space is discretised using a spectral scheme. The equations are transformed in Fourier space (Fornberg & Whitham [71]), where the nonlocal term $\mathcal{P}H$ in (4.5) is known exactly. This is the main reason why pseudospectral representation of spatial derivatives is very convenient in this case, but also because it is suitable for periodic systems (Papageorgiou et al. [40]).

4.2 Spatial discretisation using spectral methods

The spatial periodicity of the solutions H, Γ allows for them to be written in terms of Fourier series, i.e.

$$H(x, z, t) = \sum_{\substack{k_1=-\infty \\ k_1 \neq 0}}^{+\infty} \sum_{\substack{k_2=-\infty \\ k_2 \neq 0}}^{+\infty} \hat{H}_{k_1, k_2} e^{i(k_1 x + k_2 z)}, \quad (4.9a)$$

$$\Gamma(x, z, t) = \sum_{\substack{k_1=-\infty \\ k_1 \neq 0}}^{+\infty} \sum_{\substack{k_2=-\infty \\ k_2 \neq 0}}^{+\infty} \hat{\Gamma}_{k_1, k_2} e^{i(k_1 x + k_2 z)} + \bar{\Gamma}. \quad (4.9b)$$

The nonlinear terms are evaluated using the Fourier series representations (4.9) and by multiplying them together, in which case the coefficients of $e^{i(k_1 x + k_2 z)}$ are given by

$$\left(\widehat{H H_x} \right)_{k_1, k_2} = \frac{ik_1}{2} \sum_{\substack{n_1+m_1=k_1 \\ n_2+m_2=k_2}} \hat{H}_{n_1, n_2} \hat{H}_{m_1, m_2}, \quad (4.10a)$$

$$\left(\widehat{(H\Gamma)_x} \right)_{k_1, k_2} = ik_1 \sum_{\substack{n_1+m_1=k_1 \\ n_2+m_2=k_2}} \hat{H}_{n_1, n_2} \hat{\Gamma}_{m_1, m_2}. \quad (4.10b)$$

This is a spectral calculation and it is sometimes called the Fourier–spectral method or Fourier–Galerkin method, as it belongs to the family of Galerkin methods (Thomé [72]).

In practice, the spatial domain $[0, 2\pi]$ in the streamwise direction is split into $2M_x$ equidistant points and similarly the analogous domain in the spanwise direction is discretised using $2M_z$ points. The system is truncated for $|k_1| \geq M_x$, $|k_2| \geq M_z$ for suitably chosen M_x , M_z in order to achieve *spectral accuracy*⁷. The computations are based on the solution of a $8M_xM_z \times 8M_xM_z$ system for the Fourier coefficients $\hat{H}_{k_1,k_2}$, $\hat{\Gamma}_{k_1,k_2}$. Note that even when Fourier modes evolve to higher frequencies, the nonlinear part of the system is dominated by low frequency modes. This indicates that higher frequencies are “slaved” by the low frequencies, which is one of the most typical characteristics of dissipative infinite–dimensional dynamical systems (Akrivis et al. [74], Akrivis & Smyrlis [75]).

An alternative way to calculate the nonlinear convolutions is with Fast Fourier Transform (FFT) algorithms. The advantage of the use of Fourier series truncations over FFT is that the former are more accurate; however they are more expensive computationally. On the other hand, the FFT approach can introduce aliasing errors (Trefethen [73]) which lower the accuracy of the method and can cause instabilities in the numerical approximation. In the case of one–dimensional domains, the nonlinear convolution sums require $\mathcal{O}(M_x^2)$ operations, while FFT algorithms have complexity of only $\mathcal{O}(M_x \log(M_x))$ (Cooley & Tukey [76]). The one–dimensional solutions presented in the next chapter were obtained numerically using Fourier series truncations for the space discretisation (details about the calculation of the one–dimensional nonlinear terms can be found in Appendix C). However, the algorithmic complexity for two–dimensional domains increases to $\mathcal{O}(M_x^2M_z^2)$ for the Fourier–spectral method and $\mathcal{O}(M_xM_z \log(M_xM_z))$ for the FFTs; hence it was preferable to use FFT due to the prohibitive computational time required by the Fourier–spectral method.

⁷Spectral accuracy is the behaviour of the Fourier spectrum characterised by exponential decrease, until high precision is reached and rounding errors on the computer stop further improvement (Trefethen [73]).

4.3 Implicit–explicit BDF schemes

The time discretisation of the system of governing equations is performed by use of implicit–explicit Backward Differentiating Formulae (BDF). The BDF belong to the family of linearly implicit methods constructed and analysed by Akrivis & Crouzeix [77] and Akrivis, Crouzeix & Makridakis [78] for a class of nonlinear parabolic equations. The aforementioned authors proved that these numerical schemes are convergent and also that they are efficient and unconditionally stable under various conditions on the linear and the nonlinear terms of the problem.

The aim in the numerical analysis of the scheme, is firstly to rewrite the system (4.5)–(4.6) into a form that fits the class of abstract equations analysed by Akrivis & Crouzeix [77], and then to show that all the necessary conditions described in their work are fulfilled. In order to be able to prove such conditions, additional terms need to be added in equations (4.5)–(4.6), which are written as in Akrivis, Papageorgiou & Smyrlis [74]

$$H_t + \frac{c}{\nu_1} H + \nu_1 \left(\partial_x^2 + \frac{\nu_2}{\nu_1} \partial_z^2 \right)^2 H + \mathcal{P}H = -HH_x + \frac{c}{\nu_1} H + \left(\partial_x^2 + \frac{\nu_2}{\nu_1} \partial_z^2 \right) \Gamma, \quad (4.11a)$$

$$\Gamma_t - \eta \left(\partial_x^2 + \frac{\nu_2}{\nu_1} \partial_z^2 \right) \Gamma + \eta \Gamma = -(H\Gamma)_x + \eta \Gamma, \quad (4.11b)$$

with the parameter $c > 0$ to be determined later.

A similar procedure was followed for the KSE in Akrivis & Smyrlis [75] and for the dispersively modified KSE in Akrivis, Papageorgiou & Smyrlis [79]. Akrivis & Smyrlis [80] also used linearly implicit schemes to analyse a class of dispersive-dissipative systems, and Akrivis et al. [74] to study numerically a related system arising in two-phase flows. In addition to these, Akrivis, Crouzeix & Makridakis [78] used implicit–explicit multistep schemes together with finite element methods to study nonlinear parabolic problems.

Setting $\mathbf{u} = (u_1, u_2)^T = (H, \Gamma)^T$, equations (4.11) take the form of a system

$$\mathbf{u}_t + \mathcal{L}\mathbf{u} = \mathcal{B}(\mathbf{u}), \quad (4.12)$$

where

$$\mathcal{L} = \begin{pmatrix} \frac{c}{\nu_1} + \nu_1 \left(\partial_x^2 + \frac{\nu_2}{\nu_1} \partial_z^2 \right)^2 + \mathcal{P} & 0 \\ 0 & -\eta \left(\partial_x^2 + \frac{\nu_2}{\nu_1} \partial_z^2 \right) + \eta \end{pmatrix}, \quad (4.13a)$$

$$\mathcal{B}(u) = \begin{pmatrix} -u_1(u_1)_x + \frac{c}{\nu_1}u_1 + (u_2)_{xx} + \frac{\nu_2}{\nu_1}(u_2)_{zz} \\ -(u_1u_2)_x + \eta u_2 \end{pmatrix}. \quad (4.13b)$$

Separating $\mathcal{L}$ into two parts, one symmetric⁸ part $\mathcal{A}$ and one antisymmetric part $\mathcal{D}$, namely writing $\mathcal{L} = \mathcal{A} + \mathcal{D}$ with

$$\mathcal{A} = \begin{pmatrix} \mathcal{A}_1 & 0 \\ 0 & \mathcal{A}_2 \end{pmatrix}, \quad \mathcal{D} = \begin{pmatrix} \mathcal{D} & 0 \\ 0 & 0 \end{pmatrix}, \quad (4.14)$$

it is necessary to prove that the linear symmetric operator $\mathcal{A}$ is self-adjoint⁹ and positive definite¹⁰ and the nonlinear operator $\mathcal{B}$ is locally Lipschitz continuous¹¹. In this situation, the conditions in Akrivis & Crouzeix [77] are satisfied and therefore the linearly implicit schemes analysed in that study can be applied to discretise the periodic initial value problem (4.12). This will be done in Section 4.4.

For a general dispersive operator $\mathcal{D}$, the system can be discretised by A-stable

⁸An operator $\mathcal{A}$ on a Hilbert space $\mathcal{H}$ is *symmetric* (*antisymmetric*) if

$$(\mathcal{A}u, v) = \pm(u, \mathcal{A}v), \quad \forall u, v \in \mathcal{H},$$

where $(\cdot, \cdot)$ defines an inner product in $\mathcal{H}$ and the positive (negative) sign corresponds to the symmetric (antisymmetric) case.

⁹An operator $\mathcal{A}$ on a Hilbert space $\mathcal{H}$ is *self-adjoint* if it is symmetric everywhere defined.

¹⁰A symmetric operator $\mathcal{A}$ on a Hilbert space $\mathcal{H}$ is *positive definite* if

$$(\mathcal{A}u, u) \geq 0, \quad \forall u \in \mathcal{H}.$$

¹¹An operator $\mathcal{B} : X \rightarrow Y$ is *locally Lipschitz continuous* if there exists a real constant $C \geq 0$ and a neighborhood T_u of u such that

$$\|\mathcal{B}(v) - \mathcal{B}(w)\|_Y \leq C\|v - w\|_X, \quad \forall v, w \in T_u.$$

schemes but the highest attainable order of the scheme is two (Akrivis et al. [79], Akrivis & Smyrlis [80]) (this constraint is called the second Dahlquist barrier and was proved by Dahlquist in his article [81], where he also gives the definition of A–stability). The restriction of only the first and second order schemes being stable can be removed if $\mathcal{D}$ is subdominant with respect to $\mathcal{A}$ (the dominance of an operator is determined by considering the behaviour of the higher modes, i.e. for large k_1, k_2). In this case, multistep schemes of higher orders are stable and they have been analysed up to order 6 in Akrivis et al. [74] and Akrivis & Smyrlis [75]; in fact, such schemes are stable up to order 6 only (a detailed analysis of the 6 schemes applied on the Kuramoto–Sivashinsky and can also be found in Akrivis et al. [82]). This advantage of the BDF is the reason why this method is chosen to perform the numerical experiments. In what follows, the second–order accurate BDF scheme is described and implemented, but analogous results can be obtained for schemes of order $p = 1, \dots, 6$. The fourth–order Runge–Kutta (RK4) method (Kassam & Trefethen [83]) has also been analysed and applied to the system for validation purposes (the analysis is available upon request). This method is also second–order accurate and solutions obtained by the second–order BDF and the RK4 have infinitesimal relative error. However, due to the order reduction and the fact that the RK4 is more computationally expensive (it requires smaller time steps than the BDF), it was not used further in the numerical computations.

On implementing the scheme, let dt be the time step and T the final time; then $N = T/dt$ and $t_n = n dt$ for $n = 0, 1, 2, \dots, N$ are the time levels at which the solution $\mathbf{u}$ will be calculated. The second–order BDF numerical method is applied to define approximations $\mathbf{U}^n$ to $\mathbf{u}(\cdot, t_n)$ by

$$\frac{3}{2}\mathbf{U}^{n+2} + dt \mathcal{L}\mathbf{U}^{n+2} = 2\mathbf{U}^{n+1} + 2dt \mathcal{B}(\mathbf{U}^{n+1}) - \frac{1}{2}\mathbf{U}^n - dt \mathcal{B}(\mathbf{U}^n), \quad (4.15)$$

for $n = 0, 1, 2, \dots, N - 2$. It is clear from (4.15) that the linear part of the system (4.12) is discretised by an implicit scheme and the nonlinear part by an explicit one. Inserting the definitions (4.13) into equation (4.15), gives

$$\begin{aligned}
& \frac{3}{2}\mathbf{U}^{n+2} + dt \begin{pmatrix} \frac{c}{\nu_1} + \nu_1 \left(\partial_x^2 + \frac{\nu_2}{\nu_1} \partial_z^2 \right)^2 + \mathcal{P} & 0 \\ 0 & -\eta \left(\partial_x^2 + \frac{\nu_2}{\nu_1} \partial_z^2 \right) + \eta \end{pmatrix} \mathbf{U}^{n+2} \\
&= \left[2I + 2dt \begin{pmatrix} \frac{c}{\nu_1} & \left(\partial_x^2 + \frac{\nu_2}{\nu_1} \partial_z^2 \right) \\ 0 & \eta \end{pmatrix} \right] \mathbf{U}^{n+1} - \left[\frac{1}{2}I + dt \begin{pmatrix} \frac{c}{\nu_1} & \left(\partial_x^2 + \frac{\nu_2}{\nu_1} \partial_z^2 \right) \\ 0 & \eta \end{pmatrix} \right] \mathbf{U}^n \\
&\quad - 2dt \begin{pmatrix} H^{n+1} H_x^{n+1} \\ (H^{n+1} \Gamma^{n+1})_x \end{pmatrix} + dt \begin{pmatrix} H^n H_x^n \\ (H^n \Gamma^n)_x \end{pmatrix}. \quad (4.16)
\end{aligned}$$

The system (4.16) is then considered in Fourier space, where spatial discretisations are obtained. The pseudo-differential operator $\mathcal{P}$ in Fourier space becomes

$$\begin{aligned}
(\widehat{\mathcal{P}u})_{k_1, k_2} &= i\Lambda\nu_1^{-1}\mathcal{N}(k_1\sqrt{\nu_1}, k_2\sqrt{\nu_2}) \hat{u}_{k_1, k_2} \\
&= id_{k_1, k_2} \hat{u}_{k_1, k_2}, \quad k_1, k_2 \in \mathbb{Z}_+, \quad (4.17)
\end{aligned}$$

with

$$d_{k_1, k_2} = \Lambda\nu_1^{-1}\mathcal{N}(k_1\sqrt{\nu_1}, k_2\sqrt{\nu_2}). \quad (4.18)$$

To simplify the expressions, the new variable $k_\nu^2 = k_1^2 + \frac{\nu_2}{\nu_1}k_2^2$ is defined and thus the system (4.16) in Fourier space is given by

$$\begin{aligned}
& \frac{3}{2}\hat{\mathbf{U}}_{k_1, k_2}^{n+2} + dt \begin{pmatrix} \frac{c}{\nu_1} + \nu_1 k_\nu^4 + id_{k_1, k_2} & 0 \\ 0 & \eta k_\nu^2 + \eta \end{pmatrix} \hat{\mathbf{U}}_{k_1, k_2}^{n+2} = \left[2I + 2dt \begin{pmatrix} \frac{c}{\nu_1} & -k_\nu^2 \\ 0 & \eta \end{pmatrix} \right] \hat{\mathbf{U}}_{k_1, k_2}^{n+1} \\
&\quad - \left[\frac{1}{2}I + dt \begin{pmatrix} \frac{c}{\nu_1} & -k_\nu^2 \\ 0 & \eta \end{pmatrix} \right] \hat{\mathbf{U}}_{k_1, k_2}^n + 2dt \begin{pmatrix} \hat{A}_{k_1, k_2}^{n+1} \\ \hat{B}_{k_1, k_2}^{n+1} \end{pmatrix} - dt \begin{pmatrix} \hat{A}_{k_1, k_2}^n \\ \hat{B}_{k_1, k_2}^n \end{pmatrix}, \quad (4.19)
\end{aligned}$$

where $\hat{A}_{k_1, k_2}$, $\hat{B}_{k_1, k_2}$ are the Fourier coefficients of the two nonlinear terms, given by

$$\hat{A}_{k_1, k_2} = -ik_1 \mathcal{F} \left(\frac{H^2}{2} \right), \quad \hat{B}_{k_1, k_2} = -ik_1 \mathcal{F}(H\Gamma). \quad (4.20)$$

Finally, setting

$$\xi_{k_1, k_2} = \frac{3}{2} + \frac{c dt}{\nu_1} + \nu_1 dt k_\nu^4, \quad \zeta_{k_1, k_2} = \frac{3}{2} + \eta dt k_\nu^2 + \eta dt, \quad (4.21)$$

the Fourier coefficients $\hat{H}_{k_1, k_2}^{n+2}$, $\hat{\Gamma}_{k_1, k_2}^{n+2}$, $n = 0, 1, 2, \dots, N-2$ are provided by the following second order scheme

$$\begin{aligned} \hat{H}_{k_1, k_2}^{n+2} = \frac{\xi_{k_1, k_2} - i dt d_{k_1, k_2}}{\xi_{k_1, k_2}^2 + dt^2 d_{k_1, k_2}^2} & \left[\left(2 + \frac{2c dt}{\nu_1} \right) \hat{H}_{k_1, k_2}^{n+1} - 2dt k_\nu^2 \hat{\Gamma}_{k_1, k_2}^{n+1} - \left(\frac{1}{2} + \frac{c dt}{\nu_1} \right) \hat{H}_{k_1, k_2}^n \right. \\ & \left. + dt k_\nu^2 \hat{\Gamma}_{k_1, k_2}^n + 2dt \hat{A}_{k_1, k_2}^{n+1} - dt \hat{A}_{k_1, k_2}^n \right], \end{aligned} \quad (4.22a)$$

$$\hat{\Gamma}_{k_1, k_2}^{n+2} = \frac{1}{\zeta_{k_1, k_2}} \left[(2 + 2\eta dt) \hat{\Gamma}_{k_1, k_2}^{n+1} - \left(\frac{1}{2} + \eta dt \right) \hat{\Gamma}_{k_1, k_2}^n + 2dt \hat{B}_{k_1, k_2}^{n+1} - dt \hat{B}_{k_1, k_2}^n \right]. \quad (4.22b)$$

The starting value $n = 0$ of the second order method requires two initial approximations $\mathbf{U}^0$ and $\mathbf{U}^1$ in order to be applied. The approximation $\mathbf{U}^0$ can be obtained by the initial conditions by setting $\mathbf{U}^0 = (H^0, \Gamma^0)^T$, where $H^0 = H(x, z, 0)$ and $\Gamma^0 = \Gamma(x, z, 0)$. The approximation $\mathbf{U}^1$ can be evaluated by other p -order accurate schemes for $p < 2$. This can be achieved by performing one step of the implicit Euler method, which is the method chosen for this problem and is defined by

$$\mathbf{U}^1 + dt \mathcal{L} \mathbf{U}^1 = \mathbf{U}^0 + dt \mathcal{B}(\mathbf{U}^0). \quad (4.23)$$

The desired Fourier coefficients in this case are given by

$$\hat{H}_{k_1, k_2}^1 = \frac{\bar{\xi}_{k_1, k_2} - i dt d_{k_1, k_2}}{\bar{\xi}_{k_1, k_2}^2 + dt^2 d_{k_1, k_2}^2} \left[\left(1 + \frac{c dt}{\nu_1} \right) \hat{H}_{k_1, k_2}^0 - dt k_\nu^2 \hat{\Gamma}_{k_1, k_2}^0 + dt \hat{A}_{k_1, k_2}^0 \right], \quad (4.24a)$$

$$\hat{\Gamma}_{k_1, k_2}^1 = \frac{1}{\bar{\zeta}_{k_1, k_2}} \left[(1 + \eta dt) \hat{\Gamma}_{k_1, k_2}^0 + dt \hat{B}_{k_1, k_2}^0 \right], \quad (4.24b)$$

with

$$\bar{\xi}_{k_1, k_2} = 1 + \frac{c dt}{\nu_1} + \nu_1 dt k_\nu^4 = \xi_{k_1, k_2} - \frac{1}{2}, \quad \bar{\zeta}_{k_1, k_2} = 1 + \eta dt k_\nu^2 + \eta dt = \zeta_{k_1, k_2} - \frac{1}{2}. \quad (4.25)$$

4.4 Conditions in the numerical analysis

As discussed in the previous section, before applying the numerical schemes for the time discretisation, it is necessary to prove that the conditions in Akrivis & Crouzeix [77] are satisfied. The two different cases of Reynolds numbers $\mathcal{O}(\epsilon)$ and $\mathcal{O}(1)$ are going to be studied individually.

For asymptotically small Reynolds number and of the order of the film thickness $\mathcal{O}(\epsilon)$, $\mathcal{N}(k_1, k_2)$ is given by the expression (3.15) and thus the operator $\mathcal{P}$ is purely dispersive since $\mathcal{N}(-k_1, -k_2) = -\mathcal{N}(k_1, k_2)$. Denoting by $\mathcal{H}_{per}^s$ the periodic Sobolev space of order s , then the operators $\mathcal{A}_1: \mathcal{H}_{per}^4 \rightarrow L_{per}^2$, $\mathcal{A}_2: \mathcal{H}_{per}^2 \rightarrow L_{per}^2$ and the dispersive pseudo-differential operator $\mathcal{D}$ in (4.14) are defined by

$$\begin{aligned}\mathcal{A}_1 u &:= \frac{c}{\nu_1} u + \nu_1 u_{xxxx} + 2\nu_2 u_{xxzz} + \frac{\nu_2^2}{\nu_1} u_{zzzz}, \\ \mathcal{A}_2 u &:= -\eta \left(u_{xx} + \frac{\nu_2}{\nu_1} u_{zz} - u \right), \\ \mathcal{D} u &:= \mathcal{P} u.\end{aligned}\tag{4.26}$$

Both operators $\mathcal{A}_1$ and $\mathcal{A}_2$ are self-adjoint because

$$\begin{aligned}(\mathcal{A}_1 u, v) &= (u, \mathcal{A}_1 v), \quad \forall u, v \in \mathcal{H}_{per}^4, \\ (\mathcal{A}_2 u, v) &= (u, \mathcal{A}_2 v), \quad \forall u, v \in \mathcal{H}_{per}^2,\end{aligned}\tag{4.27a}$$

and are also positive definite

$$\begin{aligned}(\mathcal{A}_1 u, u) &= \frac{c}{\nu_1} \|u\|^2 + \nu_1 \|u_{xx}\|^2 + 2\nu_2 \|u_{xz}\|^2 + \frac{\nu_2^2}{\nu_1} \|u_{zz}\|^2 \geq 0, \quad \forall u \in \mathcal{H}_{per}^2, \\ (\mathcal{A}_2 u, u) &= \eta \left(\|u\|^2 + \|u_x\|^2 + \frac{\nu_2}{\nu_1} \|u_z\|^2 \right) \geq 0, \quad \forall u \in \mathcal{H}_{per}^1.\end{aligned}\tag{4.27b}$$

This result allows any choice of $c > 0$, and in the numerical calculations c was fixed to unity. Defining the inner product $(\mathbf{u}, \mathbf{v}) = (u_1, v_1) + (u_2, v_2)$ for $\mathbf{u} = (u_1, u_2)$, $\mathbf{v} = (v_1, v_2)$, then the operator $\mathcal{A}: \mathcal{H}_{per}^4 \times \mathcal{H}_{per}^2 \rightarrow L_{per}^2 \times L_{per}^2$ is defined by

$$\mathcal{A}u := \begin{pmatrix} \mathcal{A}_1 & 0 \\ 0 & \mathcal{A}_2 \end{pmatrix} \begin{pmatrix} u_1 \\ u_2 \end{pmatrix} = \begin{pmatrix} \mathcal{A}_1 u_1 \\ \mathcal{A}_2 u_2 \end{pmatrix}, \quad (4.28)$$

and is clearly self-adjoint and positive definite. The proof of $\mathcal{B}$ being locally Lipschitz continuous is very similar to the ones given in Akrivis & Smyrlis [75] and Akrivis et al. [74, 84], and therefore it will be omitted. Consequently, both of the conditions in Akrivis & Crouzeix [77] hold and the system (4.5)–(4.6) can be discretised by stable linearly implicit methods.

Writing

$$\mathcal{L}_1 = \mathcal{A}_1 + \mathcal{D} := \frac{1}{\nu_1} + \nu_1 \partial_x^4 + 2\nu_2 \partial_x^2 \partial_z^2 + \frac{\nu_2^2}{\nu_1} \partial_z^4 + \mathcal{P} \quad (4.29)$$

and utilising the asymptotic property $\mathcal{N}(k) \sim k_1 k$ as $|k| \rightarrow \infty$, clearly shows that the dispersive operator $\mathcal{D}$ is dominated by the linear operator $\mathcal{A}_1$. Consequently, higher order time-stepping schemes (up to order 6) are stable and can be used to analyse the problem in this case.

Now if the Reynolds number is of $\mathcal{O}(1)$, two different cases are identified: for long waves $\mathcal{N}(k_1, k_2)$ is given by the localised form (3.4), but in general the solution of the system (2.91) determines $\mathcal{N}(k_1, k_2)$ from (2.95). In the first case (i.e. for the localised system), the linear operators $\mathcal{A}_1$, $\mathcal{A}_2$ and $\mathcal{D}$ are introduced by

$$\begin{aligned} \mathcal{A}_1 u &:= \frac{c}{\nu_1} u + \frac{\Lambda R_e}{60} u_{xx} + \nu_1 u_{xxx} + 2\nu_2 u_{xxz} + \frac{\nu_2^2}{\nu_1} u_{zzz}, \\ \mathcal{A}_2 u &:= -\eta \left(u_{xx} + \frac{\nu_2}{\nu_1} u_{zz} - u \right), \\ \mathcal{D} u &:= 2\Lambda \left(u_x - \left(\frac{1}{15} + \frac{R_e^2}{16800} \right) u_{xxx} - \frac{1}{15} u_{xzz} \right). \end{aligned} \quad (4.30)$$

The operator $\mathcal{D}$ is antisymmetric and $(\mathcal{D}u, u) = 0$. In addition, $\mathcal{A}_2$ is the same as in the small Reynolds number case, so it is self-adjoint and positive definite. Operator $\mathcal{A}_1$ is clearly self-adjoint and its positive definiteness follows by studying

$$(\mathcal{A}_1 u, u) = \frac{c}{\nu_1} \|u\|^2 - \frac{\Lambda R_e}{60} \|u_x\|^2 + \nu_1 \|u_{xx}\|^2 + 2\nu_2 \|u_{xz}\|^2 + \frac{\nu_2^2}{\nu_1} \|u_{zz}\|^2, \quad \forall u \in \mathcal{H}_{per}^2. \quad (4.31)$$

The operator is positive definite if $\Lambda \leq 0$ for any selection of positive c (in the numerical experiments $c = 1$). If $\Lambda > 0$, use of Parseval's identity in (4.31) yields

$$\begin{aligned}
 (\mathcal{A}_1 u, u) &= 4\pi^2 \sum_{k_1=-\infty}^{+\infty} \sum_{k_2=-\infty}^{+\infty} \left(\nu_1 k_1^4 + 2\nu_2 k_1^2 k_2^2 + \frac{\nu_2^2}{\nu_1} k_2^4 - \frac{\Lambda R_e}{60} k_1^2 + \frac{c}{\nu_1} \right) |\hat{u}_{k_1, k_2}|^2 \\
 &= 4\pi^2 \nu_1 \sum_{k_1} \sum_{k_2} \left(\left(k_1^2 + \frac{\nu_2}{\nu_1} k_2^2 \right)^2 - \frac{\Lambda R_e}{60\nu_1} k_1^2 + \frac{c}{\nu_1^2} \right) |\hat{u}_{k_1, k_2}|^2 \\
 &\geq 4\pi^2 \nu_1 \sum_{k_1} \sum_{k_2} \left(k_1^4 - \frac{2\Lambda R_e}{60\nu_1} k_1^2 + \frac{c}{\nu_1^2} \right) |\hat{u}_{k_1, k_2}|^2 + 4\pi^2 \sum_{k_1} \sum_{k_2} \frac{\Lambda R_e}{60} k_1^2 |\hat{u}_{k_1, k_2}|^2.
 \end{aligned} \tag{4.32}$$

Choosing $c = \left(\frac{\Lambda R_e}{60}\right)^2$ in (4.32) results in

$$\left(\frac{\Lambda R_e}{60}\right)^2 \frac{1}{\nu_1} \|u\|^2 - \frac{\Lambda R_e}{60} \|u_x\|^2 + \nu_1 \|u_{xx}\|^2 + 2\nu_2 \|u_{xz}\|^2 + \frac{\nu_2^2}{\nu_1} \|u_{zz}\|^2 \geq \frac{\Lambda R_e}{60} \|u_x\|^2, \tag{4.33}$$

which leads to

$$(\mathcal{A}_1 u, u) \geq \frac{1}{2} \left[\left(\frac{\Lambda R_e}{60}\right)^2 \frac{1}{\nu_1} \|u\|^2 + \nu_1 \|u_{xx}\|^2 + 2\nu_2 \|u_{xz}\|^2 + \frac{\nu_2^2}{\nu_1} \|u_{zz}\|^2 \right] \geq 0. \tag{4.34}$$

For a general operator $\mathcal{P}$, the operators $\mathcal{A}_1$ and $\mathcal{D}$ can be defined as follows ($\mathcal{A}_2$ is still the same)

$$\mathcal{A}_1 u := \frac{c}{\nu_1} u + \nu_1 u_{xxxx} + 2\nu_2 u_{xxzz} + \frac{\nu_2^2}{\nu_1} u_{zzzz} + \mathcal{P}u, \quad \forall u \in \mathcal{H}_{per}^2 \tag{4.35}$$

and $\mathcal{D}u := 0$. In this case, an exact value of c such that $\mathcal{A}_1$ to be positive definite cannot be found analytically. The only possible way out of this problem is by choosing an empirical value for c and ensuring that

$$(\mathcal{A}_1 u, u) = \frac{c}{\nu_1} \|u\|^2 + \nu_1 \|u_{xx}\|^2 + 2\nu_2 \|u_{xz}\|^2 + \nu_2 \|u_{zz}\|^2 + (\mathcal{P}u, u) \geq 0, \tag{4.36}$$

at the start of every numerical simulation for a parameter set $(\nu_1, \nu_2, \Lambda, R_e, \eta, \Gamma_0)$.

5 Results for Two-dimensional Flows

Assuming that the channel is two-dimensional, the problem reduces to the case where the interface is one-dimensional. This problem was first studied by Bassom et al. [2], where the authors derived a weakly nonlinear and nonlocal system of evolution equations but solved it in the local approximation. The aim of this work is to solve the full nonlocal system and also compare nonlocal solutions to the local ones. In this chapter, the one-dimensional evolution equations are presented, together with the numerical schemes used to solve them. In addition, numerical solutions of the nonlocal model are obtained and compared to experimental interfacial shapes in the case of absence of surfactants. The linear stability properties of the system are then analysed, followed by a detailed numerical study of the dynamics of the problem. A large part of this chapter (results for $R_e = \mathcal{O}(\epsilon)$) is published in the *IMA J. Appl. Math.* (Kalogirou, Papageorgiou & Smyrlis [85]).

5.1 Evolution equations

The geometry of the flow in this case can be seen in Figure 12. The derivation of evolution equations is based on the same principles and similar scalings as the three-dimensional problem presented in Chapter 2, so it is omitted (the derivation is actually simpler in this case and details can also be found in Bassom et al. [2] and Kalogirou et al. [85]). The final evolution equations are

$$H_t + HH_x + H_{xxxx} + \frac{i\Lambda}{2\pi} \int_{-\infty}^{+\infty} \mathcal{N}(k) \hat{H}(k) e^{ikx} dk - \Gamma_{xx} = 0, \quad (5.1)$$

$$\Gamma_t + (H\Gamma)_x - \eta\Gamma_{xx} = 0, \quad (5.2)$$

and follow from (2.98)–(2.99) by setting $\partial_z = 0$. The parameters Λ and η are the same as in (2.100) and $\mathcal{N}(k)$ is now given by

$$\mathcal{N}(k) = -\frac{k}{2} F''(0), \quad (5.3)$$

where $F(y)$ is the solution of the boundary value problem (2.91) for $k_1 = k$.

The system is solved on $2L$ -periodic domains, but when transformed to 2π -periodic domains it becomes

$$H_t + HH_x + \nu H_{xxxx} + i\Lambda\nu^{-1} \sum_{k=-\infty}^{+\infty} \mathcal{N}(k\sqrt{\nu}) \hat{H}(k) e^{ikx} - \Gamma_{xx} = 0, \quad (5.4)$$

$$\Gamma_t + (H\Gamma)_x - \eta\Gamma_{xx} = 0, \quad (5.5)$$

with $\nu = \frac{\pi^2}{L^2}$. Also, all asymptotic properties of this system can be recovered from Chapter 3 by setting $k_2 = 0$ and $k = k_1$ (or $z = 0$). An important result is the localised evolution equation, which is established by use of the local approximation (3.4) with $k_2 = 0$ and is given by

$$H_t + HH_x + \nu H_{xxxx} + 2\Lambda \left(\frac{1}{\sqrt{\nu}} H_x + \frac{R_e}{120} H_{xx} - \left(\frac{1}{15} + \frac{R_e^2}{16800} \right) \sqrt{\nu} H_{xxx} \right) - \Gamma_{xx} = 0. \quad (5.6)$$

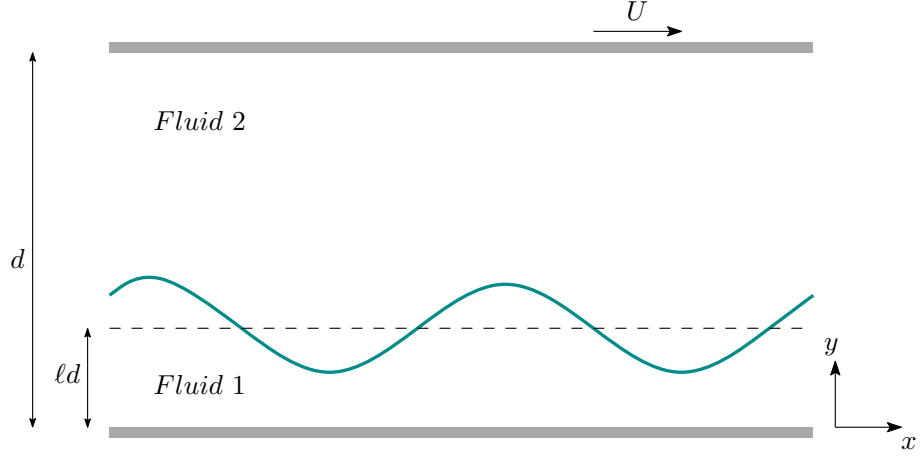


Figure 12: Geometry of the two-dimensional problem. The *dashed line* is the interface at the basic state and the *blue solid line* is the general position of the interface in the disturbed state. In the analysis, the lower fluid layer is assumed very thin in comparison to the upper layer fluid.

5.2 Conditions for numerical methods

The numerical method used for the time discretisation is once again the second-order implicit–explicit BDF scheme as described in Chapter 4, together with spectral methods for space discretisation. The scheme used for the one-dimensional system can be reduced from (4.22) by setting $k_2 = 0$ and is given by

$$\hat{H}_k^{n+2} = \frac{\xi_k - i dt d_k}{\xi_k^2 + dt^2 d_k^2} \left[\left(2 + \frac{2c dt}{\nu} \right) \hat{H}_k^{n+1} - 2dt k^2 \hat{\Gamma}_k^{n+1} - \left(\frac{1}{2} + \frac{c dt}{\nu} \right) \hat{H}_k^n + dt k^2 \hat{\Gamma}_k^n + 2dt \hat{A}_k^{n+1} - dt \hat{A}_k^n \right], \quad (5.7a)$$

$$\hat{\Gamma}_k^{n+2} = \frac{1}{\zeta_k} \left[(2 + 2\eta dt) \hat{\Gamma}_k^{n+1} - \left(\frac{1}{2} + \eta dt \right) \hat{\Gamma}_k^n + 2dt \hat{B}_k^{n+1} - dt \hat{B}_k^n \right], \quad (5.7b)$$

where

$$\hat{A}_k = -ik \mathcal{F} \left(\frac{H^2}{2} \right), \quad \hat{B}_k = -ik \mathcal{F}(H\Gamma), \quad (5.8)$$

(see also Appendix C) and

$$\xi_k = \frac{3}{2} + \frac{c dt}{\nu} + \nu dt k^4, \quad \zeta_k = \frac{3}{2} + \eta dt k^2 + \eta dt. \quad (5.9)$$

As discussed earlier, the conditions in Akrivis & Crouzeix [77] must be satisfied before applying the numerical method. For $R_e = \mathcal{O}(\epsilon)$, $\mathcal{N}(k)$ is an odd function of k and the operator $\mathcal{P}$ is dispersive. In order to show that $\mathcal{A}: \mathcal{H}_{per}^4 \times \mathcal{H}_{per}^2 \rightarrow \mathcal{L}_{per}^2 \times \mathcal{L}_{per}^2$ is self-adjoint and positive definite ($\mathcal{H}_{per}^s$ is the periodic Sobolev space of order s), it is enough to show these conditions for $\mathcal{A}_1$ and $\mathcal{A}_2$. In this case, the operators $\mathcal{A}_1: \mathcal{H}_{per}^4 \rightarrow \mathcal{L}_{per}^2$, $\mathcal{A}_2: \mathcal{H}_{per}^2 \rightarrow \mathcal{L}_{per}^2$ and the antisymmetric operator $\mathcal{D}$ are defined by

$$\mathcal{A}_1 u := \frac{c}{\nu} u + \nu u_{xxxx}, \quad \mathcal{A}_2 u := -\eta(u_{xx} - u), \quad \mathcal{D}u := \mathcal{P}u. \quad (5.10)$$

Obviously, both $\mathcal{A}_1$ and $\mathcal{A}_2$ are self-adjoint and positive definite operators for any choice of $c > 0$ (in the numerical calculations $c = 1$). The proof of $\mathcal{B}$ being locally Lipschitz continuous is omitted because it is very similar to that presented in Akrivis et al. [74].

Therefore, both of the conditions in Akrivis & Crouzeix [77] hold and the system (5.4)–(5.5) can be discretised by linearly implicit methods. Having in mind the asymptotic property $\mathcal{N}(k) \sim k^2$ as $|k| \rightarrow \infty$, operator $\mathcal{A}_1$ dominates the dispersive term $\mathcal{D}$ and thus time-stepping schemes of order up to 6 are stable.

Moving on to the case of $R_e = \mathcal{O}(1)$, for long waves the linear operators $\mathcal{A}_1$, $\mathcal{A}_2$ and $\mathcal{D}$ are introduced by

$$\begin{aligned} \mathcal{A}_1 u &:= \frac{c}{\nu} u + \frac{\Lambda R_e}{60} u_{xx} + \nu u_{xxxx}, & \mathcal{A}_2 u &:= -\eta(u_{xx} - u), \\ \mathcal{D}u &:= 2\Lambda \left(u_x - \left(\frac{1}{15} + \frac{R_e^2}{16800} \right) u_{xxx} \right). \end{aligned} \quad (5.11)$$

Clearly, $\mathcal{D}$ is antisymmetric with $(\mathcal{D}u, u) = 0$. Moreover, both $\mathcal{A}_1$ and $\mathcal{A}_2$ are self-adjoint and $\mathcal{A}_2$ is also positive definite. For $\mathcal{A}_1$ it follows that

$$(\mathcal{A}_1 u, u) = \frac{c}{\nu} \|u\|^2 - \frac{\Lambda R_e}{60} \|u_x\|^2 + \nu \|u_{xx}\|^2, \quad \forall u \in \mathcal{H}_{per}^2. \quad (5.12)$$

From this equality it is obvious that if $\Lambda \leq 0$ then $\mathcal{A}_1$ is positive definite for any $c \geq 0$, but if $\Lambda > 0$ the operator can become positive definite for a specific choice of the constant c . This is achieved by using Parseval's formulas and choosing $c = \left(\frac{\Lambda R_e}{60} \right)^2$.

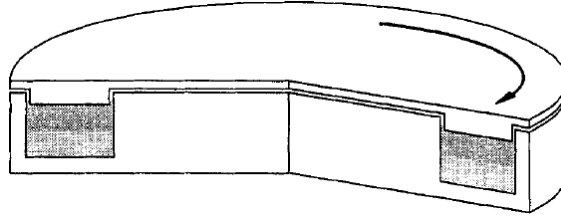


Figure 13: Experimental device, as used by Barthelet, Charru & Fabre (taken from Barthelet et al. [46], p.26). The channel is bent into an annular ring so that its ends meet and the fluid is dragged by the plate motion.

For a general operator $\mathcal{P}$, an analogous result proving the positive definiteness of $\mathcal{A}_1$ can be found for

$$c = \left(\Lambda \nu^{-1/2} \left| \min \left(\Im(F''(0)) \right) \right| \right)^2 \quad (5.13)$$

(for a detailed proof of this result see Appendix D).

5.3 Absence of surfactant: comparison with experiment

Before solving the model equations numerically with the goal of investigating the dynamics of the flow, the objective is to first examine whether the derived model captures the essential features of the interface. To that end, numerical solutions of the model will be obtained and compared with experimental data. Due to the absence of experiments performed on two-layer Couette flows with insoluble surfactants, the model will be first simplified for the situation where the interface is clean of surfactants. In this case, an experiment considering the interfacial instabilities arising in a two-fluid Couette flow in a channel was performed by Barthelet, Charru & Fabre [46] and will be used for qualitative comparisons with numerical simulations.

The device used to investigate the development of the interface was a channel of rectangular cross-section, bent into an annular ring so that its ends meet (Figure 13). The fluids motion was driven by the upper plate rotation around the axis of the ring, as indicated in the figure, and the position of the interface was measured with a probe situated in the middle of the cross-section. The mean diameter of the channel was $D = 400$ mm, its width $W = 40$ mm and the channel depth was $d = 20$ mm. The lower fluid used in the experiment was a mixture of distilled water and glycerine in

Table 1: Physical parameters of the problem, as used in the two-fluid channel flow experiment by Barthelet et al. [46] and in the numerical simulations of the model equation describing the flow dynamics.

Parameter	Experiment	Numerical Simulations
Diameter	$D = 0.4$ m	
Width	$W = 0.04$ m	
Depth	$d = 0.02$ m	
Surface tension	$\gamma = 0.03$ Pa·m	
Viscosity (thick fluid)	$\mu_1 = 0.0108$ Pa·s	μ'_2
Viscosity (thin fluid)	$\mu_2 = 0.0297$ Pa·s	μ'_1
Density (thick fluid)	$\rho_1 = 1142$ kg·m ⁻³	ρ'_2
Density (thin fluid)	$\rho_2 = 846$ kg·m ⁻³	ρ'_1 (taken equal to ρ'_2)
Viscosity ratio	$m = \frac{\mu_2}{\mu_1} = 2.76$	$m' = \frac{1}{m} = 0.3623$
Density ratio	$r = \frac{\rho_2}{\rho_1} = 0.741$	$r' = 1$
Depth ratio	$h = \frac{h_2}{h_1} = 0.25$	$h' = \frac{h'_1}{h'_2} = \frac{\epsilon}{1-\epsilon} \approx \epsilon$

proportions 42 – 58% and the upper fluid was a mineral oil. The physical properties of the fluids are given in Table 1, together with the related choice of parameters used in the numerical calculations.

Even though their experimental device was three-dimensional, Barthelet et al. [46] were only interested in studying interfacial instabilities that arise due to the shearing motion (the channel width was much smaller than its length so that the waves develop in the longitudinal direction only). Thus their setup can be described by the two-dimensional flow configuration on the left panel of Figure 14. The experiments were performed for various values of the layer thickness $h = h_2/h_1$, but the only case which is relevant to the comparisons here is for $h = 0.25$, corresponding to the upper fluid being relatively thin compared to the lower fluid. In order to cast the problem studied here (where the lower fluid is the thin one) similar to the experiment's configuration, it is assumed that the lower plate moves and the whole system is reflected about the x -axis (see right panel in Figure 14). In this case, the fluid viscosities and densities must be also interchanged, so that the properties of the thin fluid (2) and thick

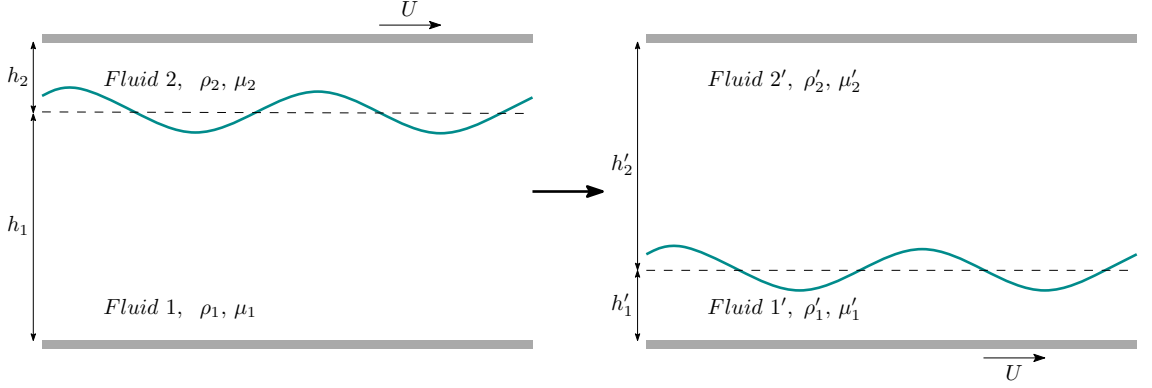


Figure 14: Flow configuration in experiment and mathematical modelling. Left panel: experimental setup, thin fluid on top and upper plate moving. Right panel: modelling setup, thin fluid on bottom and lower plate moving.

fluid (1) in the experiment to match the thin fluid (1') and thick fluid (2') in the mathematical model (see also Table 1). The reflection of the system corresponds to using the symmetry $H \rightarrow -H$ in the evolution equation (5.4), resulting in

$$H_t - HH_x + \nu H_{xxxx} + i\Lambda\nu^{-1} \sum_{k=-\infty}^{+\infty} \mathcal{N}(k\sqrt{\nu}) \hat{H}(k) e^{ikx} = 0. \quad (5.14)$$

Here, the function $\mathcal{N}(k)$ is still defined by (5.3), where $F(y)$ is the solution of the linear Orr–Sommerfeld boundary value problem (2.91) in the upper layer fluid (for $k_1 = k$) with a base flow velocity $\overline{U}'_2 = 1 - y$ instead of $\overline{U}_2 = y$ (because the lower plate is now moving). Note that the predictions of the linear stability of equation (5.14) are consistent with the results of Yih [1], which suggest instability of the flow if the thin film is the more viscous fluid ($\Lambda > 0$) and stability otherwise ($\Lambda \leq 0$).

The problem is non-dimensionalised according to (2.34), using the depth of the channel d as the characteristic length scale and the upper plate U as the velocity scale. A spatially periodic solution is then sought with period equal to about $L_w = 230$ mm. Assuming that in non-dimensional variables the solution is $2L$ -periodic, then $2L = L_w/d \approx 11.5$ and in the numerical computations the bifurcation parameter ν has the value $\nu = (\frac{\pi}{L})^2 = 0.3$. Moreover, the density ratio is set to $r' = 1$ and a “new” viscosity ratio is defined as $m' = 1/m = 0.3623$, which when used in (2.100)

Table 2: Parameter values used in the five comparisons with the experiments. The five ratios U/U_L are obtained from the experimental paper by Barthelet et al. [46], where $U_L = 0.138$ m/s.

U/U_L	1.06	1.13	1.33	1.58	1.77
U	0.146 m/s	0.156 m/s	0.184 m/s	0.218 m/s	0.244 m/s
Re_2	309	330	389	461	516
Re_1	112	120	141	167	187
We	16.24	18.48	25.66	36.07	45.25
Ca	0.145	0.154	0.182	0.216	0.242

gives $\Lambda = 0.11$ (with $Ca_0 = 0.16$). What is left is to find the Reynolds number in the upper layer, which is necessary for the calculation of the nonlocal term and it is given by

$$Re_2 = \frac{\rho'_2 U d}{\mu'_2} = \frac{\rho_1 U d}{\mu_1}. \quad (5.15)$$

The only missing parameter here is the upper plate velocity U , which is taken from the experimental paper for five different experiments corresponding to different upper plate speeds. These are given in Table 2, together with the corresponding Reynolds numbers in each fluid, and the Weber and Capillary numbers (notice that the order of the Capillary number, as well as the viscosity ratio m' , are in agreement with the scalings in (2.69)).

The final solution obtained from the numerical simulations is a travelling wave of the form $H(x - ct)$. The wave is rescaled back to the original dimensional variables by applying a series of transformations: first the transformation in (4.1) to revert from 2π -periodic to $2L$ -periodic domains, followed by (2.97) to invert the canonical rescaling, then (2.80) to remove the Galilean transformation and slow time scale and finally (2.34) to go back to dimensional units. Eventually, the position of the interface is evaluated at $x = 0$ and is given by

$$S = -d \left[\epsilon + \epsilon^2 \frac{\sqrt{\nu}}{3Ca_0 m'} H \left(-\frac{\overline{U}'_1(\epsilon) U \sqrt{\nu}}{d} t \right) \right], \quad (5.16)$$

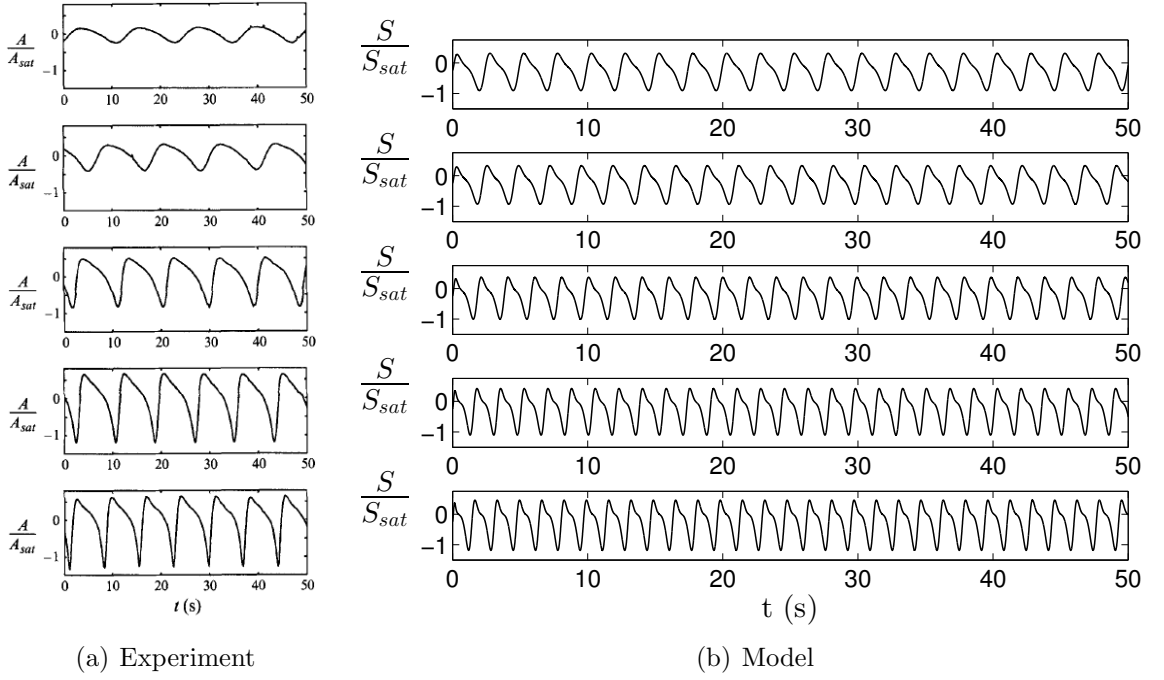


Figure 15: Position of the interface at a fixed point. (a) Experimental shapes obtained by Barthelet, Charru & Fabre (taken from Barthelet et al. [46], p.36), and (b) interfacial shapes obtained numerically by solving model equation (5.14). The five plots correspond to the values of upper plate speeds or Reynolds numbers given in Table 2.

where the base flow in fluid (1') is found to be $\overline{U}'_1 = \frac{1-\epsilon}{1-\epsilon(1-m)}$.

Interestingly, Barthelet & Charru [86] also attempted to compare their experimental results with empirical model equations that have been derived by other researchers (Hooper & Grimshaw [28], Charru & Fabre [30]) to describe the time evolution of the interface in two-layer Couette flows. The evolution equations they used were of the Kuramoto–Sivashinsky type and they discussed that a Kuramoto–Sivashinsky–Korteweg–de Vries equation (which included the extra term u_{xxx} representing linear dispersion) contains all essential features of the interfacial instability and thus it is the most attractive in describing the wave shapes. Indeed, their numerical simulations confirmed this assumption. However, the model equation (5.14) used here is distinct from the ones used by Barthelet & Charru [86] since it includes the effect of inertia in the upper layer fluid, so it is expected to provide a better agreement with the experimental results of Barthelet et al. [46].

Figure 15 shows the time evolution of (a) experimental and (b) numerical interfacial waves evaluated at a fixed point, for the five different configurations shown in Table 2. The wave amplitudes are normalised with the saturated amplitude of the wave for the largest Reynolds number, i.e. for $Re_2 = 516$. Notice that the waves plotted in the two panels have similar shapes, consisting of steeper wave fronts and sharp troughs. However, the experimental waves become much steeper as the Reynolds number increases and their amplitudes more than double. This is not observed in the numerical solutions, which also seem to have much shorter wavelength than the experimental ones. This discrepancy could be attributed to the fact that the depth ratio $h = 0.25$ is relatively large for the asymptotic model to be precise (which is valid for arbitrarily small ϵ). Nonetheless, this study aims for a qualitative comparison and it is satisfying to see that the numerical solutions reproduce the wave shapes and manage to capture the trends of increasing amplitude and decreasing period for larger Reynolds numbers, as seen in the experiments.

Based on the above observations, it is expected that the asymptotic model will be able to reproduce shorter waves observed in the experiment for larger upper plate speeds, but this was not attempted. On a final note, there is work in progress which consists of direct numerical simulations (DNS) on two-layer Couette flows and aims to compare the numerical solutions obtained by the asymptotic model and the DNS.

5.4 Linear stability theory

Coming back to the problem of two-fluid flows in the presence of surfactants, the aim now is to solve the evolution equations numerically. Before introducing numerical solutions of the problem, the linear stability properties of the system (5.1)–(5.2) are presented. Perturbing about the uniform states $H = 0$, $\Gamma = \Gamma_0$, normal mode solutions are sought in the form (Drazin [87])

$$H(x, t) = \delta (c_1 e^{ikx + \sigma t} + c.c.), \quad \Gamma(x, t) = \Gamma_0 + \delta (c_2 e^{ikx + \sigma t} + c.c.). \quad (5.17)$$

Here δ is an arbitrary infinitesimal parameter, k is the wavenumber which is real, σ is the amplification rate which is complex and can also be written as $\sigma_{\text{R}} + i\sigma_{\text{I}}$, $c_{1,2}$ are complex constants and c.c. denotes complex conjugates. Substituting (5.17) into (5.1)–(5.2), results in the following dispersion relation

$$\sigma^2 + (k^4 + i\Lambda\mathcal{N}(k) + \eta k^2) \sigma + (\eta k^6 + i\eta\Lambda\mathcal{N}(k)k^2 - i\Gamma_0 k^3) = 0. \quad (5.18)$$

This is a quadratic equation for σ , so there exist two normal modes. Positive real part of the growth rate provides the condition for instability, i.e. $\sigma_{\text{R}} = \Re(\sigma) > 0$. For sufficiently large k , $\mathcal{N}(k) \sim k^2$ and both modes become negative ($\sigma_{1\text{R}} \sim -\eta k^2$, $\sigma_{2\text{R}} \sim -k^4$), therefore the flow becomes stable above a cut-off wavenumber value; this short wave stabilisation is due to surface tension effects. Therefore it is sufficient to look for positive growth rates at the vicinity of $k = 0$ to determine whether the flow is unstable.

For equal-viscosity fluids, i.e. $\Lambda = 0$, the growth rates for $k \ll 1$ are given by

$$\sigma_{1,2\text{R}} = \pm \sqrt{\frac{\Gamma_0}{2}} k^{3/2} - \frac{\eta}{2} k^2 + \dots, \quad (5.19)$$

where the plus sign corresponds to $\sigma_{1\text{R}}$ and the minus sign to $\sigma_{2\text{R}}$. Figure 16 shows the two growth rates for $\Lambda = 0$ and $\Gamma_0 = 1$, $\eta = 1$, where the black line corresponds to the unstable growth rate $\sigma_{1\text{R}}$ and the red line to the stable growth rate $\sigma_{2\text{R}}$. Therefore the flow in this case is unstable. It can become stable if $\eta \rightarrow \infty$, which corresponds to infinite surfactant diffusivity and thus a uniform surfactant distribution at the interface (equivalently, this is possible in the absence of surfactant, i.e. $\Gamma_0 \rightarrow 0$). Increasing Γ_0 leads to the completely opposite effect, that is the unstable region becomes larger. In the case when $\eta \rightarrow 0$, both growth rates tend to zero for large wavenumbers (one through positive and one through negative values) and this makes the problem ill-posed since there is no dissipation at large scales.

On the contrary, for $\Lambda \neq 0$ and for small wavenumbers (long waves), using the asymptotic result $\mathcal{N}(k) \approx 2k + \frac{iR_e}{60} k^2 + \left(\frac{2}{15} + \frac{R_e^2}{8400}\right) k^3$ in the dispersion relation, yields the growth rates

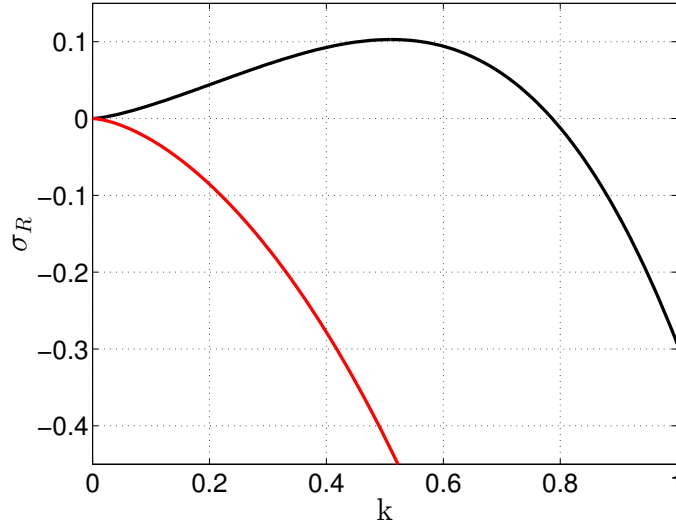


Figure 16: Growth rates for $\Lambda = 0$, $\Gamma_0 = 1$, $\eta = 1$. The black line corresponds to the unstable growth rate σ_{1R} and the red line to the stable growth rate σ_{2R} .

$$\sigma_{1R} = \frac{(\Gamma_0 - 2\eta\Lambda)}{2\Lambda}k^2 + \mathcal{O}(k^3), \quad \sigma_{2R} = \frac{(R_e\Lambda^2 - 30\Gamma_0)}{60\Lambda}k^2 + \mathcal{O}(k^3). \quad (5.20)$$

If the film is more viscous than the upper fluid, i.e. $\Lambda > 0$, the flow is unstable if (and only if, as shown in Bassom et al. [2])

$$\Gamma_0 - 2\eta\Lambda > 0 \quad \text{or} \quad R_e\Lambda^2 - 30\Gamma_0 > 0. \quad (5.21)$$

The first condition is the same as in the case of Stokes flow ($R_e = 0$), while the second condition is never satisfied in that case; thus the Stokes flow is only unstable if $\Lambda < \frac{\Gamma_0}{2\eta}$. Physically, the first instability condition can be satisfied by either having a sufficiently large initial surfactant concentration Γ_0 or small surfactant diffusion coefficient η , or by decreasing the viscosity difference between the two fluids. The second condition is physically possible by either imposing considerable viscosity contrast between the two fluids, by having a sufficiently large Reynolds number or by decreasing the initial concentration of the surfactant.

If the film is less viscous than the upper fluid, i.e. $\Lambda < 0$, then the first normal mode is always stable to small wavenumber perturbations and the second normal

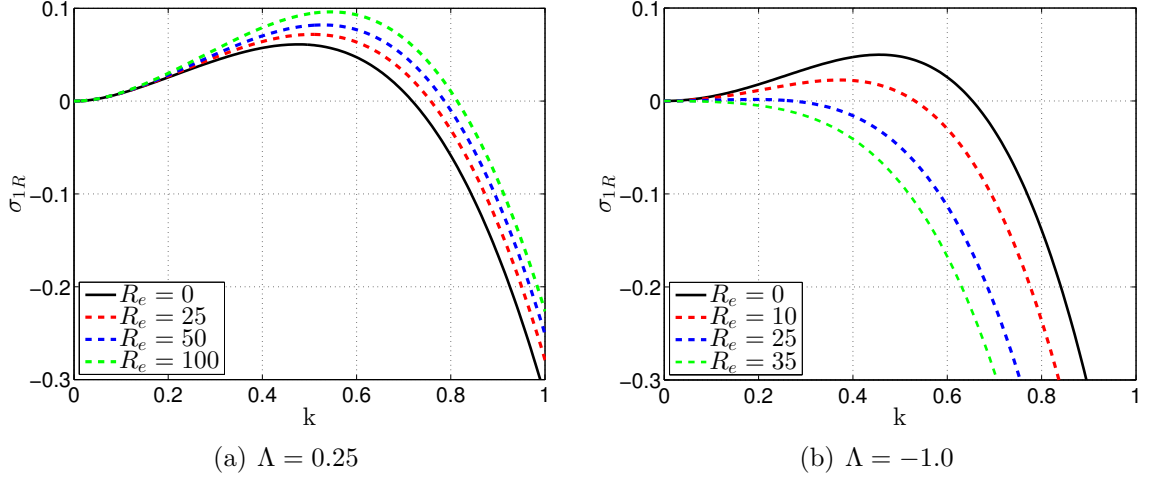


Figure 17: Effect of the Reynolds number on unstable growth rates, for $\Gamma_0 = 1$, $\eta = 1$. (a) Positive $\Lambda = 0.25$: increasing $R_e = 0, 25, 50, 100$ leads to larger unstable region. (b) Negative $\Lambda = -1.0$: increasing $R_e = 0, 10, 25, 35$ now shrinks the unstable region and eventually stabilises the problem above a cut-off Reynolds number value.

mode is unstable if

$$R_e \Lambda^2 - 30 \Gamma_0 < 0. \quad (5.22)$$

In the case of $R_e = 0$, condition (5.22) is always satisfied and therefore the Stokes flow is always unstable if the film is the less viscous fluid.

The effect of the Reynolds number on the stability of the problem can be seen in Figure 17 for $\Gamma_0 = 1$, $\eta = 1$. In particular, the unstable growth rates are plotted as functions of the wavenumber k , for Reynolds numbers $R_e = 0, 25, 50, 100$. Clearly, when Λ is positive (equal to 0.25 in panel (a)), increasing R_e increases the unstable region. This is also verified when looking at the cut-off wavenumbers below which the flow becomes stable, which also increase as the Reynolds number increases and are given by $k_c = 0.7182, 0.7575, 0.7865, 0.8137$, respectively. The opposite effect occurs in the case of negative Λ , as seen in panel (b) for $\Lambda = -1.0$.

What follows is an investigation of the effect of Λ on the stability. This is illustrated in Figure 18(a) for $R_e = 0$, $\Gamma_0 = 1$, $\eta = 1$. Increasing negative Λ leads to increase in the unstable growth, but then as Λ crosses to positive values the maximum growth starts decreasing and eventually becomes stable for $\Lambda > 0.25$.

Additionally, a comparison between the growth rates obtained from the nonlocal

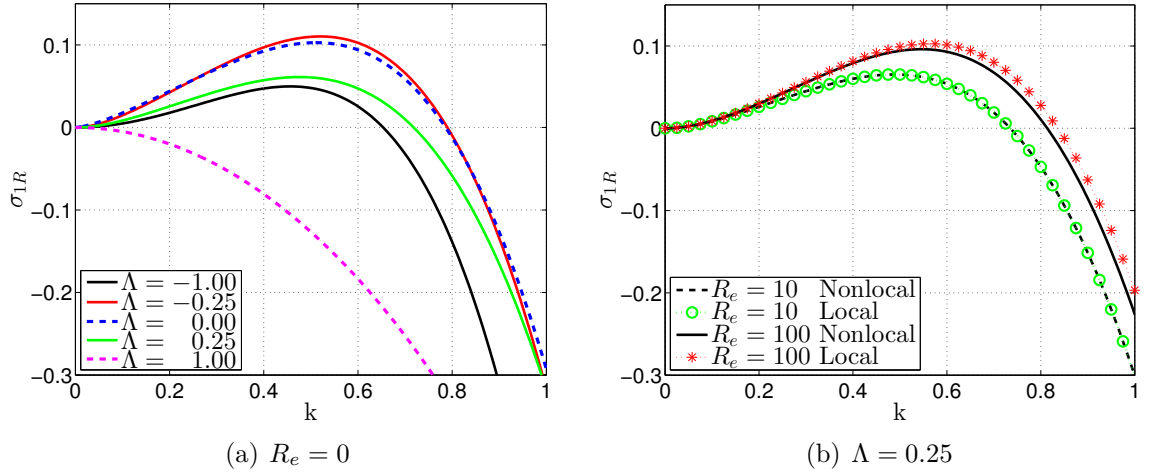


Figure 18: (a) Effect of the Λ on unstable growth rates, for $R_e = 0$, $\Gamma_0 = 1$, $\eta = 1$. (b) Comparison between local and nonlocal systems for $\Lambda = 0.25$, $\Gamma_0 = 1$, $\eta = 1$ and for $R_e = 10$ (black dashed & green) and $R_e = 100$ (black solid & red).

and local problems is performed. For the nonlocal problem, $\mathcal{N}(k)$ is given by (5.3) and the growth rates can only be found numerically. These are then compared graphically with the growth rates (5.20) obtained from the local system, as seen for example in Figure 18(b) for $\Lambda = 0.25$ and for Reynolds numbers $R_e = 10$ and $R_e = 100$. It is observed that for long waves the curves corresponding to the growth rates of the two systems are indistinguishable. However, for short waves the curves are identical for small Reynolds numbers only and start deviating as the Reynolds number grows. This suggests that solving the problem in its full nonlocal form is preferable and will reflect the dynamics of the system better than its local approximation.

The instability conditions (5.21), (5.22) are summarised in the stability diagram in Figure 19. One observation from the diagram is that instability always exists for $\Lambda = 0$ at any Reynolds number. This is in agreement with the findings of Frenkel & Halpern [31] and Halpern & Frenkel [32], who stated that Marangoni instability exists even for fluids with equal viscosities. Moreover, increasing $\Lambda > 0$ destabilises the flow above the critical value $(30\Gamma_0/R_e)^{1/2}$ (i.e. beyond the curve $R_e\Lambda^2 = 30\Gamma_0$). Decreasing $\Lambda < 0$ leads to the opposite effect, suggesting a viscosity stratification stabilisation of the Marangoni instability. Interestingly, there is a region in the parameter space where long wavelength perturbations are stable, even in the presence of surfactant and

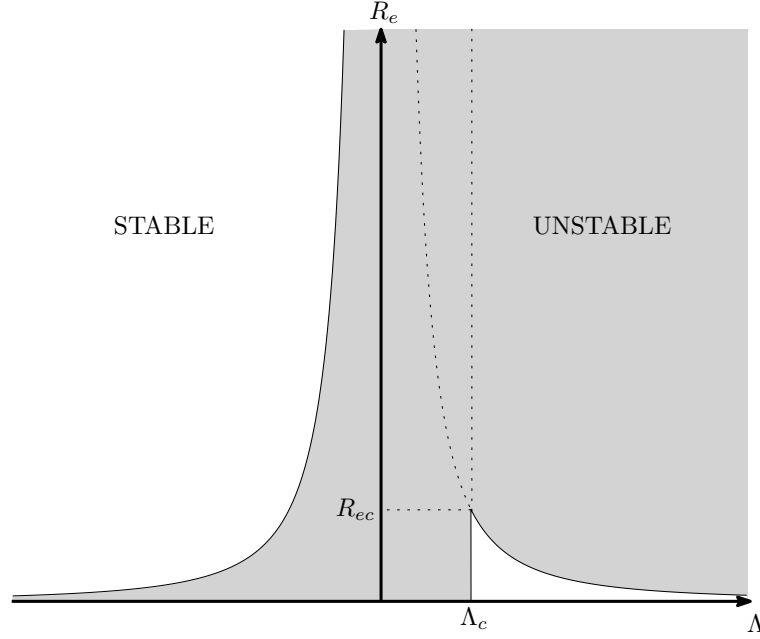


Figure 19: Stability diagram showing regions of stability (white) and instability (grey) in the Λ – R_e parameter space. The critical points are $\Lambda_c = \Gamma_0/2\eta$ and $R_{ec} = 120\eta^2/\Gamma_0$.

inertia; this happens if $R_e\Lambda^2/30 < \Gamma_0 < 2\eta\Lambda$. As shown by Yih [1], the surfactant-free flow is unstable for any $\Lambda > 0$, $R_e > 0$, therefore this suggests that the presence of surfactant can also stabilise some flow configurations.

Another remark is that for $R_e = 0$ the flow is unstable as long as Λ remains smaller than the critical value $\Lambda_c = \Gamma_0/2\eta$. An increase in the Reynolds number destabilises the flow if $\Lambda > 0$ and stabilises the flow if $\Lambda < 0$, as already seen in Figure 17. This result verifies the suggestions of various authors that inertial effects increase the growth of the surfactant-induced Marangoni instability and therefore produce new regions of instability, if the film is more viscous than the overlying fluid (Pozrikidis [34], Blyth & Pozrikidis [35], Frenkel & Halpern [36]). The short wave stabilisation seen in Figures 16, 17, 18 is due to surface tension effects (Hooper & Boyd [20]), represented by the H_{xxxx} term in the evolution equation for the film thickness.

The instability conditions are used numerically to identify regions in parameter space where instability and non-trivial dynamics are expected. Such calculations are presented in the next section.

5.5 Numerical experiments

Due to the complex dynamical phenomena, several diagnostics are used in the evaluation of the different attractors computed numerically. One useful tool is the energy of the solution $H(x, t)$ (or L_2 -norm), defined by

$$E(t) := \|H(\cdot, t)\|_{L_2}^2 = \int_0^{2\pi} H^2(x, t) dx. \quad (5.23)$$

The energy can be used in phase-plane constructions $(E(t), \dot{E}(t))$ and Poincaré maps (or return maps) satisfying $\dot{E}(t) = 0$. Such data analysis helps in characterising the dynamical behaviour of the system.

The calculation of $\dot{E}(t)$ is obtained by multiplying (5.4) by H and integrating over a period, yielding

$$\dot{E}(t) = -2\nu \|H_{xx}\|^2 - 2(H, \mathcal{P}H) + 2 \int_0^{2\pi} H \Gamma_{xx} dx, \quad (5.24)$$

where $(\cdot, \cdot)$ denotes an inner product in the L_2 space. This is computed with spectral accuracy using Parseval's formulas. The values of minima (or maxima) in the energy $E(t)$ are then estimated by a second-order polynomial interpolation to find the roots of $\dot{E}(t) = 0$. Afterwards, return maps are constructed by plotting curves in $\mathbb{R}^2$ consisting of the points (E_n, E_{n+1}) , $n = 1, \dots$, where E_n is the n th minimum of the energy signal $E(t)$. The obtained geometrical object provides information about the attractor. If the return map contains just one point, the flow is time-periodic with one minimum in the $E(t)$ signal; in this case, the period of oscillations is estimated by the difference between two consecutive minima. Continuous-looking curves that fill up with points as n increases indicate quasi-periodic behaviour analogous to the flow on a torus, while foldings and self-similarity provide strong evidence for chaos (Bergé et al. [88]).

For parameter values that support travelling wave solutions, the phase speed c is calculated numerically by assuming wave solutions of permanent form given by $H(x, t) = H(x - ct)$, $\Gamma(x, t) = \Gamma(x - ct)$. Inserting these into equation (5.5), multi-

plying by Γ_x and integrating over a period (Tseluiko & Papageorgiou [48]), yields the following expression

$$c = \frac{\int_0^{2\pi} \Gamma_x (H\Gamma)_x dx}{\int_0^{2\pi} \Gamma_x^2 dx}. \quad (5.25)$$

The computation of the wavespeed c in (5.25) is spectrally accurate. More precisely, a travelling wave is taken to exist and to have constant speed c_0 if

$$\limsup_{t \rightarrow \infty} \frac{\int_0^{2\pi} \Gamma_x (H\Gamma)_x dx}{\int_0^{2\pi} \Gamma_x^2 dx} = c_0. \quad (5.26)$$

5.5.1 Asymptotically small Reynolds number: $R_e = \mathcal{O}(\epsilon)$

Solutions of the initial value problem are calculated starting from the initial conditions

$$H(x, 0) = \frac{1}{10} \nu^{-1/2} \sin x, \quad \Gamma(x, 0) = \Gamma_0 \nu^{-1/2}. \quad (5.27)$$

The weight factor $\nu^{-1/2}$ is used such that for simulations performed for different ν (and for all other parameters fixed), the undisturbed physical film thickness and base surfactant concentration are of the same size regardless of the periodic length of the domain L (keeping in mind transformation (4.1)).

All the results that follow in this section were calculated for initial surfactant concentration $\Gamma_0 = 1$ and for surfactant diffusion coefficient $\eta = 1$, therefore the flow is linearly unstable if and only if $\Lambda < 0.5$ (based on the analysis in Section 5.4). The flow for equal viscosity fluids ($\Lambda = 0$) was studied first, in which case solutions saturate away from the trivial state for $\nu < 0.618$. This case has been studied in detail by Bassom et al. [2], who investigated the effect of surfactant diffusivity η and initial surfactant concentration Γ_0 on the solutions. They reported existence of multimodal travelling wave families whose spatial periods depend on the initial conditions and the number of unstable modes in the problem.

Interestingly, the first bifurcation point ν_0 such that for $\nu > \nu_0$ solutions return to the base states and for $\nu < \nu_0$ unstable solutions appear, can be found analytically

from the dispersion relation¹² as explained next. A sufficient condition for instability is given by picking $k = 1$ and ensuring that $\Re(\sigma) > 0$ (if $k = 0$ then $\sigma = 0$), hence to find the neutral point ν_0 it is sufficient to set $\Re(\sigma) = 0$. A few steps of algebra then yield a fourth-order polynomial in ν , which has only one positive real solution: ν_0 . In the case $\Lambda = 0$, the polynomial is given by

$$\nu^4 + 2\eta\nu^3 + \eta^2\nu^2 - \frac{\Gamma_0^2}{\eta} = 0, \quad (5.28)$$

and the solution ν_0 is found to be

$$\nu_0 = -\frac{\eta}{2} + \frac{(\eta^3 + 4\Gamma_0\sqrt{\eta})^{1/2}}{2\sqrt{\eta}}. \quad (5.29)$$

Taking $\Gamma_0 = 1$, $\eta = 1$ for example, gives $\nu_0 = \frac{-1+\sqrt{5}}{2}$ which is equal to 0.618 and matches the value found numerically.

Figure 20 demonstrates the variation of the bifurcation point ν_0 against η for fixed $\Gamma_0 = 1$ (panel (a)) and against Γ_0 for fixed $\eta = 1$ (panel (b)). Clearly, in the limits $\eta \rightarrow 0$ and $\eta \rightarrow \infty$, ν_0 becomes asymptotically large or small, respectively. The asymptotic behaviour of ν_0 for large η is $\nu_0 \sim \eta^{-3/2}$ (obtained asymptotically by (5.28) by balancing the last two terms), also confirmed by the logarithmic inset plot in Figure 20(a). This physically means that increasing the surfactant diffusivity leads to a uniform surfactant distribution at the interface and thus an increasingly stable flow. On the other hand, for small enough η , ν_0 grows similarly to $\nu_0 \sim \eta^{-1/4}$ and this makes the problem ill-posed with no large scale dissipation. Furthermore, in the absence of surfactant $\Gamma_0 = 0$ the flow is stable (corresponding to $\nu_0 = 0$ as seen in Figure 20(b)). As Γ_0 increases the value of ν_0 also increases, hence making the region of instability larger (the asymptotic behaviour of ν_0 for large Γ_0 is $\nu_0 \sim \Gamma_0^{1/2}$, obtained by balancing the first and last terms in equation (5.28)).

The solutions that arise as soon as the parameter ν crosses the first bifurcation

¹²This dispersion relation is obtained by linearising the system (5.4)–(5.5) and is slightly different from (5.18), which was obtained by linearisation of (5.1)–(5.2). Here periodic solutions are considered and thus the normal modes are characterised by integer wavenumbers $k \in \mathbb{Z}_+$.

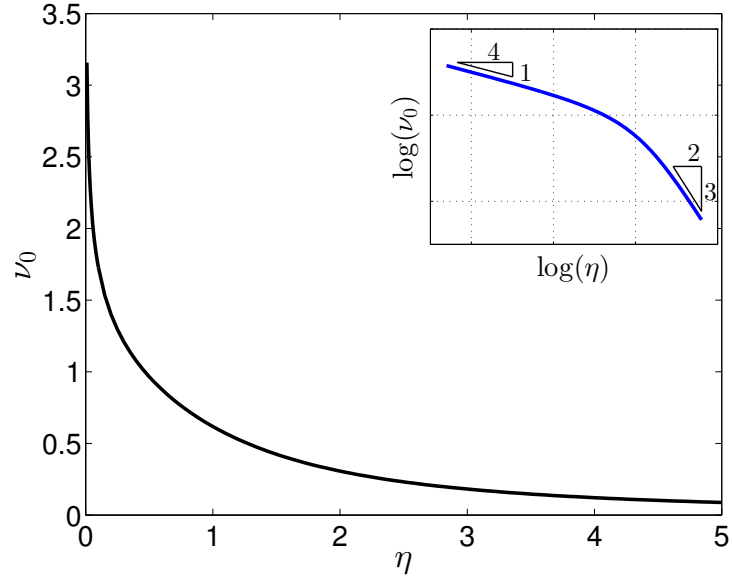
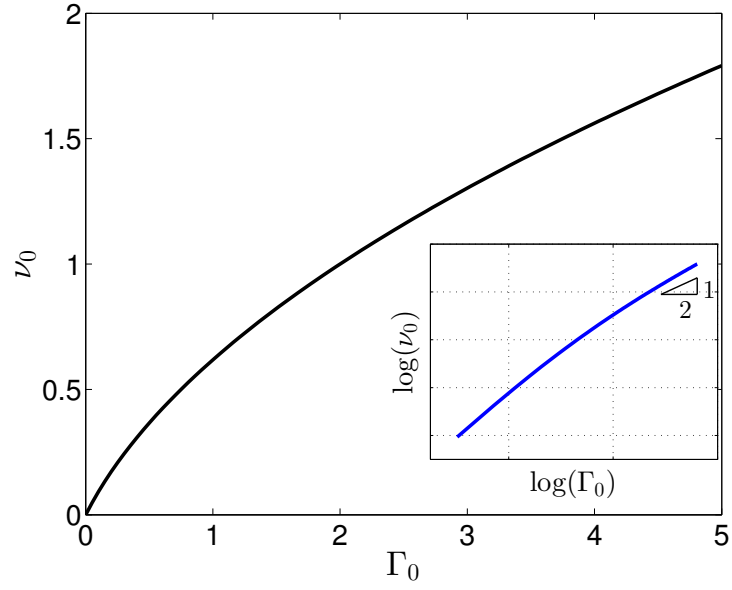
(a) Fixed $\Gamma_0 = 1$.(b) Fixed $\eta = 1$.

Figure 20: Variation of the bifurcation point ν_0 against η and Γ_0 , for $\Lambda = 0$. Inset figures show logarithmic plots depicting the analytically predicted slopes at different limits.

point ν_0 can be obtained analytically by bifurcation techniques. Right after the bifurcation occurs, the first nontrivial solutions that arise are travelling waves, which can be constructed by considering solutions of the form $H = H(x - ct)$, $\Gamma = \Gamma(x - ct)$. In this case the system (5.4)–(5.5) becomes

$$-cH' + HH' + \nu H'''' - \Gamma'' = 0, \quad (5.30a)$$

$$-c\Gamma' + (H\Gamma)' - \eta\Gamma'' = 0. \quad (5.30b)$$

Expanding H, Γ in Fourier series

$$H = \sum_{k=1}^{\infty} (H_k^s \sin kx + H_k^c \cos kx), \quad (5.31a)$$

$$\Gamma = \Gamma_0^c + \sum_{k=1}^{\infty} (\Gamma_k^s \sin kx + \Gamma_k^c \cos kx), \quad (5.31b)$$

and writing the parameter $\nu = \nu_0 - \epsilon$ for $\epsilon \ll 1$, then it can be found that the coefficients of $\cos kx, \sin kx$ have amplitudes $\epsilon^{k/2}$, $\forall k \in \mathbb{N}$. This argument is based on similar results about the steady states of the one-dimensional Kuramoto–Sivashinsky equation near the bifurcation point $\nu = 1$ (Frisch et al. [89]). Opposed to the KS case, here the bifurcation point ν_0 will be found as part of the solution and unsurprisingly it will reduce to (5.29). Therefore H, Γ and the wave speed c are expanded in powers of $\epsilon^{1/2}$ as follows

$$H = \epsilon^{1/2} H_1 + \mathcal{O}(\epsilon), \quad \Gamma = \Gamma_0^c + \epsilon^{1/2} \Gamma_1 + \mathcal{O}(\epsilon), \quad c = c_0 + \epsilon^{1/2} c_1 + \mathcal{O}(\epsilon), \quad (5.32)$$

with the Fourier modes given by

$$H_1 = H_1^s \sin(x + \phi), \quad \Gamma_1 = \Gamma_1^s \sin(x) + \Gamma_1^c \cos(x). \quad (5.33)$$

In these expansions, ϕ is the phase and is there due to translational invariance of the solution; it has an arbitrary value and is taken equal to $\phi = 0$ without loss of generality. In addition, Γ_0^c comes from the initial conditions and is actually a function

of ν_0 and ϵ ,

$$\Gamma_0^c = \Gamma_0 \nu^{-1/2} = \Gamma_0 (\nu_0 - \epsilon)^{-1/2} = \Gamma_0 \nu_0^{-1/2} \left(1 + \frac{\epsilon}{2\nu_0} + \mathcal{O}(\epsilon^2) \right). \quad (5.34)$$

Substituting expansions (5.32) into the system (5.30) and considering the $\mathcal{O}(\epsilon^{1/2})$ equations, the eigenvalues c_0 and ν_0 can be found explicitly by solving the following two equations

$$c_0^3 + \eta^2 c_0 + \eta \Gamma_0 \nu_0^{-1/2} = 0, \quad \nu_0 = \frac{c_0^2}{\eta}. \quad (5.35)$$

A simple algebraic calculation gives $\nu_0^{-1/2} = -\frac{\sqrt{\eta}}{c_0}$, where the negative sign was chosen instead of the positive because otherwise the final solution for c_0 would be complex. Finally, c_0 is found as the unique negative real solution of the equation

$$c_0^4 + \eta^2 c_0^2 - \eta^{3/2} \Gamma_0 = 0. \quad (5.36)$$

The exact solution for $\Gamma_0 = 1$, $\eta = 1$ is found to be $c_0 = -0.7862$ and the bifurcation point is $\nu_0 = 0.618$; these values were confirmed numerically by solving the initial value problem.

A final representative example for the equal-viscosity fluids case $\Lambda = 0$ is presented in Figure 21 for $\nu = 0.1$. In panel (a) the energy of the solution is demonstrated, which initially oscillates and after about 25 time units it saturates to a constant value. The wave speed has a similar behaviour and for $t > 25$ it reaches the constant value of approximately -0.7365 ; this can be seen in panel (b). Three snapshots of the interfacial and surfactant saturated waves are illustrated in panels (c) and (d) respectively, for the times $t = 98, 100, 102$.

In what follows, the outcomes of the numerical experiments for $\Lambda \neq 0$ are demonstrated in the direction of identifying the effect of the nonlocal term. To begin with, the case of positive Λ is studied. Taking $\Lambda = 0.25$, the flow is found to be linearly unstable for $\nu < 0.515$. This bifurcation point could be also obtained from the dispersion relation as in the simpler case of $\Lambda = 0$; the analytical expression for ν_0 is the unique positive real root of a fourth-order polynomial in ν , which is given in

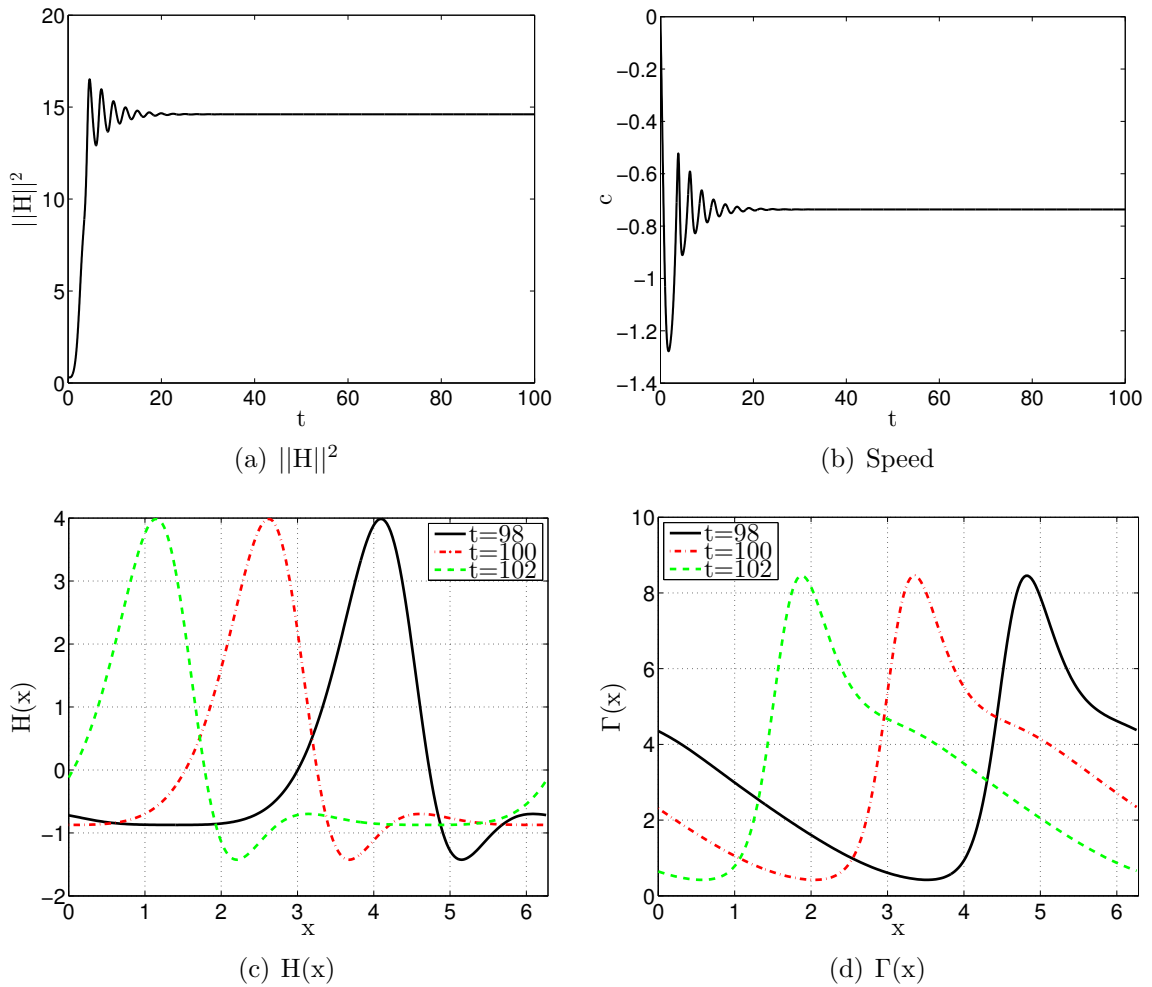


Figure 21: Travelling wave solutions obtained for $\nu = 0.1$, $R_e = 0$, $\Lambda = 0$, $\Gamma_0 = 1$, $\eta = 1$. (a) L_2 -norm of solution $H(x)$ saturating to a constant energy value. (b) Time evolution of the travelling wave speed c . (c) Interfacial profiles $H(x)$ taken at times $t = 98$ (black), $t = 100$ (red), $t = 102$ (green). (d) Surfactant profiles $\Gamma(x)$ taken at times $t = 98, 100, 102$ (black, red, green lines respectively).

Table 3: Dynamical behaviour of solutions for different values of ν and for $R_e = 0$, $\Lambda = 0.25$, $\Gamma_0 = 1$, $\eta = 1$. Key to solution types: TW – travelling waves; PTW – periodic travelling waves in time; QP – quasi-periodic in time; C – chaotic in time.

ν	Solution type	ν	Solution type
0.5–0.096	TW	0.008–0.007	TW
0.095–0.089	PTW	0.006	PTW
0.088–0.017	TW	0.005	TW
0.016–0.015	PTW	0.004	PTW
0.014–0.011	TW	0.003–0.002	QP
0.010–0.009	PTW	0.001	C

Appendix E for a general Reynolds number R_e . For values of ν larger than 0.515, large-time solutions are expected to tend to trivial steady states; non-trivial dynamics arise below this critical value. Extensive large-time numerical experiments were performed for different values of the domain parameter ν and are displayed in Table 3 for the range of values $0.001 \leq \nu \leq 0.5$. The different attractors named in the table are: TW – travelling waves of fixed form and constant speed; PTW – periodic travelling waves that experience time-periodic oscillations (namely after each period of oscillation the solution returns to its original form but is shifted spatially by a constant amount); QP – quasi-periodic oscillations in time; C – chaotic oscillations in time.

For values of ν close to the bifurcation point $\nu_0 = 0.515$ and for a relatively broad range of values $\nu < \nu_0$, the solutions saturate to steady-state travelling waves; oscillations (if they exist) in the energy signal decay and the norms reach a plateau, either via a region of decaying oscillations or monotonically. An example of travelling wave solutions is provided in Figure 22 for $\nu = 0.2$. The constant energy value is reached after about 15 time units, as observed in panel (a); the saturated wave profiles at time $t = 100$ can be seen in panel (b). At the value $\nu = 0.095$, a Hopf bifurcation takes place generating time-periodic travelling waves. These solutions have energy that oscillates in time and they can be simply identified when looking at the phase plane by the closed curve (periodic cycle) that forms after a long period of

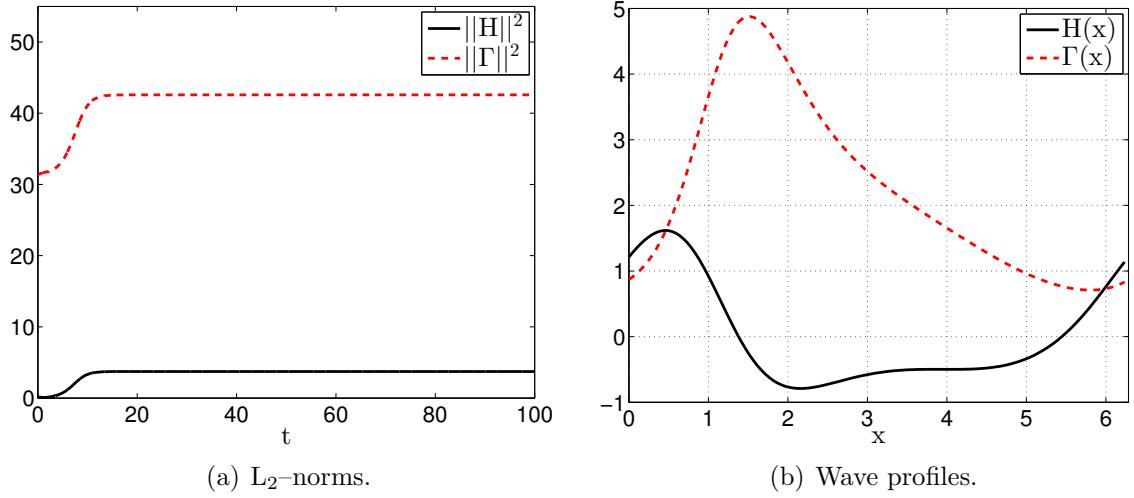


Figure 22: Travelling wave L_2 -norms and solution profiles for $\nu = 0.2$, $R_e = 0$, $\Lambda = 0.25$, $\Gamma_0 = 1$, $\eta = 1$. The saturated interfacial (solid black) and surfactant (dashed red) wave profiles in panel (b) are taken at time $t = 100$.

evolution. Figure 23 portrays this development for $\nu = 0.09$, where panel (a) depicts the energy $E(t)$ for $100 < t < 500$ and panel (b) the phase plane $(E(t), \dot{E}(t))$ in the same time interval. The final solution profiles at $t = 500$ can be seen in panel (c).

As ν decreases, travelling wave windows are interchanged with time-periodic windows and the pattern continues until $\nu = 0.003$. For $\nu \leq 0.003$, the dynamics of the flow enter more complex regimes. Figures 24 and 25 illustrate such complex solutions for $\nu = 0.002$ and $\nu = 0.001$, which exhibit quasi-periodicity and chaos, respectively. Panels (a) in both figures show the L_2 -norms in the time intervals $900 < t < 1000$, which are characterised by aperiodic fluctuations in the energy signal (Molenaar et al. [90]), and panels (b) present the corresponding profiles at the final time $t = 1000$. The flow for $\nu = 0.002$ is quasi-periodic according to the return map in Figure 24(c) which consists of dense curves, while for $\nu = 0.001$ the dispersal of the points and the foldings in the return map in Figure 25(c) suggest that the flow is chaotic.

Results for the case of a less viscous film compared to the overlying fluid, i.e. negative Λ , are considered next. For $\Lambda = -1.0$, for example, the dynamical behaviour of the flow is similar to the results of Table 3. While $\nu < 0.427$, windows supporting travelling waves are obtained, separated by windows supporting time-periodic trav-

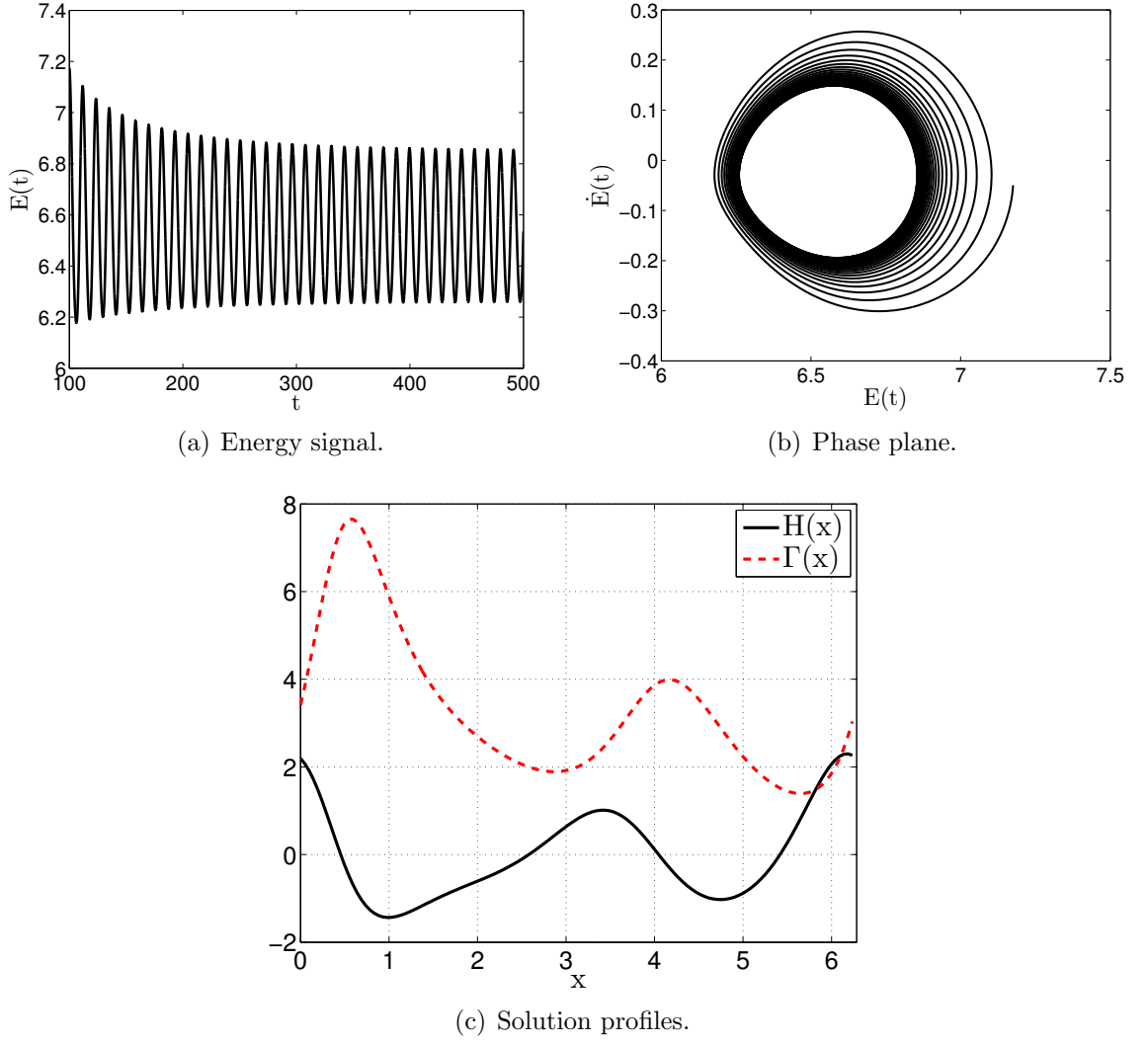


Figure 23: Time-periodic travelling wave solutions for $\nu = 0.09$, $R_e = 0$, $\Lambda = 0.25$, $\Gamma_0 = 1$, $\eta = 1$. (a) Energy signal is oscillating between two constant values. (b) Phase plane, which tends to a limit cycle in this case. (c) Interfacial (solid black) and surfactant (dashed red) solution profiles taken at time $t = 500$.

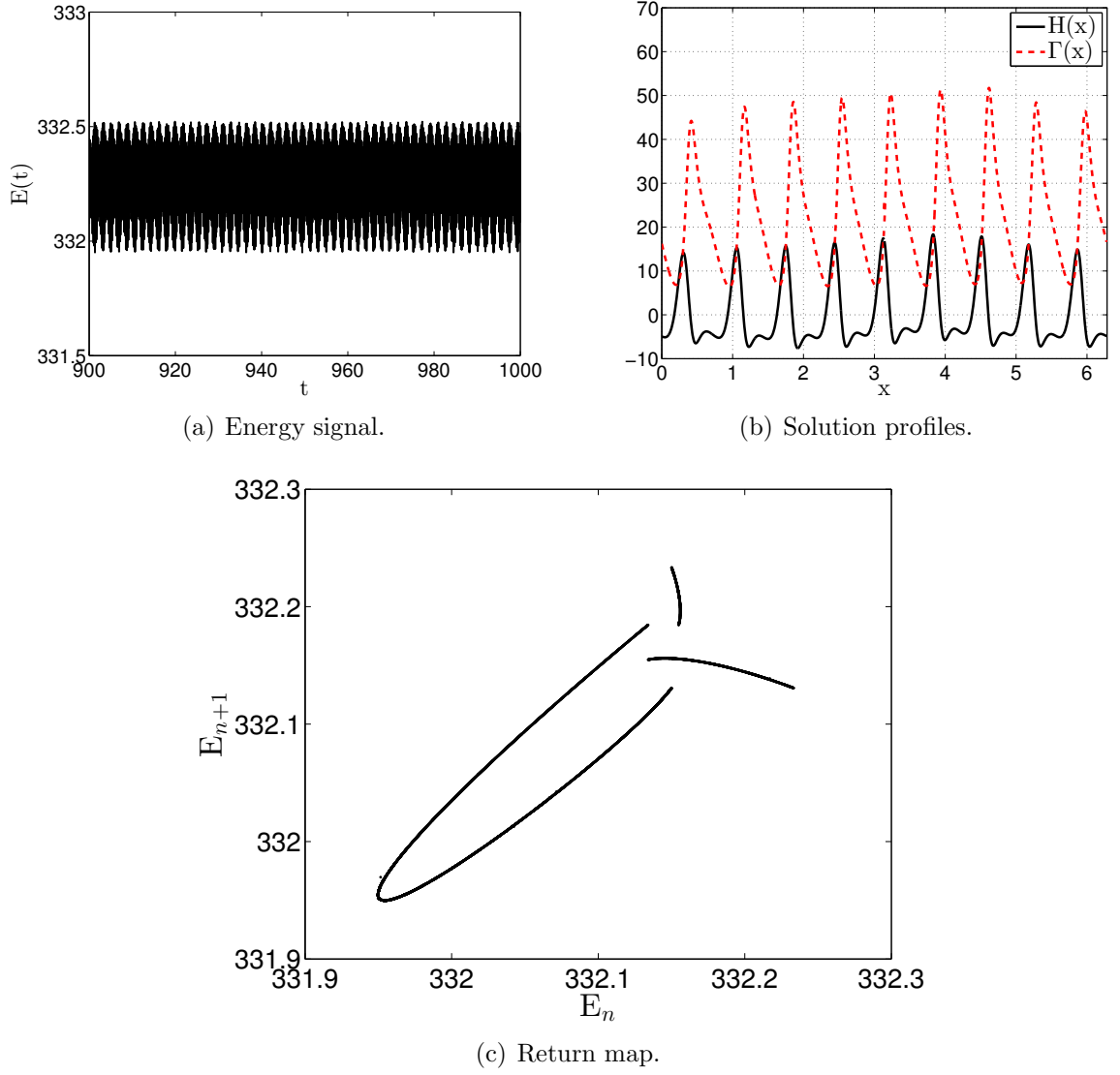


Figure 24: Quasi-periodic solutions obtained for $\nu = 0.002$, $R_e = 0$, $\Lambda = 0.25$, $\Gamma_0 = 1$, $\eta = 1$. (a) Energy signal. (b) Interfacial (solid black) and surfactant (dashed red) solution profiles taken at time $t = 1000$. (c) Return map consisting of dense curves.

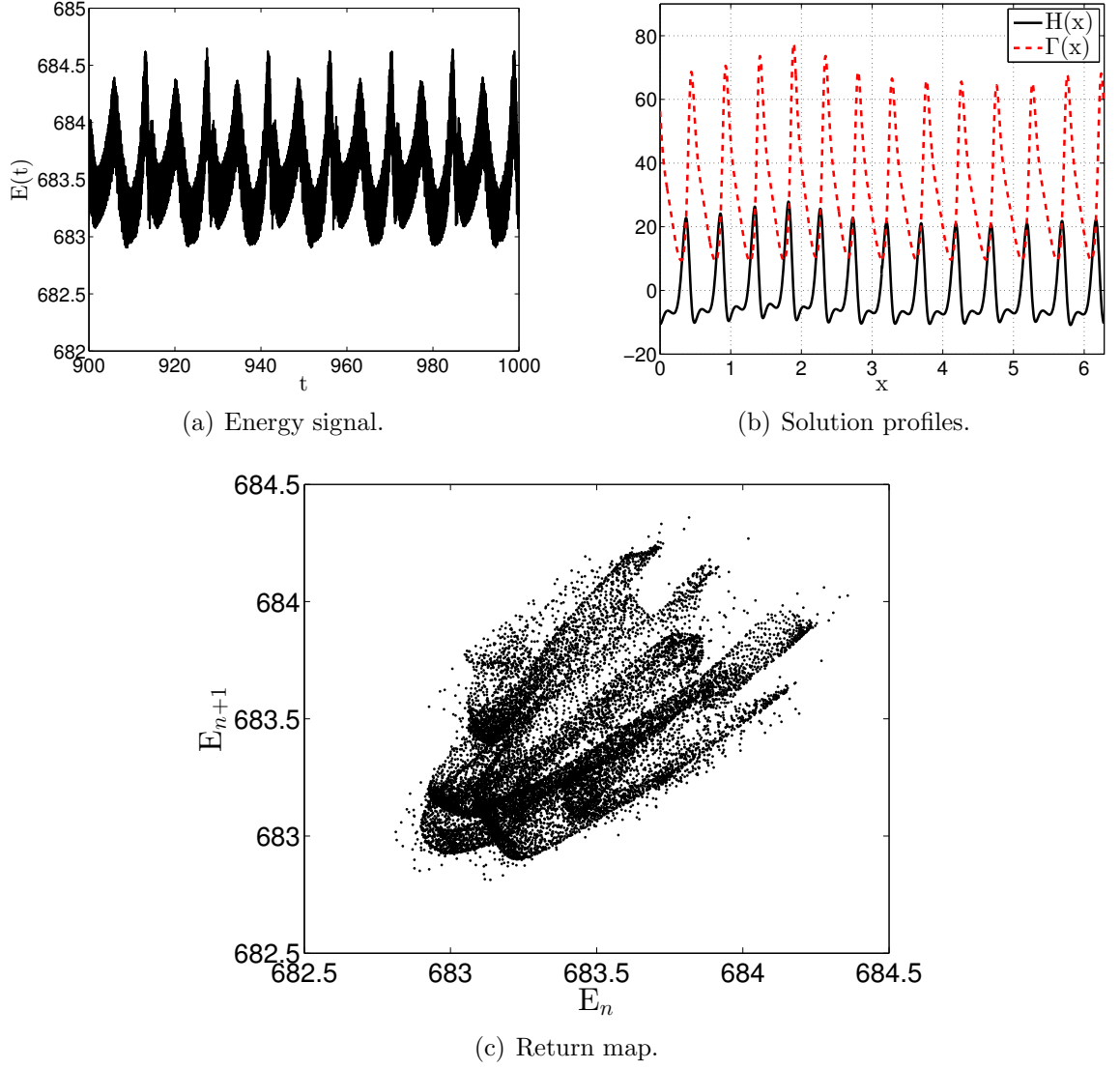


Figure 25: Chaotic solutions obtained for $\nu = 0.001$, $R_e = 0$, $\Lambda = 0.25$, $\Gamma_0 = 1$, $\eta = 1$. (a) Energy signal. (b) Interfacial (solid black) and surfactant (dashed red) solution profiles taken at time $t = 1000$. (c) Return map consisting of foldings.

elling waves and more intricate structures emerge as $\nu \rightarrow 0$. Figure 26 displays some characteristics of the solutions for fixed negative $\Lambda = -1.0$ and decreasing ν . In Figure 26(a) the variation of the wavespeed c with ν is shown for all computed windows where travelling waves are found. Figure 26(b) demonstrates the variation of the period of oscillation with ν for solutions taken from all the time-periodic windows. The travelling wave speed, where travelling waves exist and are stable, is negative and monotonically decreasing with decreasing ν . It also appears to diverge as $\nu \rightarrow 0$ (clearly, the system is ill-posed if $\nu = 0$). When time-periodic travelling waves are supported, the period of oscillation is altered non-monotonically but for sufficiently small ν it appears to decrease to smaller values as ν decreases towards 0.

The effect of the viscosity ratio on the behaviour of the solutions is investigated next and results for varying Λ and different but fixed values of ν are presented in Figure 27. Relatively large values $\nu = 0.1, 0.15, 0.2$ are selected in order to track the characteristics of stable travelling waves. The variation of the speed c is plotted in panel (a) and the corresponding final L_2 -norm of the solution (after oscillations completely fade out) in panel (b), both against Λ in the range $-5.0 \leq \Lambda \leq 0.5$. One remarkable feature in Figure 27(a) is that the wavespeeds are negative and decrease monotonically with Λ . While $|\Lambda|$ remains relatively small (about $-0.2 \leq \Lambda \leq 0.5$), smaller values of ν generate slower travelling waves, but as $|\Lambda| \gg 1$ smaller ν produce waves which travel faster to the left, in agreement with the result in Figure 26(a). Moreover, there is a finite window of values of Λ which support non-trivial waves, according to Figure 27(b). The window size increases as ν decreases but is found to remain bounded as long as stable travelling waves develop at large times. Note that the seemingly pathological behaviour of Figure 27(a) of negative and linearly decreasing speeds as Λ is decreased, is associated with wave amplitudes that shrink to zero so that the branches terminate at a finite value of Λ . Sample travelling wave profiles for $\nu = 0.1$ and for $\Lambda = 0.25, 0.0, -0.25, -1.0$ are given in Figures 28(a)–(d). The non-monotonic behaviour of Figure 27(b) is observed by looking at the wave amplitudes which increase at first and then start decreasing, with $\Lambda = -0.25$ profiles containing the most energy.

The final set of results provides a comparison between solutions of the nonlocal

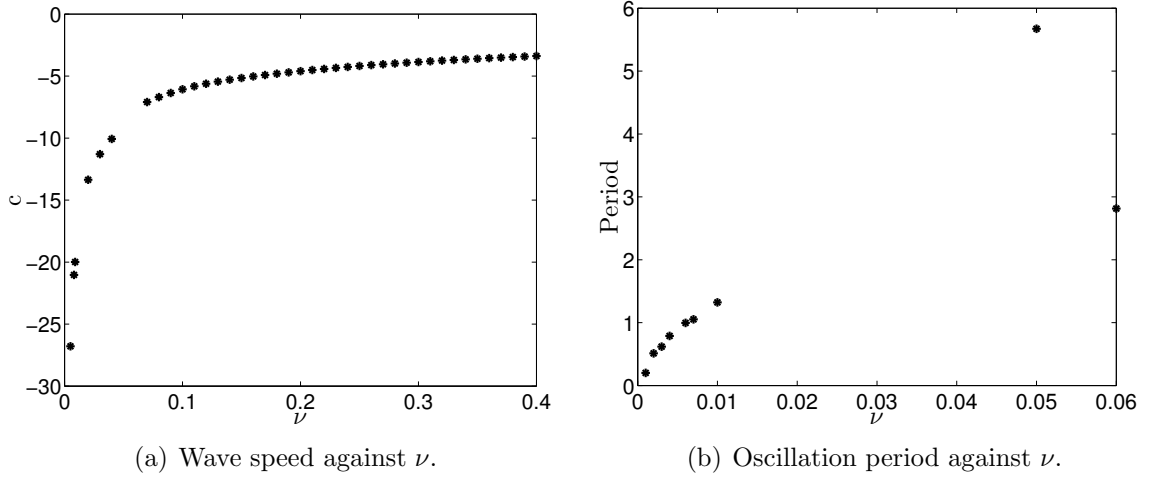


Figure 26: Characteristics of (a) travelling wave speeds and (b) periods of oscillation of time-periodic travelling waves, for $R_e = 0$, $\Lambda = -1.0$, $\Gamma_0 = 1$, $\eta = 1$.

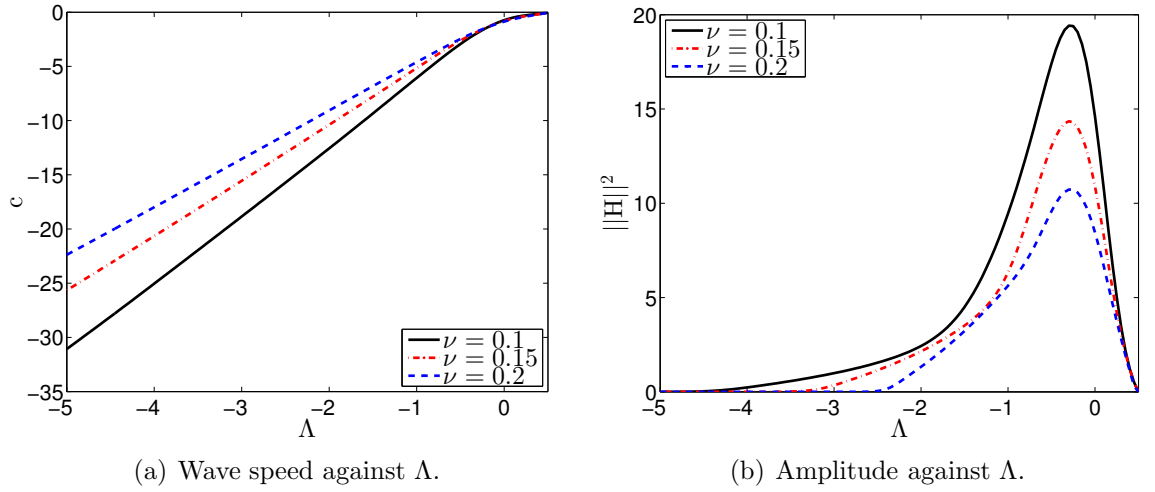


Figure 27: Properties of travelling wave solutions for relatively large ν , $R_e = 0$, $\Gamma_0 = 1$, $\eta = 1$. (a) Travelling wave speed against Λ , and (b) wave amplitude against Λ .

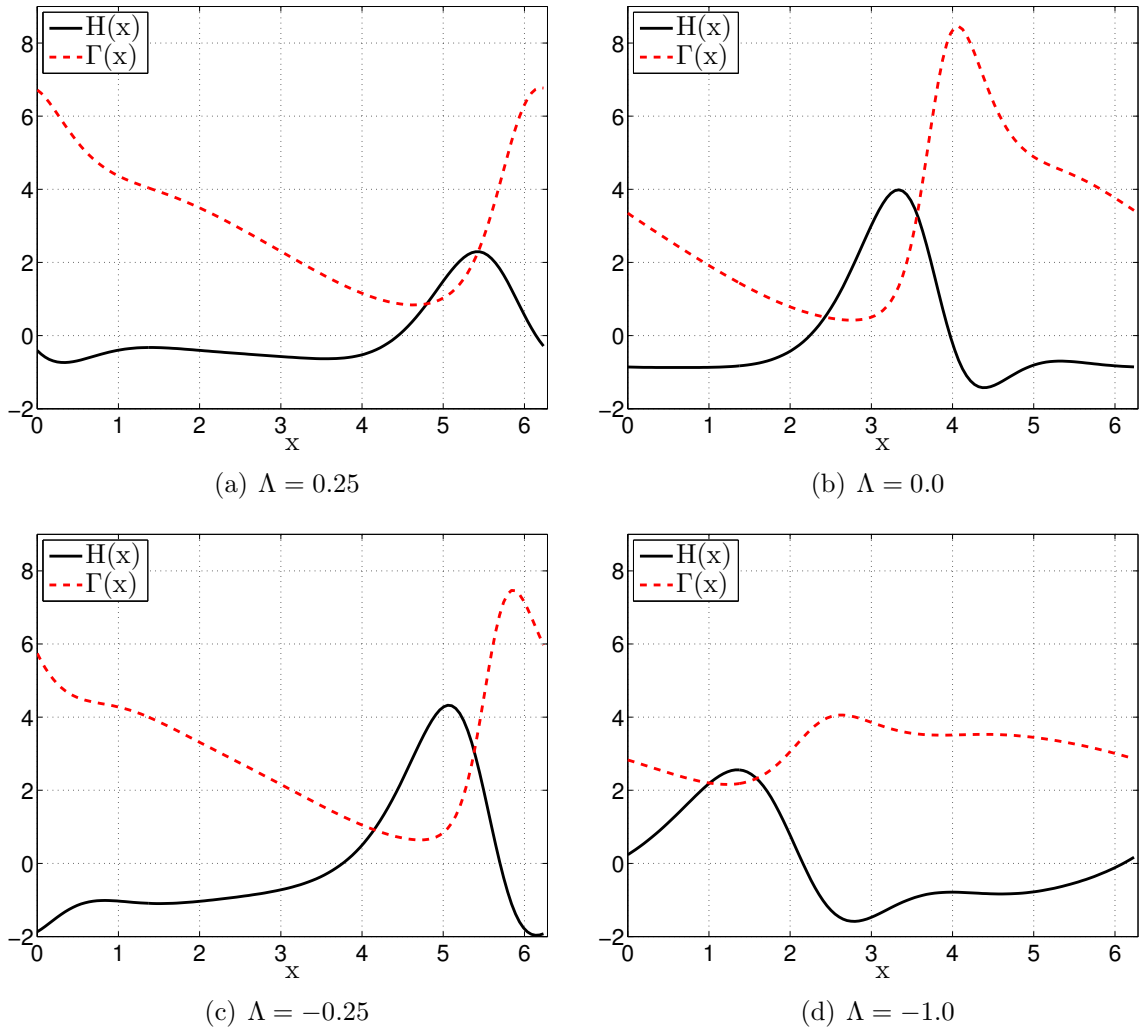


Figure 28: Wave profiles $H(x)$ (solid black) and $\Gamma(x)$ (dashed red) for four different values of Λ and for $\nu = 0.1$, $R_e = 0$, $\Gamma_0 = 1$, $\eta = 1$.

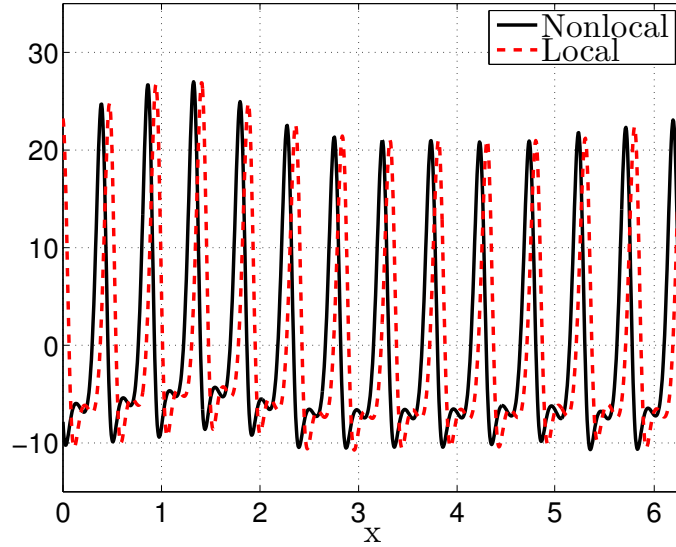


Figure 29: Comparison of the saturated wave profiles $H(x)$ resulting from nonlocal (solid black) and local (dashed red) systems for $\nu = 0.001$, $R_e = 0$, $\Lambda = 0.25$, $\Gamma_0 = 1$, $\eta = 1$.

system (5.4)–(5.5) and the corresponding local one that uses the small wavenumber approximation (3.4) (for $R_e = 0$ and $k_2 = 0$), leading to the localised evolution equation (5.6). Considering the case $\Lambda = 0.25$ and $\nu = 0.001$, which supports chaotic solutions according to Table 3, the two systems are solved with the same initial conditions and the solutions $H(x)$ are compared at time $t = 1000$. The two resulting interfacial solution profiles are plotted in Figure 29 with the solid black and dashed red curves corresponding to the nonlocal and local problems, respectively. The main difference is a small phase shift between the two profiles leading to the conclusion that the two solution trajectories remain close and appear to have the same essential geometrical features. The amount of the phase shift has been found to increase as ν decreases as would be expected intuitively.

5.5.2 Finite Reynolds number: $R_e = \mathcal{O}(1)$

Turning to the case of moderate Reynolds numbers, numerical experiments were performed for initial value problems with initial conditions identical to (5.27) in order to examine the effect of the presence of inertia on flow stability. To that end, many

numerical tests were carried out for different values of ν and R_e , whereas all other parameters were kept fixed. For $R_e \neq 0$, the flow is unstable if $\Lambda < 0.5$ or $R_e \Lambda^2 > 30$ when the film is the more viscous fluid ($\Lambda > 0$) or if $R_e \Lambda^2 < 30$ when the upper fluid is more viscous ($\Lambda < 0$). Numerical solutions of the dispersion relation indicate that instability occurs below a critical value ν_0 , depending on the value of the Reynolds number (see also Figure 17). This ν_0 can be also obtained analytically by linearising problem (5.4)–(5.5) and setting $k = 1$ in the resulting dispersion relation. The outcome is a fourth-order polynomial in ν similar to (5.28) (given in Appendix E), which has a unique real and positive solution ν_0 . The variation of ν_0 with R_e and Λ is in line with the observations from the stability diagram in Figure 19. Its value grows with R_e for positive Λ and decays for negative Λ . Moreover, for negative and decreasing Λ the value of ν_0 decreases, suggesting again a viscosity stratification stabilisation of the Marangoni instability. If Λ is positive and increasing, the opposite effect takes place (viscosity destabilisation). The physical effect of shear in the cases where the film or the upper layer fluid is the more viscous, and the destabilising mechanism due to viscosity stratification, have been described in detail by Charru & Hinch [27] and was summarised in the introduction in Chapter 1.

The case of positive Λ is studied first. Taking $\Lambda = 0.25$ and $R_e = 25$, the flow is linearly unstable for $\nu < 0.575$. For values of ν larger or equal than $\nu_0 = 0.575$, large-time solutions tend to trivial steady states; non-trivial dynamics arise below this critical value. Extensive large-time numerical experiments were performed for different values of the domain parameter ν and are displayed in Table 4 for the range of values $0.001 \leq \nu \leq 0.6$. The new characteristic here is the appearance of periodic travelling waves with m distinct minima in one time period of the energy signal $E(t)$, noted as PTW[m] in the table. This behaviour is verified by the return map which contains m points. The period of oscillation in this case is calculated by finding the difference between $(m + 1)$ consecutive minima. As ν becomes smaller tending to 0, large-time solutions are trapped into the basin of attraction of complex attractors, namely quasi-periodic and chaotic attractors.

For a relatively broad range of values of ν smaller than the bifurcation point $\nu_0 = 0.575$, steady-state travelling wave solutions emerge; oscillations (if they exist)

Table 4: Dynamical behaviour of the solutions for different values of ν and for $R_e = 25$, $\Lambda = 0.25$, $\Gamma_0 = 1$, $\eta = 1$. ST stands for stable flow, PTW[m] corresponds to time-periodic solutions with m distinct minima in one time period of the $E(t)$ signal, QP indicates quasi-periodic flows, and C chaotic flows.

ν	Solution type	ν	Solution type
0.6	ST	0.022–0.018	PTW[1]
0.574–0.118	TW	0.017	QP
0.117–0.111	PTW[2]	0.016–0.014	TW
0.110–0.096	PTW[1]	0.013–0.012	PTW[1]
0.095–0.046	TW	0.011	TW
0.045–0.037	PTW[1]	0.010	PTW[56]
0.036	PTW[2]	0.009–0.003	QP
0.035	PTW[12]	0.002	C
0.034–0.023	TW	0.001	QP

in the energy signal decay, leading to a constant energy level. At the value $\nu = 0.117$, the steady-state traveling waves lose stability by a Hopf bifurcation leading to time-periodic travelling waves. As ν decreases from 0.117 to 0.111, the energy signal $E(t)$ has two minima in each time period. At $\nu = 0.11$ another bifurcation occurs to give oscillations with one minimum in every period in the graph of $E(t)$. As ν decreases further, travelling wave windows are interchanged with time-periodic windows and the pattern persists until $\nu = 0.01$ (with the exception of $\nu = 0.017$ in which case the flow is quasi-periodic).

Characteristic time-periodic solutions are presented in Figure 30. The figure depicts results obtained for $\nu = 0.037$, 0.036, 0.035, which correspond to PTW[1], PTW[2] and PTW[12] respectively. The panels on the left show the three energies in the same time interval $409 < t < 443.4$ (for reasons that will become apparent later) and the panels on the right illustrate the corresponding phase planes. All the phase planes consist of closed curves confirming the periodicity of the solutions, but the number of turns attained increases as ν decreases. The solution for $\nu = 0.037$ has period approximately 1.8, with the energy $E(t)$ exhibiting one maximum and one

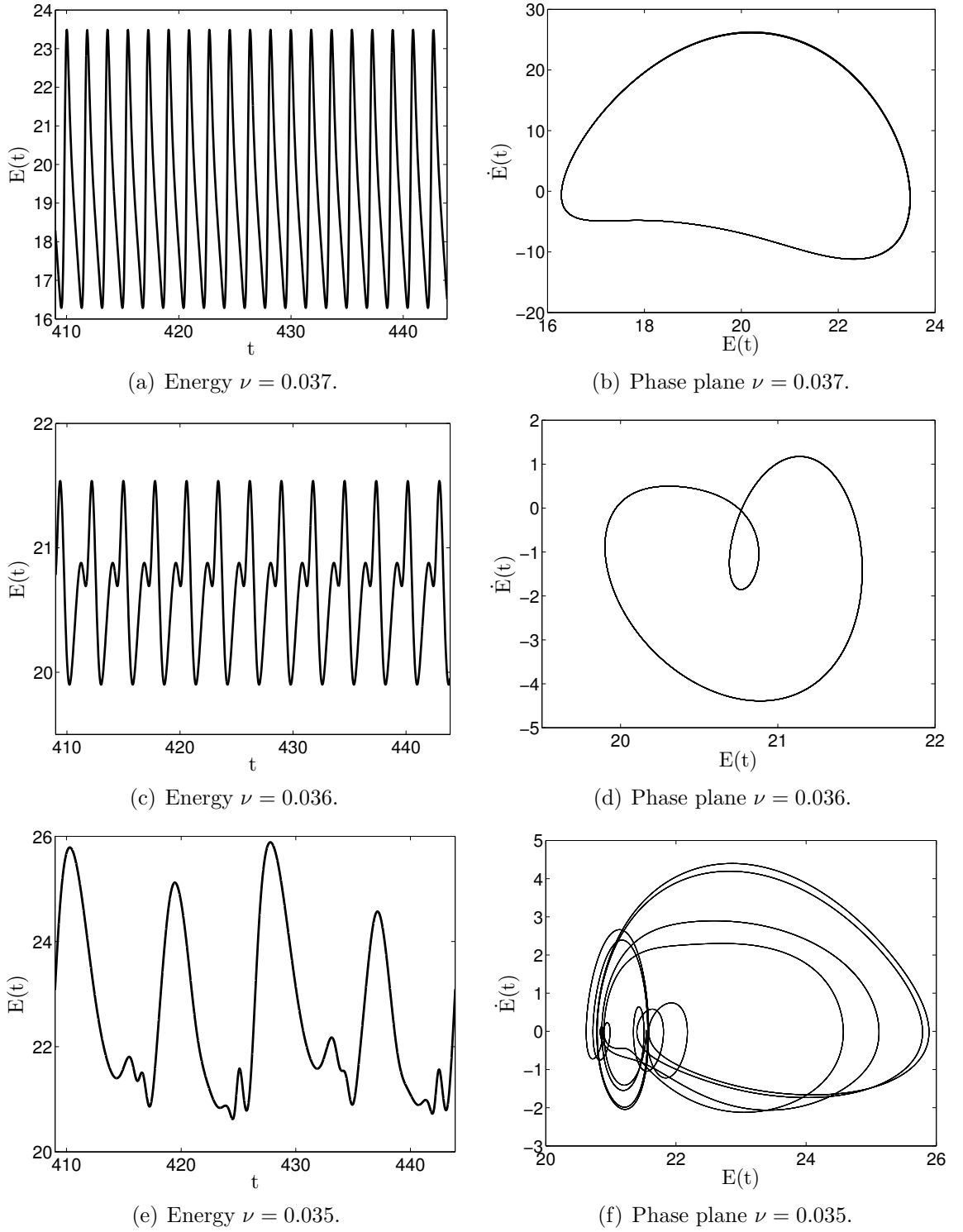


Figure 30: Energies and phase planes of time-periodic travelling wave solutions obtained for $R_e = 25$, $\Lambda = 0.25$, $\Gamma_0 = 1$, $\eta = 1$. (a)–(b) correspond to PTW[1] solutions obtained for $\nu = 0.037$, (c)–(d) to PTW[2] solutions that arise for $\nu = 0.036$, and (e)–(f) correspond to PTW[12] solutions obtained for $\nu = 0.035$.

minimum over one period (Figure 30(a)). At the two extrema the derivative of the energy is zero $\dot{E}(t) = 0$, which can also be seen in the phase plane in Figure 30(b). Similarly, the period of the solution for $\nu = 0.036$ is about 2.8 and the energy attains two maxima and two minima in one period (Figure 30(c)). The curve in the phase plane in Figure 30(d) has four points where $\dot{E}(t) = 0$, two corresponding to the energy maxima and the other two to the energy minima. The last case for $\nu = 0.035$ is more complicated, with a period equal to 34.9 and 12 maxima (or minima) in each time period. The energy plot in Figure 30(e) shows exactly one period of oscillation and the corresponding phase plane is portrayed in Figure 30(f).

Representative plots of the interfacial and surfactant wave profiles for all computed windows where travelling waves are found are provided in Figure 31. In the first window which supports travelling waves, the waves are fully modal, meaning that they contain all Fourier modes. In panel (a) the wave profiles are demonstrated for $\nu = 0.2$. In the second travelling-wave window the solutions become bimodal, i.e. they are travelling waves with nonzero Fourier modes in the spectrum $k = 2n$, n integer (Tilley et al. [91]). In this case, the waves have period $2\pi/2$, as shown in panel (b) for $\nu = 0.09$. As ν decreases, higher modal travelling waves arise in the next travelling-wave windows from Table 4, namely trimodal, tetramodal and pentamodal solutions. These are waves periodic in space with periods $2\pi/3$, $2\pi/4$ and $2\pi/5$, respectively (the nonzero Fourier modes are multiples of 3, 4 or 5). Panels (c)–(e) illustrate this behaviour for $\nu = 0.03$, 0.015, 0.011, which belong to the trimodal, tetramodal and pentamodal windows, respectively. Note that in Figure 31 as ν is reduced the amplitude of the travelling waves increases from 2.59 for the fully modal waves to 4.16 for bimodal, 7.13 for trimodal, 9.87 for tetramodal and 11.83 for the pentamodal waves.

Another notable feature in all the plots in Figure 31 is that the surfactant concentration becomes locally maximum or minimum in the vicinities where $H = 0$ (this feature will also appear in Figure 36 that will follow). To explain this physically, the interfacial velocity is considered, which is given by

$$u_I = \overline{U}_I(\epsilon) + m\epsilon^2 H + \epsilon^3 U_1 + \mathcal{O}(\epsilon^4). \quad (5.37)$$

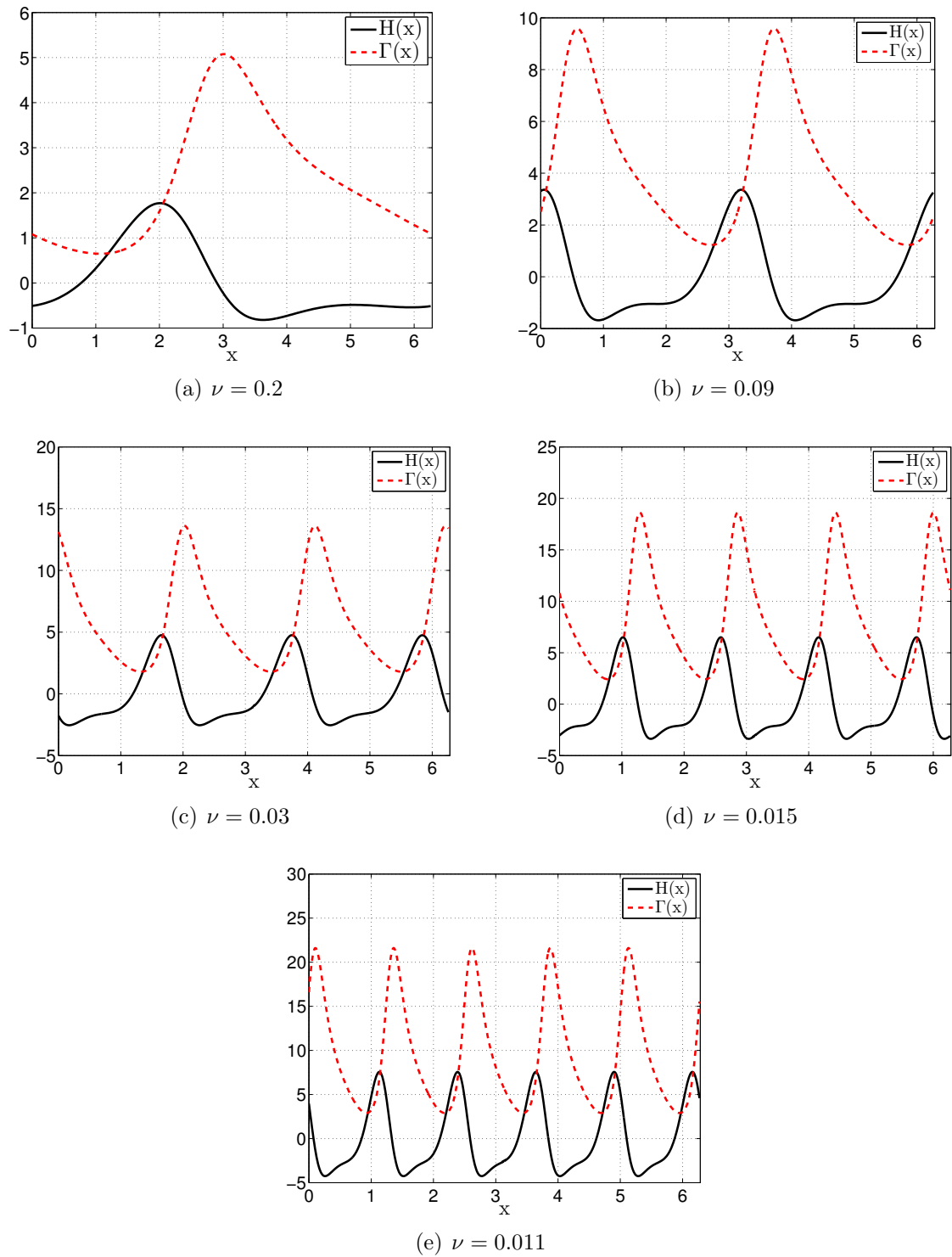


Figure 31: Wave profiles $H(x)$ (solid black) and $\Gamma(x)$ (dotted red) taken at time $t=100$, for $R_e = 25$, $\Lambda = 0.25$, $\Gamma_0 = 1$, $\eta = 1$. The five panels depict solutions for $\nu = 0.2, 0.09, 0.03, 0.015, 0.011$. Each panel corresponds to a n -modal travelling wave with period $2\pi/n$, $n = 1, \dots, 5$, respectively.

It is clear that the interfacial velocity perturbation at leading order $\mathcal{O}(\epsilon^2)$ is equal to mH . This means that whenever there is a position $x = x^*$ such that $H(x^*) = 0$, $H > 0$ for $x < x^*$ and $H < 0$ for $x > x^*$, then the local flow for $x < x^*$ is positive and for $x > x^*$ is negative. This results in the surfactant to get accumulated in the vicinity of the point x^* , thus yielding a local maximum in Γ . Before every surfactant maximum concentration point there is an interfacial maximum and an interfacial minimum after. If $H < 0$ for $x < x^*$ and $H > 0$ for $x > x^*$, then the opposite situation occurs; the flow now has reversed direction compared to the previous case and the surfactant concentration attains a local minimum in the vicinity of $x = x^*$. The accumulation of surfactant near x^* causes variations in the surfactant concentration, which in turn give rise to surface tension gradients. These gradients create Marangoni stresses which then drive the spreading of surfactant molecules away from regions of high surfactant concentration (Matar & Craster [5]).

When ν becomes small enough and close to 0 the flow gets attracted to complex dynamical behaviour, mainly quasi-periodicity but also chaos. Figures 32 and 33 demonstrate the results for $\nu = 0.007$ and $\nu = 0.002$, for which the corresponding flows are quasi-periodic and chaotic respectively. Panels (a) in both figures depict large-time solutions and panels (b) portray the energy spectra $|\hat{E}_k|^2$, where $\hat{E}_k$ are the Fourier coefficients of the energy signal. Moreover, in panels (c) the return maps of the solutions are demonstrated. The dense curve created by the minima points and illustrated in the return map in Figure 32(c), as well as the number of dominant frequencies (more than one) in the energy spectrum in Figure 32(b) confirm the quasi-periodicity of the flow for $\nu = 0.007$ (Ott [92]). On the other hand, for $\nu = 0.002$ the foldings in the return map (Figure 33(c)) and the “broad band” noise around the dominant frequencies in the energy spectrum (Figure 33(b)) indicate a chaotic behaviour (Molenaar et al. [90], Hall & Papageorgiou [93]).

Results for negative Λ are presented next. For $\Lambda = -0.25$, for example, the flow is unstable for Reynolds numbers $R_e < 480$, therefore the Reynolds number is fixed to $R_e = 25$ in the numerical experiments. For these parameter values, the flow is linearly unstable for $\nu < 0.55$. Solutions mostly develop into travelling waves, except for ν in the range $0.049 - 0.053$ where solutions are time-periodic travelling waves.

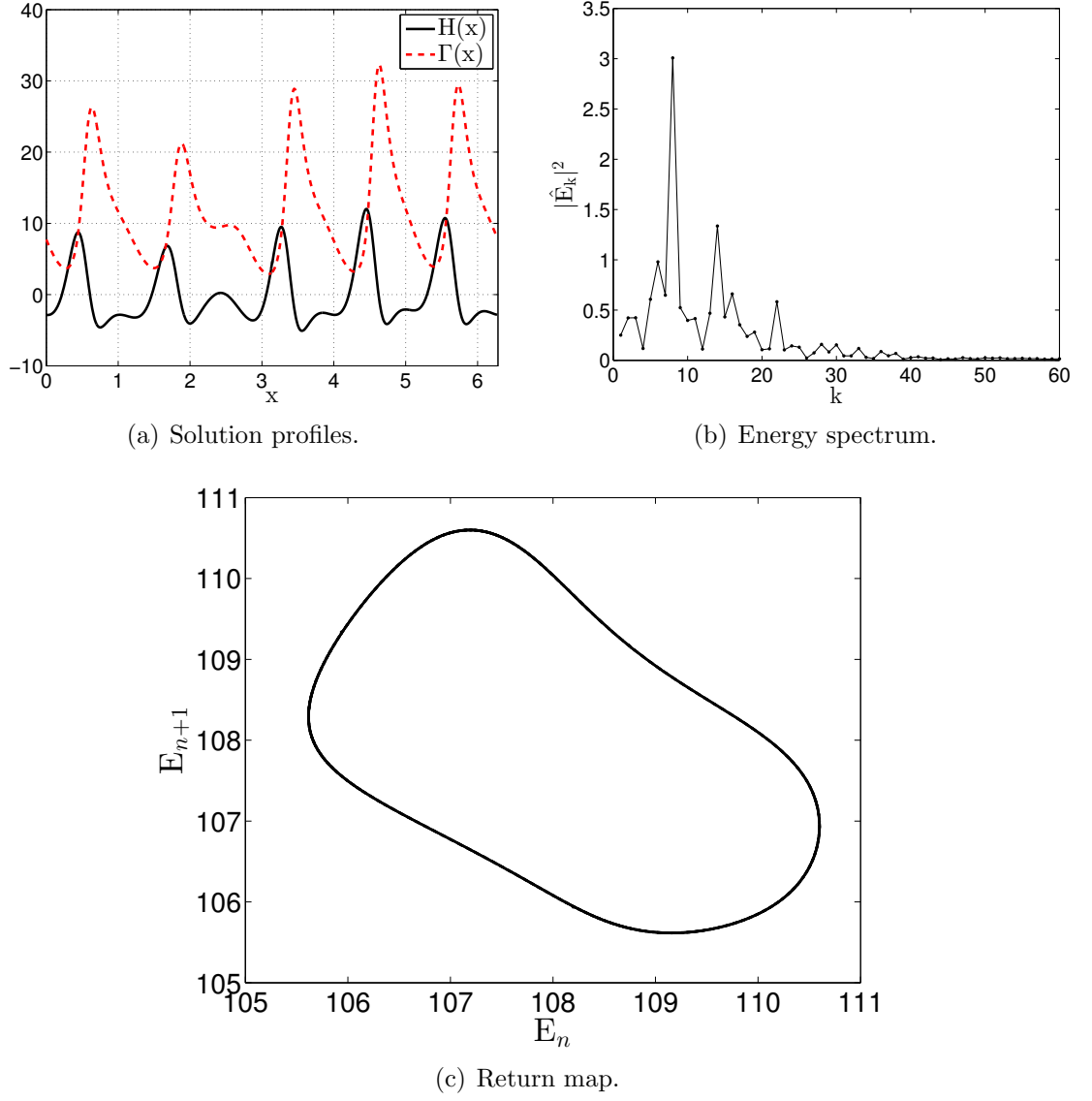


Figure 32: Quasi-periodic solutions obtained for $\nu = 0.007$, $R_e = 25$, $\Lambda = 0.25$, $\Gamma_0 = 1$, $\eta = 1$. (a) Interfacial (solid black) and surfactant (dashed red) solution profiles taken at time $t = 1000$. (b) Energy spectrum $|\hat{E}_k|^2$ against k . (c) Return map consisting of a curve densely filled with points.

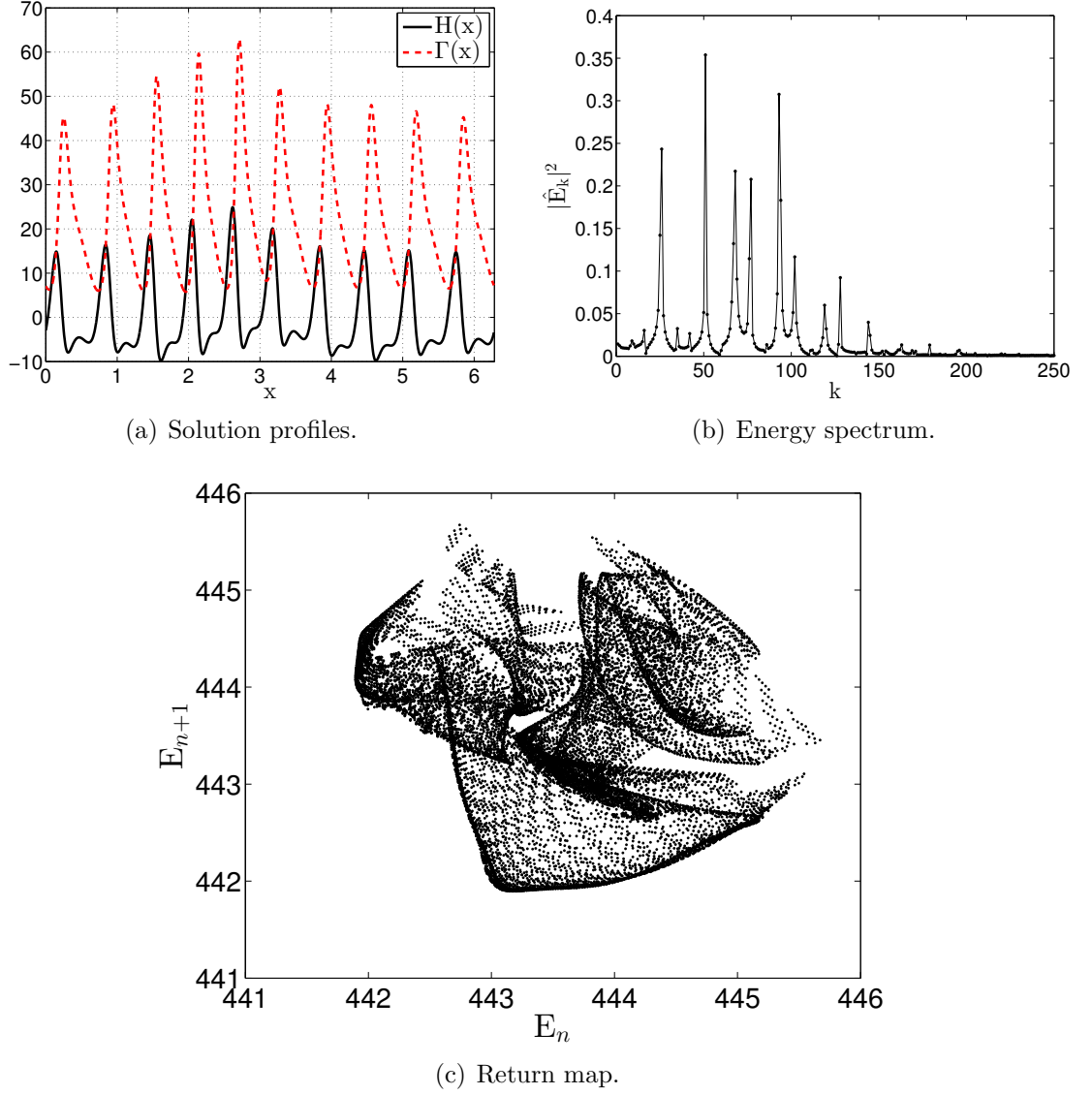


Figure 33: Chaotic solutions obtained for $\nu = 0.002$, $R_e = 25$, $\Lambda = 0.25$, $\Gamma_0 = 1$, $\eta = 1$. (a) Interfacial (solid black) and surfactant (dashed red) solution profiles taken at time $t = 1000$. (b) Energy spectrum $|\hat{E}_k|^2$ against k . (c) Return map consisting of foldings.

Numerical calculations were performed for ν as small as $\nu = 0.01$, but no intricate structures were observed. Figure 34(a) demonstrates the variation of the wavespeed with decreasing ν for solutions taken from all the travelling wave windows. In Figure 34(b) the plot of variation of the period of oscillation with ν is shown for all computed windows where time-periodic waves are found. The divergence of the travelling wave speed as $\nu \rightarrow 0$ is similar to the case $R_e = 0$ seen before. In the small window where time-periodic waves are supported, the period of oscillation increases monotonically (almost linearly) as ν decreases.

In order to identify the effect of the Reynolds number on the characteristics of the flow, results for fixed ν are considered hereafter. For $\nu = 0.1$, for example, numerical calculations were performed for the range of Reynolds number values $0 \leq R_e \leq 100$. For $0 \leq R_e \leq 4$ and $31 \leq R_e \leq 100$, solutions develop into travelling waves and the wavespeed c is shown in Figure 35(a). In the range $5 \leq R_e \leq 30$, periodic travelling waves emerge; the period of oscillation is calculated and illustrated in Figure 35(b). Obviously, in each of the travelling wave windows the wavespeed is negative and increases monotonically with the Reynolds number. In the second window, though, the waves travel to the left much faster. Furthermore, the period of oscillation (when time-periodic travelling waves are supported) decreases monotonically as the Reynolds number increases from 5 to 30. The period discontinuity at about $R_e = 10$ indicates that the solutions enter a different time-periodic attractor.

The final results presented in this section concern the study of the effect of R_e and Λ on the flow; this is done by picking parameter values from the unstable regions in the stability diagram in Figure 19 and plotting the corresponding solutions. The critical points in the stability diagram for $\Gamma_0 = 1$, $\eta = 1$ become $\Lambda_c = 0.5$ and $R_{ec} = 120$. Three different Reynolds numbers $R_e = 50, 150, 300$ are used and for each case three values of Λ are chosen; sample interfacial and surfactant wave profiles are plotted in Figure 36 for $\nu = 0.1$. It is seen that for fixed $R_e < 120$ the wave amplitudes increase for negative or zero Λ , but then start decreasing when Λ crosses to positive values (and eventually diminish for $\Lambda \geq \Lambda_c$). When the Reynolds number is greater than $R_{ec} = 120$, the amplitude increases as Λ increases. Another observation is that for a fixed $\Lambda < 0$, the amplitude of the profiles decreases as R_e increases, since in this

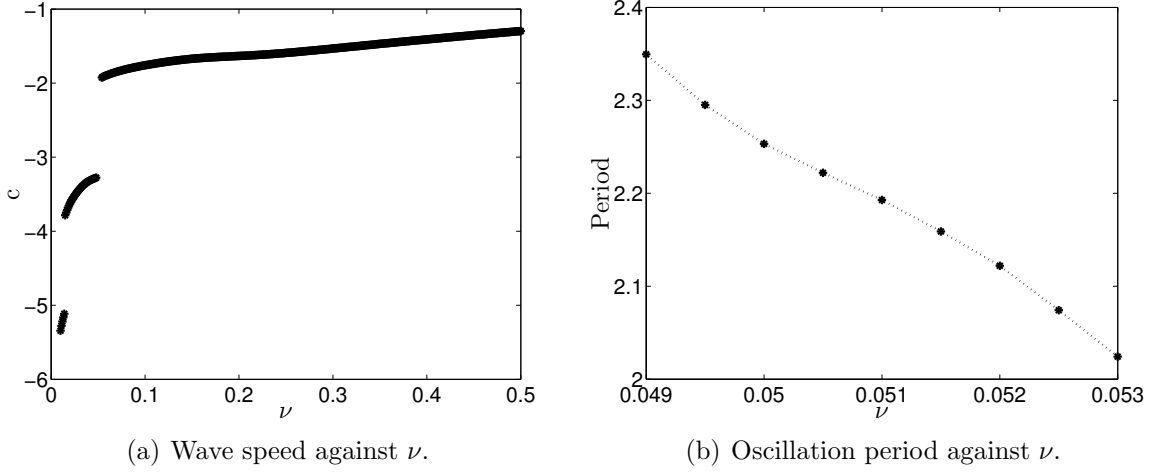


Figure 34: Characteristics of (a) travelling wave speeds and (b) periods of oscillation of time-periodic travelling waves, for $R_e = 25$, $\Lambda = -0.25$, $\Gamma_0 = 1$, $\eta = 1$.

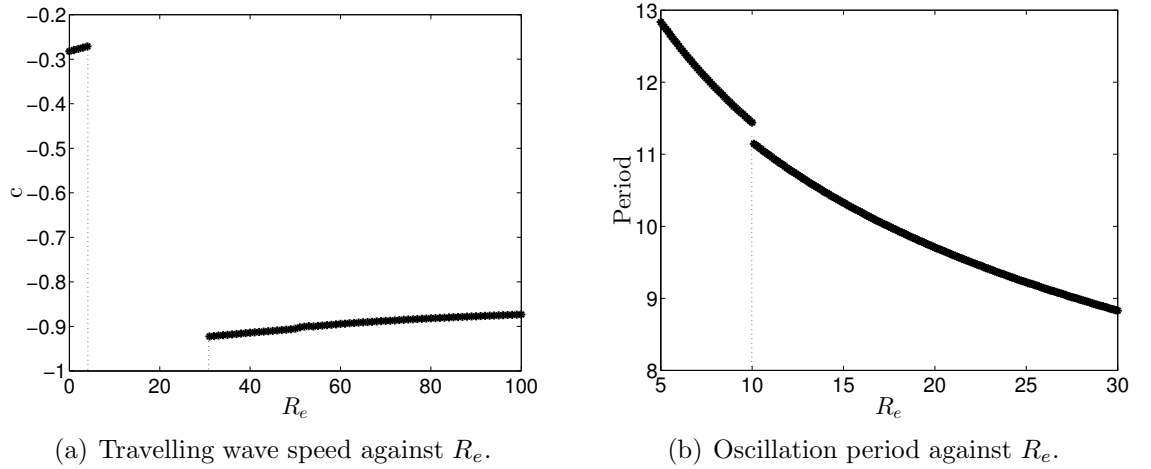


Figure 35: Characteristics of (a) travelling wave speeds and (b) periods of oscillation of time-periodic travelling waves, for $\nu = 0.1$, $\Lambda = 0.25$, $\Gamma_0 = 1$, $\eta = 1$. The Reynolds number in (a) is in the range $0 \leq R_e \leq 4$ and $31 \leq R_e \leq 100$, and in (b) in the range $5 \leq R_e \leq 30$.

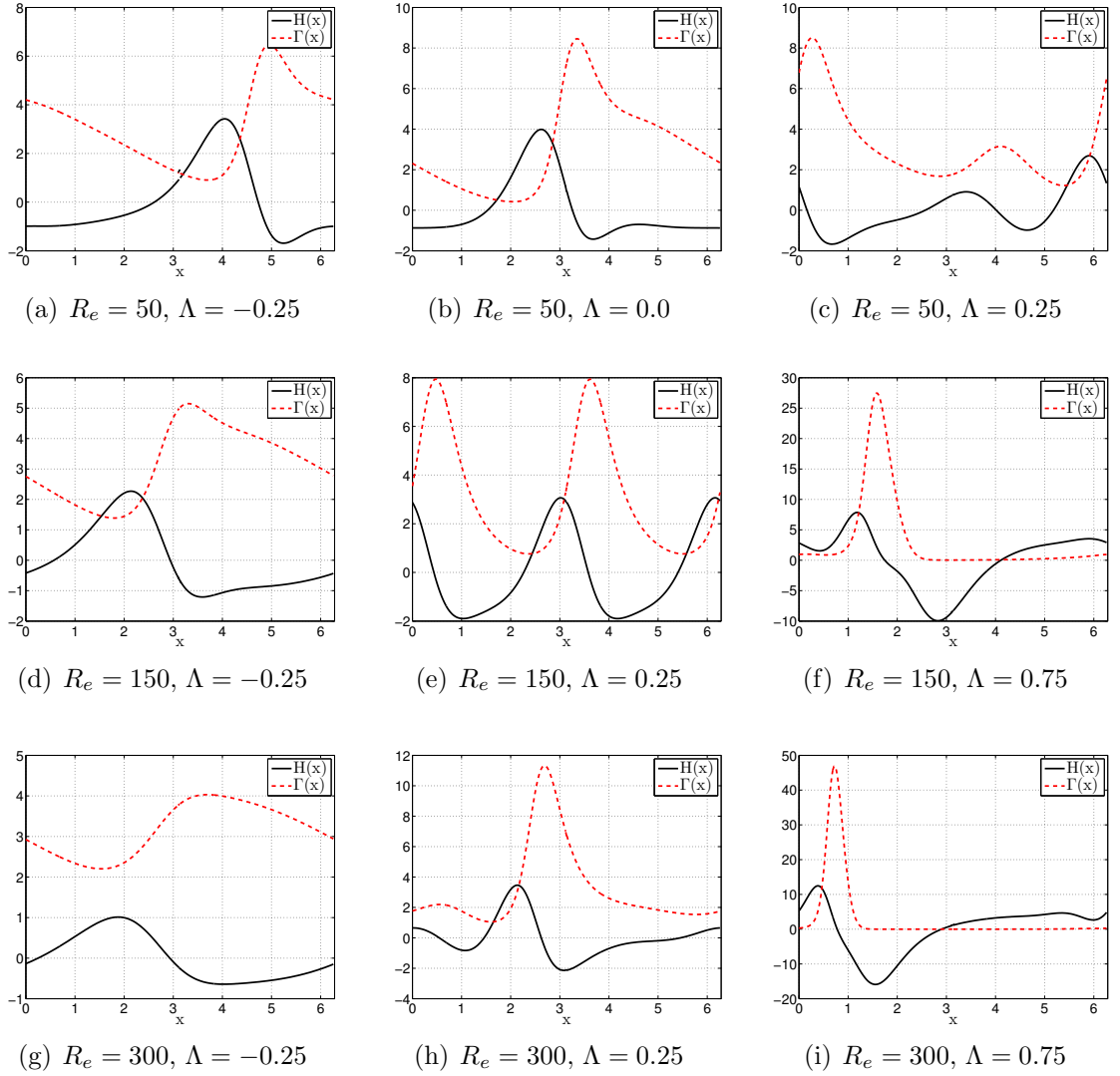


Figure 36: Representative wave profiles $H(x)$ (solid black) and $\Gamma(x)$ (dashed red) for $\nu = 0.1$, $\Gamma_0 = 1$, $\eta = 1$, for different values of Λ and $R_e = 50$ (top row), $R_e = 150$ (middle row), $R_e = 300$ (bottom row).

case the Reynolds number has a stabilising effect on the flow. On the other hand, if $\Lambda > 0$ and fixed, increasing the Reynolds number leads to an increase of the wave amplitude. All the above results are in agreement with the remarks from the stability diagram in Section 5.4.

6 Results for Three-dimensional Flows

The interface is now a two-dimensional surface and the evolution equations are the ones derived in Chapter 2. The objective of this chapter is to address the stability of one-dimensional travelling wave solutions to spanwise perturbations. This is done via a linear stability analysis and nonlinear numerical computations. The aim is to investigate whether a Squire's type theorem is valid in two-layer Couette flows with surfactants. The results presented in this chapter, together with part of the previous chapter (results for $R_e = \mathcal{O}(1)$) form an article in preparation (Kalogirou & Papageorgiou [94]).

6.1 Linear stability theory

Firstly, the linear stability properties of the system (2.98)–(2.99) will be presented.

Linear solutions H , Γ are written in a normal mode form

$$H(x, z, t) = \delta \left(c_1 e^{i(k_1 x + k_2 z) + \sigma t} + c.c. \right), \quad (6.1a)$$

$$\Gamma(x, z, t) = \Gamma_0 + \delta \left(c_2 e^{i(k_1 x + k_2 z) + \sigma t} + c.c. \right), \quad (6.1b)$$

where k_1, k_2 are the wavenumbers in x - and z -directions respectively, and $\sigma = \sigma_R + i\sigma_I$ is the amplification rate as before. Substituting the normal modes (6.1) into the system (2.98)–(2.99), results in the following dispersion relation

$$\sigma^2 + (k^4 + i\Lambda\mathcal{N}(k_1, k_2) + \eta k^2) \sigma + (\eta k^6 + i\eta\Lambda\mathcal{N}(k_1, k_2)k^2 - i\Gamma_0 k_1 k^2) = 0, \quad (6.2)$$

where $k = \sqrt{k_1^2 + k_2^2}$. Growth rates are damped for large enough $k_{1,2}$, so looking for positive growth in the vicinity of $(k_1, k_2) = (0, 0)$ is sufficient to find regions of instability in parameter space. For equal-viscosity fluids ($\Lambda = 0$), long wave approximations ($k_1, k_2 \ll 1$) give the growth rates

$$\sigma_{1,2R} = \pm \sqrt{\frac{\Gamma_0}{2}} k_1^{1/2} k - \frac{\eta}{2} k^2 + \dots \quad (6.3)$$

The first growth rate σ_{1R} is positive at leading order, so the flow is always unstable in this case (as long as $\Gamma_0 \neq 0$). For $\Lambda \neq 0$, the expansion (3.4) of $\mathcal{N}(k_1, k_2)$ is used into the dispersion relation, yielding the growth rates

$$\sigma_{1R} = \frac{(\Gamma_0 - 2\eta\Lambda)}{2\Lambda} k^2 + \mathcal{O}(k^3), \quad \sigma_{2R} = \frac{(R_e\Lambda^2 - 30\Gamma_0)}{60\Lambda} k_1^2 - \frac{\Gamma_0}{2\Lambda} k_2^2 + \mathcal{O}(k^3). \quad (6.4)$$

The three-dimensional flow is unstable if one of the growth rates in (6.4) is positive, which in the case of a more viscous film ($\Lambda > 0$) is true if

$$\Gamma_0 - 2\eta\Lambda > 0 \quad \text{or} \quad R_e\Lambda^2 - 30\Gamma_0 > 0. \quad (6.5)$$

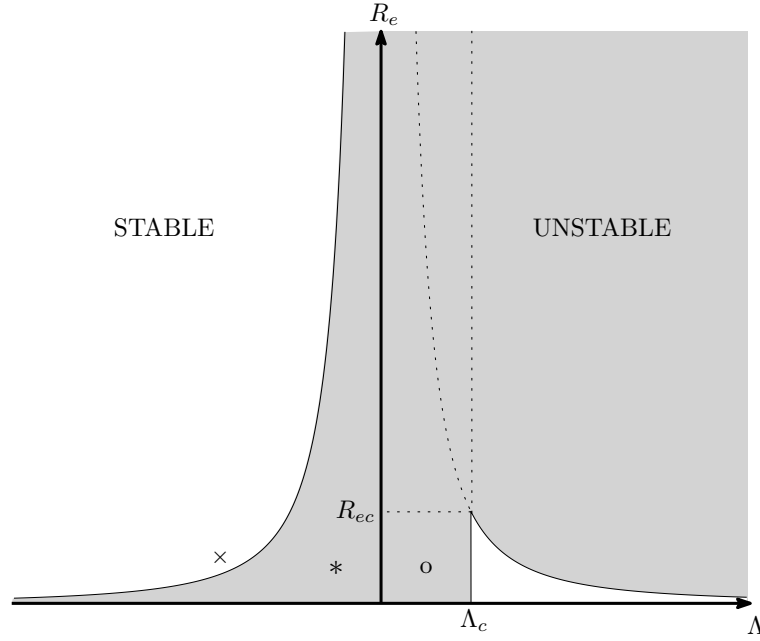


Figure 37: Stability diagram in the $\Lambda - R_e$ parameter space corresponding to two-dimensional flows (repetition of Figure 19). Regions of stability are shown with white and regions of instability with grey colour, while the critical points are given by $\Lambda_c = \Gamma_0/2\eta$ and $R_{ec} = 120\eta^2/\Gamma_0$. The three points ‘o’, ‘*’ and ‘x’ are points of interest in the numerical simulations.

While the first instability condition in (6.5) is obvious, the second condition is explained as follows: looking back to the stability diagram from the two-dimensional flow case (Figure 37), the critical curves are given by $\Lambda = 0.5$ and $R_e = 30\Gamma_0/\Lambda^2$ (for positive Λ). The asymptotic curve will now become $R_e = \frac{30\Gamma_0}{\Lambda^2} \left(1 + \frac{k_2^2}{k_1^2}\right)$, which for non-zero values of k_1, k_2 is shifted upwards compared with the original curve in the diagram (corresponding to $k_2 = 0$). Hence the case $k_2 = 0$ provides the largest instability region. In Figure 38(a), the positive part of the unstable growth rate is plotted versus k_1, k_2 for $Re = 25$, $\Lambda = 0.25$, $\Gamma_0 = 1$, $\eta = 1$ and in this case the maximum growth occurs on the axis $k_2 = 0$.

For negative Λ (less viscous film) the first normal mode is always stable to small wavenumber perturbations and the second normal mode can be unstable even if $R_e\Lambda^2 - 30\Gamma_0 > 0$, i.e. even when the two-dimensional flow is stable. Based on the same reasoning as before, the stability curve (for negative Λ) will shift upwards, creating a larger instability region. This result is also confirmed by Figure 38(b),

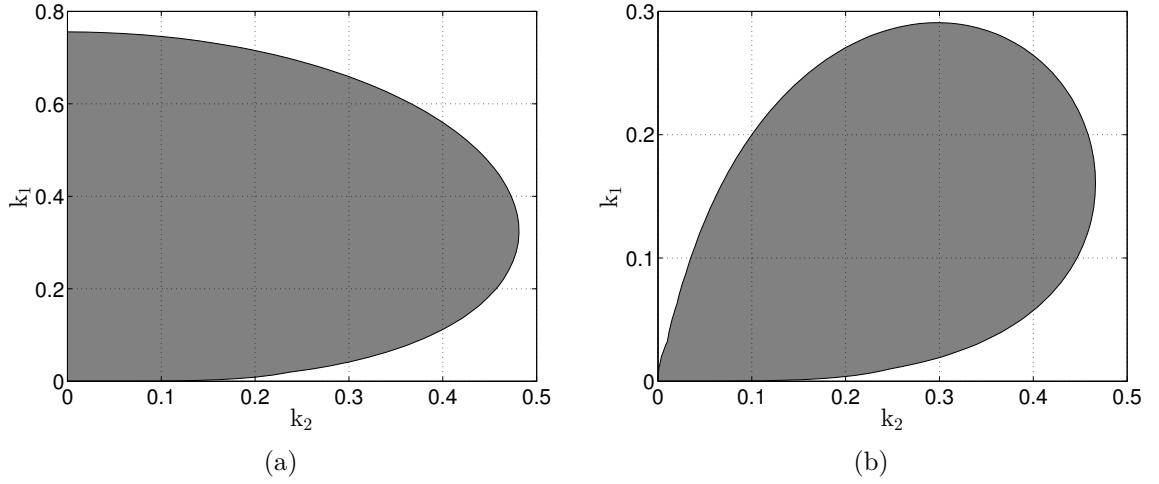


Figure 38: Regions of instability (grey) and stability (white) plotted against k_1, k_2 for $\Gamma_0 = 1, \eta = 1$. (a) $Re = 25, \Lambda = 0.25$, corresponding to the unstable point ‘o’ on the stability diagram in Figure 37. (b) $Re = 35, \Lambda = -1.0$, corresponding to the stable point ‘x’ on the stability diagram in Figure 37.

where the unstable growth rate is plotted versus k_1, k_2 for $Re = 35, \Lambda = -1.0$, $\Gamma_0 = 1, \eta = 1$. The choice of parameter values is such that the corresponding two-dimensional flow is stable (notice that for $k_2 = 0$ there is no instability region) and the three-dimensional is unstable.

6.2 Squire's theorem for $Re = \mathcal{O}(\epsilon)$

In his famous theorem about the stability of a viscous fluid flow in a parallel channel, Squire [95] stated that *for any three-dimensional unstable mode there is an associated more unstable two-dimensional mode*. An analogous result for two-fluid parallel flows was proved by Hesla et al. [96], where the authors showed that if a three-dimensional perturbation (two-dimensional interface) is unstable then a two-dimensional perturbation exists and is more unstable. Consequently, in these cases it is sufficient to consider only two-dimensional perturbations in order to study the stability of a problem. The main objective of this section is to investigate the validity of a Squire's type theorem in two-fluid channel flows with surfactants.

As discussed in the previous section, for order one Reynolds numbers it is not

possible to prove a Squire's theorem because for $\Lambda < 0$ a three-dimensional perturbation is more unstable than a two-dimensional one. However, for asymptotically small Reynolds numbers the theorem is valid, as shown below. Considering the local system (i.e. using (3.4)), the dispersion relation is written as

$$\sigma^2 + p_1(k_1, k_2)\sigma + p_0(k_1, k_2) = 0, \quad (6.6)$$

where $p_0(k_1, k_2)$ and $p_1(k_1, k_2)$ are polynomials given by

$$\begin{aligned} p_0(k_1, k_2) &= k^4 + 2i\Lambda k_1 - \frac{\Lambda R_e}{60} k_1^2 + \frac{2i\Lambda}{15} k_1 k^2 + \frac{i\Lambda R_e^2}{8400} k_1^3 + \eta k^2, \\ p_1(k_1, k_2) &= \eta k^6 + 2i\eta\Lambda k_1 k^2 - \frac{\eta\Lambda R_e}{60} k_1^2 k^2 + \frac{2i\eta\Lambda}{15} k_1 k^4 + \frac{i\eta\Lambda R_e^2}{8400} k_1^3 k^2 - i\Gamma_0 k_1 k^2. \end{aligned} \quad (6.7)$$

The positive growth rate is then equal to

$$\sigma_1 = -\frac{p_1}{2} + \frac{\sqrt{p_1^2 - 4p_0}}{2}. \quad (6.8)$$

The goal is to find the critical point (k_1^*, k_2^*) where the positive growth rate has a local (and global) maximum. This can be done by finding a (k_1^*, k_2^*) where

$$\frac{\partial \sigma_1}{\partial k_1} = 0, \quad \frac{\partial \sigma_1}{\partial k_2} = 0, \quad (6.9a)$$

$$\frac{\partial^2 \sigma_1}{\partial k_1^2} \frac{\partial^2 \sigma_1}{\partial k_2^2} - \frac{\partial^2 \sigma_1}{\partial k_1 \partial k_2} > 0, \quad \frac{\partial^2 \sigma_1}{\partial k_1^2} < 0. \quad (6.9b)$$

It can be proved that $\frac{\partial \sigma_1}{\partial k_2} = 0$ at $k_2 = 0$ only, and also that $\frac{\partial \sigma_1}{\partial k_1} = 0$ for a $k_1^* \neq 0$. At the point $(k_1^*, 0)$, the second derivative criterion (6.9b) also holds. Therefore the positive growth rate σ_1 has its only maximum there and its real part $\sigma_{1R} = \Re(\sigma_1)$ becomes maximum at the same point. As an example, in the case of $\Lambda = 0.25$, $\Gamma_0 = 1$, $\eta = 1$ the critical point is $(k_1^*, k_2^*) = (0.4757, 0)$, hence the perturbations corresponding to $k_2 = 0$ are the most unstable, which is the required result. Therefore it is sufficient to study the two-dimensional flow in this case.

Direct numerical solutions of the dispersion relation confirm the above result. For

asymptotically small Reynolds number the maximum growth rate is obtained for zero k_2 , but for order one Reynolds numbers the positive growth rate attains its maximum value at a point $(k_1^*, k_2^*) \neq (0, 0)$.

6.3 Stability of travelling waves

Before presenting numerical results of the system (4.5)–(4.6), it is necessary to explain the diagnostics used to classify the solutions. The energy of the solution $H(x, z, t)$ is now generalised to a double integral by

$$E(t) := \|H(\cdot, \cdot, t)\|_{L_2}^2 = \int_0^{2\pi} \int_0^{2\pi} H^2(x, z, t) dx dz. \quad (6.10)$$

To calculate $\dot{E}(t)$, equation (4.5) is multiplied by H and integrated over a period, yielding

$$\begin{aligned} \dot{E}(t) = & -2\nu_1 \|H_{xx}\|^2 - 4\nu_2 \|H_{xz}\|^2 - 2\frac{\nu_2^2}{\nu_1} \|H_{zz}\|^2 - 2(H, \mathcal{P}H) \\ & + 2 \int_0^{2\pi} \int_0^{2\pi} H \left(\Gamma_{xx} + \frac{\nu_2}{\nu_1} \Gamma_{zz} \right) dx dz, \end{aligned} \quad (6.11)$$

where again $(\cdot, \cdot)$ is the inner product in L_2 . This formula is used to construct phase-planes and return maps to help analyse the attractors of the system, as described before for the one-dimensional problem (see p.109).

The interest is to obtain numerical solutions of the two-dimensional problem and then study their stability under spanwise perturbations. For relatively small channel lengths, the solutions are one-dimensional travelling waves characterised by constant energy and given by the form $\overline{H}(x - c\tau)$, $\overline{\Gamma}(x - c\tau)$ (τ is the final time of the one-dimensional simulation); these are the solutions whose stability will be investigated next.

The system of PDEs (4.5)–(4.6) is solved with initial condition consisting of random spanwise perturbations of the one-dimensional travelling wave solution, i.e.

$$H(x, z, 0) = \overline{H}(x - c\tau) + \mathcal{R}(z), \quad \Gamma(x, z, 0) = \overline{\Gamma}(x - c\tau) + \mathcal{R}(z), \quad (6.12)$$

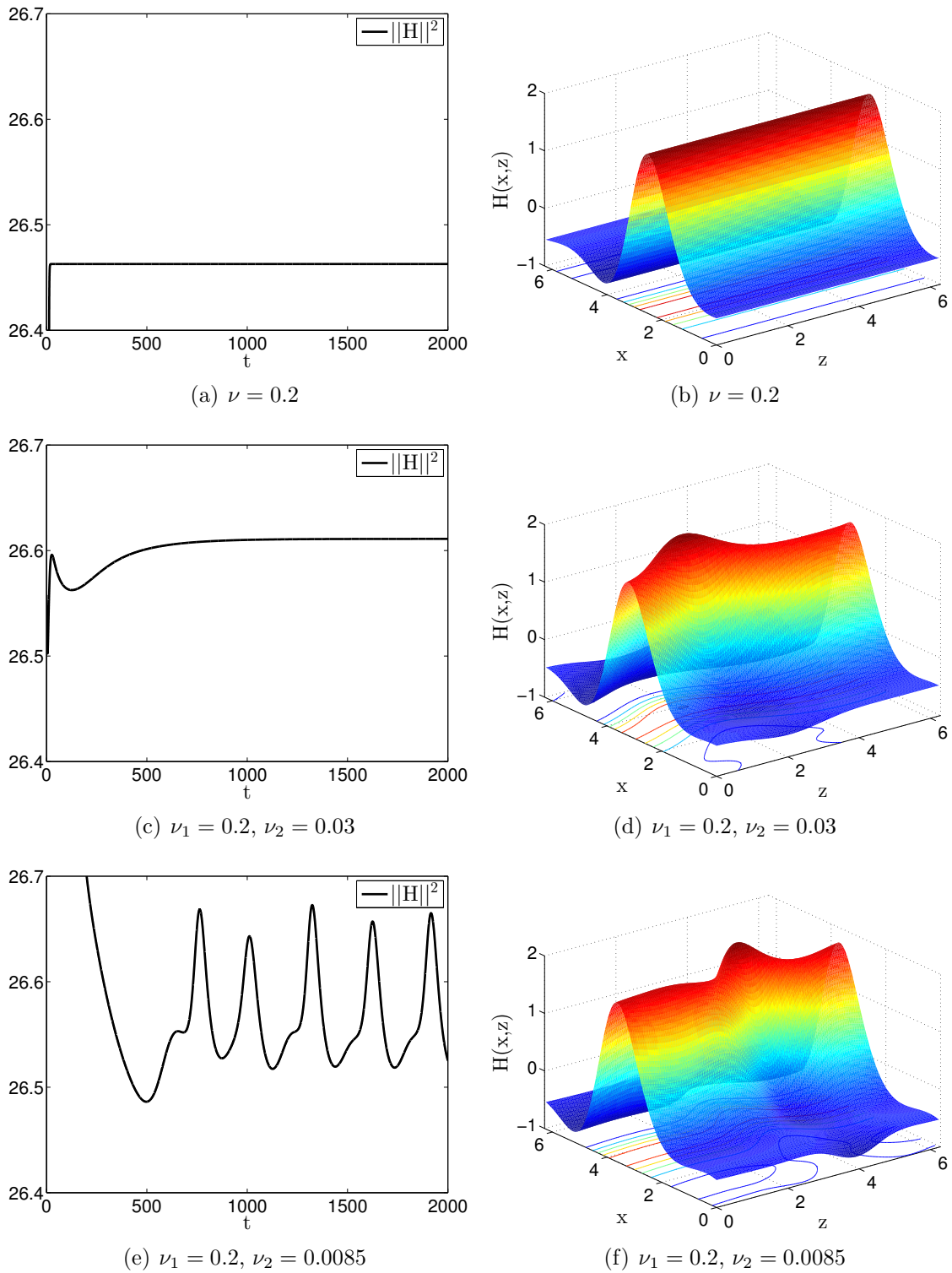


Figure 39: Energy of the solutions and interfacial profiles for $Re = 25$, $\Lambda = 0.25$, $\Gamma_0 = 1$, $\eta = 1$. (a)–(b) $\nu = 0.2$: one-dimensional travelling wave. (c)–(d) $\nu_1 = 0.2$, $\nu_2 = 0.03$: secondary instability stable in time. (e)–(f) $\nu_1 = 0.2$, $\nu_2 = 0.0085$: secondary instability unstable in time. All profiles are taken at time $t = 2000$.

where

$$\mathcal{R}(z) = \sum_{m=1}^N (\alpha_m \sin mz + \beta_m \cos mz), \quad (6.13)$$

with $N = 5$ and random Fourier coefficients $\alpha_m, \beta_m \in [-0.1, 0.1]$. Figure 39 demonstrates the solutions for $Re = 25$, $\Lambda = 0.25$, $\Gamma_0 = 1$, $\eta = 1$, which corresponds to point ‘o’ on the stability diagram in Figure 37. The first set of panels (a)–(b) show the L_2 –norm and profile of the one–dimensional problem for $\nu = 0.2$. Keeping $\nu_1 = 0.2$ fixed and allowing ν_2 to decrease, the effect of the spanwise perturbations on the one–dimensional travelling wave solution is studied. Starting from $\nu_2 = 0.2$ and until about $\nu_2 = 0.06$, the travelling wave solution does not get affected and remains one–dimensional. Beyond that value, two–dimensional structures appear that are stable in time and travel with the wave in the direction of the flow. A representative solution is given in panels (c)–(d) for $\nu_2 = 0.03$. Decreasing ν_2 further gives rise to unsteady two–dimensional structures; this can be seen in panels (e)–(f) for $\nu_2 = 0.0085$. The solution is still travelling in the streamwise direction, but is now changing its shape periodically in time.

A measure of two–dimensionality was also calculated by taking the difference of the L_2 –norms of the travelling wave solutions for every ν_2 ,

$$d(H, \overline{H}) = ||H(x, z, t)||^2 - ||\overline{H}(x - c\tau)||^2. \quad (6.14)$$

The result is shown in Figure 40 against ν_2^{-1} for the values of ν_2 which support travelling wave solutions. For $0.06 \leq \nu_2 \leq 0.2$ the measure is zero, depicting that the waves remain one–dimensional and travelling. For smaller values of ν_2 , two–dimensional waves emerge and become more visible as ν_2 decreases. This pattern continues until about $\nu_2 = 0.03$, below which the waves lose stability in time.

A similar behaviour can be seen in Figure 41 for $Re = 25$, $\Lambda = -0.25$, $\Gamma_0 = 1$, $\eta = 1$ (corresponding to point ‘*’ on the stability diagram in Figure 37). The only difference now is that the equation describing the evolution of the interface in a flow without surfactant is stable (panels (a)–(b), $\nu = 0.25$) and the flow becomes destabilised due to the presence of surfactant. In panels (c)–(d) the one–dimensional

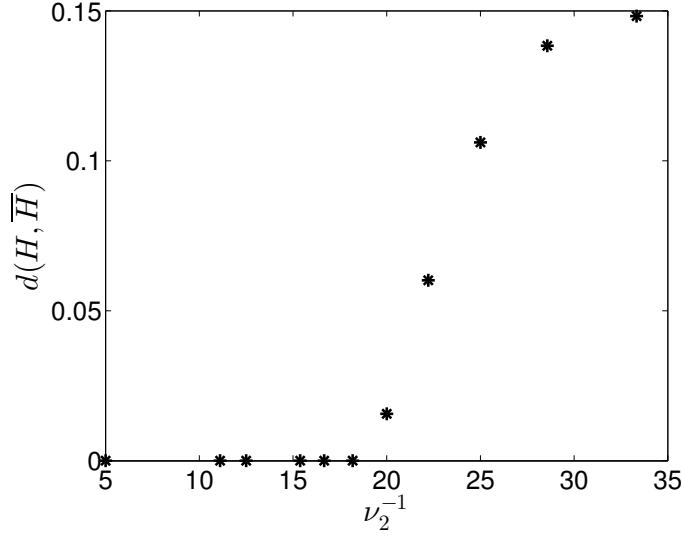


Figure 40: Measure of two-dimensionality defined in (6.14) against ν_2^{-1} , for $\nu_1 = 0.2$ and $Re = 25$, $\Lambda = 0.25$, $\Gamma_0 = 1$, $\eta = 1$. H is the two-dimensional interfacial solution and $\bar{H}$ corresponds to the one-dimensional travelling wave solution obtained for the same parameter values.

travelling wave solution obtained for $\nu = 0.25$ is shown. Finally, panels (e)–(f) illustrate the solution for $\nu_1 = 0.25$, $\nu_2 = 0.01$, which in this case is a travelling wave with a secondary instability.

Perhaps the most interesting case occurs when the three-dimensional flow is unstable but the corresponding two-dimensional flow is stable. A representative example is given in Figure 42 for $\nu_1 = \nu_2 = 0.05$ and $Re = 35$, $\Lambda = -1.0$, $\Gamma_0 = 1$, $\eta = 1$. The analogous two-dimensional problem with $\nu = 0.05$ (and the same values of the remaining parameters) is stable and corresponds to point ‘ $\times$ ’ on the stability diagram in Figure 37. As can be seen in Figure 42, the solutions are travelling waves defined by

$$\begin{aligned} H(x, z, t) &= H(x + c \sin \theta t, z - c \cos \theta t), \\ \Gamma(x, z, t) &= \Gamma(x + c \sin \theta t, z - c \cos \theta t), \end{aligned} \quad (6.15)$$

(c and θ are defined as in Figure 57(a), Section 9.4 in Chapter 9 to follow, with the difference that c has upright direction and θ increases in the anti-clockwise direction).

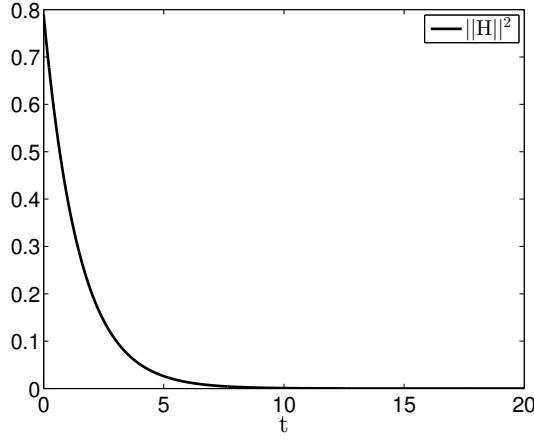
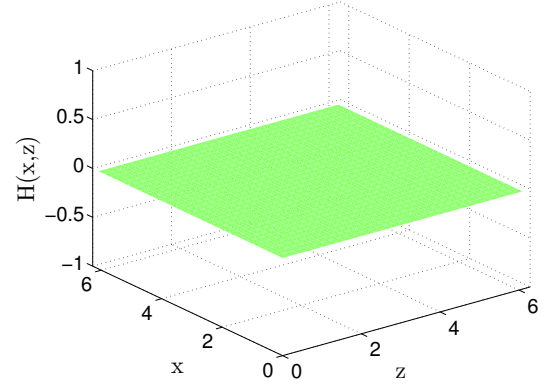
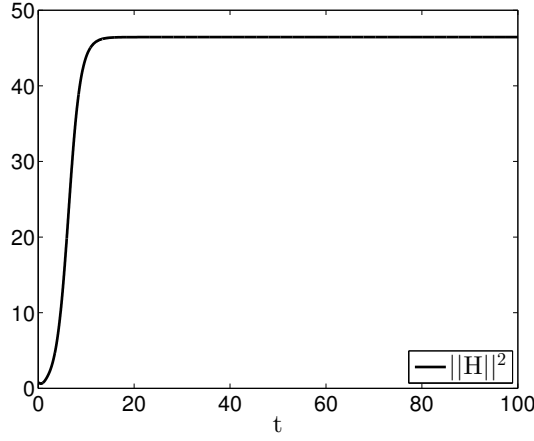
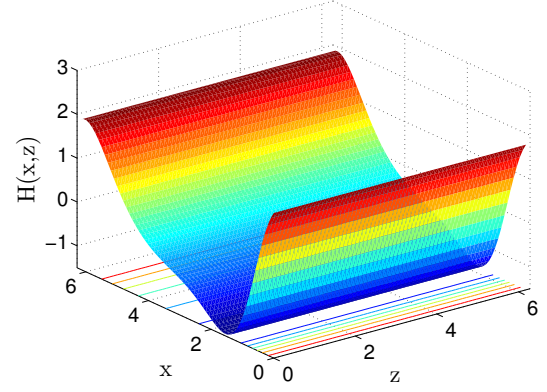
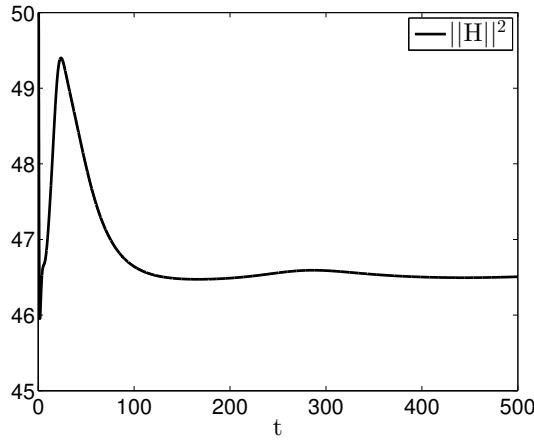
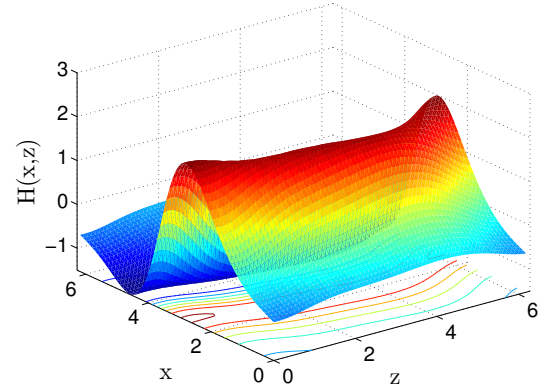
(a) $\nu = 0.25$ (b) $\nu = 0.25$ (c) $\nu = 0.25$ (d) $\nu = 0.25$ (e) $\nu_1 = 0.25, \nu_2 = 0.01$ (f) $\nu_1 = 0.25, \nu_2 = 0.01$

Figure 41: Interfacial energies and profiles for $Re = 25$, $\Lambda = -0.25$, $\Gamma_0 = 1$, $\eta = 1$. (a)–(b) $\nu = 0.25$: stable flow without surfactants. (c)–(d) $\nu = 0.25$: surfactant-induced one-dimensional instability. (e)–(f) $\nu_1 = 0.25, \nu_2 = 0.01$: secondary structure arising, resulting in a fully two-dimensional instability.

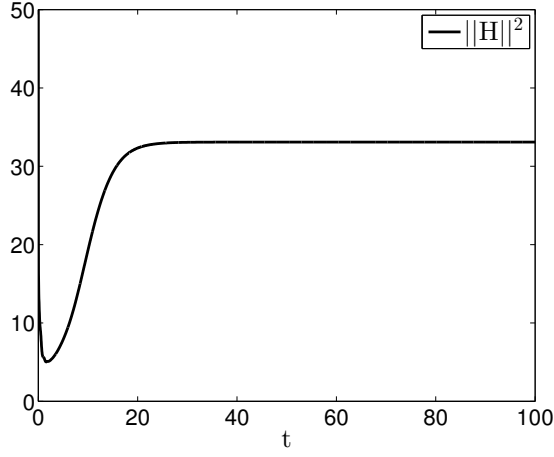
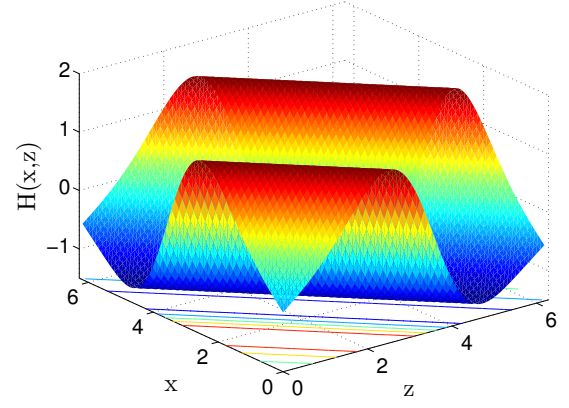
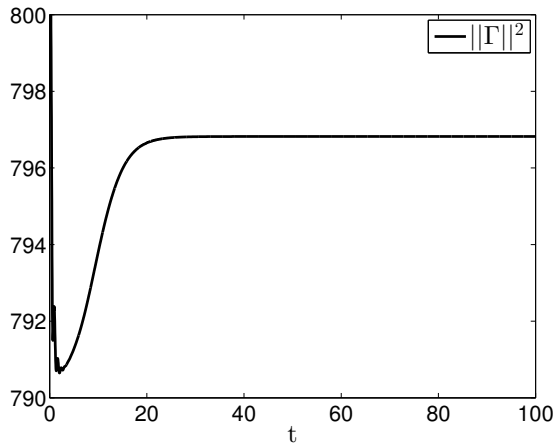
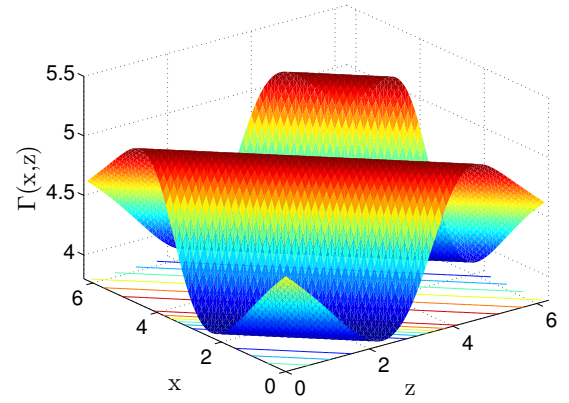
(a) L_2 -norm $\|H\|^2$ (b) Profile $H(x,z)$ (c) L_2 -norm $\|\Gamma\|^2$ (d) Profile $\Gamma(x,z)$

Figure 42: (a)–(b) Interfacial L_2 -norms $\|H\|^2$ and profiles $H(x,z)$ taken at the final time $t = 100$. (c)–(d) Surfactant concentration L_2 -norms $\|\Gamma\|^2$ and profiles $\Gamma(x,z)$ at $t = 100$. The parameter values used are $\nu_1 = \nu_2 = 0.05$ and $Re = 35$, $\Lambda = -1.0$, $\Gamma_0 = 1$, $\eta = 1$. The profiles in panels (b) and (d) are taken at time $t = 100$. The corresponding one-dimensional problem with $\nu = 0.05$ is stable.

An interesting feature of this particular example is that the waves are one-dimensional and in a rotated frame of reference; in fact, the wave is a function of $x+z$ and travelling in a direction of $\theta = 45^\circ$ with the shearing motion. This observation is in line with the linear stability results and the shift of the stability curve to create a greater instability region (see Figure 37).

In what follows, the stability of nonlinear one-dimensional travelling waves is studied. Assume that for some fixed parameter values and some ν the system (5.4)–(5.5) admits travelling wave solutions $\overline{H}(\xi)$, $\overline{\Gamma}(\xi)$, with $\xi = x - c\tau$. Two-dimensional solutions $H(\xi, z, t)$, $\Gamma(\xi, z, t)$ are then introduced, formed by the one-dimensional travelling waves $\overline{H}$, $\overline{\Gamma}$ and small perturbations $\tilde{H}$, $\tilde{\Gamma}$, i.e.

$$H(\xi, z, t) = \overline{H}(\xi) + \tilde{H}(\xi, z, t), \quad (6.16)$$

$$\Gamma(\xi, z, t) = \overline{\Gamma}(\xi) + \tilde{\Gamma}(\xi, z, t).$$

Substituting these solutions into the two-dimensional system of equations (4.5)–(4.6), results in the following linear system satisfied by the perturbations

$$\tilde{H}_t + \left(\overline{H}\tilde{H}\right)_\xi + \nu_1 \left(\partial_\xi^2 + \frac{\nu_2}{\nu_1}\partial_z^2\right)^2 \tilde{H} + \mathcal{P}\tilde{H} - \left(\partial_\xi^2 + \frac{\nu_2}{\nu_1}\partial_z^2\right) \tilde{\Gamma} = 0, \quad (6.17a)$$

$$\tilde{\Gamma}_t + \left(\overline{H}\tilde{\Gamma}\right)_\xi + \left(\overline{\Gamma}\tilde{H}\right)_\xi - \eta \left(\partial_\xi^2 + \frac{\nu_2}{\nu_1}\partial_z^2\right) \tilde{\Gamma} = 0. \quad (6.17b)$$

The small perturbations $\tilde{H}$, $\tilde{\Gamma}$ are resolved into normal modes in the z -direction as follows

$$\tilde{H} = f(\xi)e^{\lambda t}e^{ik_2 z}, \quad \tilde{\Gamma} = g(\xi)e^{\lambda t}e^{ik_2 z}, \quad (6.18)$$

where λ is an eigenvalue (growth rate) and the eigenfunctions f , g are 2π -periodic in ξ . The latter satisfy the system

$$\lambda f + \left(\overline{H}f\right)_\xi + \nu_1 \left(\partial_\xi^2 - \frac{\nu_2}{\nu_1}k_2^2\right)^2 f + \hat{\mathcal{P}}_{k_2}f - \left(\partial_\xi^2 - \frac{\nu_2}{\nu_1}k_2^2\right) g = 0, \quad (6.19a)$$

$$\lambda g + \left(\overline{H}g\right)_\xi + \left(\overline{\Gamma}f\right)_\xi - \eta \left(\partial_\xi^2 - \frac{\nu_2}{\nu_1}k_2^2\right) g = 0. \quad (6.19b)$$

The linear convolutions are calculated by writing the solutions in their Fourier series representation

$$\begin{aligned}\overline{H}(\xi) &= \sum_{k_1} \widehat{H}(k_1) e^{ik_1\xi}, & \overline{\Gamma}(\xi) &= \sum_{k_1} \widehat{\Gamma}(k_1) e^{ik_1\xi}, \\ f(\xi) &= \sum_{k_1} \widehat{f}(k_1) e^{ik_1\xi}, & g(\xi) &= \sum_{k_1} \widehat{g}(k_1) e^{ik_1\xi},\end{aligned}\quad (6.20)$$

and seeking solutions of the system in Fourier space, i.e. finding the eigenvalues λ that satisfy the set of equations

$$-\lambda \widehat{f}(k_1) = ik_1 \left(\widehat{Hf} \right) + \nu_1 \left(k_1^2 + \frac{\nu_2}{\nu_1} k_2^2 \right)^2 \widehat{f}(k_1) + \widehat{\mathcal{P}}_{k_1, k_2} \widehat{f}(k_1) + \left(k_1^2 + \frac{\nu_2}{\nu_1} k_2^2 \right) \widehat{g}(k_1), \quad (6.21a)$$

$$-\lambda \widehat{g}(k_1) = ik_1 \left(\widehat{Hg} \right)_\xi + ik_1 \left(\widehat{\Gamma f} \right) + \eta \left(k_1^2 + \frac{\nu_2}{\nu_1} k_2^2 \right) \widehat{g}(k_1). \quad (6.21b)$$

This is a linear system for the $4M_x$ unknowns $\widehat{f}(k_1)$, $\widehat{g}(k_1)$ and thus there exist $4M_x$ eigenvalues. Due to the translational invariance of the problem, there is always one eigenvalue satisfying $\lambda = 0$ (Longhi [97]). The condition for instability is provided by satisfying $\Re(\lambda) > 0$ for at least one eigenvalue and for positive integer values of k_2 . In practice, setting $k_2 = 1$ and looking for at least one eigenvalue with positive real part is a sufficient condition for two-dimensional instability (because the system is long wave unstable).

The above formulas are used to study the stability of the travelling wave branches in Figure 35(a). It is found that the two branches are unstable to streamwise as well as spanwise perturbations. The instability to streamwise perturbations is in the sense that different large-time solutions arise to different initial value problems. To see that, the following initial condition is used for the interfacial perturbation, to include an additional unstable mode

$$H(x, 0) = \frac{1}{10} \nu^{-1/2} (\sin x + 0.5 \cos 2x), \quad (6.22)$$

(the initial surfactant concentration is constant and the same as in (5.27)). Solu-

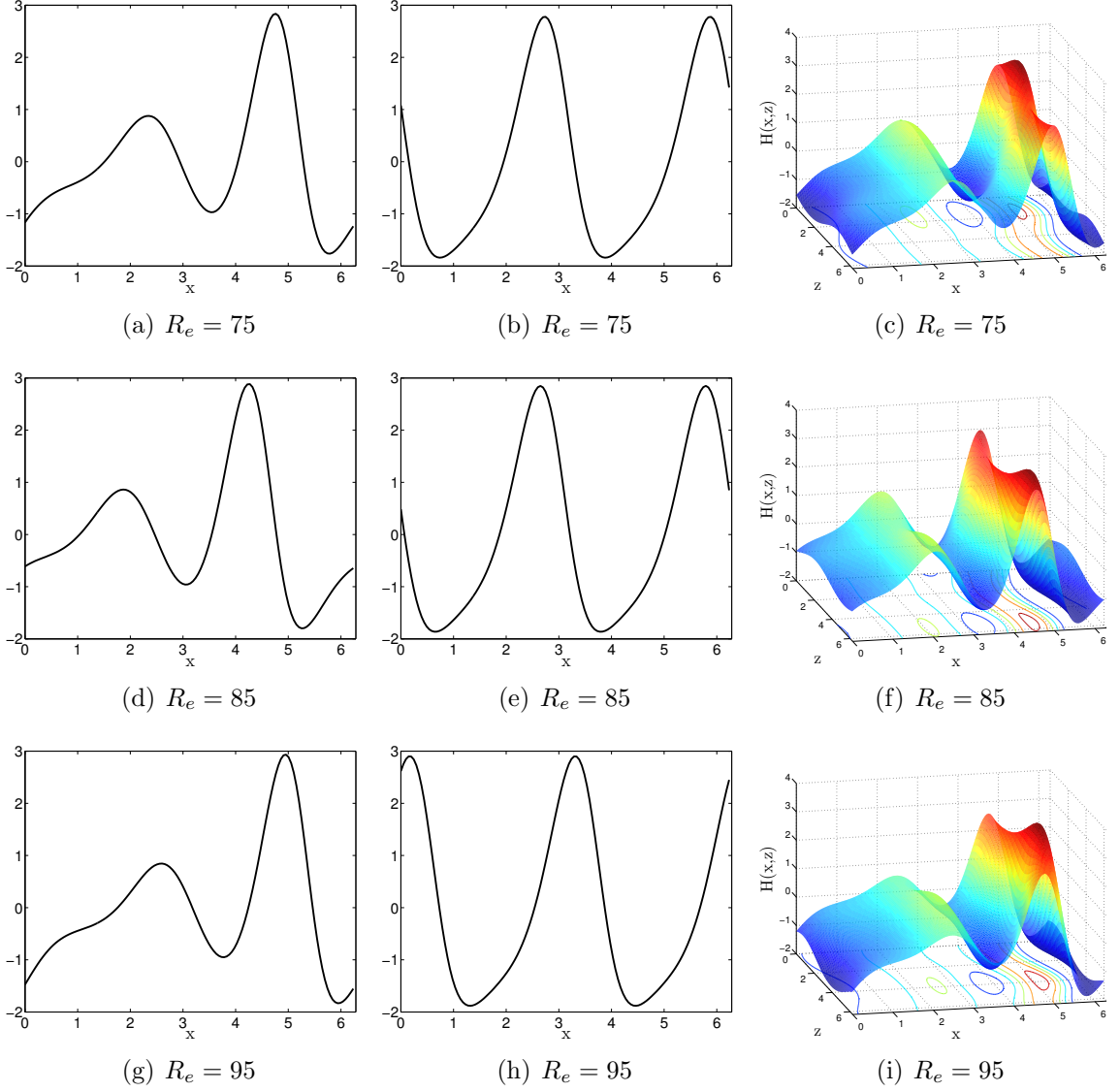


Figure 43: Interfacial profiles for $\nu = 0.1$, $\Lambda = 0.25$, $\Gamma_0 = 1$, $\eta = 1$ and $R_e = 75$ (top row), $R_e = 85$ (middle row), $R_e = 95$ (bottom row). The profiles in the first column are obtained from the one-dimensional initial value problem with the initial conditions (5.27). The corresponding profiles in the second column are obtained with initial conditions (6.22). The third column depicts fully two-dimensional solutions for $\nu_1 = \nu_2 = 0.1$.

tions obtained with initial conditions (6.22) are compared to the ones corresponding to initial conditions (5.27) for different values of the Reynolds number taken from both branches in Figure 35(a). Representative results corresponding to the second branch with $31 \leq R_e \leq 100$ are presented next (similar results hold for R_e in the range $0 \leq R_e \leq 4$). The interfacial travelling wave solutions obtained with initial conditions (5.27) and (6.22) are shown on the left and middle columns of Figure 43 respectively, for $\nu = 0.1$ and $R_e = 75, 85, 95$ (the rest of the parameters have the same values as in Figure 35(a)). It is observed that the two solutions are different, confirming the instability of the former. Note that the three profiles obtained for different R_e have similar features, with the only difference being a slight increase in the amplitude as the Reynolds number increases. The right column in Figure 43 depicts two-dimensional interfacial waves for $\nu_1 = \nu_2 = 0.1$ and $R_e = 75, 85, 95$, obtained with initial conditions (6.12), i.e. perturbing about the travelling wave solutions on the left panels. The resulting waves are clearly fully two-dimensional due to the development of secondary instabilities and this verifies the instability of the one-dimensional solutions to spanwise perturbations.

7 Conclusions

This chapter provides a summary of the work presented in the first part of the thesis, regarding the problem of two-fluid shear flows with surfactants. The summary is followed by a discussion of the main results and novel findings. Finally, possible future developments and extensions of this work are described, including the problem of two-layer channel flow with soluble surfactants in the film.

7.1 Summary of research

This thesis focuses on a two-layer shear flow and the evolution of its surfactant-laden interface. The problem is tackled analytically and numerically towards investigating the effects of inertia and the presence of surfactant on the stability of the flow. The mathematical modelling is performed based on assumptions motivated by the various applications of this problem, which suggest considering a thin lower fluid layer and dilute surfactant concentrations. The significantly smaller size of the film thickness compared to its length suggests the use of lubrication techniques, in which case inertial effects in the film are negligible. A set of coupled weakly nonlinear evolution equations is then derived, which describe the spatiotemporal evolution of the film thickness and its local surfactant concentration. Inertial effects in the thick fluid layer are taken into account via a nonlocal integral term, which couples the film and upper fluid dynamics. A localised approximation of the evolution equation for the film is obtained in the appropriate asymptotic limit. The model evolution equation captures essential features of long interfacial waves that have been observed in two-fluid Couette flow experiments in the absence of surfactants.

Accurate numerical methods based on linearly implicit BDF schemes are studied and implemented. In order to analyse the dynamical behaviour of the system, extensive numerical experiments are performed for a large range of parameter values, specifically for domains that become increasingly longer. Two special cases regarding the size of the Reynolds number (R_e) in the upper layer fluid are considered separately: R_e asymptotically small and of the order of the film thickness, and R_e of order one. Numerical solutions corresponding to the two-dimensional problem are first obtained and their stability to spanwise perturbations is then investigated by fixing the length of the channel and increasing its width. The characteristics of the solutions obtained are described in detail in the next section. In what follows, an interpretation of the results is also given, together with a discussion of the physical mechanisms associated with this problem.

7.2 Discussion of main findings

The nonlocal model derived here includes all physical processes involved in a two-fluid shear flow. These include the inertial long wave destabilisation of a two-layer Couette flow by any non-zero Reynolds number, however small (Yih [1]). This instability only exists if the thin fluid is more viscous than the overlying fluid, otherwise the flow is stable at any Reynolds number (Hooper [22]). Addition of surfactant can destabilise the flow even in the absence of inertia, irrespectively of which fluid is more viscous and even when there are no viscosity differences (Frenkel & Halpern [31], Halpern & Frenkel [32]). Moreover, inertial effects increase the growth of the surfactant-induced Marangoni instability and therefore produce new regions of instability (Pozrikidis [34], Blyth & Pozrikidis [35], Frenkel & Halpern [36]). Interestingly, it is possible to have a stable flow with both surfactant and inertia present for relatively large viscosity ratios. In this case, viscous forces are much stronger than inertial and Marangoni forces, providing a viscosity stratification stabilisation of the flow.

The problem is characterised by long wave instability, either due to inertial or Marangoni forces (both physical quantities are represented by second order diffusive terms in the film thickness evolution equation). It is interesting to note that in the axisymmetric problem studied by Kas-Danouche et al. [8], the long wave destabilisation was due to the contribution of azimuthal curvature and occurred even in the absence of inertia or surfactant. The nonlinear term in the evolution equation is responsible for energy redistribution from long waves to short waves (Bassom et al. [2]). In addition, surface tension is responsible for the stabilisation of all short waves (Hooper & Boyd [20]) and it is represented by the fourth order capillary term in the evolution equation.

The physical mechanism driving the surfactant-induced Marangoni instability is the following: areas of high surfactant concentration are characterised by low surface tension, which tends to increase the surface area. Thus the surrounding high surface tension fluid pulls more strongly on the low surface tension fluid, leading to the development of surface tension gradients and causing the fluid to flow away from such regions. Therefore the interfacial wave is expected to develop a trough close to

the region of surfactant accumulation and this explains the out-of-phase profiles of the interfacial and surfactant concentration waves.

Perhaps most importantly, this work provides a theory that compares well with two-fluid Couette flow experimental phenomena. The nonlocal model captures interfacial wave structures observed in shear flow experiments (Barthelet et al. [46]) and reproduces important features for relatively high values of inertia. It is found that increased inertia causes an increase in the amplitude and decrease in the period of the wave, similarly to the experimental results. However, a discrepancy of the wave frequency is noticed, with numerically obtained waves having much smaller wavelength than the experimental ones.

For the first time, numerical simulations have been carried out to solve the full nonlocal system of evolution equations and classify the dynamics over a range of parameters. Results show that as the length of the system increases, the solutions become unstable to long wavelength perturbations (Frenkel & Halpern [38]). Large-time solutions are mostly nonlinear travelling waves or time-periodic travelling waves. As ν becomes smaller, travelling waves give rise to more complex dynamics including quasi-periodic and chaotic oscillations in time. The existence of intricate phenomena for asymptotically small Reynolds number have not been previously found in the work of Bassom et al. [2]. The results of Bassom et al. only reveal travelling wave solutions and the authors discuss that the dynamics are simpler in this case because of the absence of the destabilising term H_{xx} from the evolution equation. Their argument is based on the fact that in the axisymmetric problem studied by Kas-Danouche et al. [8] the H_{xx} term appears in the evolution equation even at asymptotically small Reynolds number, causing richer flow dynamics.

In addition, numerical calculations reveal that solutions of the nonlocal and local systems have similar dynamical behaviour, even if they get attracted by complex attractors. The essential difference is the existence of a phase shift between the solutions, which is enhanced as $\nu \rightarrow 0$ (similar result was found in Smyrlis & Papa-georgiou [45] for a KS-type equation). This result also shows that complex solutions can develop from the local system, which have not been reported by Bassom et al. [2]. Moreover, for relatively large and fixed ν , travelling wave solutions which tend to triv-

ial steady states for large enough $|\Lambda|$ are supported, forming a viscosity stratification stabilisation of the Marangoni instability.

For finite values of the Reynolds number, a computational case study reveals the existence of travelling waves, periodic travelling waves, quasi-periodic and chaotic solutions. A notable travelling wave feature is that successive travelling wave windows have their spatial period successively decreased. An important difference between the results for $R_e = 0$ and $R_e = 25$ is that the flow gets attracted to chaotic dynamical behaviour for $\nu = 0.001$ and $\nu = 0.002$, respectively. Having in mind the definition of ν , this corresponds to systems of approximate lengths $2L \approx 200$ and $2L \approx 140$, respectively. Physically, this means that when inertia is absent chaotic phenomena arise if the length of the channel is about 200 times larger than the depth of the channel. Consequently greater inertial effects cause the development of chaotic solutions in shorter channels.

Lastly, the novelty of this work also lies in the investigation of the stability of the three-dimensional flow. For vanishing Reynolds number, a Squire's type theorem is valid and consequently it is sufficient to study only the two-dimensional problem in this case, which is the most unstable. Most importantly, it is established that in the presence of inertia one-dimensional travelling waves can be unstable to spanwise perturbations. In particular, these travelling waves are found to remain one-dimensional while the channel's width is relatively small, but as the width of the channel increases secondary instabilities emerge and the waves become fully two-dimensional. As soon as the secondary instabilities arise, they are stable in time and travel with the waves in the direction of the flow; they eventually lose stability and become time-periodic for wide enough channels.

7.3 Future work

7.3.1 Travelling wave bifurcations

One possible extension of the results obtained in this work is the numerical construction of travelling waves by considering solutions of the form $H = H(x - ct)$,

$\Gamma = \Gamma(x - ct)$ and using them to solve the nonlinear system (5.4)–(5.5) (a similar procedure was performed by Tilley et al. [91] while investigating the effect of electric fields on travelling waves arising in planar liquid sheets, reported by Matsuuchi [98] and Mehring & Sirignano [99]). Substituting the Fourier representation (5.31) of the solutions and truncating the series after a sufficiently large number M , gives a nonlinear system for the Fourier coefficients of the solutions. The system for $k = 1, \dots, M$ is given by

$$\begin{aligned} -ckH_k^s + \nu k^4 H_k^c + P_k^c + k^2 \Gamma_k^c - F_k^c &= 0, \\ ckH_k^c + \nu k^4 H_k^s + P_k^s + k^2 \Gamma_k^s - F_k^s &= 0, \\ -ck\Gamma_k^s + \eta k^2 \Gamma_k^c - G_k^c &= 0, \\ ck\Gamma_k^c + \eta k^2 \Gamma_k^s - G_k^s &= 0, \end{aligned} \tag{7.1}$$

where

$$\begin{aligned} P_k^c &= \frac{\Lambda \nu^{-1/2}}{2} k \left(H_k^c \Im \left(F''(0) \right) - H_k^s \Re \left(F''(0) \right) \right), \\ P_k^s &= \frac{\Lambda \nu^{-1/2}}{2} k \left(H_k^c \Re \left(F''(0) \right) + H_k^s \Im \left(F''(0) \right) \right), \end{aligned} \tag{7.2}$$

and $F_k^c, F_k^s, G_k^c, G_k^s$ are the Fourier modes of the nonlinear terms. This is a system of $4M$ equations with $4M + 1$ unknowns, the extra unknown being the travelling wave speed c . To make the solution of the problem unique, the translational invariance of the solutions is used, which provides an additional condition and thus reduces the number of unknowns by one. This extra condition can be arbitrary and in this case the choice is $H_1^c = 0$. Finally, Newton's method is applied on the above system.

The interest lies in the examination of possible existence of multiple states at the same parameter values (this phenomenon is caused by the nonlinearity). Such bifurcation branches have already been found by use of a continuation method (see Figure 44 for an example of travelling wave branches obtained for $R_e = 25, \Lambda = 0.25$). The method used includes obtaining a solution from the time-dependent code for some ν for which travelling waves are supported and then using this solution as the

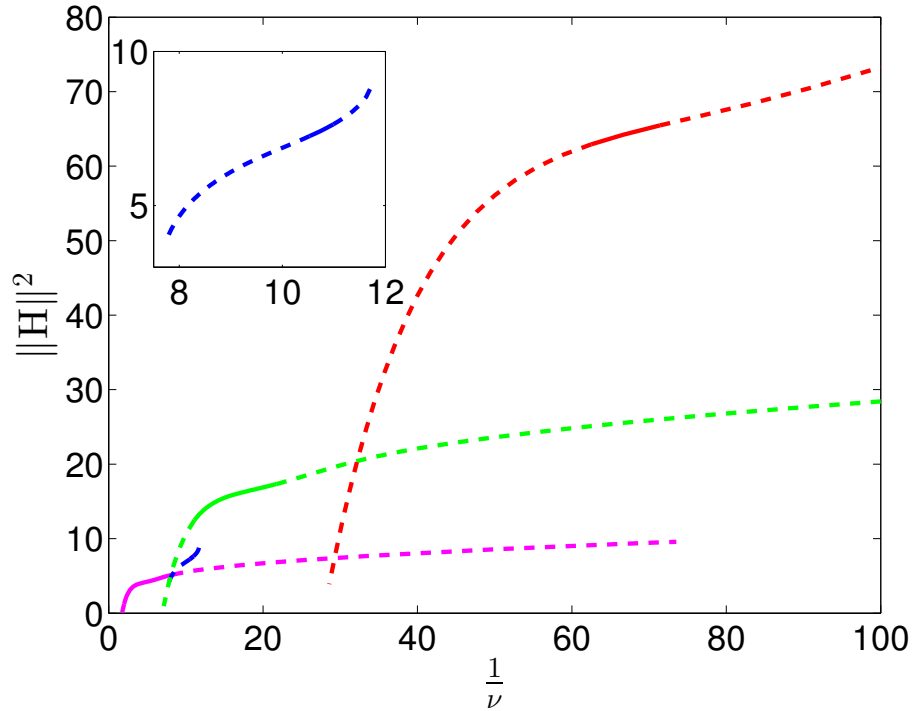


Figure 44: Travelling wave bifurcation branches obtained for $R_e = 25$, $\Lambda = 0.25$, $\Gamma_0 = 1$, $\eta = 1$. The figure shows the final constant energy value against $\frac{1}{\nu}$, while the inset depicts a magnification of the branch in blue. Continuous lines correspond to solutions obtained from the time-dependent code and dashed lines to continuations.

initial guess for the Newton's method with $\nu + \Delta\nu$. The latter solution is then used as an initial guess for the next iteration of the Newton's method. However, this method fails at some points, where the solutions possibly become quasi-periodic. In this case a more sophisticated method must be applied for an extensive search of all possible branches and this is possible by using the software package *AUTO* (Doedel [100]), which is suitable for continuation and bifurcation problems.

The branches obtained by continuation techniques correspond to unstable solutions, whereas the solutions resulting from the time-dependent code are stable. A natural extension of this work would be the stabilisation of the unstable solutions using feedback control (for similar studies on stabilisation of the Kuramoto–Sivashinsky equation see Armaou & Christofides [101] and Christofides & Armaou [102]).

7.3.2 Stability of travelling waves

Another possible development is the investigation of the stability of the different travelling wave solutions. Of particular interest is the study of the modulational stability of multimodal travelling waves, i.e. waves of period $\frac{2\pi}{m}$, $m = 2, 3, \dots$. This can be achieved by perturbing the m -modal wave with a small perturbation of period $\frac{2\pi}{p}$, $p \leq m$, and using this as initial condition for a numerical simulation with the same parameter values. A similar strategy was followed by Tilley et al. [91] when studying the dynamics of electrified films. The authors constructed these travelling waves numerically and showed that they are unstable to long wavelength modulational perturbations. The examination of the stability of travelling waves is motivated by previous studies concerning the modulational stability of solutions of the Kuramoto–Sivashinsky equation, including travelling waves (Barker et al. [103]) and steady states (Frisch et al. [89], Kevrekidis et al. [104]). It has been demonstrated that these steady state solutions can be constructed based on a similarity property (Smyrlis & Papageorgiou [11]) and their modulational stability was studied by using homogenisation theory (Frisch et al. [89], Papageorgiou et al. [105]).

7.3.3 Existence & analyticity of solutions

The systems of evolution equations derived here fall in the general class of dissipative infinite dimensional dynamical systems. To complement the numerical study provided in this thesis, analytical proofs are still required on the existence, well-posedness and analyticity of solutions (analytic periodic functions are characterized by exponentially decaying Fourier modes). However, in this case such proofs are challenging because the evolution equations form a system of coupled PDEs.

There are several related studies in the area, particularly for the well-known Kuramoto–Sivashinsky equation (Collet et al. [106, 107], Goodman [108], Frankel & Roytburd [109, 110]) and nonlocal Kuramoto–Sivashinsky equations arising in interfacial electrohydrodynamics (Tseluiko & Papageorgiou [111]). Robinson [112] and Temam [113] also proved existence and uniqueness of solutions of the KSE, based on similar ideas to proofs regarding existence and uniqueness of solutions of the Navier–

Stokes equations. Moreover, the KSE and a larger class of generalised Burgers equations consisting of a quadratic nonlinearity and a linear parabolic part, were proved to be well-posed (Tadmor [114]) and thus admitting a unique solution continuously dependent on its initial data. In fact, Tadmor [114] proved that his results can be extended to any equation of the KS-type with a nonlocal term of order greater than $3/2$.

Consequently, the required proofs for existence, well-posedness and analyticity of the solutions H, Γ of the system describing the evolution of a surfactant-laden interface can be based on the same principles followed for similar proofs for the scalar solution u of the Kuramoto–Sivashinsky equation.

7.3.4 Turbulent shear flows

The formation of different river landforms due to sediment transport is an important element in the science of geomorphology. Fowler [47] studied this problem from a mathematical point of view, by considering the interaction of a fluid flow with an erodible substrate. Of particular interest was the formation of dunes, which are observed as variations in channel profile in the direction of the flow and occur extensively in river flow (other types of bedform are ripples and anti-dunes). Such patterns are formed through an erosional instability of the uniform state when water flows down a straight channel.

To describe the problem mathematically, a model of rapid and turbulent shear flow over a slightly wavy boundary needs to be adopted. The limit of large Reynolds number is associated with a very small friction factor and is the relevant limit in such applications. A simple mathematical model can be therefore formulated by considering a two-fluid channel flow in the turbulent flow regime, with the lower fluid layer close to the bed of the river considered very thin. The equation describing the evolution of the film thickness in the large Reynolds number limit is given by

$$u_t + uu_x + u_{xxx} + R_e^{\frac{1}{3}} \mathcal{P}u = 0, \quad (7.3)$$

with

$$\hat{\mathcal{P}}_k = \frac{3}{2} Ai(0) e^{\frac{i\pi}{6}} k^{\frac{4}{3}}. \quad (7.4)$$

Here, the asymptotic expression (3.25) for function $\mathcal{N}(k)$ in the large R_e limit is used (for $k_2 = 0$ and $k_1 = k$). Note that the same asymptotic solution of the Orr–Sommerfeld equation is derived by Fowler [47] to describe a turbulent shear flow over a flat riverbed.

Since the Reynolds number is large, the nonlocal term dominates in the evolution equation. Balancing the orders of magnitude of the nonlinear and nonlocal terms, results in

$$u^2 \sim R_e^{\frac{1}{3}} u \implies u \sim R_e^{\frac{1}{3}}. \quad (7.5)$$

Therefore the following transformations are introduced

$$t = R_e^{-\frac{1}{3}} \tau, \quad u = R_e^{\frac{1}{3}} U, \quad (7.6)$$

and the evolution equation for the film thickness becomes

$$U_\tau + UU_x + \nu_R U_{xxxx} + \mathcal{P}U = 0, \quad (7.7)$$

with $\nu_R = R_e^{-\frac{1}{3}}$. The final evolution equation is then solved in $[0, L]$ periodic domains for a fixed value of the period L . However, as the Reynolds number increases, the solution u also increases. The interface is perturbed as $S = \epsilon + \epsilon^2 u$ and for $u \sim \frac{1}{\epsilon}$, i.e. $\epsilon \sim R_e^{-\frac{1}{3}}$, the weakly nonlinear theory eventually breaks down (not valid for arbitrarily small ϵ) leading to flow separation.

7.3.5 Soluble surfactants

One possible future development of the subject is to allow for the surfactant to migrate into the bulk of the film, which can happen in the case in which the surfactant is soluble in the bulk. Studies about the dynamics of soluble surfactants on a thin film have been carried out by Jensen & Grotberg [19] and Halpern & Grotberg [115]. Assuming the surfactant initially present as an interface monolayer, it then desorbs

from the interface and diffuses across the film (it is also assumed that the lower plate is completely impermeable to surfactant). The latter surfactant transport is controlled by both the bulk and interface distributions, which are described by two convection–diffusion equations. The bulk and interface surfactant concentrations are coupled through a boundary condition at the interface (Jensen & Grotberg [19], Halpern & Grotberg [115]). This boundary condition helps in determining an equation of state known as the Gibbs adsorption equation, which provides the dependence of the surface tension on the interfacial surfactant concentration *on equilibrium* (some famous equations of state include the Langmuir, Frumkin, Henry and Sheludko isotherms, see Pozrikidis [57] and Craster et al. [116]). The bulk surfactant concentration is crucial in the problem because above the *critical micelle concentration* (CMC), surfactant monomers form into micelles; hence two distinct cases have to be considered:

- Bulk concentrations below the CMC

The surfactant transport in this case is controlled by two convection–diffusion equations describing the variations of surfactant concentration at the interface Γ and in the bulk C (it is assumed that the surfactant is only present in one phase). These are given by

$$\frac{\partial \Gamma}{\partial t} - \frac{\partial \mathbf{r}}{\partial t} \cdot \nabla_s \Gamma + \nabla_s \cdot (\Gamma \mathbf{u}_s) + \Gamma \kappa (\mathbf{u}_I \cdot \mathbf{n}) = \mathcal{D}_s (\nabla_s^2 \Gamma) + q_{\text{rc}}, \quad (7.8)$$

$$\frac{\partial C}{\partial t} + \mathbf{u} \cdot \nabla C = \mathcal{D}_b (\nabla^2 C), \quad (7.9)$$

where $\mathcal{D}_s$, $\mathcal{D}_b$ denote the surface and bulk surfactant diffusivities, respectively. The term q_{rc} describes the sorption kinetics and incorporates the flux of surfactant between the interface and the bulk. The surfactant flux also provides coupling between the interface and bulk convection–diffusion equation and it is given by

$$q_{\text{rc}} = k_a C \left(1 - \frac{\Gamma}{\Gamma_\infty} \right) - k_d \Gamma. \quad (7.10)$$

Here, the parameters k_a and k_d are the interfacial adsorption/desorption rates, respectively.

To make the problem non-dimensional, in addition to the transformations in (2.34), the following transformations are also used

$$C \rightarrow C_\infty C, \quad q_{\text{rc}} \rightarrow \frac{\Gamma_\infty U}{d} q_{\text{rc}}, \quad (7.11)$$

where C_∞ is the uniform bulk concentration in the undisturbed state. The dimensionless surfactant flux is given by

$$q_{\text{rc}} = Bi \left(K_s C (1 - \Gamma) - \Gamma \right), \quad (7.12)$$

with the Biot number Bi (Wang et al. [117]) and the non-dimensional parameter K_s defined by

$$Bi = k_d \frac{d}{U}, \quad K_s = \frac{k_a C_\infty}{k_d \Gamma_\infty}. \quad (7.13)$$

- Bulk concentrations above the CMC

In addition to the interfacial surfactant convection–diffusion equation, now there are two coupled equations describing the concentration of bulk monomers C and micelles M , given by (Craster et al. [116])

$$\frac{\partial C}{\partial t} + \mathbf{u} \cdot \nabla C - \mathcal{D}_b (\nabla^2 C) = -n q_{\text{CM}}, \quad (7.14)$$

$$\frac{\partial M}{\partial t} + \mathbf{u} \cdot \nabla M - \mathcal{D}_m (\nabla^2 M) = q_{\text{CM}}. \quad (7.15)$$

Here $\mathcal{D}_b$, $\mathcal{D}_m$ denote the bulk monomer and micelle diffusivities, respectively, and the surfactant flux is now equal to

$$q_{\text{CM}} = k_m C^n - k_n M, \quad (7.16)$$

with k_m being the rate at which a micelle M is created in the bulk phase from n monomers, and k_n the rate of breakup of a micelle into n monomers. The flux is non-dimensionalised as in (7.11) and it becomes

$$q_{\text{CM}} = K_b (C^n - M), \quad (7.17)$$

where the new dimensionless parameters are

$$K_b = k_n \frac{d}{U}, \quad C_\infty = \left(\frac{k_n}{nk_m} \right)^{\frac{1}{(n-1)}}. \quad (7.18)$$

Finally, the evolution equations will be derived using lubrication theory (Craster & Matar [13]), since the thickness of the film is significantly smaller than its length. The two cases (below and above the CMC) will first be applied in two-dimensional flows and then the theory will be extended to three dimensions.

Part II

Two-dimensional Kuramoto–Sivashinsky Equation

8 Introduction

In this chapter, the well-known Kuramoto–Sivashinsky equation (KSE) is introduced as a model equation arising in several physical contexts. An overview of known results for its one-dimensional version is then given, followed by the motivation for studying the two-dimensional KSE. This study is pursued here and it is based on the lack of analytical or numerical studies on the equation in higher dimensions. The structure of the second part of the thesis then follows, with a short description of the content of every chapter therein.

The Kuramoto–Sivashinsky equation (KSE) in its most general form is given by

$$u_t + \frac{1}{2} |\nabla u|^2 + \Delta u + \Delta^2 u = 0, \quad (8.1)$$

where $u = u(\mathbf{x}, t)$, $(\mathbf{x}, t) \in \mathbb{R}^2 \times \mathbb{R}_+$. The equation was first derived by Homsy [118] and Nepomnyashchii [119] in their studies on thin film flows down an inclined plane. It was later rederived by Kuramoto [120] while investigating diffusion-induced chaos in reaction systems, and Sivashinsky [121, 122, 123] while studying flame front propagation. The 2D KSE is of interest because its differentiated version in two spatial dimensions forms a system related to the surfactant-free interfacial evolution equation derived in the previous part of the thesis. Also, both PDEs include a similar type of nonlinearity and a fourth order linear dissipation. The KSE has received significant attention in its one-dimensional form both analytically and numerically and an overview of the main results is provided next.

8.1 One-dimensional KS equation

In spatial dimension one, the 1D Kuramoto–Sivashinsky equation is mainly known in its differentiated form

$$\begin{aligned} u_t + uu_x + u_{xx} + u_{xxxx} &= 0, \quad (x, t) \in \mathbb{R} \times \mathbb{R}_+, \\ u(x + 2L, t) &= u(x, t), \\ u(x, 0) &= u_0(x), \end{aligned} \quad (8.2)$$

which has been studied extensively in the past decades. It forms a model for complex spatiotemporal dynamics in spatially extended systems, hence it has attracted a plethora of interest. The 1D KSE describes the asymptotic behaviour of many physical problems. In addition to describing flame-front instabilities (Sivashinsky [122]), it also arises in fluid dynamics problems, for example in two-phase flows (Papageorgiou et al. [40], Tilley et al. [91]) and free surface thin film flows (Hooper & Grimshaw [28], Sivashinsky & Michelson [124]). Moreover, it is found to emerge in various ap-

plications in physics, including plasma physics (Cohen et al. [125]), ion sputtering (Cuerno & Barabási [126]) and chemical physics for propagation of concentration waves (Kuramoto [120], Kuramoto & Tsuzuki [127]).

There have been numerous studies of the 1D KSE with $2L$ –periodic boundary conditions, both theoretical [106, 107, 108, 109, 110, 114, 128] as well as numerical [9, 11, 89, 124, 129]. The results show that the KSE is one of the simplest partial differential equations exhibiting a particularly complex dynamical behaviour associated with chaotic dynamics as the spatial length increases (Tseluiko & Papageorgiou [111]). It has a convective Burgers–type nonlinearity which provides a transfer of energy between the active and dissipative modes. The essential features of the dynamics of the system are captured well by a finite dimensional dynamical system of ordinary differential equations for the Fourier modes (Hyman et al. [129]). The number of degrees of freedom is at least as large as the number of linearly unstable Fourier modes (Akrivis et al. [79], Constantin et al. [130]), and often two or three in practice (Charru [131]).

Considering the 1D KS equation with periodic initial conditions with period $2L$, Tadmor [114] proved that it admits a unique smooth solution (that remains $2L$ –periodic), continuously dependent on its initial data. In addition to this, much of the analytical work regarding the 1D KSE has involved establishing how the energy (defined by the L_2 –norm of the solution $\|u\|_{L_2}$) scales with the length of the domain. Assuming that the domain $[0, 2L]$ is bounded, it is found that large–time solutions are bounded by an absorbing ball with L –dependent radius (in L_2 and higher Sobolev spaces). This result is called *dissipativity* and is one of the significant features of the KSE. The radius of this absorbing ball has been found to be a power of L ,

$$\limsup_{t \rightarrow \infty} \|u\|_{L_2} = \mathcal{O}(L^p), \quad (8.3)$$

with the first value of p ever obtained being $5/2$ for odd–parity solutions (Nicolaenko et al. [128]). The radius of the absorbing ball has been dramatically improved over the years by various researchers, as can be seen in Table 5. However, the best known analytic bound of $\mathcal{O}(L^p)$ for $p > 5/6$ does not yet approach the optimal bound

Table 5: Optimal bounds for the L_2 -norm of the solutions of the one-dimensional Kuramoto–Sivashinsky equation. The best known analytic bound overestimates the optimal bound found numerically.

Authors	Year	Bound	Comments
Nicolaenko et al. [128]	1985	$\mathcal{O}(L^{5/2})$	Valid only for odd initial data
Il'yashenko [133]	1992	$\mathcal{O}(L^{7/2})$	Removed the oddness assumption
Goodman [108]	1994	$\mathcal{O}(L^{5/2})$	Valid for general periodic solutions
Collet et al. [106]	1993	$\mathcal{O}(L^{8/5})$	Valid for all mean-zero functions
Jolly et al. [134]	2000	$\mathcal{O}(L^{3/2})$	Expressed as a function of L
Bronski & Gambill [135]	2006	$\mathcal{O}(L^{3/2})$	Based on Lyapunov functions
Giacomelli & Otto [136]	2005	$\mathcal{O}(L^{3/2})$	Proved by the entropy method
Otto [137]	2009	$\mathcal{O}(L^{5/6+})$	For all exponents greater than $\frac{5}{6}$
Wittenberg & Holmes [132]	1999	$\mathcal{O}(L^{1/2})$	Obtained numerically

$\mathcal{O}(L^{1/2})$, found numerically by Wittenberg & Holmes [132].

Furthermore, solutions were proved to be analytic in x in a strip around the real axis of width

$$\beta_w \geq CL^{-16/25}, \quad (8.4)$$

with C a constant independent of L . This estimate was proved by Collet et al. [107] and it is the lower rigorous bound. The analyticity of the solution implies that the high frequency part of the spectrum has the form

$$|\hat{u}(k; t)| = \mathcal{O}\left(e^{-CL^{-16/25} \frac{\pi}{L} |k|}\right), \quad (8.5)$$

where $|\hat{u}(k; t)|$ is the k^{th} Fourier coefficient of $u(x, t)$. Numerical computations, though, suggest the presence of a stronger bound independent of L (Collet et al. [107], Wittenberg & Holmes [132]), such that the solutions satisfy

$$\limsup_{t \rightarrow \infty} \sum_{k \in \mathbb{Z}} e^{2\beta_w \frac{\pi}{L} |k|} |\hat{u}(k; t)|^2 \leq \text{const.}, \quad (8.6)$$

with $\beta_w \approx 3.5$ (Akrivis & Smyrlis [75], Collet et al. [107]).

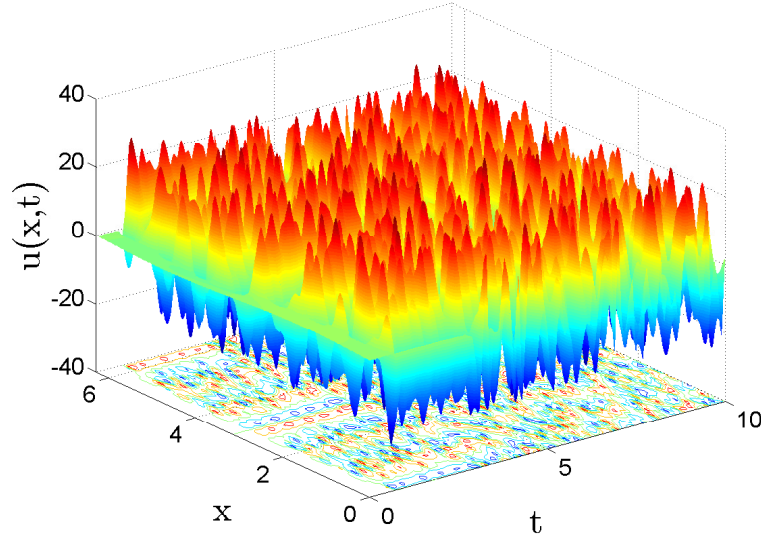


Figure 45: Typical solution $u(x, y)$ of the one-dimensional Kuramoto–Sivashinsky equation exhibiting chaotic dynamics for a domain length of $2L = 60$.

Moreover, as the solution enters the chaotic regime, it remains of $\mathcal{O}(1)$ and it adds more oscillations as L increases. It was proved by Kukavica [138] that the number of rapid oscillations of the solutions is universally bounded by an expression exponential in L . This bound was later improved by Grujić [139] to an expression essentially algebraic in L , more specifically of $\mathcal{O}(L^{41/25} \log L)$. These analytical results provide bounds that are not sharp and overestimate the optimal bound. A clear picture is provided by the numerical experiments, which show that the number of rapid oscillations of the solutions as L increases is of $\mathcal{O}(L)$ and the distance between oscillations is $\mathcal{O}(1)$.

In addition to establishing how the energy scales with the system size, there have been several notable studies examining how the solution itself changes with the system size. For domain lengths smaller than 2π , the 1D KSE is stable and solutions return to the trivial state for any choice of initial conditions, i.e. $\limsup_{t \rightarrow \infty} \|u\|_{L_2} = 0$. As the domain length $2L$ increases above the bifurcation point 2π , the zero solution loses stability to a unimodal steady state, which in turn becomes unstable to multi-modal steady states, travelling waves, oscillatory and chaotic solutions for larger L . The transition to chaos occurs through a period doubling cascade that follows the

Feigenbaum scenario (Papageorgiou & Smyrlis [9], Smyrlis & Papageorgiou [10, 11]). For sufficiently large L , the solution becomes dynamically disordered and gets trapped into a chaotic attractor (see Figure 45 for an example of a chaotic solution obtained for $2L = 60$). In fact, the chaotic dynamics are extensive with local dynamics being asymptotically independent of L for $L \gg 1$, according to Wittenberg & Holmes [132]. The authors also showed that the energy is equipartitioned among the Fourier modes in the large scale region; such notions are described in more detail later.

8.2 Two-dimensional KS equation

Despite the rich dynamics observed in the 1D KS, the number of studies of the KS in higher dimension is somewhat limited. The question of global regularity for the Kuramoto–Sivashinsky in higher dimensions is still an open problem in nonlinear analysis. The first attempts for proving some analytical results about boundedness, analyticity and stability of the two-dimensional KSE were by Sell & Taboada [140] and Molinet [141]. Both authors assumed that the domain was very thin in the y -direction, which makes the problem “almost” one-dimensional. In Sell & Taboada [140], the authors have shown the existence of a bounded absorbing set in $\mathcal{H}_{per}^1([0, 2\pi] \times [0, 2\pi\epsilon])$ for ϵ small enough. In Molinet [141] this result is improved by showing that

$$\limsup_{t \rightarrow \infty} \|u\|_{L_2} \leq \mathcal{O}(L_x^{8/5} L_y^{1/2}), \quad (8.7)$$

on the bounded domain $(0, 2L_x) \times (0, 2L_y)$ with some restrictions on the initial data and for domain sizes $2L_x \geq 2\pi$, $0 < 2L_y < 2\pi$ satisfying

$$\left(1 - \left(\frac{L_y}{2\pi}\right)^2\right)^{-\frac{4}{9}} L_y \leq C L_x^{-67/35}. \quad (8.8)$$

In the meantime, a few related studies on two-dimensional equations of the KS-type have been reported. Demirkaya & Stanislavova [142] investigated the long-time behaviour of radially symmetric solutions of the KSE in a shell domain; they proved that there exists a time independent bound for the L_2 -norm of the solu-

tion. Demirkaya [143] also proved global well-posedness of a variation of the two-dimensional KSE, under specific assumptions. Moreover, Cao & Titi [144] have shown that the only locally integrable stationary solutions of the one- and two-dimensional version of (8.1) are the trivial constant solutions. In addition, Michelson [145] proved the existence of a nontrivial radial steady solution of the two-dimensional problem, that is asymptotically periodic.

One can have the slightly varied KSE in two spatial dimensions

$$u_t + \frac{1}{2} (u_x^2 + \alpha u_y^2) + (u_{xx} + \beta u_{yy}) + \Delta^2 u = 0, \quad (8.9)$$

with initial condition

$$u(x, y, 0) = u_0(x, y), \quad (8.10)$$

and periodic boundary conditions

$$u(x + 2L_x, y, t) = u(x, y + 2L_y, t) = u(x, y, t), \quad (8.11)$$

where α and β are real parameters controlling the anisotropy of the nonlinear and the linear terms. The anisotropic equation in (8.9) was derived by Cuerno & Barabási [126] to describe the nonlinear evolution of surfaces eroded by ion bombardment, also containing a noise term which represented stochastic arrivals of ions. It was also studied by Rost & Krug [146] for different combinations of the signs of α and β . Note that the coefficient α in (8.9) can never become zero when $\beta \neq 0$. In such a case, taking $\alpha = 0$ would make the nonlinear term u_y^2 disappear, thus making the equation “linear” with respect to y . The u_x^2 nonlinear term would transfer energy from the destabilizing term u_{xx} to the stabilizing term u_{xxxx} , but nothing could stop the exponential growth of unstable modes in y (due to the unstable term u_{yy}).

The above equation (8.9) for $\alpha = \beta = 0$, when differentiated with respect to x becomes

$$v_t + vv_x + v_{xx} + \Delta^2 v = 0, \quad (8.12)$$

with $v = u_x$. This is a model equation arising in falling film applications, often

including a dispersive term Δv_x (e.g. see the studies by Saprykin et al. [147] and Toh et al. [148]). Considering equation (8.12) with equal spatial lengths $L_x = L_y = L$, Pinto [149] showed that solutions are bounded for all positive times in the L_2 space and other $\mathcal{H}^m$ spaces. In the same paper the existence of a global attractor with finite dimension was also proved. The estimate for the L_2 -norm upper bound was found to be

$$\limsup_{t \rightarrow \infty} \|v\|_{L_2} \leq \mathcal{O}(L^{12} \log L). \quad (8.13)$$

Pinto [150] also showed time analyticity for solutions of the same equation (8.12). The bound (8.13) is far from optimal and was significantly improved numerically in the work by Akrivis et al. [84], who established the apparently optimal bound of $\mathcal{O}(L^2)$.

Furthermore, it can be proved that solutions of the isotropic equation with $\alpha = \beta$ positive and $\mathcal{O}(1)$ are bounded and mostly develop into travelling waves or become of oscillatory or chaotic type. The symmetric case $\alpha = \beta = 1$, which reduces to the initial equation (8.1), is considered hereafter.

8.3 Aims of this study

The combination of numerical and analytical work on the one-dimensional Kuramoto–Sivashinsky equation provides a clear understanding of its dynamics and their properties. The interesting families of solutions arising from the 1D KS equation, especially the extensive chaotic dynamics, as well as the lack of a clear understanding of the analogous two-dimensional equation are the main reasons for pursuing this study. Although there is a growing body of analytical work for the multi-dimensional Kuramoto–Sivashinsky, there has yet to be a complementary numerical study. Therefore this work is devoted to an exhaustive numerical study of the two-dimensional KS equation.

In the following chapter, a full characterisation of the solutions that arise for different domain sizes is performed by identifying the different attractors and describing their characteristics. It is found that many results extend from the one-dimensional

to the two-dimensional case, including the hierarchy of bifurcations. In addition, to complement and motivate further analytical studies, the energy of the solution is examined in the chaotic regime. Both the dependence of the energy on the system size and how the energy spectrum depends on wavenumber are established. It is shown that equipartition of energy holds in the chaotic regime (for the differentiated version of the equation) and that the energy spectrum is fully symmetric and isotropic. The behaviour of the spectrum is found to depend crucially on the nature of the nonlinearity.

The structure of the second part of the thesis is as follows: Chapter 9 introduces doubly periodic solutions and presents the linear stability properties of the equation. It also provides optimal energy bounds and results proving equipartition of energy and extensive dynamics for the differentiated version of the equation. In the same chapter, detailed numerical results are presented for a large range of domains lengths. Finally, Chapter 10 summarises the main results and findings of this study.

The results presented in this part of the thesis form an article in preparation (Kalogirou, Papageorgiou & Keaveny [151]).

9 Numerical experiments

The aim of this chapter is to provide the mean-zero version of the 2D KSE, which will be the basic equation to be solved numerically. In addition, the linear stability properties of the problem are presented and the numerical methods used are briefly discussed. Optimal energy bounds of the two-dimensional Kuramoto–Sivashinsky equation are also obtained. Furthermore, equipartition of energy and extensive dynamics in the chaotic regime are demonstrated for the differentiated version of the equation. Detailed numerical results for an exhaustive range of domain lengths then follow and the various attractors that arise are described. Solution types include steady states, travelling waves, time-periodic bursts, quasi-periodic and chaotic solutions.

9.1 KS equation on periodic domains

The two-dimensional Kuramoto–Sivashinsky equation is solved numerically on $2L_x \times 2L_y$ -periodic domains, i.e. for solutions satisfying

$$u(x + 2L_x, y, t) = u(x, y + 2L_y, t) = u(x, y, t). \quad (9.1)$$

However, equation (8.1) is not a mean-zero equation as the one-dimensional analogue (8.2) is. To see that, (8.1) is integrated over the domain to yield an equation for the evolution of the mean of u , which is defined by

$$\bar{u}(t) = \frac{1}{4L_x L_y} \int_0^{2L_x} \int_0^{2L_y} u(x, y, t) dx dy. \quad (9.2)$$

The time evolution of the mean $\bar{u}(t)$ is described by the following equation

$$\frac{d}{dt} \bar{u}(t) = -\frac{1}{8L_x L_y} \int_0^{2L_x} \int_0^{2L_y} |\nabla u|^2 dx dy. \quad (9.3)$$

From (9.3) it can be seen that the mean of u grows at least algebraically in time. Thus it is useful to make the equation mean-zero before solving it numerically, in order to avoid dealing with solutions oscillating around a nonzero mean value, which also grows in time (a similar approach was also followed by Hyman et al. [129] for the 1D KSE). This is possible since the nonlinearity does not contribute to the mean and also the mean does not contribute to the dynamics of the other modes (or the other modes to the dynamics of the mean). To achieve this, the $(k_1, k_2) = (0, 0)$ mode is zeroed out which gives the mean of u by definition of Fourier coefficients, i.e. $\hat{u}(0, 0) = \bar{u}(t) = 0$. Therefore, the actual equation solved numerically is the following mean-zero equation for $v(x, y, t) = u(x, y, t) - \bar{u}(t)$,

$$v_t + \frac{1}{2} \left(|\nabla v|^2 - \frac{1}{4L_x L_y} \int_0^{2L_x} \int_0^{2L_y} |\nabla v|^2 dx dy \right) + \Delta v + \Delta^2 v = 0. \quad (9.4)$$

As done with the 1D KS equation, the mean can also be removed by differentiating (8.1) and casting it in a mean-zero form. Many researchers [140, 141, 142, 144] used

a similar technique for the 2D KSE by differentiating it with respect to x and y and reached a system of two mean-zero equations (similar to the 1D analogue equation (8.2)). The system is obtained by setting $U_1 = u_x$ and $U_2 = u_y$ and using the fact that $U_{1y} = U_{2x}$, transforming (8.1) into

$$\mathbf{U}_t + (\mathbf{U} \cdot \nabla) \mathbf{U} + \Delta \mathbf{U} + \Delta^2 \mathbf{U} = 0, \quad (9.5)$$

where $\mathbf{U} = (U_1, U_2)^T$. Using again the property $U_{1y} = U_{2x}$ converts the system (9.5) into

$$\mathbf{U}_t + \frac{1}{2} \nabla (\mathbf{U} \cdot \mathbf{U}) + \nabla (\nabla \cdot \mathbf{U}) + \nabla (\Delta (\nabla \cdot \mathbf{U})) = 0. \quad (9.6)$$

Taking the curl of equation (9.6) and using the fact that the curl of a gradient is zero, gives the conservation of curl $\mathbf{U}$ in time, i.e. $(\nabla \times \mathbf{U})_t = \mathbf{0}$. The initial conditions $\mathbf{U}^0 = (U_1^0, U_2^0)$ must be chosen such that they satisfy $\nabla \times \mathbf{U}^0 = (0, U_{2x}^0 - U_{1y}^0) = \mathbf{0}$ to ensure that $\text{curl } \mathbf{U} = \text{curl } \mathbf{U}^0$ remains zero throughout the numerical experiments. However, during the numerical calculations $\text{curl } \mathbf{U}$ was growing in time, eventually tending to a constant of about 10^{-7} which is larger than desired (a value of 10^{-16} is essentially zero in double-precision accuracy). Thus it was decided to return to the single equation (8.1) and work with its mean-zero version (9.4).

Finally, it is common to rescale the Kuramoto–Sivashinsky into domains with length 2π , so the two-dimensional equation considered here is rescaled into the domain $[0, 2\pi] \times [0, 2\pi]$ via the transformations

$$x \rightarrow \frac{L_x}{\pi} x, \quad y \rightarrow \frac{L_y}{\pi} y, \quad t \rightarrow \left(\frac{L_x}{\pi} \right)^2 t. \quad (9.7)$$

The transformed equation is given by

$$u_t + \frac{1}{2} |\nabla_\nu u|^2 + \Delta_\nu u + \nu_1 \Delta_\nu^2 u = 0, \quad (9.8)$$

where

$$\nabla_\nu = \left(\partial_x, \frac{\nu_2}{\nu_1} \partial_y \right), \quad \Delta_\nu = \partial_x^2 + \frac{\nu_2}{\nu_1} \partial_y^2, \quad (9.9)$$

are the transformed operators and

$$\nu_1 = \left(\frac{\pi}{L_x}\right)^2, \quad \nu_2 = \left(\frac{\pi}{L_y}\right)^2, \quad (9.10)$$

are bifurcation parameters that play an important role in the dynamics; they decrease as L_x, L_y increase respectively, introducing more unstable modes in the dynamics. The corresponding rescaled mean-zero equation for $v(x, y, t) = u(x, y, t) - \bar{u}(t)$ is

$$v_t + \frac{1}{2} \left(|\nabla_\nu v|^2 - \frac{1}{4\pi^2} \int_0^{2\pi} \int_0^{2\pi} |\nabla_\nu v|^2 dx dy \right) + \Delta_\nu v + \nu_1 \Delta_\nu^2 v = 0. \quad (9.11)$$

Note that with solutions of (9.11) in hand, one can easily transform back to solutions of the unscaled problem on the doubly periodic domain $[0, 2L_x] \times [0, 2L_y]$. The unscaled solutions are used in several places in the sequel and this interchange is quite straightforward.

9.2 Linear stability

Performing a linear stability analysis before solving the problem numerically can be useful in order to provide the region of instability in parameter space. Perturbing about the uniform state $v = 0$, a normal mode solution is sought in the form

$$v(x, y, t) = \delta \left(e^{i(n_1 x + n_2 y) + \sigma t} + c.c. \right), \quad (9.12)$$

where n_1, n_2 are non-zero integer wavenumbers in the x - and y -directions respectively, δ is infinitesimal, σ is the complex amplification rate and c.c. denotes complex conjugates. Substituting (9.12) into (9.11), results in the following dispersion relation

$$\sigma = \left(n_1^2 + \frac{\nu_2}{\nu_1} n_2^2 \right) (1 - \nu_1 n_1^2 - \nu_2 n_2^2). \quad (9.13)$$

From this equation it can be seen that the solution $v = 0$ is unstable if the growth rate σ is positive, which is possible if

$$\nu_1 n_1^2 + \nu_2 n_2^2 < 1. \quad (9.14)$$

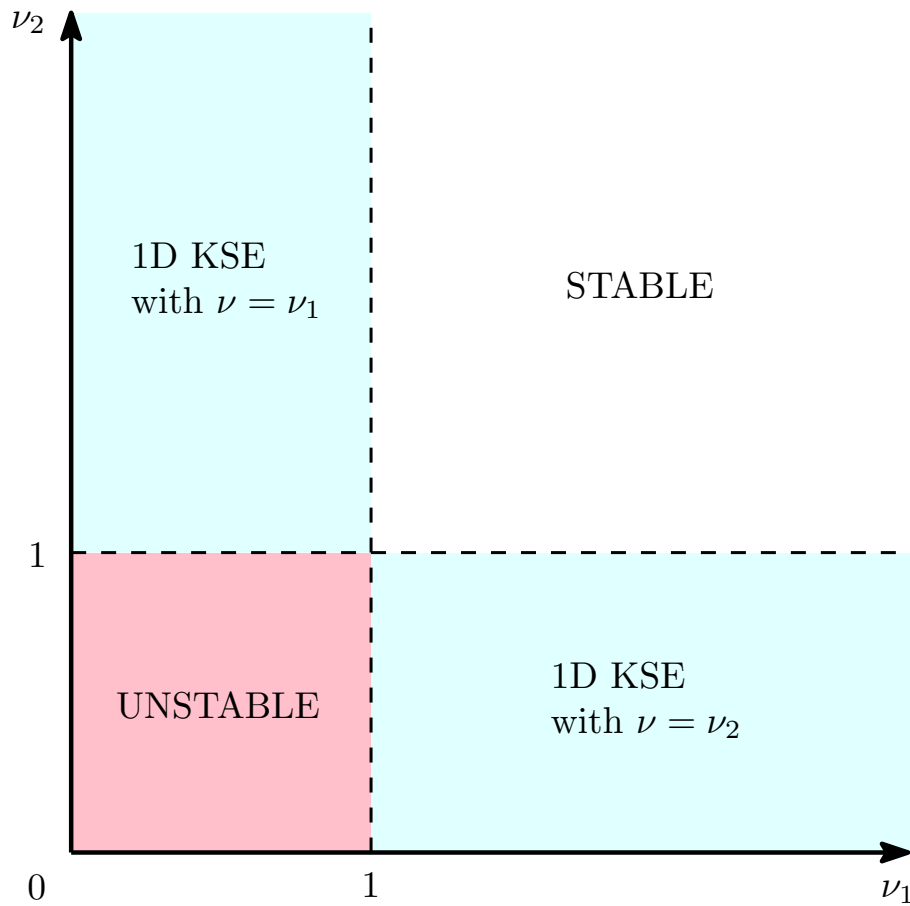


Figure 46: Stability diagram for the two-dimensional Kuramoto-Sivashinsky equation, showing regions of stability and instability depending on the values of ν_1, ν_2 . The equation is stable when both $\nu_1, \nu_2 > 1$. If only one of ν_1, ν_2 is smaller than 1, then dynamics are described by the 1D KSE with ν equal to ν_1 or ν_2 , whichever is smaller than 1. If both $\nu_1, \nu_2 < 1$ then the solutions are completely two-dimensional.

The condition (9.14) determines the domain of instability in the ν_1, ν_2 parameter space for every choice of wavenumbers (n_1, n_2) . Equivalently, it gives the unstable modes (n_1, n_2) for all values of ν_1, ν_2 . It therefore establishes the parameter regime that is of interest and serves for finding suitable initial conditions (which provide the range of unstable modes in the problem). The stability properties of the problem are outlined in Figure 46 and explained in detail below.

For $\nu_1 > 1$ and $\nu_2 > 1$, condition (9.14) cannot be satisfied for any $n_1, n_2 \in \mathbb{Z}_+$, thus all solutions are stable and decay to zero after a short time. If at least one of ν_1 or ν_2 is less than unity, the initial conditions provide the range of unstable modes. For instance, if the initial condition is $u(x, y, 0) = \sin(x+y)$ where $n_1 = 1$ and $n_2 = 1$, then a positive growth rate is ensured if $\nu_1 + \nu_2 < 1$ (with equality corresponding to a diagonal line connecting $\nu_1 = 1$ and $\nu_2 = 1$ on the diagram in Figure 46). A choice of an initial condition independent of y , results in the instability condition being independent of ν_2 . In addition to that, the solution v remains independent of y for all times. In this case the time evolution of the 2D KSE is the same as the 1D KSE with $\nu = \nu_1$. Similar observations apply in the case of x -independent initial conditions in which case the solution remains independent of x for all subsequent times and is essentially the same as the one obtained from the 1D KSE with $\nu = \nu_2$.

Based on the above arguments, which are summarised in Figure 46, the initial condition used in the numerical experiments was chosen carefully so that it lies in the shaded square created by lines $\nu_1 = 1$ and $\nu_2 = 1$. To be more specific, the following initial condition was used in all the numerical calculations

$$v(x, y, 0) = \sin(x + y) + \sin(x) + \sin(y). \quad (9.15)$$

This gives three unstable modes $(n_1, n_2) = (1, 1), (1, 0), (0, 1)$ and rich dynamical behaviour, including quasi-periodic and chaotic solutions, which will be presented in the next sections.

The initial value problem (9.11), (9.15) is solved numerically using a pseudospectral Fourier method. The space discretisation is achieved by writing the solution in terms of Fourier series (this is possible because of periodicity of the solution) and

considering a system of ordinary differential equations for a finite number of Fourier modes. The spatial domain $[0, 2\pi]$ in the x -direction is split into $2M_x$ equidistant points and similarly the domain in the y -direction is discretised using $2M_y$ points. The resulting ODEs are then integrated in time using a second-order stable and accurate BDF scheme. The numerical analysis and details about the method are described in Appendix F.

9.3 Energy equipartition in chaotic regime

Before presenting the numerical results and all the different solutions that arise as ν_1 and ν_2 vary, the statistical properties of the chaotic regime are explored. It will be shown in Section 9.4 which follows that large-time solutions exhibit spatiotemporal chaotic behaviour for small values of ν_1, ν_2 (equivalently large values of L_x, L_y). The study of the properties of the chaotic solutions is important in order to establish energy bounds as the system size increases.

Many authors in the past have shown interest in studying how the energy density and spectrum of the one-dimensional KSE depend on the system size as it becomes larger. Their results suggest that the average energy density is bounded independently of the system size L and that the energy is equipartitioned between low wavenumbers. Similar properties are investigated here for the 2D KSE for large enough values of L_x, L_y (it is equivalent to studying the limit $\nu_1, \nu_2 \rightarrow 0$, but the statistical properties of the chaotic regime are better observed against L_x, L_y). This is achieved by solving equation (9.4) in the domain $[0, 2L_x] \times [0, 2L_y]$ in the limit $L_x, L_y \rightarrow \infty$ (usually taken ≥ 30 in computations). The energy is defined to be

$$E(L_x, L_y, t) = \int_0^{2L_x} \int_0^{2L_y} v^2(x, y, t) dx dy. \quad (9.16)$$

The rapid oscillations of the solutions suggest a universal bound for both space and time averages of the solutions (Giacomelli & Otto [136]), therefore it is reasonable to study how the time-average of the energy varies as the system size increases.

Additionally, the averaged energy spectrum is given by

$$S(k_1, k_2) = 4L_x L_y \langle |\hat{v}(k_1, k_2, t)|^2 \rangle = \frac{1}{T_2 - T_1} \int_{T_1}^{T_2} 4L_x L_y |\hat{v}(k_1, k_2, t)|^2 dt, \quad (9.17)$$

which is normalised by being multiplied by $4L_x L_y$. Here, $\langle \cdot \rangle$ denotes time-average and $T_2 > T_1$ are sufficiently large times chosen so that the solution enters the chaotic attractor and the total duration $T_2 - T_1$ is large enough to obtain convergence to a time-average value. Note also that the *physical* spectrum $S(k_1, k_2)$ is equal to the *canonical* spectrum $S_\pi(n_1, n_2)$ coming from the rescaled equation in $[0, 2\pi] \times [0, 2\pi]$ domains, which can be verified as follows¹³

$$S(k_1, k_2) = 4L_x L_y \langle |\hat{v}(k_1, k_2, t)|^2 \rangle = \frac{2\pi}{\sqrt{\nu_1}} \frac{2\pi}{\sqrt{\nu_2}} \langle |\hat{v}(n_1, n_2, \nu_1 t)|^2 \rangle = S_\pi(n_1, n_2). \quad (9.18)$$

The one-dimensional case has been studied by various authors [129, 132, 152], as discussed in the introduction. Their results are reproduced here and summarised in Figure 47. Figure 47(a) shows the time-averaged energy $\langle E(L, t) \rangle$, where the energy is now given by

$$E(L, t) = \|v\|_{L_2}^2 = \int_0^{2L} v^2(x, t) dx. \quad (9.19)$$

As reported in Wittenberg & Holmes [132], it can be seen that $\langle E(L, t) \rangle$ is asymptotically proportional to the system size L (this conclusively suggests that the solution v remains of $\mathcal{O}(1)$ as L increases). This means that the energy density $\frac{1}{L} \langle E(L, t) \rangle$ is finite as $L \rightarrow \infty$. The numerically observed upper bound for the L_2 -norm

$$\limsup_{t \rightarrow \infty} \|v\|_{L_2} \leq cL^{1/2}, \quad (9.20)$$

provides the smallest exponent and has not yet been obtained analytically; the best available analytic bound is $\mathcal{O}(L^{5/6+})$ (Otto [137]) (c.f. earlier comments).

¹³Having transformations (9.7) in mind, it follows that a two-dimensional perturbation of wavenumbers $n_1, n_2 \in \mathbb{Z}$ in the canonical domain $[0, 2\pi] \times [0, 2\pi]$ corresponds to a perturbation of wavenumbers $k_1 = n_1 \sqrt{\nu_1}$, $k_2 = n_2 \sqrt{\nu_2}$ in the physical domain $[0, 2L_x] \times [0, 2L_y]$.

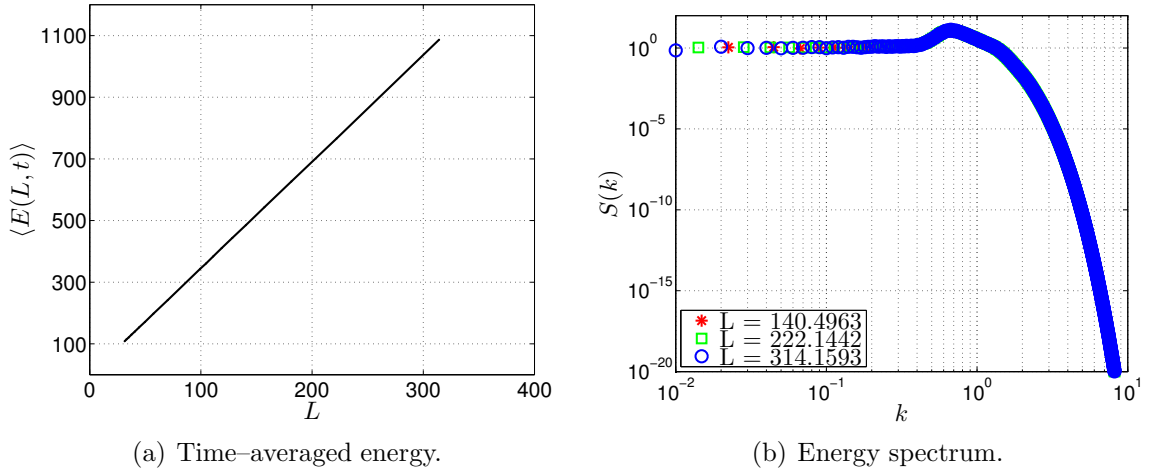


Figure 47: Statistical characteristics of the solutions of the one-dimensional Kuramoto–Sivashinsky equation in the chaotic regime. (a) Average energy growing linearly with L . (b) Energy spectrum independent of the value of L in the small wavenumber region.

Figure 47(b) also shows the spectral energy

$$S(k) = 2L \langle |\hat{v}(k, t)|^2 \rangle, \quad (9.21)$$

plotted against $k = \frac{n\pi}{L}$, $n \in \mathbb{Z}$, for three different domain lengths $2L$ approximately equal to 280, 445 and 630, all of which yield chaotic solutions. It can be seen that the spectral energy is flat in the large scale region, hence it has an invariant distribution among the small wavenumbers; this property is called *equipartition* of energy. In the same region, the energy spectrum also has the same density and distribution independently of the value of L . This is in line with the feature of the 1D KS showing *extensive dynamics*, that is, the large system can be decomposed into smaller subsystems which essentially have the same behaviour. Most of the energy is contained into the small wavenumbers, and dissipation leads to an exponential decay at large wavenumbers. An energy peak occurs at approximately $k \sim \frac{1}{\sqrt{2}}$, which coincides with the most unstable mode predicted by linear stability¹⁴.

¹⁴The linear growth rate for the 1D KSE is $\sigma = k^2 - k^4 = \left(\frac{n\pi}{L}\right)^2 \left(1 - \left(\frac{n\pi}{L}\right)^2\right)$, which provides instability for long waves, i.e. if $k < 1$, and reaches its maximum at $k = \frac{1}{\sqrt{2}}$.

In this study, the aim is to obtain analogous results for the two-dimensional problem. More specifically, large-time solutions are computed for the following three cases of L_x, L_y :

Case i: $L_x = L_y = L$ and $L \gg 1$

Similarly to the 1D case, here the equation is solved over square domains that increase in size. The time-averaged energy $\langle E(L, L, t) \rangle$ is plotted against L^2 in Figure 48(a) and the result is clearly linear. Plotting the energy against L in a logarithmic scale plot returns a linear relationship, and using a least squares fit of the line returns a value of 2.0203. This allows drawing the conclusion

$$\langle E(L, L, t) \rangle \sim cL^2, \quad L \gg 1, \quad (9.22)$$

where c is a positive constant independent of L .

Case ii: $L_x = 10L_y = 10L$ and $L \gg 1$

This case is similar to *Case i*, but the domain is now rectangular and 10 times longer than wide. The result is again $\langle E(10L, L, t) \rangle = \mathcal{O}(L^2)$. Though not shown, a slope of about 1.9667 is obtained by a least squares fit of the data in logarithmic scales.

Case iii: L_y fixed, $L_x \gg 1$

Here the domain is a rectangle with fixed width L_y and increasing length L_x . For two fixed values of $L_y = \sqrt{2}\pi$ and $L_y = 2\pi$ the averaged energy is plotted against $L_x L_y$ and the result can be seen in Figure 48(b). Note that both values of L_y are greater than π and thus there exist unstable y modes in the problem. An estimation of the slopes is calculated using least squares and they are found to be approximately 1.0120 for $L_y = \sqrt{2}\pi$ and 1.0116 for $L_y = 2\pi$. Consequently it is shown that when one of the two domain lengths is fixed and the other is increased, then the average energy scales with the dimension that is varied and the dynamics are analogous to 1D ones.

The next set of results provide the characteristics of the energy spectrum in the chaotic regime for domain sizes chosen from *Cases i* or *ii*. The numerically computed

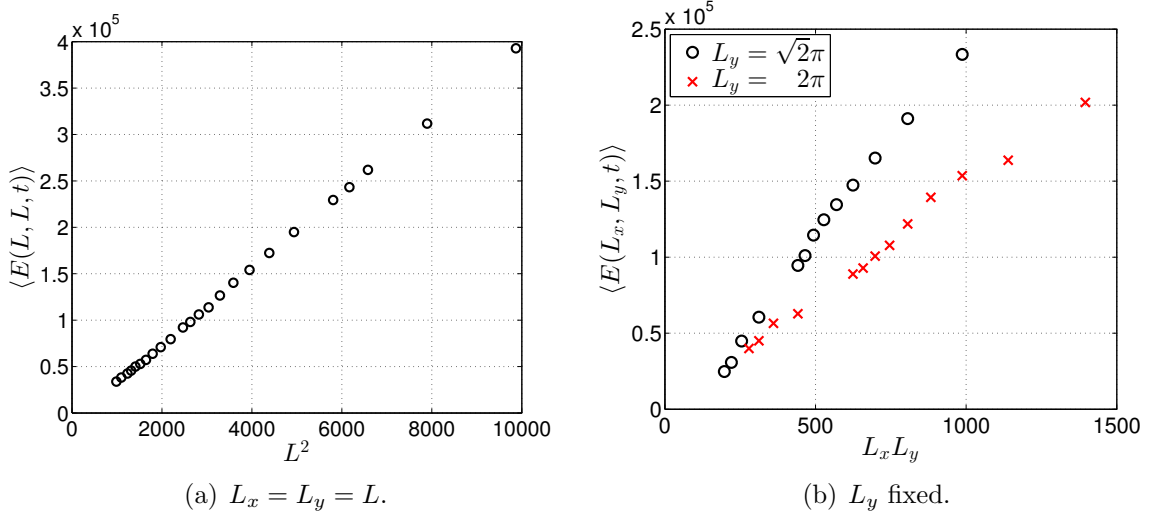


Figure 48: Time-average of the energy of the two-dimensional Kuramoto–Sivashinsky equation. (a) Equal domain lengths $L_x = L_y = L$ with $L \gg 1$, in which case the energy grows proportionally to L^2 . (b) Increasingly longer square domains with $L_x \gg 1$ and L_y fixed. Two cases considered for $L_y = \sqrt{2}\pi$ (crossmarks) and $L_y = 2\pi$ (circles); in both cases the energy is proportional to L_x .

spectrum is shown in Figure 49(a) against

$$k = \sqrt{k_1^2 + k_2^2} = \sqrt{\left(\frac{n_1\pi}{L_x}\right)^2 + \left(\frac{n_2\pi}{L_y}\right)^2}, \quad (9.23)$$

where $n_1, n_2 \in \mathbb{Z}$, for two different sets of (L_x, L_y) . It can be seen that the two spectra have the same form for both sets of (L_x, L_y) , as observed in the case of the one-dimensional Kuramoto–Sivashinsky equation (Toh [153]). A notable difference from the 1D case is the small wavenumber behaviour of the spectrum; it behaves like $S(k_1, k_2) \sim k^{-2}$ instead of reaching a constant value. The factor of k^{-2} is attributed to the form of the nonlinearity in equation (9.4) being v_x^2 instead of vv_x (like the 1D KS), and it originates because the latter nonlinearity comes from differentiation of the former; a more detailed argument follows.

It should be first noted that the well-known 1D KS equation (8.2) is actually a differentiated version of the original equation (8.1) derived by Kuramoto and Sivashinsky. Therefore the differentiated 1D KSE spectrum presented in Figure 47(b) has an

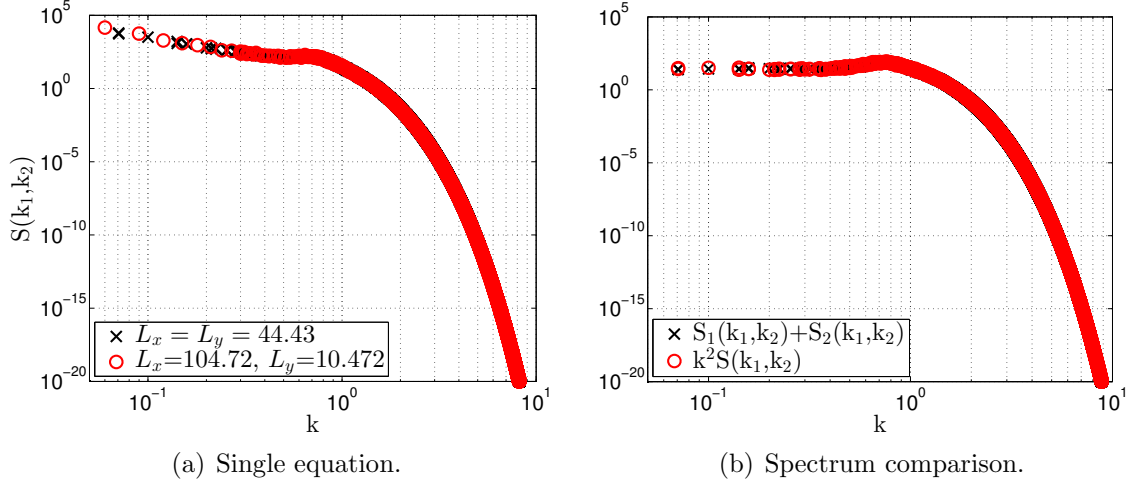


Figure 49: Energy spectrum of the two-dimensional Kuramoto–Sivashinsky equation. (a) Spectrum obtained by the single equation for two different sets of (L_x, L_y) , namely $L_x = L_y = \frac{\pi}{\sqrt{0.005}} = 44.43$ and $L_x = 10L_y = \frac{\pi}{\sqrt{0.0009}} = 104.72$. (b) Comparison between spectrum $k^2 S(k_1, k_2)$ obtained by the single equation (9.4) and the sum of the spectra $S_1(k_1, k_2) + S_2(k_1, k_2)$ from the system (9.5), for $L_x = L_y = \frac{\pi}{\sqrt{0.005}} = 44.43$.

additional factor of $|ik|^2 = k^2$, compared to the spectrum of the non-differentiated equation (8.1). A similar behaviour as the one seen in Figure 49(a) was also reported by Yamada and Kuramoto [154] for the one-dimensional KSE, where the authors studied the equation in its non-differentiated form. Consequently, when looking at the two-dimensional problem (9.4), the solution v should be missing a k^2 factor when compared to the differentiated ones $U_1 = v_x$, $U_2 = v_y$ coming from system (9.5). Indeed, in Fourier space,

$$|\widehat{U}_{1k}|^2 = |(\widehat{v}_x)_k|^2 = |ik_1 \widehat{v}_k|^2 = k_1^2 |\widehat{v}_k|^2, \quad (9.24a)$$

$$|\widehat{U}_{2k}|^2 = |(\widehat{v}_y)_k|^2 = |ik_2 \widehat{v}_k|^2 = k_2^2 |\widehat{v}_k|^2, \quad (9.24b)$$

so adding them together gives

$$|\widehat{U}_{1k}|^2 + |\widehat{U}_{2k}|^2 = (k_1^2 + k_2^2) |\widehat{v}_k|^2 = k^2 |\widehat{v}_k|^2. \quad (9.25)$$

Figure 49(b) illustrates a comparison between the spectrum $k^2 S(k_1, k_2)$ resulting from

the single equation (9.4) and the sum of the two spectra $S_1(k_1, k_2) + S_2(k_1, k_2)$ coming from the system (9.5), for $L_x = L_y = \frac{\pi}{\sqrt{0.005}}$. Here $S_i(k_1, k_2) = \langle |\widehat{U}_{ik}|^2 \rangle$, $i = 1, 2$. The infinitesimal difference between the two confirms what is shown in (9.25).

It remains to explain why the two-dimensional spectrum is a function of the magnitude of the wavenumber $k = \sqrt{k_1^2 + k_2^2}$ only, as observed in Figure 49. In order to prove this, equation (9.4) is first considered in Fourier space and then being multiplied by $\hat{v}_k^*$ (stars * denote complex conjugates), to yield

$$\hat{v}_k^* \left((\hat{v}_k)_t + \frac{1}{2} \left(\widehat{|\nabla v|^2} \right)_k - (k^2 - k^4) \hat{v}_k \right) = \hat{c}_0. \quad (9.26)$$

Taking complex conjugate gives

$$\hat{v}_k \left((\hat{v}_k^*)_t + \frac{1}{2} \left(\widehat{|\nabla v|^2} \right)_k^* - (k^2 - k^4) \hat{v}_k^* \right) = \hat{c}_0^*. \quad (9.27)$$

Here, $\hat{c}_0$ is the $(0, 0)$ Fourier coefficient of the integral term $\frac{1}{4L_x L_y} \int_0^{2L_x} \int_0^{2L_y} |\nabla v|^2 dx dy$, which is a real function of t only and thus $\hat{c}_0^* = \hat{c}_0$. Adding (9.26) and (9.27) together and averaging in time, results in

$$\frac{d}{dt} \langle |\hat{v}_k|^2 \rangle + \left\langle \hat{v}_k^* \left(\widehat{|\nabla v|^2} \right)_k + \hat{v}_k \left(\widehat{|\nabla v|^2} \right)_k^* \right\rangle - 2(k^2 - k^4) \langle |\hat{v}_k|^2 \rangle = 2 \langle \hat{c}_0 \rangle. \quad (9.28)$$

Here, the time-derivative term $\frac{d}{dt} \langle |\hat{v}_k|^2 \rangle$ is zero because the time-average over different (large) times is the same, and the right hand side term is independent of k . Thus $\langle |\hat{v}_k|^2 \rangle$ will only be a function of k if the nonlinear term $\left\langle \hat{v}_k^* \left(\widehat{|\nabla v|^2} \right)_k + \hat{v}_k \left(\widehat{|\nabla v|^2} \right)_k^* \right\rangle$ only depends on k . As a consistency check, this term was calculated numerically and was also found to be a function of k only.

One would probably ask why the averaged energy spectrum is isotropic with respect to k_1, k_2 . The answer is given below by studying an *asymmetric* equation similar to the 2D KSE and noting that the 2D KSE is fully *symmetric* with respect to x and y . The results provide evidence that the behaviour of the spectrum is completely linked to the nature of the nonlinearity. The following KS-type equation

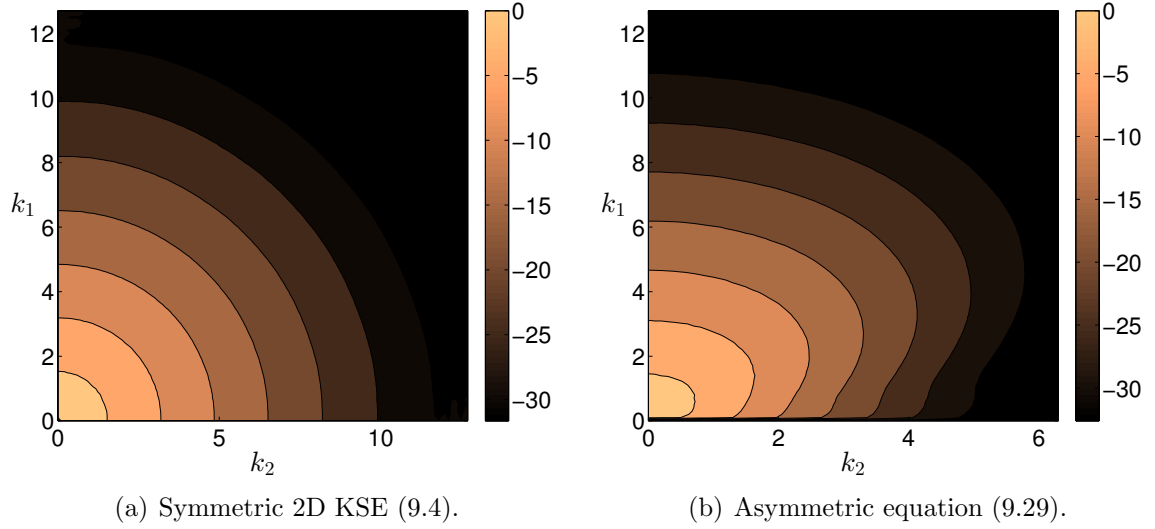


Figure 50: Energy spectrum obtained by (a) the symmetric 2D KSE (9.4) and (b) the asymmetric KS-type equation (9.29), for $L_x = L_y = \frac{\pi}{\sqrt{0.01}} = 31.416$.

$$v_t + vv_x + v_{xx} + \Delta^2 v = 0, \quad (9.29)$$

lacks symmetry in both the nonlinear and linear terms, and is a right choice for an asymmetric equation that would have similar dynamics to the standard 2D KSE. It arises from falling film applications with surface tension and it was studied by various authors (Akrivis et al. [84], Toh et al. [148], Indireshkumar & Frenkel [155]), sometimes in the presence of a dispersive term $\delta\Delta(v_x)$.

Indeed, the spectrum of the above equation is non-symmetric and can be seen and compared to the symmetric 2D KSE spectrum in Figure 50. Panel (a) illustrates a top view of the $S(k_1, k_2)$ surface against k_1 and k_2 , and panel (b) shows the corresponding result for the asymmetric equation (9.29). Both panels are for system lengths $L_x = L_y = \frac{\pi}{\sqrt{0.01}}$. Note that it is not necessary to have $L_x = L_y$ to obtain a radially symmetric spectrum of the equation (9.4), but it is also symmetric for $L_x \neq L_y$.

In fact, the radius of the absorbing ball in L_2 was computed for square domains with $L_x = L_y = L$ and for L sufficiently large (this work is part of an article by Akrivis, Kalogirou, Papageorgiou & Smyrlis [84], submitted to the *IMA J. Numer. Anal.*). The initial condition $v(x, y, 0)$ is taken to consist of a large range of linearly

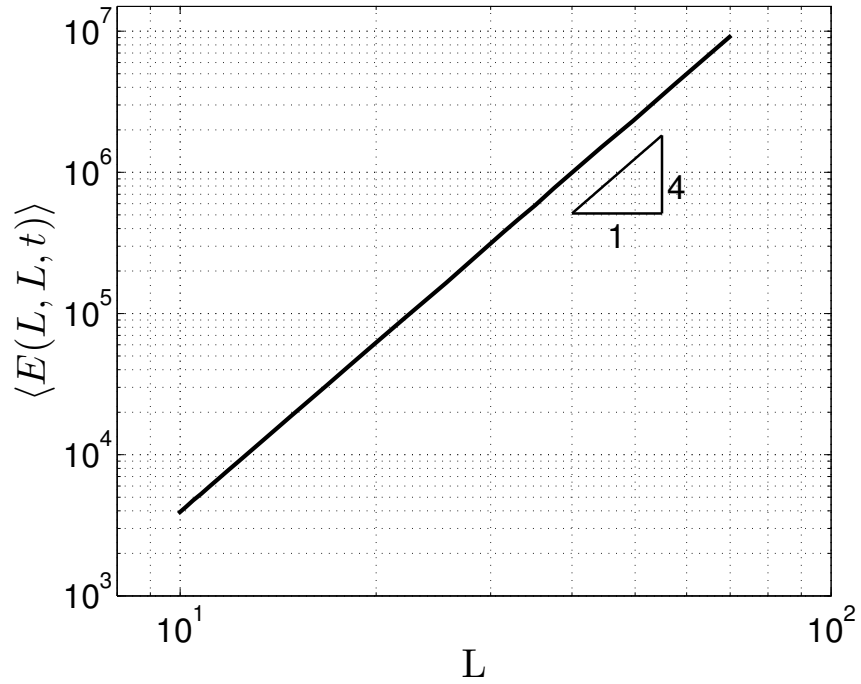


Figure 51: Log-log plot of the time-averaged energy against L , for the solutions obtained by the asymmetric KS-type equation (9.29). The slope of the line is approximately equal to 4.

unstable Fourier modes with random amplitudes. The averaged energy is plotted as a function of L using logarithmic scales in Figure 51. The slope of $\langle E(L, L, t) \rangle$ was obtained using a least squares fit of the data presented in Figure 51 to obtain a value of 3.9865. This strongly suggests that

$$\langle E(L, L, t) \rangle \sim cL^4, \quad L \gg 1, \quad (9.30)$$

for a constant $c > 0$ independent of L . Surprisingly, this bound is different from the corresponding bound in (9.22) for the symmetric 2D KS equation. The reason this result is observed is because the solution in this case grows proportionally to L for $L \gg 1$, in contrast to known results for the 1D KS equation which suggest that $u = \mathcal{O}(1)$ for $L \gg 1$. Consequently, further work is required in order to explain this remarkable behaviour.

9.4 Numerical solutions and dynamics

Numerical results that arise by solving initial value problems are presented next in the direction of identifying the various dynamics of the solutions. The initial value problem (9.11), (9.15) is solved for a range of parameter values ν_1, ν_2 in the unstable region predicted by linear stability, namely for $0 < \nu_1, \nu_2 \leq 1$. Many different types of solutions arise, including complex dynamics as $\nu_1, \nu_2 \rightarrow 0$, which will be described in detail later in this section. For the one-dimensional equation, numerical studies as $\nu \rightarrow 0$ have shown the existence of a wide range of attractors. For relatively large values of ν in the range $0.3 < \nu < 1$, steady states solutions are found. Smaller values of ν give rise to travelling waves, time-periodic bursts and finally chaos for about $\nu = 0.12115$, via a period-doubling route and according to the Feigenbaum scenario (Papageorgiou & Smyrlis [9], Smyrlis & Papageorgiou [10, 11]). For the two-dimensional equation, though, the domain of instability provides infinitely many routes leading to chaotic dynamics. In this case, transition to chaos depends on the path in parameter space (ν_1, ν_2) . Two different paths are examined as part of this study and the results will be presented later; these are $\nu_1 = \nu_2 = \nu$ with $\nu \rightarrow 0$, and $\nu_2 \rightarrow 0$ with ν_1 fixed.

Numerical simulations are carried out over the unstable range of ν_1 and ν_2 with step size 0.05 and solutions are classified over this region. A useful symmetry of the 2D KSE about $\nu_1 = \nu_2$ (under a space and a time scale transformation) is used to reduce the domain over which solutions are calculated numerically.

<u>Parameter values</u>		<u>Solution</u>
(ν_1, ν_2)	$\longrightarrow$	$u(x, y, t)$
(ν_2, ν_1)	$\longrightarrow$	$u\left(y, x, \frac{\nu_2}{\nu_1}t\right)$

That is, if $u(x, y, t)$ is the solution obtained for the parameter set (ν_1, ν_2) , then the one corresponding to (ν_2, ν_1) is $u\left(y, x, \frac{\nu_2}{\nu_1}t\right)$ (the property can be clearly seen by multiplying through the equation by $\frac{\nu_1}{\nu_2}$). This feature is used in the numerical computations to reduce the computational domain by half, namely only solutions corresponding to $\nu_1 \geq \nu_2$ are calculated and the ones for $\nu_1 < \nu_2$ are obtained through the above

symmetry. The numerical results are summarised in the phase diagram in Figure 52 and all the different states are noted by different coloured circles. The diagram includes a relatively large region of steady states (SS), starting from the bifurcation point $(\nu_1, \nu_2) = (1, 1)$ and covering almost half of the computational domain. Steady state solutions are followed by travelling waves (TW) or time-periodic waves (TP), including periodic homoclinic bursts (PHoB) and periodic heteroclinic bursts (PHeB). For relatively small values of ν_1, ν_2 , more complex solutions arise, which are characterised by quasi-periodic (QP) or chaotic (C) oscillations in time. Chaotic solutions also appear in the form of chaotic homoclinic bursts (CHoB) or chaotic heteroclinic bursts (CHeB).

In what follows, the various types of solutions presented in Figure 52 are characterised and analysed in detail. The analysis will first focus on different cuts from the phase diagram that might be similar to the one-dimensional KSE for $\nu \rightarrow 0$, stating the similarities and differences with the 1D case. Afterwards, the different states will be considered, starting from steady states, going to travelling waves, then to various time-periodic bursts and finally to quasi-periodicity and chaos. The different attractors found numerically will be evaluated using several helpful tools, including the energy of the solution defined by

$$E(t) := \|v(\cdot, \cdot, t)\|_{L_2}^2 = \int_0^{2\pi} \int_0^{2\pi} v^2(x, y, t) dx dy. \quad (9.31)$$

Note that the above energy definition is related to one presented in (9.16) for $2L_x \times 2L_y$ -periodic domains by $E(t) = \sqrt{\nu_1} \sqrt{\nu_2} E(L_x, L_y, t)$. The calculation of $\dot{E}(t)$ is obtained by multiplying (9.11) by v and integrating over a period, yielding

$$\begin{aligned} \dot{E}(t) = 2\|v_x\|^2 + 2\frac{\nu_2}{\nu_1}\|v_y\|^2 - 2\nu_1\|v_{xx}\|^2 - 4\nu_2\|v_{xy}\|^2 - 2\frac{\nu_2^2}{\nu_1}\|v_{yy}\|^2 \\ - \int_0^{2\pi} \int_0^{2\pi} \left(v_x^2 + \frac{\nu_2}{\nu_1} v_y^2 \right) v dx dy. \end{aligned} \quad (9.32)$$

The computations of $E(t)$ and $\dot{E}(t)$ are both performed with spectral accuracy and are used in phase-plane constructions $(E(t), \dot{E}(t))$ and return maps consisting of the

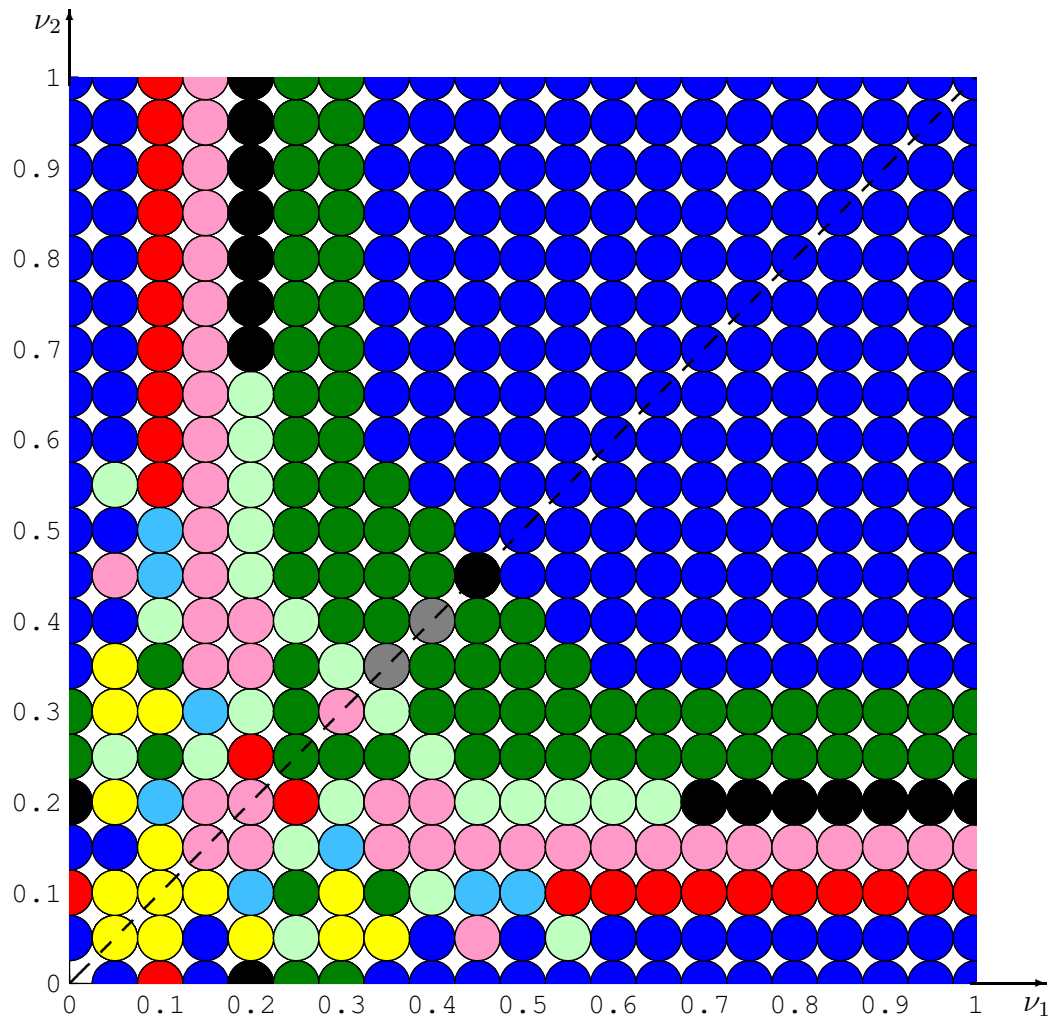


Figure 52: Parameter space diagram classifying the various solution types obtained from the two-dimensional Kuramoto–Sivashinsky equation, for parameter values in the range $0 < \nu_1, \nu_2 \leq 1$.

Key to colours:

● Steady states (SS)	● Periodic homoclinic bursts (PHoB)	● Chaotic homoclinic bursts (CHoB)
● Travelling waves (TW)	● Periodic heteroclinic bursts (PHeB)	● Chaotic heteroclinic bursts (CHeB)
● Time-periodic waves (TP)	● Quasi-periodic solutions (QP)	● Chaotic solutions (C)

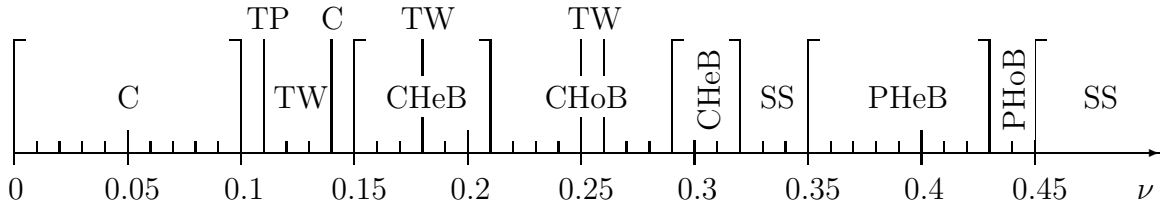


Figure 53: Dynamical behaviour of solutions obtained for $\nu_1 = \nu_2 = \nu$. Key to solution types abbreviations: SS – steady states, PHoB – periodic-homoclinic bursts, PHeB – periodic heteroclinic bursts, TW – travelling waves, TP – time-periodic solutions, CHoB – chaotic homoclinic bursts, CHeB – chaotic heteroclinic bursts, C – chaotic solutions.

minimum points of $\dot{E}(t) = 0$, denoted by E_n , $n = 1, 2, \dots$ (for more details, see Section 5.5).

To begin with, extensive numerical calculations are performed on square domains, namely for $\nu_1 = \nu_2$, with step size 0.01. An outline of the various solution types obtained for different $\nu = \nu_1 = \nu_2$ is given in the schematic diagram in Figure 53. The first solutions to emerge are steady states for parameter values $0.45 \leq \nu < 1$. For $0.43 < \nu < 0.45$, the fixed point attractor overlaps with a time-periodic attractor and for smaller $0.35 \leq \nu \leq 0.45$ it competes with another fixed point, to give periodic heteroclinic bursts in the energy plot. The first chaotic solutions arise for ν as high as 0.32, which are then interchanged with travelling wave windows to follow a transition to chaos as ν decreases further. This route to chaos does not appear to follow the pattern of period-doubling as in the case of the one-dimensional KSE (Papageorgiou & Smyrlis [9], Smyrlis & Papageorgiou [11]). A notable characteristic of the chaotic solutions is that they remain $\mathcal{O}(1)$ as ν decreases but the number of oscillations in the profiles becomes increasingly larger (a similar result holds for the 1D KS and it was proved analytically that the number of rapid spatial oscillations increases linearly with the system size (Grujić [139])).

In order to investigate the development of the solutions in the limit $\nu_2 \rightarrow 0$, the region for small but fixed ν_1 between $0 < \nu_1 \leq 0.35$ and $\nu_2 \leq \nu_1$ is also particularly emphasised. The aim is to examine if for a fixed ν_1 , two-dimensional solutions obtained for $\nu_2 \rightarrow 0$ reduce to the solution of the one-dimensional KSE with $\nu = \nu_1$ (or

Table 6: Dynamical behaviour of solutions for $0 < \nu_1 \leq 0.35$ and $\nu_2 < 0.05$. The solutions in the limit $\nu_2 \rightarrow 0$ do not reduce to the one-dimensional KSE with $\nu = \nu_1$. For a key to solution types see the caption of Figure 53. The new solution type in this table is TP[m], which indicates a time-periodic solution with m distinct minima in one time period of the energy signal.

$\nu_2 \backslash \nu_1$	0.05	0.10	0.15	0.20	0.25	0.30	0.35
0.04	C	C	TP[1]	C	C	C	C
0.03	C	C	QP	C	TP[1]	C	C
0.02	C	C	C	C	TW	TP[3]	C
0.01	C	C	C	C	TP[5]	C	C
0.005	C	C	C	C	TP[1]	C	C
1D KSE $\nu = \nu_1$	SS	CHoB	SS	PHoB	TW	TW	SS

equivalently, the 2D KS solution for $\nu_2 = 0$). The results are summarised in Table 6. It can be seen that as ν_2 decreases, solutions are mostly chaotic and they do not reduce to the given solution type obtained by the 1D KSE for $\nu = \nu_1$, hence the above intuitive guess does not hold (the limit $\nu_2 \rightarrow 0$ is not continuous). Two representative return maps are shown in Figure 54. Panel (a) corresponds to a quasi-periodic solution obtained for $(\nu_1, \nu_2) = (0.15, 0.03)$ and the quasi-periodicity is verified by the continuous-looking curves in the plot. The return map of the solution obtained for $(\nu_1, \nu_2) = (0.25, 0.04)$ is illustrated in panel (b), which is surmised to be chaotic due to the foliations seen in the plot.

The various attractors already mentioned and presented in the phase diagram in Figure 52 will be further studied and analysed. The main solution types in the diagram are steady states, travelling waves, time-periodic solutions, quasi-periodic and chaotic solutions. The characteristics of all these states are described in detail in the rest of this chapter.

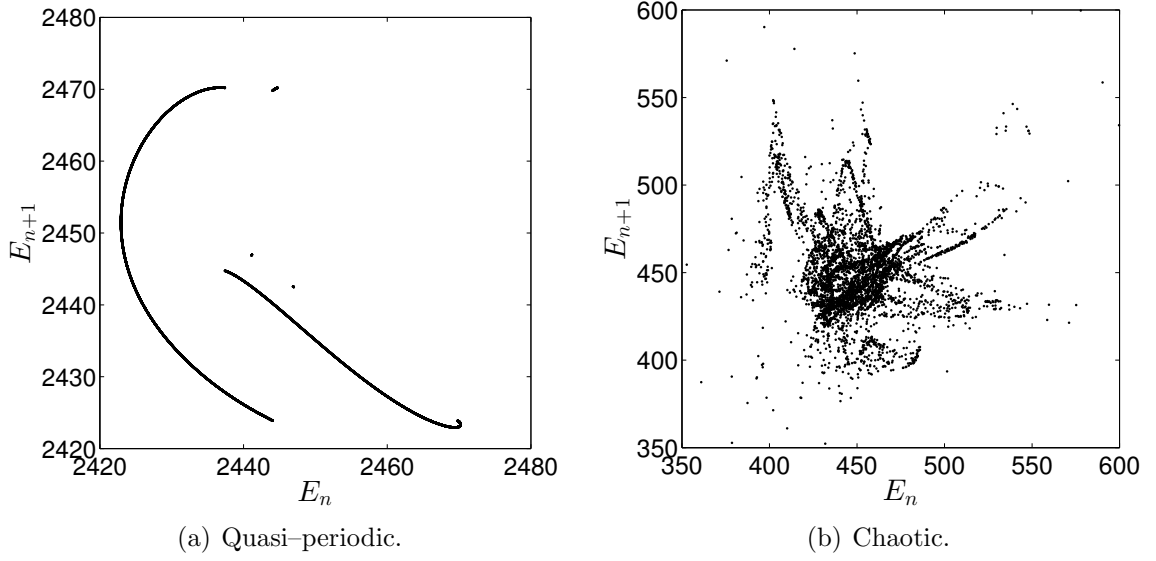


Figure 54: Return maps confirming the complex dynamics of (a) a quasi-periodic solution obtained for $(\nu_1, \nu_2) = (0.15, 0.03)$, and (b) a chaotic solution obtained for $(\nu_1, \nu_2) = (0.25, 0.04)$.

• Steady states

For $\nu_1 > 1, \nu_2 > 1$ the solutions are linearly stable and are attracted to the trivial state $v = 0$. At $\nu_1 = 1, \nu_2 = 1$ the first bifurcation occurs, leading to non-trivial solutions. In a large region enclosed roughly within the lines $\nu_1 = 0.35, \nu_2 = 0.35$ and $\nu_1 + \nu_2 = 0.95$, the solutions are unimodal steady states, namely the profiles are independent of time, with relatively small energy. Near the bifurcation point $(\nu_1, \nu_2) = (1, 1)$ one can write

$$\nu_1 = 1 - \alpha_1 \epsilon, \quad \nu_2 = 1 - \alpha_2 \epsilon, \quad (9.33)$$

for $\alpha_1, \alpha_2 > 0$ and $\epsilon \ll 1$. The equation satisfied by steady state solutions close to the bifurcation point $(1, 1)$ is the following

$$\frac{1}{2} \left(v_x^2 + \frac{1 - \alpha_2 \epsilon}{1 - \alpha_1 \epsilon} v_y^2 \right) - \frac{1}{2} \frac{1}{4\pi^2} \int_0^{2\pi} \int_0^{2\pi} |\nabla_\epsilon v|^2 dx dy + \Delta_\epsilon v + (1 - \alpha_1 \epsilon) \Delta_\epsilon^2 v = 0, \quad (9.34)$$

with $\nabla_\epsilon = \left(\partial_x, \frac{1 - \alpha_2 \epsilon}{1 - \alpha_1 \epsilon} \partial_y \right)$ and $\Delta_\epsilon = \partial_x^2 + \frac{1 - \alpha_2 \epsilon}{1 - \alpha_1 \epsilon} \partial_y^2$.

In a relevant study by Frisch et al. [89], the authors obtained analytic expressions for the steady state solutions of the 1D KSE, which are invariant under Galilean transformation. The authors showed that only modes $k = \pm 1$ and ± 2 are relevant to leading order in ϵ . A similar procedure can be adopted here to obtain analytical solutions for the steady states of the 2D KSE. This is done by considering the system of equations (9.5) (after transforming it to $2\pi \times 2\pi$ -periodic domains) and obtaining analytical solutions for U_1, U_2 (it is easier to work with the system in this case because it is already written in a mean-free form). The system under this concept transforms into

$$U_1 U_{1x} + \frac{1 - \alpha_2 \epsilon}{1 - \alpha_1 \epsilon} U_2 U_{1y} + \Delta_\epsilon U_1 + (1 - \alpha_1 \epsilon) \Delta_\epsilon^2 U_1 = 0, \quad (9.35a)$$

$$U_1 U_{2x} + \frac{1 - \alpha_2 \epsilon}{1 - \alpha_1 \epsilon} U_2 U_{2y} + \Delta_\epsilon U_2 + (1 - \alpha_1 \epsilon) \Delta_\epsilon^2 U_2 = 0. \quad (9.35b)$$

The solutions U_1, U_2 are then expanded in powers of $\epsilon^{1/2}$ and all the coefficients are written as Fourier series (this is possible because solutions are $2\pi \times 2\pi$ -periodic). The series are written in terms of $\sin(m(x + \theta))$, $\sin(m(y + \phi))$, $m \in \mathbb{Z}_+$ and θ, ϕ are the phase shifts in x and y respectively. Substituting the expansions into (9.35) and also ensuring that resonant terms disappear, the final expressions for U_1, U_2 are obtained and are given by

$$U_1 = -2 (12\alpha_1 \epsilon)^{1/2} \sin(x + \theta) - 2\alpha_1 \epsilon \sin(2(x + \theta)) - 12 \left(\frac{\alpha_1 \epsilon}{12} \right)^{3/2} \sin(3(x + \theta)) + \mathcal{O}(\epsilon^2), \quad (9.36a)$$

$$U_2 = -2 (12\alpha_2 \epsilon)^{1/2} \sin(y + \phi) - 2\alpha_2 \epsilon \sin(2(y + \phi)) - 12 \left(\frac{\alpha_2 \epsilon}{12} \right)^{3/2} \sin(3(y + \phi)) + \mathcal{O}(\epsilon^2). \quad (9.36b)$$

Interestingly, the analytical expressions for U_1 and U_2 show that they are functions of independent variables, i.e. $U_1 = U_1(x)$, $U_2 = U_2(y)$. If U_1, U_2 were functions of both x and y , that would have prevented the matching of coefficients of terms with the same order. From the above analytical solutions it is obvious that $n_1 = 1$, $n_2 = 1$ are the first modes to become unstable after the crossing at the critical point into the unstable region (similarly to the result for the 1D KSE by Frisch et al. [89]). The analytical expression for v is obtained by using the fact that $U_1 = u_x = v_x$ and

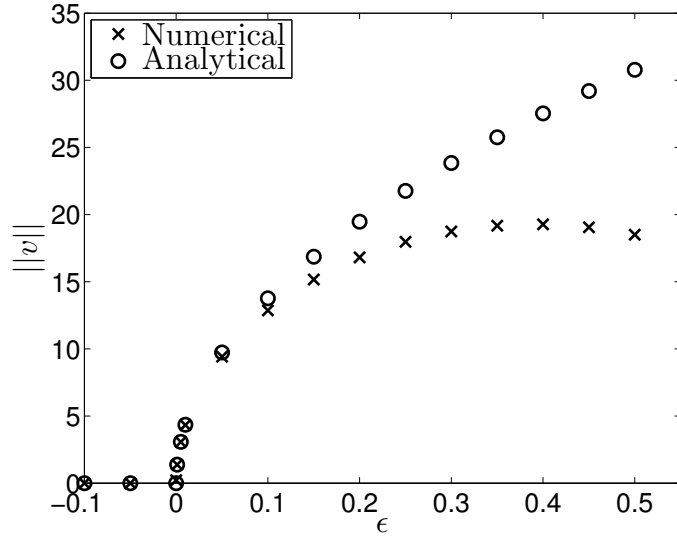


Figure 55: Energy $\|v\|$ of steady states against ϵ . Comparison between numerical solution (crosses) and the analytical solution (circles) given in (9.40), up to order $\epsilon^{1/2}$.

$U_2 = u_y = v_y$. Integrating $U_1(x)$ and $U_2(y)$ yields

$$v = \int U_1(x) dx + f_1(y) = \int U_2(y) dy + f_2(x), \quad (9.37)$$

with the functions of integration f_1, f_2 given by

$$f_1(y) = \int U_2(y) dy, \quad f_2(x) = \int U_1(x) dx. \quad (9.38)$$

Therefore the final analytical solution v is found to be

$$v = \int U_1(x) dx + \int U_2(y) dy, \quad (9.39)$$

or equally, using (9.36),

$$\begin{aligned} v = & 2(12\epsilon)^{1/2} \left[\alpha_1^{1/2} \cos(x + \theta) + \alpha_2^{1/2} \cos(y + \phi) \right] \\ & + \epsilon \left[\alpha_1 \cos(2(x + \theta)) + \alpha_2 \cos(2(y + \phi)) \right] \\ & + 4 \left(\frac{\epsilon}{12} \right)^{3/2} \left[\alpha_1^{3/2} \cos(3(x + \theta)) + \alpha_2^{3/2} \cos(3(y + \phi)) \right] + \mathcal{O}(\epsilon^2). \end{aligned} \quad (9.40)$$

A pointwise comparison between the analytical solution (9.40) and the numerical solution obtained by solving equation (9.34) is performed with very good agreement between the two. Figure 55 shows a bifurcation diagram of the final constant value of the norm $\|v\|_{L_2}$ against parameter ϵ for $\theta = \phi = 0$ (these phase values were fixed and the initial value problem was solved with initial condition determined from preliminary experiments, such that the numerical and analytical solutions to have the same phase). The analytical solution (9.40) up to order $\epsilon^{1/2}$ is given with crosses and the solution obtained numerically is represented by circles. The two are identical and zero for negative values at ϵ , since in that case the solutions return to the trivial state and the L_2 -norms tend to zero, i.e. $\limsup_{t \rightarrow \infty} \|v(\cdot, \cdot, t)\|_{L_2} = 0$. The difference between analytically and numerically obtained norms is infinitesimal for $\epsilon \ll 1$ and increases as ϵ grows. Three numerical solution profiles for $\epsilon = 0.05, 0.1, 0.2$ can be seen in Figure 56, taken at $t = 100$. An increase in the respective amplitudes is observed for increasing values of ϵ , growing from 6 at $\epsilon = 0.05$, to 8.2 at $\epsilon = 0.1$ and 10.7 at $\epsilon = 0.2$.

A different branch of steady state solutions appears again for smaller $\nu_2 = 0.05$ and for ν_1 in the range $0.6 \leq \nu_1 \leq 1$ (see Figure 52). Solutions in this steady attractor have much larger energy, with values starting from 645.4 at $\nu_1 = 1$. Though not shown here, the energy varies non-monotonically with ν_1 ; it increases for decreasing ν_1 and reaches the value 1432.05 at $\nu_1 = 0.7$, and it then starts decreasing and becomes equal to 1365.51 at $\nu_1 = 0.6$.

• *Travelling waves*

For $\nu_2 = 0.25, \nu_2 = 0.3$ and $0.55 \leq \nu_1 \leq 1$ and also in the region $0.7 \leq \nu_1 + \nu_2 \leq 0.9$, the solutions develop into travelling waves with constant phase speed. When looking at the time evolution of a fixed point on the wave profile, contours are created which are straight and parallel lines (see, for example, Figure 57(b)). To analyse this behaviour, solutions $v(x, y, t)$ are written in a travelling wave form as

$$v(x, y, t) = v(x + c \sin \theta t, y - c \cos \theta t) = v(\chi, \psi), \quad (9.41)$$

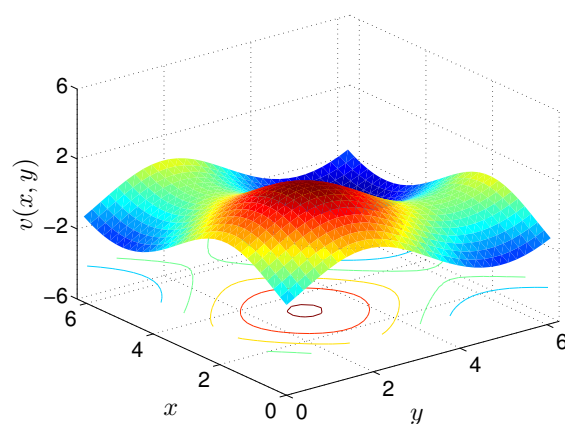
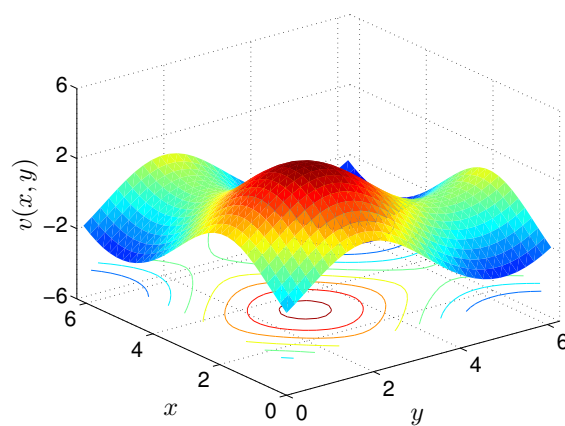
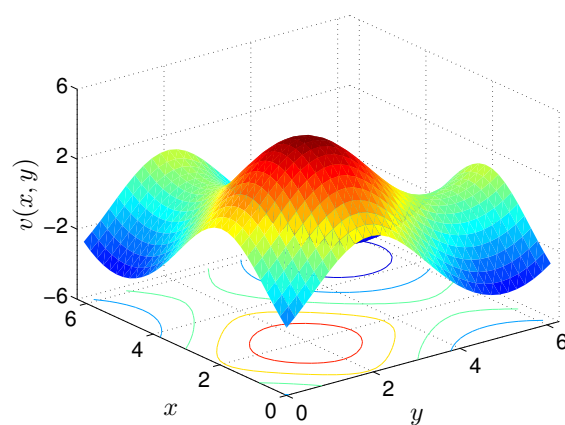
(a) $\epsilon = 0.05$ (b) $\epsilon = 0.1$ (c) $\epsilon = 0.2$

Figure 56: Steady state profiles $v(x, y)$ taken at time $t = 100$ for three different values of ϵ , corresponding to $\nu_1 = \nu_2 = 0.95, 0.9, 0.8$.

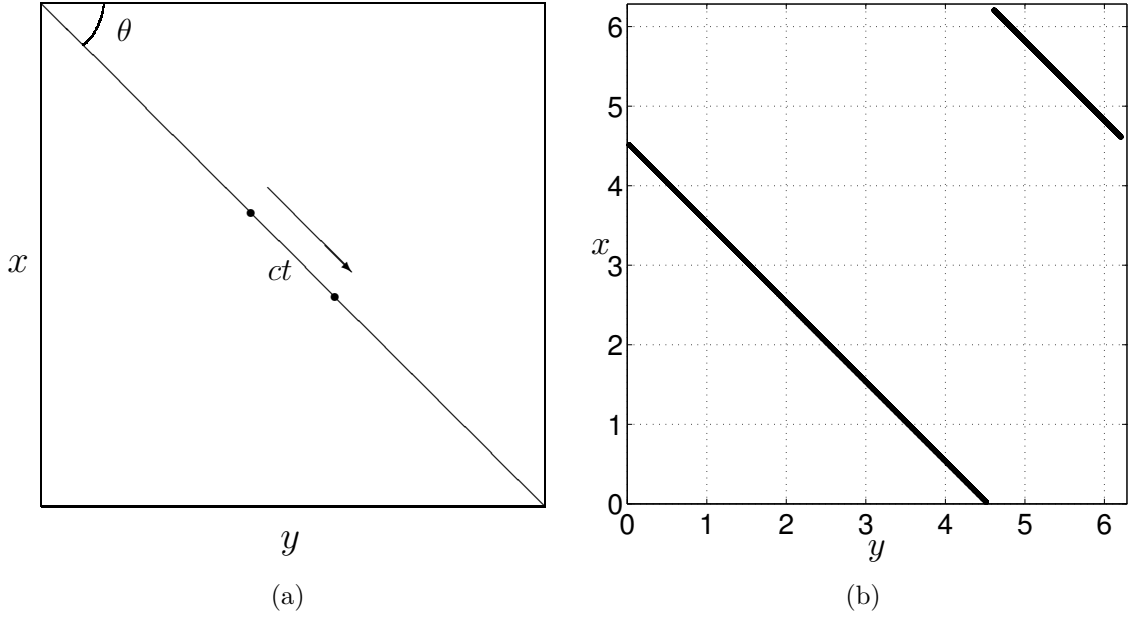


Figure 57: (a) Sample contour created as a wave travels in a two-dimensional domain with speed c , creating an angle θ with the y -axis. (b) Location of $\max(v)$ in space for a travelling wave obtained for $\nu_1 = \nu_2 = 0.25$.

where c is the constant wave speed, θ is the angle to the y -axis (Figure 57(a)) and χ, ψ are new variables defined by

$$\chi = x + c \sin \theta t, \quad \psi = y - c \cos \theta t. \quad (9.42)$$

Using the chain rule, the following transformations are obtained

$$\partial_t = c \sin \theta \partial_\chi - c \cos \theta \partial_\psi, \quad \partial_x = \partial_\chi, \quad \partial_y = \partial_\psi. \quad (9.43)$$

Inserting these transformations into equation (9.11), results in the following equation satisfied by travelling wave solutions

$$c \sin \theta v_\chi - c \cos \theta v_\psi + \frac{1}{2} \left(v_\chi^2 + \frac{\nu_2}{\nu_1} v_\psi^2 \right) - \frac{1}{2} \frac{1}{4\pi^2} \int_0^{2\pi} \int_0^{2\pi} |\nabla_{\chi,\psi} v|^2 dx dy + \Delta_{\chi,\psi} v + \nu_1 \Delta_{\chi,\psi}^2 v = 0, \quad (9.44)$$

where $\nabla_{\chi,\psi} = \left(\partial_\chi, \frac{\nu_2}{\nu_1} \partial_\psi \right)$ and $\Delta_{\chi,\psi} = \partial_\chi^2 + \frac{\nu_2}{\nu_1} \partial_\psi^2$.

In order to find the wavespeed c and angle θ , equation (9.44) is multiplied by v_χ and v_ψ , respectively. It is then integrated across the domain, to yield

$$c \sin \theta \int_0^{2\pi} \int_0^{2\pi} v_\chi^2 d\chi d\psi - c \cos \theta \int_0^{2\pi} \int_0^{2\pi} v_\chi v_\psi d\chi d\psi + \frac{1}{2} \int_0^{2\pi} \int_0^{2\pi} v_\chi \left(v_\chi^2 + \frac{\nu_2}{\nu_1} v_\psi^2 \right) d\chi d\psi = 0, \quad (9.45a)$$

$$c \sin \theta \int_0^{2\pi} \int_0^{2\pi} v_\chi v_\psi d\chi d\psi - c \cos \theta \int_0^{2\pi} \int_0^{2\pi} v_\psi^2 d\chi d\psi + \frac{1}{2} \int_0^{2\pi} \int_0^{2\pi} v_\psi \left(v_\chi^2 + \frac{\nu_2}{\nu_1} v_\psi^2 \right) d\chi d\psi = 0. \quad (9.45b)$$

Then the following expressions are calculated:

- $\sin \theta \times (9.45a) + \cos \theta \times (9.45b)$
- $\cos \theta \int_0^{2\pi} \int_0^{2\pi} v_\psi^2 d\chi d\psi \times (9.45a) + \sin \theta \int_0^{2\pi} \int_0^{2\pi} v_\chi^2 d\chi d\psi \times (9.45b).$

The two resulting equations are combined together to eliminate the speed c and find θ . The angle θ is given by the formula

$$\theta = \tan^{-1} \left(\frac{A_\chi \int_0^{2\pi} \int_0^{2\pi} v_\psi^2 d\chi d\psi - A_\psi \int_0^{2\pi} \int_0^{2\pi} v_\chi v_\psi d\chi d\psi}{A_\chi \int_0^{2\pi} \int_0^{2\pi} v_\chi v_\psi d\chi d\psi - A_\psi \int_0^{2\pi} \int_0^{2\pi} v_\chi^2 d\chi d\psi} \right), \quad (9.46)$$

with

$$A_\chi = \frac{1}{2} \int_0^{2\pi} \int_0^{2\pi} v_\chi \left(v_\chi^2 + \frac{\nu_2}{\nu_1} v_\psi^2 \right) d\chi d\psi, \quad A_\psi = \frac{1}{2} \int_0^{2\pi} \int_0^{2\pi} v_\psi \left(v_\chi^2 + \frac{\nu_2}{\nu_1} v_\psi^2 \right) d\chi d\psi. \quad (9.47)$$

Finally, the speed c can be found by inserting (9.46) into (9.45a) and is given by the following formula

$$c = \frac{A_\chi}{\cos \theta \int_0^{2\pi} \int_0^{2\pi} v_\chi v_\psi d\chi d\psi - \sin \theta \int_0^{2\pi} \int_0^{2\pi} v_\chi^2 d\chi d\psi}. \quad (9.48)$$

Expressions (9.46) and (9.48) can be computed with spectral accuracy by use of

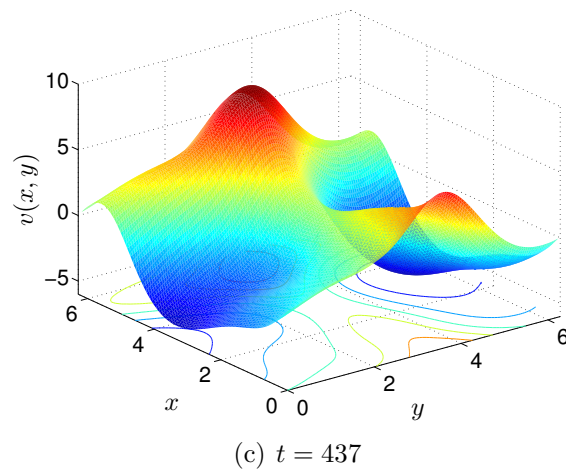
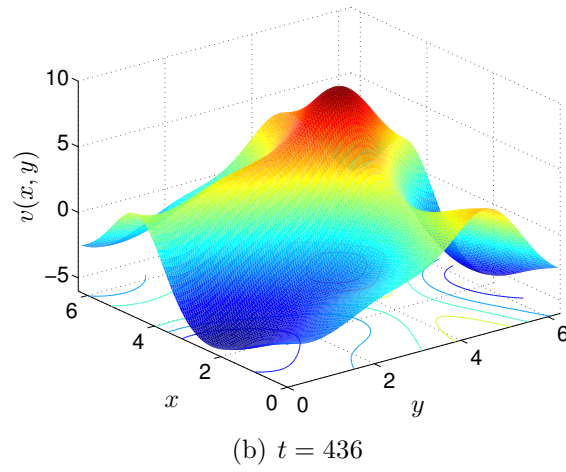
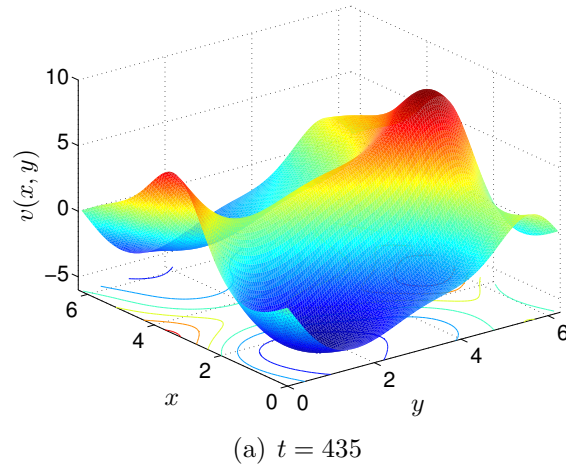


Figure 58: Travelling wave profiles $v(x, y)$ at three consecutive times $t = 435, 436, 437$, obtained for $\nu_1 = \nu_2 = 0.25$.

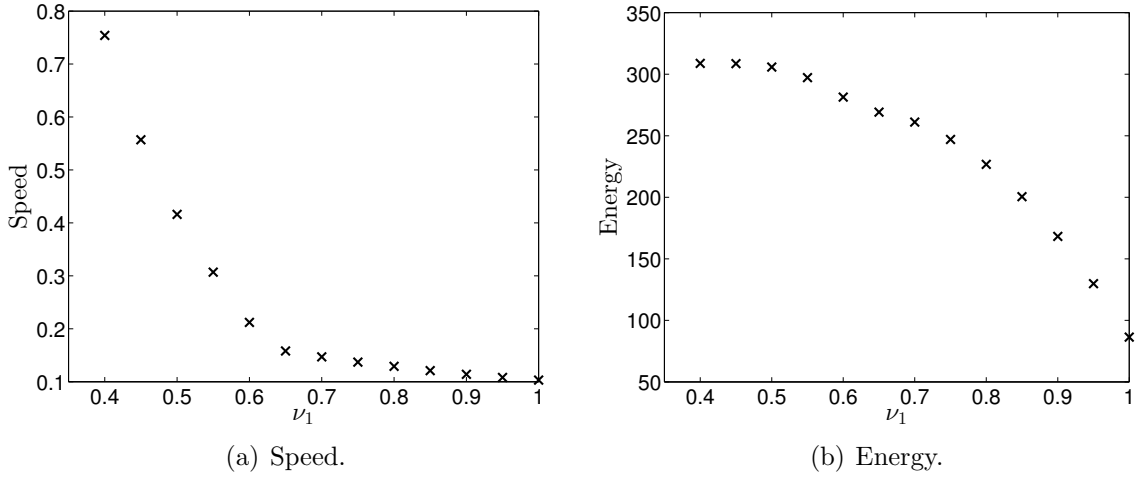


Figure 59: Characteristics of travelling waves obtained for ν_1 in the range $0.4 \leq \nu_1 \leq 1$ and fixed $\nu_2 = 0.3$. (a) Travelling wave speed against ν_1 , and (b) saturated wave energy against ν_1 .

Parseval's formulas. As a typical example, a travelling wave is obtained for $\nu_1 = \nu_2 = 0.25$, in which case the wavespeed c and angle θ are found numerically to be $c = -1.151$ and $\theta = \frac{\pi}{4}$. Another way to find the speed of the travelling wave and also to get the desired contours in space, is to pick one point (x^*, y^*) of the solution $v(x, y)$ and follow its Lagrangian evolution. This is done by choosing the global maximum of the solution $\max(v)$ and keeping track of its locations (x^*, y^*) at every time unit. These points are then plotted in Figure 57(b). The profiles for three consecutive times $t = 435, 436, 437$ are also illustrated in Figure 58. In this specific case of $\nu_1 = \nu_2 = 0.25$, the wave maximum follows a periodic motion in space with a period of 2π . In most other cases of travelling waves, e.g. for $(\nu_1, \nu_2) = (0.45, 0.3)$, the spatial motion is quasi-periodic and the contour lines in the $x - y$ space are dense.

Furthermore, on the lines $\nu_2 = 0.25$, $\nu_2 = 0.3$ the wave speed c is positive and increases monotonically with decreasing ν_1 . The wavespeed variation with respect to ν_1 is demonstrated in Figure 59(a) for fixed $\nu_2 = 0.3$. Moreover, for the same fixed value of ν_2 the wave energy also increases as ν_1 becomes smaller (Figure 59(b)), whereas for $\nu_2 = 0.25$ it increases at first and then starts decreasing after $\nu_1 = 0.6$.

Table 7: Periods of oscillation of time-periodic solutions of the 2D KSE, obtained for $\nu_2 = 0.2$ and decreasing ν_1 . For $0.7 \leq \nu_1 \leq 1$ periodic homoclinic bursts arise, giving place to time-periodic solutions for smaller ν_1 in the range $0.45 \leq \nu_1 \leq 0.65$.

ν_1	1.00	0.95	0.90	0.85	0.80	0.75	0.70
Per	126.75	119	113.5	108.75	102.3	96.15	89.9
ν_1	0.65	0.60	0.55	0.50	0.45		
Per	2.79	2.66	2.57	2.54	2.68		

• *Time periodic solutions*

For fixed $\nu_2 = 0.2$ and $0.7 \leq \nu_1 \leq 1$, a time-periodic attractor coalesces with a fixed point attractor. Solutions are periodic homoclinic bursts, which are characterised by constant energy plateaus disturbed by bursts periodically appearing in time. A representative example of this behaviour is given in Figure 60 for $(\nu_1, \nu_2) = (0.8, 0.2)$. Two typical profiles are illustrated in panels (a)–(b) and the energy and phase plane are shown in panels (c) and (d), respectively. Clearly, the phase plane is a closed curve which confirms the periodicity of the attractor. The profiles between the bursts are steady states, x -unimodal and y -bimodal. This means that the nonzero Fourier modes are the ones for all $n_1 \in \mathbb{Z}$ but only even $n_2 = 2m_2$, $m_2 \in \mathbb{Z}$. In the region symmetric with respect to $\nu_1 = \nu_2$, the nonzero modes are only $n_1 = 2m_1$, $m_1 \in \mathbb{Z}$, $n_2 \in \mathbb{Z}$, also confirming the symmetry described above with respect to x and y . The characteristic profiles in Figures 60(a)–(b) are taken from a constant energy state and an energy peak, at times $t = 360$ and $t = 381$, respectively. The period of oscillation decreases as ν_1 becomes smaller and is given in the first part of Table 7.

On the same line $\nu_2 = 0.2$ but for smaller values of ν_1 between $0.45 \leq \nu_1 \leq 0.65$, solutions are time-periodic with their energy oscillating rapidly in time. An example of such solution for $(\nu_1, \nu_2) = (0.5, 0.2)$ is shown in Figure 61. Three profiles at times $t = 139, 141.54, 144.08$ are plotted in panels (a)–(c) and the energy is demonstrated in panel (d). Also, the phase plane depicted in panel (e) is a closed cycle in this case. The period of oscillation of the energy is equal to 2.54 for the parameter values used in

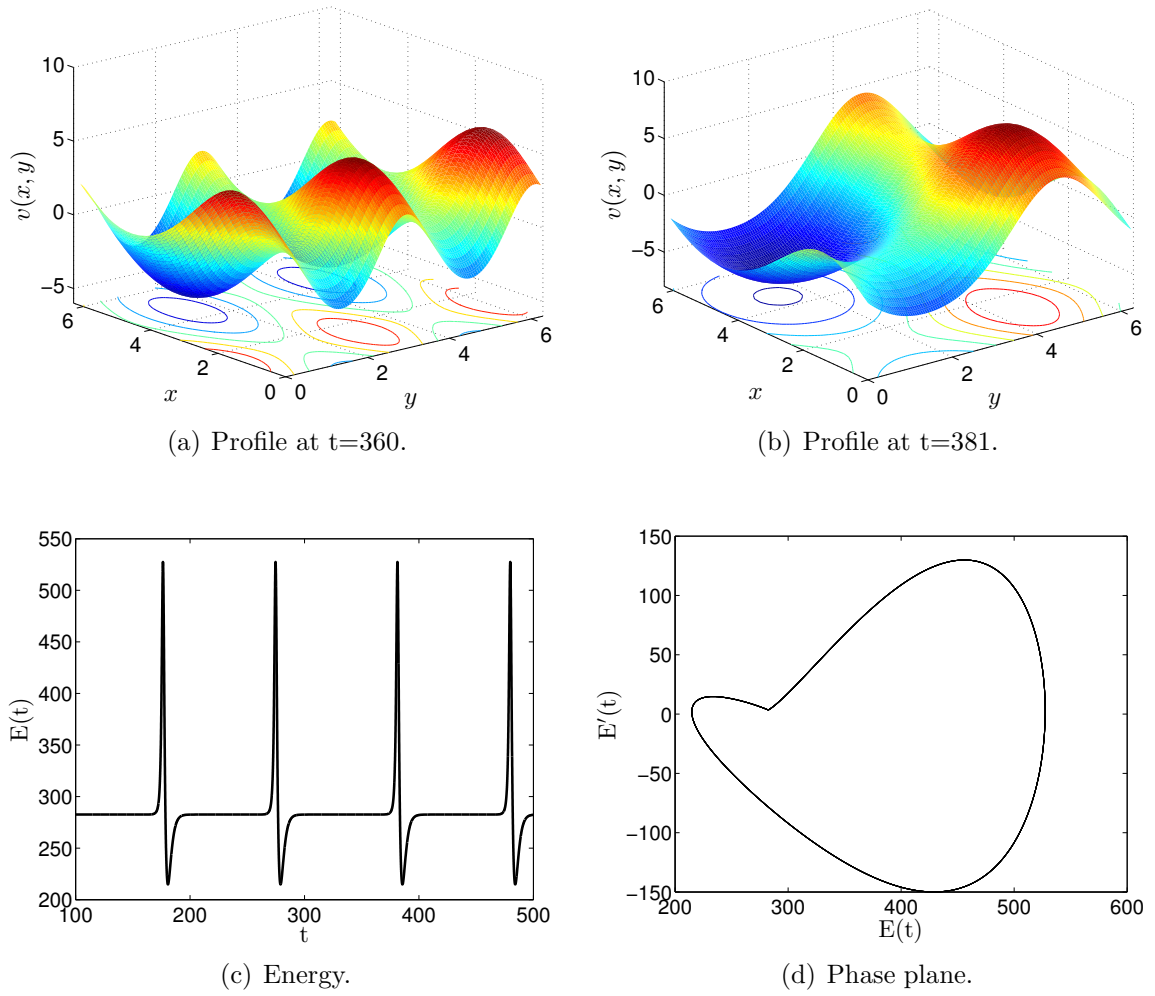


Figure 60: Representative profiles, energy and phase plane of a periodic homoclinic solution obtained for $(\nu_1, \nu_2) = (0.8, 0.2)$. Profiles in (a)–(b) are taken at times $t = 360$, 381 and correspond to a constant energy plateau and a burst, respectively.

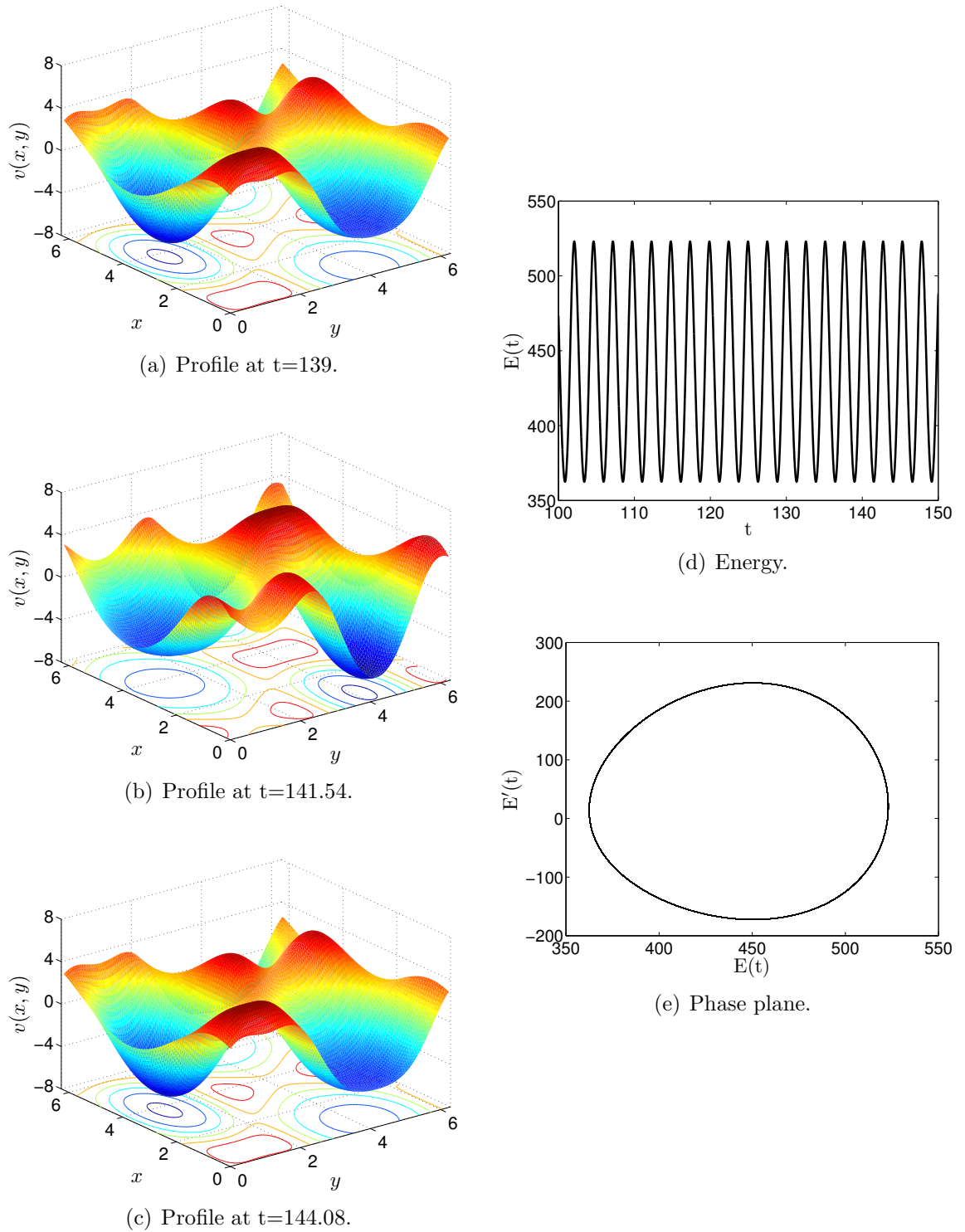


Figure 61: Profiles, energy and phase plane of a time-periodic solution obtained for $(\nu_1, \nu_2) = (0.5, 0.2)$. Profiles in panels (a)–(c) are taken at times $t = 139, 141.54, 144.08$ and correspond to one period of oscillation between each of them.

this example. Between each one of the profiles in panels (a)–(c) the energy completes one period of oscillation, though the shape of the solution profile returns to its initial form after two periods of oscillation. This is also confirmed by looking at the time evolution of the solution at a fixed point (i.e. by tracking $v(\pi, \pi, t)$ for example), which has a period twice that its energy signal. This behaviour is interesting because it is not obvious why the energy of a time-periodic solution would have twice the frequency (this requires specific conditions on the Fourier modes of the energy signal). It is found that all solutions on the line $\nu_2 = 0.2$ have this distinctive feature. Note that these solutions do not travel in space, but only change their shape periodically in time. The oscillation periods of solutions on this line are given in the second part of Table 7. The periods in this case are much smaller than the ones from the periodic homoclinic bursts described earlier. For $\nu_1 + \nu_2 < 0.65$ it is found that the time-periodic solutions are also travelling, meaning that after each period of oscillation the profiles return to their initial shape but shifted by a constant amount.

- *Quasi-periodicity and chaos*

For smaller $\nu_2 = 0.15$ and $0.35 \leq \nu_1 \leq 1$, the solutions get attracted by a chaotic attractor. In this case the chaotic attractor coincides with two fixed points, as the energy switches between two different plateaus and exhibits chaotic bursts in between. These types of solutions are called chaotic heteroclinic bursts. Figure 62 demonstrates representative plots of a chaotic heteroclinic solution obtained for $(\nu_1, \nu_2) = (0.85, 0.15)$. Panels (a)–(c) present the solution profiles at the times $t = 1100, 1230, 1300$, while panels (d)–(e) depict the corresponding energy and phase plane. The latter confirms the aperiodic nature of the solution, since the phase plane is not a closed repeating curve. Moreover, it can be seen that the profiles are y –bimodal on the lower constant energy levels (panel (c)) and totally unimodal on the upper constant energy levels (panel (a)) and on the bursts (panel (b)). Note that for this particular example, only 12 Fourier modes are active in the x –direction (greater than machine precision 10^{-16}), while in the y –direction 30 modes are needed. This result is particularly important because it verifies that chaotic solutions behave according to low-modal

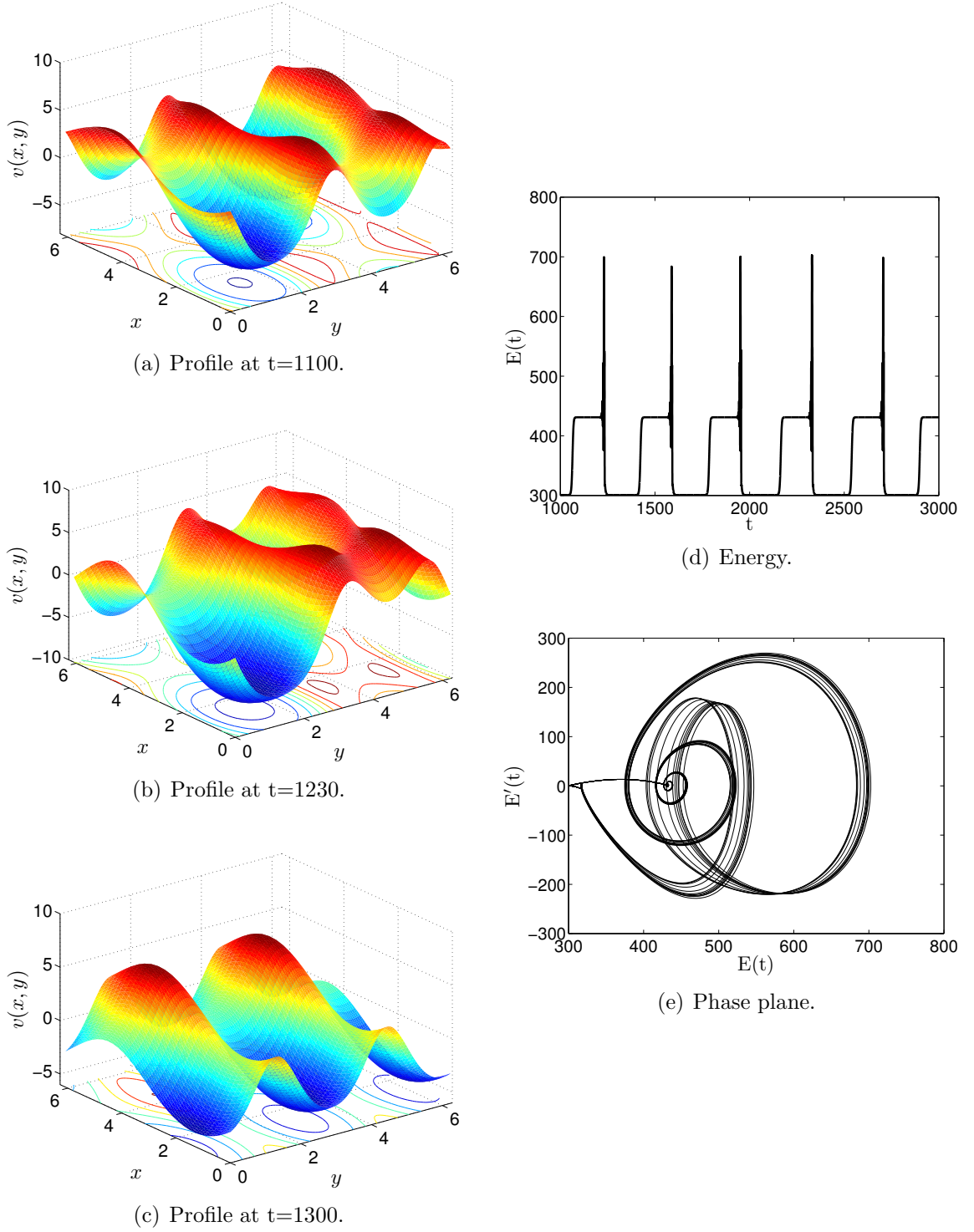


Figure 62: Profiles, energy and phase plane of a chaotic heteroclinic solution obtained for $(\nu_1, \nu_2) = (0.85, 0.15)$. Typical profiles corresponding to an upper constant energy state, a chaotic burst and a lower state are shown in (a)–(c) and are taken at times $t = 1100, 1230, 1300$, respectively.

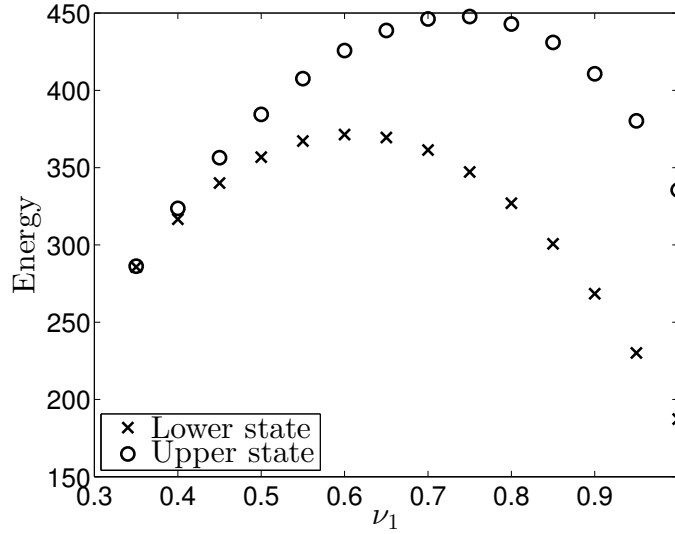


Figure 63: Energies of a chaotic heteroclinic attractor obtained for decreasing ν_1 and fixed $\nu_2 = 0.15$. Crossmarks denote energy values on lower branches and circles on upper branches. The heteroclinic attractor reduces to a homoclinic one at about $\nu_1 = 0.35$.

dynamics (similarly to the 1D KS result, see Papageorgiou & Smyrlis [9]).

Additionally, from $\nu_1 = 1$ and decreasing values of ν_1 , the energies of the lower and upper states increase monotonically until about $\nu_1 = 0.6$. However, as ν_1 decreases further, the energies on both states start decreasing and at $\nu_1 = 0.35$ the two states coalesce into a single state with energy value equal to 286. This behaviour can be better seen in Figure 63, where the energies of both states are plotted against ν_1 .

Another family of chaotic solutions is observed for $\nu_2 = 0.1$ and $0.55 \leq \nu_1 \leq 1$, for which values the solutions become chaotic homoclinic bursts with constant energy between each burst. Though not shown here, profiles are y -bimodal only and the constant energy value increases from 132.5 at $\nu_1 = 1$ to 316.64 at $\nu_1 = 0.6$ but then decreases to 312.45 at $\nu_1 = 0.55$. Moreover, the return maps are characterised by self-similarity, verifying the chaotic behaviour of the bursts.

As ν_1, ν_2 decrease further, solutions are characterised by more complex structures, including quasi-periodicity. A typical profile of a quasi-periodic solution can be seen in Figure 64(a) for $(\nu_1, \nu_2) = (0.45, 0.1)$, taken at a large time $t = 15000$. The corresponding energy is shown in Figure 64(b). Quasi-periodicity is similar to quasi-

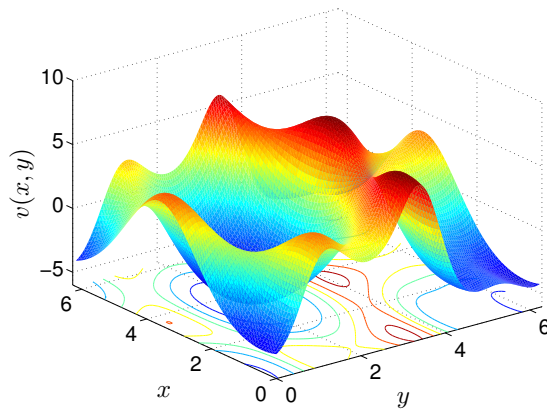
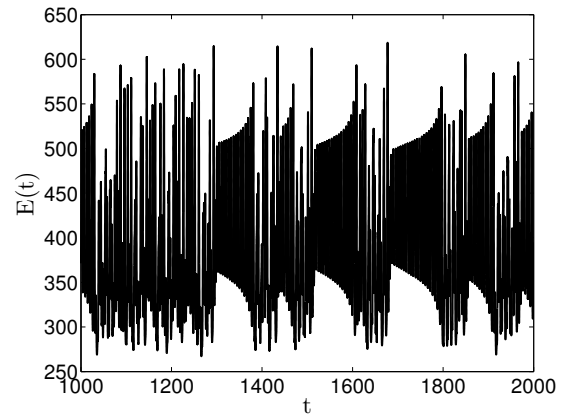
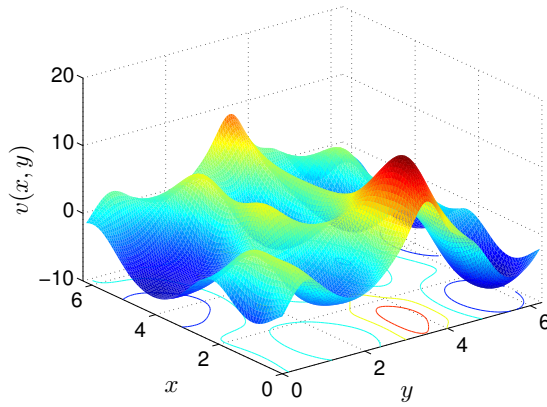
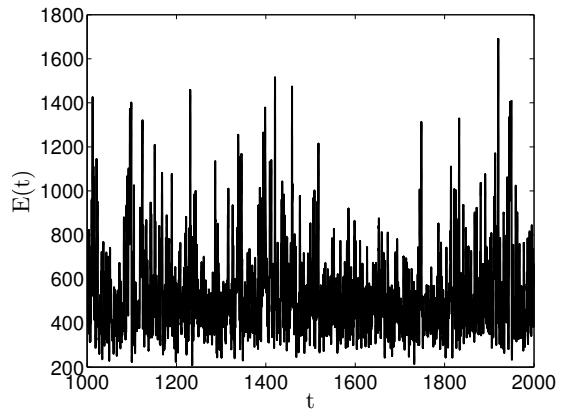
(a) Profile $(\nu_1, \nu_2) = (0.45, 0.1)$.(b) Energy $(\nu_1, \nu_2) = (0.45, 0.1)$.(c) Profile $(\nu_1, \nu_2) = (0.2, 0.05)$.(d) Energy $(\nu_1, \nu_2) = (0.2, 0.05)$.

Figure 64: Quasi-periodic and chaotic solution profiles and energies. (a)–(b) Quasi-periodic attractor for $(\nu_1, \nu_2) = (0.45, 0.1)$. (c)–(d) Chaotic attractor for $(\nu_1, \nu_2) = (0.2, 0.05)$. Both solution profiles are taken at a large time $t = 15000$.

periodic flows on a torus and the return map consists of continuous-looking curves densely filled with points (similar to Figure 54(a)). As $\nu_1, \nu_2 \rightarrow 0$ solutions are mainly chaotic. This chaotic attractor does not emerge through homoclinic or heteroclinic bursting like before and has a more complicated structure. Figures 64(c)–(d) demonstrate a characteristic profile (at a large time $t = 15000$) and the time evolution of the energy of a chaotic solution obtained for parameter values $(\nu_1, \nu_2) = (0.2, 0.05)$. The return map of the solution usually provides useful information about the attractor, but in this case it looks like a cloud and consists of unrecognisable patterns.

10 Conclusions

This chapter summarises the aims and achievements of the work in the second part of the thesis, concerning the study of the two-dimensional Kuramoto–Sivashinsky equation. Most importantly, the main conclusions drawn from this work are highlighted and the extension of well-known results for the one-dimensional Kuramoto–Sivashinsky equation to the two-dimensional equation are emphasised. Finally, some future directions are discussed.

10.1 Summary of this study

The second part of this thesis was devoted to an extensive numerical study of the two-dimensional Kuramoto–Sivashinsky equation. The Kuramoto–Sivashinsky equation is well-known, as it arises in various physical applications. It describes, for instance, the evolution of disturbed flame fronts or unstable fluid interfaces. Despite the numerous analytical and numerical studies of the equation in one spatial dimension, there is only a limited number of studies (mostly analytical) on the KS equation in two-dimensions. This work is therefore motivated by the absence of a clear understanding of how the interesting dynamics and different families of solutions extend to higher dimensions.

A detailed numerical investigation of the solutions is carried out, including a full characterisation of the different attractors that arise. Non-trivial solutions emerge beyond critical domain sizes that can be predicted using linear theory, and they evolve to more complicated structures as the domain becomes increasingly larger. Solution types for varying domain sizes include steady states, travelling waves, time-periodic bursts, quasi-periodic and chaotic solutions. In the chaotic regime, it is established that the energy is equally distributed among the small Fourier modes (long waves) and the behaviour of the spectrum is found to depend crucially on the nature of the nonlinearity. Optimal bounds that depend on the size of the domain are also numerically obtained for the energy of the equation.

10.2 Discussion of main results

The work carried out as part of this thesis forms the first complete computational study on the two-dimensional Kuramoto–Sivashinsky equation. The 2D KS is solved numerically after being rescaled to have zero mean. This is possible because the mean (zero mode) does not contribute to the dynamics of the other modes. The linear properties of the mean-free equation are studied by linearising around the zero steady solution. By doing so, an instability condition is obtained, which in turn determines the region of instability in parameter space ν_1, ν_2 . The bifurcation parameters $\nu_1,$

ν_2 depend on the inverse of the domain sizes L_x, L_y squared, and they initiate non-trivial solutions below the critical values $\nu_1 < 1, \nu_2 < 1$. These critical values are analogous to the critical boundary $\nu < 1$ that holds for the one-dimensional equation (Smyrlis & Papageorgiou [10]). Interestingly, if only one of ν_1 or ν_2 is smaller than 1, then the large-time solution is identical to the corresponding one-dimensional KSE solution obtained with ν equal to the ν_1 or ν_2 that is smaller than unity (therefore the 2D equation studied analytically on thin domains by Sell & Taboada [140] and Molinet [141] is essentially equivalent to the 1D KS).

As ν_1, ν_2 decrease, more unstable modes are introduced into the dynamics of the problem. This helps to determine the initial condition, chosen such that at least a few modes lie in the region of instability. The initial condition must depend on both x and y , otherwise the solutions evolve to undesired one-dimensional structures. The preferred initial condition (9.15) includes three unstable modes and thus it introduces numerous interesting dynamical phenomena.

A large number of numerical experiments of the initial value problem are performed for a wide range of parameter values ν_1, ν_2 in the unstable regime, in order to obtain quantitative characteristics of the dynamics. A symmetry property of the equation is invoked to reduce the size of the domain of interest (the instability region) and shows that half of the solutions are obtainable from the solutions at exchanged x, y and ν_1, ν_2 . For relatively large ν_1, ν_2 , unimodal steady state solutions arise similarly to the one-dimensional KS. For values close to the first bifurcation point $(\nu_1, \nu_2) = (1, 1)$, analytical solutions are obtained by following the asymptotic analysis of Frisch et al. [89] for the 1D KS and are compared to numerical solutions with very good agreement. For moderate values of ν_1, ν_2 , travelling waves or time-periodic solutions emerge. The travelling waves are fully two-dimensional and follow a periodic or quasi-periodic spatial motion analogous to motion on a torus. Time-periodic solutions appear in the form of periodic homoclinic or heteroclinic bursts, or solutions with shapes rapidly oscillating with time (note that again, such solutions also appear in the 1D case as well, see Smyrlis & Papageorgiou [11]).

Of particular interest in this study is the characterisation of transition to chaos as the bifurcation parameters ν_1, ν_2 shrink to zero. The two-dimensional nature of the

computational domain allows for the possibility of infinitely many different routes to chaos. More specifically, the cuts $\nu_1 = \nu_2 = \nu$ and ν_1 fixed with $\nu_2 \rightarrow 0$ are explored; results indicate that the transition to chaos is via quasi-periodicity and does not appear to follow the pattern of period-doubling found in the case of the 1D KS (Papageorgiou & Smyrlis [9], Smyrlis & Papageorgiou [11]). More computations are needed to fully explore such differences.

Furthermore, the statistical properties of the chaotic solutions are studied in order to establish energy bounds as the system size increases. It is established numerically that the average energy is asymptotically proportional to the system size, similar to the one-dimensional case (Wittenberg & Holmes [132]). For the differentiated version of the equation (a system of two equations in this case – see (9.5)), the total energy is defined by the sum of the two energies of the differentiated solutions v_x , v_y and it is shown to be equipartitioned among the Fourier modes in large scales. In fact, the dynamics of the two-dimensional Kuramoto–Sivashinsky appear to be extensive as in that the local dynamics are asymptotically independent of the system size. Additionally, the energy spectrum is found to depend crucially on the nature of the nonlinearity. For the symmetric 2D KSE the spectrum is isotropic, but for other asymmetric two-dimensional equations of the KS-type this is not true.

10.3 Future directions

The present work is the first numerical study on the two-dimensional Kuramoto–Sivashinsky equation and encourages further analytical study. In particular, proofs regarding existence, analyticity and boundedness of the solution of the two-dimensional Kuramoto–Sivashinsky equation are still missing. The studies by Sell & Taboada [140] and Molinet [141] provide some of the required results for thin domains, but there is a lack of analytical works for arbitrary domain sizes. Therefore this study could provide an insight towards the open challenges.

Finally, future work on this problem could include the effect of dispersion, which can be introduced by adding the term Δu_x in the equation. This is motivated by known results for the one-dimensional KS which prove that dispersion can regularise

chaotic dynamics into travelling wave pulses (Akrivis et al. [79], Kawahara [156]). In two-dimensions, Saprykin et al. [147] studied the asymmetric 2D KS equation (8.12) and constructed travelling waves by assuming solutions of permanent form $u(x, y, t) = u(x - ct, y)$. In a related study, Akrivis et al. [84] managed to regularise chaotic solutions into stable travelling waves by increasing dispersion. These waves, however, eventually lost stability at higher values of dispersion. Their results suggest that most of the travelling waves obtained by Saprykin et al. [147] are unstable in the sense that they may not emerge as large-time solutions to the initial value problem. This feature of the two-dimensional problem is quite distinct from the behaviour in the one-dimensional case, where even moderate amounts of dispersion produce stable travelling wave pulses. Consequently, an extensive computational study of the dispersive 2D KS equation would be of much value to the field.

Appendix

A Numerical solution of the boundary value problem (2.91)

The boundary value problem (2.91) can be solved numerically using finite difference methods. This method provides approximations for the derivatives of $F(y)$ by making use of Taylor series expansions. More specifically, the central difference approximations to the first, second and fourth derivatives are

$$\begin{aligned} F'(y_n) &= \frac{F(y_{n+1}) - F(y_{n-1}))}{2h} + \mathcal{O}(h^2), \\ F''(y_n) &= \frac{F(y_{n+1}) - 2F(y_n) + F(y_{n-1}))}{h^2} + \mathcal{O}(h^2), \\ F^{(iv)}(y_n) &= \frac{F(y_{n+2}) - 4F(y_{n+1}) + 6F(y_n) - 4F(y_{n-1}) + F(y_{n-2}))}{h^4} + \mathcal{O}(h^2), \end{aligned} \quad (\text{A.1})$$

where $h = \frac{1}{N}$ and the points $\{y_n\}_0^N$ form a partition of $[0, 1]$ and are defined by

$$y_n = nh, \quad n = 0, 1, \dots, N. \quad (\text{A.2})$$

Setting

$$f(y) = -(2k^2 + ik_1 R_e y), \quad g(y) = ik_1 k^2 R_e y + k^4, \quad (\text{A.3})$$

and symbolising F_n, f_n, g_n as the approximations of $F(y_n), f(y_n), g(y_n)$ respectively, produces at leading order (terms of $\mathcal{O}(h^2)$ are dropped) the difference equation

$$\frac{F_{n+2} - 4F_{n+1} + 6F_n - 4F_{n-1} + F_{n-2}}{h^4} + f_n \frac{F_{n+1} - 2F_n + F_{n-1}}{h^2} + g_n F_n = 0, \quad (\text{A.4})$$

which is used to compute numerical approximations to the ODE (2.91a). This can be arranged in a system of linear equations for $n = 1, 2, \dots, N-1$, given by

$$F_{n+2} - (4 - h^2 f_n) F_{n+1} + (6 - 2h^2 f_n + h^4 g_n) F_n - (4 - h^2 f_n) F_{n-1} + F_{n-2} = 0. \quad (\text{A.5})$$

The above $(N-1)$ equations together with the four boundary conditions provide $(N+3)$ equations for the $(N+3)$ unknowns $F_{-1}, F_0, \dots, F_N, F_{N+1}$. The boundary conditions (2.91b) using finite difference approximations are written as

$$\begin{aligned}
F(0) = 0 &\Rightarrow F_0 = 0, \\
F'(0) = 1 &\Rightarrow \frac{F_1 - F_{-1}}{2h} = 1 \Leftrightarrow F_1 - F_{-1} = 2h, \\
F(1) = 0 &\Rightarrow F_N = 0, \\
F'(1) = 0 &\Rightarrow \frac{F_{N+1} - F_{N-1}}{2h} = 0 \Leftrightarrow F_{N+1} = F_{N-1}.
\end{aligned} \tag{A.6}$$

Hence, the problem reduces to the numerical solution of a $(N + 3) \times (N + 3)$ penta-diagonal system of the form

$$\mathbf{A}\mathbf{F} = \mathbf{b}, \tag{A.7}$$

where

$$\mathbf{A} = \begin{pmatrix} 0 & 1 & 0 & & \dots & & 0 \\ -1 & 0 & 1 & 0 & \dots & & 0 \\ 1 & \ell_1 & d_1 & u_1 & 1 & & \vdots \\ 0 & \ddots & \ddots & \ddots & \ddots & \ddots & \\ \vdots & & 1 & \ell_{N-1} & d_{N-1} & u_{N-1} & 1 \\ 0 & & \dots & 0 & -1 & 0 & 1 \\ 0 & & \dots & & 0 & 1 & 0 \end{pmatrix}, \quad \mathbf{F} = \begin{pmatrix} F_{-1} \\ F_0 \\ F_1 \\ \vdots \\ F_N \\ F_{N+1} \end{pmatrix}, \quad \mathbf{b} = \begin{pmatrix} 0 \\ 2h \\ 0 \\ \vdots \\ 0 \\ 0 \end{pmatrix} \tag{A.8}$$

and

$$\begin{aligned}
d_n &= 6 - 2h^2 f_n + h^4 g_n, \\
u_n = \ell_n &= -(4 - h^2 f_n), \quad n = 1, 2, \dots, N - 1.
\end{aligned} \tag{A.9}$$

B Proof of asymptotic properties of $\mathcal{J}_{1,2}$, $\mathcal{L}_{1,2}$

The asymptotic results used in Section 3.4 are based on asymptotic properties of Airy functions. Specifically, for $R_e \rightarrow \infty$ the integral $\mathcal{J}_1$ becomes

$$\begin{aligned} \mathcal{J}_1 &\sim \frac{1}{2k} \int_0^1 e^{-ks} \text{Ai} \left(k_1^{\frac{1}{3}} R_e^{\frac{1}{3}} e^{\frac{i\pi}{6}} s \right) ds \\ &\sim \frac{1}{2k} \int_0^\epsilon e^{-ks} \text{Ai} \left(k_1^{\frac{1}{3}} R_e^{\frac{1}{3}} e^{\frac{i\pi}{6}} s \right) ds \\ &\quad + \frac{1}{2k} \int_\epsilon^1 \frac{1}{2\sqrt{\pi}} \left(k_1^{\frac{1}{3}} R_e^{\frac{1}{3}} e^{\frac{i\pi}{6}} s \right)^{-\frac{1}{4}} e^{-ks} e^{-\frac{2}{3} \left(k_1^{1/3} R_e^{1/3} e^{i\pi/6} s \right)^{\frac{3}{2}}} ds, \end{aligned} \quad (\text{B.1})$$

where $\epsilon \gg R_e^{-1/3}$. In the second integral above, the Airy function $\text{Ai}(x)$ is replaced by its leading order asymptotic expansion for large argument $x \rightarrow \infty$ (Abramowitz [157]). The latter integral tends to zero as the Reynolds number tends to infinity.

In the first integral though, s is in the interval $[0, \epsilon]$ so it is useful to apply the transformation $\xi = R_e^{\frac{1}{3}} s$, where ξ is an order one variable, which gives

$$\begin{aligned} \mathcal{J}_1 &\sim \frac{1}{2k} \int_0^{\epsilon R_e^{1/3}} e^{-k R_e^{-\frac{1}{3}} \xi} \text{Ai} \left(k_1^{\frac{1}{3}} e^{\frac{i\pi}{6}} \xi \right) R_e^{-\frac{1}{3}} d\xi \\ &\sim \frac{1}{2k} R_e^{-\frac{1}{3}} \int_0^\infty \text{Ai} \left(k_1^{\frac{1}{3}} e^{\frac{i\pi}{6}} \xi \right) d\xi \\ &\sim \frac{1}{2k} R_e^{-\frac{1}{3}} k_1^{-\frac{1}{3}} e^{-\frac{i\pi}{6}} \int_0^\infty \text{Ai}(\xi) d\xi. \end{aligned} \quad (\text{B.2})$$

Using the fact that $\int_0^\infty \text{Ai}(\xi) d\xi = \frac{1}{3}$ (Abramowitz [157]) implies the following result

$$\mathcal{J}_1 \sim \frac{1}{6} R_e^{-\frac{1}{3}} k^{-1} k_1^{-\frac{1}{3}} e^{-\frac{i\pi}{6}}. \quad (\text{B.3})$$

Following a similar procedure, the asymptotic result for $\mathcal{L}_1$ is obtained and is the same as that for $\mathcal{J}_1$. However, for the integrals involving the Airy function $\text{Bi}(x)$, the result is different due to the exponential asymptotic behaviour of $\text{Bi}(x)$ for $x \rightarrow \infty$ (Abramowitz [157]). In particular,

$$\begin{aligned}
\mathcal{J}_2 &\sim \frac{1}{2k} \int_0^1 e^{-ks} \operatorname{Bi} \left(k_1^{\frac{1}{3}} R_e^{\frac{1}{3}} e^{\frac{i\pi}{6}} s \right) ds \\
&\sim \frac{1}{2k} \int_0^1 \frac{1}{2\sqrt{\pi}} \left(k_1^{\frac{1}{3}} R_e^{\frac{1}{3}} e^{\frac{i\pi}{6}} s \right)^{-\frac{1}{4}} e^{-ks} e^{\frac{2}{3} \left(k_1^{1/3} R_e^{1/3} e^{i\pi/6} s \right)^{\frac{3}{2}}} ds.
\end{aligned} \tag{B.4}$$

This is of the order $o\left(e^{R_e^{1/2}}\right)$. It can be shown that $\mathcal{L}_2$ is of the same order, hence both integrals are exponentially growing as $R_e \rightarrow \infty$.

As a result, the integral ratios that appear in equations (3.22) are both $\mathcal{O}(1)$ quantities,

$$\frac{\mathcal{J}_1}{\mathcal{L}_1} = \mathcal{O}(1) \quad \text{and} \quad \frac{\mathcal{J}_2}{\mathcal{L}_2} = \mathcal{O}(1). \tag{B.5}$$

C Nonlinear terms in Fourier space

A spatially 2π -periodic solution (H, Γ) of the system (5.4)–(5.5) is written the form

$$\begin{aligned} H(x, t) &= \sum_{\substack{k=-\infty \\ k \neq 0}}^{+\infty} \hat{H}_k(t) e^{ikx}, \\ \Gamma(x, t) &= \sum_{k=-\infty}^{+\infty} \hat{\Gamma}_k(t) e^{ikx}, \end{aligned} \quad (\text{C.1})$$

where $\hat{\Gamma}_0(t) = \bar{\Gamma}$ is equal to the spatial mean of Γ (function H has a zero spatial mean, therefore $\hat{H}_0 = 0$). The nonlinear terms $-HH_x$ and $-(H\Gamma)_x$ in (5.8), which are necessary in the analysis of the numerical scheme in Section 5.2, are expressed as

$$\begin{aligned} -HH_x &= \sum_{\substack{k=-\infty \\ k \neq 0}}^{+\infty} \hat{A}_k(t) e^{ikx}, \\ -(H\Gamma)_x &= \sum_{\substack{k=-\infty \\ k \neq 0}}^{+\infty} \hat{B}_k(t) e^{ikx}. \end{aligned} \quad (\text{C.2})$$

In practice, the series are truncated after a sufficiently large number of modes M , therefore the Fourier coefficients $\hat{A}_k(t)$ and $\hat{B}_k(t)$ are given by

$$\hat{A}_k(t) = -\frac{ik}{2} \begin{cases} \sum_{n=1}^{M-1-k} \hat{H}_{-n} \hat{H}_{k+n} + \sum_{\substack{n=1 \\ n \neq k}}^{M-1} \hat{H}_n \hat{H}_{k-n} & \text{if } k > 0 \\ \sum_{\substack{n=1 \\ n \neq -k}}^{M-1} \hat{H}_{-n} \hat{H}_{k+n} + \sum_{n=1}^{M-1+k} \hat{H}_n \hat{H}_{k-n} & \text{if } k < 0, \end{cases} \quad (\text{C.3})$$

$$\hat{B}_k(t) = -ik \begin{cases} \hat{\Gamma}_0 \hat{H}_k + \sum_{n=1}^{M-1-k} \hat{H}_{-n} \hat{\Gamma}_{k+n} + \sum_{\substack{n=1 \\ n \neq k}}^{M-1} \hat{H}_n \hat{\Gamma}_{k-n} & \text{if } k > 0 \\ \hat{\Gamma}_0 \hat{H}_{-k} + \sum_{\substack{n=1 \\ n \neq -k}}^{M-1} \hat{H}_{-n} \hat{\Gamma}_{k+n} + \sum_{n=1}^{M-1+k} \hat{H}_n \hat{\Gamma}_{k-n} & \text{if } k < 0, \end{cases} \quad (\text{C.4})$$

for $k = -M + 1, \dots, M - 1$.

D Positive definiteness of $\mathcal{A}_1$ for a pseudo-differential operator $\mathcal{P}$

In general, a 2π -periodic function u with Fourier coefficients $\hat{u}_k$ is written as

$$u(x) = \sum_{\substack{k=-\infty \\ k \neq 0}}^{+\infty} \hat{u}_k e^{ikx}, \quad \hat{u}_k = \frac{1}{2\pi} \int_0^{2\pi} u(x) e^{-ikx} dx. \quad (\text{D.1})$$

Then the nonlocal term can be written as

$$(\mathcal{P}u, u) = \int_0^{2\pi} \left(\sum_k \sum_n i\Lambda\nu^{-1} \mathcal{N}(k\sqrt{\nu}) \hat{u}_k \hat{u}_n e^{i(k+n)x} \right) dx. \quad (\text{D.2})$$

The above integral is non-zero only if $n = -k$, i.e.

$$\begin{aligned} (\mathcal{P}u, u) &= 2\pi i\Lambda\nu^{-1} \sum_{\substack{k=-\infty \\ k \neq 0}}^{+\infty} \mathcal{N}(k\sqrt{\nu}) \hat{u}_k \hat{u}_{-k} \\ &= 2\pi i\Lambda\nu^{-1} \left[\sum_{k=-\infty}^{-1} \mathcal{N}(k\sqrt{\nu}) \hat{u}_k \hat{u}_{-k} + \sum_{k=1}^{+\infty} \mathcal{N}(k\sqrt{\nu}) \hat{u}_k \hat{u}_{-k} \right] \\ &= 2\pi i\Lambda\nu^{-1} \sum_{k=1}^{\infty} (\mathcal{N}(k\sqrt{\nu}) + \mathcal{N}(-k\sqrt{\nu})) \hat{u}_k \hat{u}_{-k} \\ &= 2\pi i\Lambda\nu^{-1} \sum_{k=1}^{\infty} (\mathcal{N}(k\sqrt{\nu}) - \overline{\mathcal{N}(k\sqrt{\nu})}) \hat{u}_k \overline{\hat{u}_k} \\ &= 2\pi i\Lambda\nu^{-1} \sum_{k=1}^{\infty} 2i\Im(\mathcal{N}(k\sqrt{\nu})) |\hat{u}_k|^2 \\ &= 2\pi\Lambda\nu^{-1/2} \sum_{k=1}^{\infty} k\Im(F''(0)) |\hat{u}_k|^2. \end{aligned} \quad (\text{D.3})$$

Taking the complex conjugate of (2.91) and applying the transformation $k \rightarrow -k$, provides the condition $\mathcal{N}(-k) = -\overline{\mathcal{N}(k)}$ used in the above calculation. Moreover, $\hat{u}_k = \overline{\hat{u}_{-k}}$ because the function u is real-valued.

Numerical solutions of (2.91) show that $\Im(F''(0)) \leq 0$. Thus if $\Lambda \leq 0$, $(\mathcal{P}u, u) \geq 0$

and setting

$$\mathcal{A}_1 u := \frac{c}{\nu} u + \nu u_{xxx} + \mathcal{P}u, \quad \mathcal{D}u := 0, \quad (\text{D.4})$$

(with $c = 1$) and $\mathcal{A}_2$ defined as in (5.11), ensures that $\mathcal{A}$ is a self-adjoint and positive definite operator. If $\Lambda > 0$ the same definition for $\mathcal{A}_1$ and $\mathcal{D}$ is used again, but now c must be chosen appropriately to ensure the positive definiteness of $\mathcal{A}_1$. Using the lower bound $\Im(F''(0)) \geq -\left|\min\left(\Im(F''(0))\right)\right| = -F_{im}$ in the above expression for $(\mathcal{P}u, u)$ and inserting the result in

$$(\mathcal{A}_1 u, u) = \frac{c}{\nu} \|u\|^2 + \nu \|u_{xx}\|^2 + (\mathcal{P}u, u), \quad (\text{D.5})$$

yields

$$\begin{aligned} \frac{c}{\nu} \|u\|^2 + \nu \|u_{xx}\|^2 + (\mathcal{P}u, u) &\geq 2\pi \sum_{k=-\infty}^{+\infty} \left(\nu k^4 + \frac{c}{\nu} \right) |\hat{u}_k|^2 - 2\pi \sum_{k=1}^{\infty} \Lambda \nu^{-1/2} F_{im} k |\hat{u}_k|^2 \\ &= 4\pi \sum_{k=1}^{\infty} \left(\nu k^4 - \frac{\Lambda \nu^{-1/2}}{2} F_{im} k + \frac{c}{\nu} \right) |\hat{u}_k|^2 \\ &\geq 4\pi \sum_{k=1}^{\infty} \left(\nu k^4 - \frac{\Lambda \nu^{-1/2}}{2} F_{im} k^2 + \frac{c}{\nu} \right) |\hat{u}_k|^2 \\ &= 4\pi \nu \sum_{k=1}^{\infty} \left(k^4 - \frac{2\Lambda \nu^{-1/2}}{\nu} F_{im} k^2 + \frac{c}{\nu^2} \right) |\hat{u}_k|^2 \\ &\quad + 3 \sum_{k=1}^{\infty} 2\pi \Lambda \nu^{-1/2} F_{im} k^2 |\hat{u}_k|^2. \end{aligned} \quad (\text{D.6})$$

Choosing the constant c to be equal to $c = (\Lambda \nu^{-1/2} F_{im})^2$ makes the first term in the last step a perfect square and converts the above estimation into (see also (D.3))

$$\frac{(\Lambda \nu^{-1/2} F_{im})^2}{\nu} \|u\|^2 + \nu \|u_{xx}\|^2 + (\mathcal{P}u, u) \geq -3(\mathcal{P}u, u), \quad (\text{D.7})$$

leading to the lower bound

$$(\mathcal{A}_1 u, u) \geq \frac{3}{4} \left(\nu \|u_{xx}\|^2 + \frac{(\Lambda \nu^{-1/2} F_{im})^2}{\nu} \|u\|^2 \right) \geq 0. \quad (\text{D.8})$$

E Analytical solution of the bifurcation point ν_0

The solutions of the system (5.4)–(5.5) return to the trivial state for $\nu > \nu_0$ and become unstable for $\nu < \nu_0$. The bifurcation point ν_0 can be obtained analytically by linearising the problem and picking $k = 1$ in the resulting dispersion relation. The analytical expression for ν_0 is the unique positive real root of the following fourth-order polynomial in ν

$$\nu^4 + c_3\nu^3 + c_2\nu^2 + c_1\nu + c_0 = 0. \quad (\text{E.1})$$

The coefficients $c_{0,1,2,3}$ are functions of the parameters R_e , Λ , Γ_0 , η and are given by

$$\begin{aligned} c_3 &= 2\eta - \frac{\Lambda R_e}{20} + \Lambda^2 \left(\frac{2}{15} + \frac{R_e^2}{8400} \right)^2, \\ c_2 &= \eta^2 + \frac{8\Lambda^2}{15} + 3 \left(\frac{\Lambda R_e}{60} \right)^2 - \frac{\Lambda R_e}{15} \left(\eta + \frac{\Lambda^2}{15} \right) + 2\Lambda^2 \frac{R_e^2}{8400} \left(2 - \frac{1}{15} \frac{\Lambda R_e}{60} \right) \\ &\quad - \left(\frac{2}{15} + \frac{R_e^2}{8400} \right) \left(\frac{\Lambda \Gamma_0}{\eta} + \Lambda^2 \frac{\Lambda R_e}{60} \frac{R_e^2}{8400} \right), \\ c_1 &= 4\Lambda^2 \left(1 - \frac{\Lambda R_e}{60} \frac{R_e^2}{8400} \right) + \left(\frac{\Lambda R_e}{60} \right)^2 \left(2\eta - \frac{\Lambda R_e}{60} \right) - \frac{\Lambda R_e}{60} \left(\eta^2 + \frac{8\Lambda^2}{15} \right) \\ &\quad - 2\Lambda \frac{\Gamma_0}{\eta} + \Lambda \frac{\Gamma_0}{\eta} \left(\eta + \frac{\Lambda R_e}{60} \right) \left(\frac{2}{15} + \frac{R_e^2}{8400} \right), \\ c_0 &= \frac{1}{30\eta} (\Gamma_0 - 2\eta\Lambda) (R_e\Lambda^2 - 30\Gamma_0). \end{aligned} \quad (\text{E.2})$$

Note that when $\Lambda = 0$ the above polynomial reduces to the one in (5.28).

F Numerical methods for the 2D KS equation

The two-dimensional Kuramoto–Sivashinsky equation was solved numerically using implicit–explicit BDF schemes. In order to fit the class of abstract equations analysed by Akrivis & Crouzeix [77], equation (9.11) is first written as in Akrivis et al. [84]

$$v_t + \mathcal{L}v = \mathcal{B}(v), \quad (\text{F.1})$$

with

$$\mathcal{L} = c + \Delta_\nu + \nu_1 \Delta_\nu^2, \quad \mathcal{B}(v) = cv - \frac{1}{2} \left(v_x^2 + \frac{\nu_2}{\nu_1} v_y^2 \right) + \frac{1}{2} m_v(t), \quad (\text{F.2})$$

where $c > 0$ and $m_v(t)$ is the integral term in (9.11), which is a function of t only. For the symmetric operator $\mathcal{L}$ it is necessary to prove that it is self-adjoint and positive definite and for the nonlinear operator $\mathcal{B}$ that is locally Lipschitz continuous, in order for the conditions in Akrivis & Crouzeix [77] to be satisfied. Obviously, $\mathcal{L}$ is self-adjoint and for $v \in \mathcal{H}_{per}^4$, the periodicity of the function provides that

$$(\mathcal{L}v, v) = c\|v\|^2 - \|v_x\|^2 - \frac{\nu_2}{\nu_1} \|v_y\|^2 + \nu_1 \|v_{xx}\|^2 + 2\nu_2 \|v_{xy}\|^2 + \frac{\nu_2^2}{\nu_1} \|v_{yy}\|^2. \quad (\text{F.3})$$

Using the Parseval's theorem and Young's inequality¹⁵, the following relation is obtained for positive constants ϵ_1, ϵ_2

$$\|v_x\|^2 \leq \frac{1}{4\epsilon_1} \|v\|^2 + \epsilon_1 \|v_{xx}\|^2, \quad \|v_y\|^2 \leq \frac{1}{4\epsilon_2} \|v\|^2 + \epsilon_2 \|v_{yy}\|^2. \quad (\text{F.4})$$

Inserting (F.4) into (F.3), leads to

$$(\mathcal{L}v, v) \geq \left(c - \frac{1}{4\epsilon_1} - \frac{1}{4\epsilon_2} \frac{\nu_2}{\nu_1} \right) \|v\|^2 + 2\nu_2 \|v_{xy}\|^2 + (\nu_1 - \epsilon_1) \|v_{xx}\|^2 + \frac{\nu_2}{\nu_1} (\nu_2 - \epsilon_2) \|v_{yy}\|^2. \quad (\text{F.5})$$

¹⁵The Young's inequality in its general form states that for any non-negative real numbers a and b and positive real numbers p and q such that $\frac{1}{p} + \frac{1}{q} = 1$, then

$$ab \leq \frac{a^p}{\epsilon p} + \frac{\epsilon b^q}{q}.$$

The inequality is applied in formulas (F.4) with $p = q = 2$ and $\epsilon = 2\epsilon_1$ or $\epsilon = 2\epsilon_2$.

Choosing

$$\epsilon_1 = \frac{\nu_1}{2}, \quad \epsilon_2 = \frac{\nu_2}{2} \quad \text{and} \quad c - \frac{1}{4\epsilon_1} - \frac{1}{4\epsilon_2} \frac{\nu_2}{\nu_1} = 1, \quad (\text{F.6})$$

yields the value of c for which the operator $\mathcal{L}$ is positive definite, namely

$$c = 1 + \frac{1}{\nu_1}. \quad (\text{F.7})$$

The proof of $\mathcal{B}$ being locally Lipschitz continuous is very similar to the one given in Akrivis et al. [84] for a similar operator. Therefore both of the conditions in Akrivis & Crouzeix [77] hold and the equation (9.11) can be discretised by linearly implicit methods, which are proved to be stable and convergent.

Considering the second-order BDF as given in (4.15) and defining approximations V^n to $v(\cdot, \cdot, t_n)$ for $n = 0, 2, \dots, N-2$ and $N = T/dt$, $t_n = n dt$ (T is the final time and dt is the time step), spatial discretisations of the Fourier modes are obtained and are given by

$$\begin{aligned} \hat{V}_{k_1, k_2}^{n+2} = \frac{1}{\xi_{k_1, k_2}} & \left[(2 + 2c dt) \hat{V}_{k_1, k_2}^{n+1} - \left(\frac{1}{2} + c dt \right) \hat{V}_{k_1, k_2}^n + 2dt \left(\hat{A}_{k_1, k_2}^{n+1} + \frac{\nu_2}{\nu_1} \hat{B}_{k_1, k_2}^{n+1} \right) \right. \\ & \left. - dt \left(\hat{A}_{k_1, k_2}^n + \frac{\nu_2}{\nu_1} \hat{B}_{k_1, k_2}^n \right) \right], \end{aligned} \quad (\text{F.8})$$

where

$$\hat{A}_{k_1, k_2} = -\mathcal{F} \left(\frac{1}{2} v_x^2 \right), \quad \hat{B}_{k_1, k_2} = -\mathcal{F} \left(\frac{1}{2} v_y^2 \right), \quad (\text{F.9})$$

and

$$\xi_{k_1, k_2} = \frac{3}{2} + c dt - dt \left(k_1^2 + \frac{\nu_2}{\nu_1} k_2^2 \right) + \nu_1 \left(k_1^2 + \frac{\nu_2}{\nu_1} k_2^2 \right)^2. \quad (\text{F.10})$$

For $n = 0$, one step of the implicit Euler method is performed in order to obtain approximation for V^1 using the known approximation for V^0 , given by the initial conditions.

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