Shearing Flows in Liquid Crystal Models

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Abstract

The liquid crystal phase is a phase of matter between the solid and liquid phase whose flow is characterized by a velocity field and a director field which describes locally the orientation of the liquid crystal. In this work we explore shearing flows in two related continuum models of liquid crystals. The first is a phenomenological model of frictional forces in a geological fault, which is motivated by the second model, the Leslie-Ericksen continuum theory of liquid crystals.

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Contents

Chapter 1

Introduction

In this work we explore shearing flows of liquid crystals in the context of both the Leslie-Ericksen continuum theory of nematic liquid crystals and a simplified phenomenological continuum model for nematic liquid crystals proposed to describe frictional forces in geological faults. The phenomenological model is a simplification of the Leslie-Ericksen continuum theory, but still captures the underlying dynamics.

1.1 Liquid Crystals

The liquid crystal phase is a phase of matter between the liquid and solid phases. They have flow properties of liquids, but because the molecules possess a highly anisotropic structure they also exhibit properties of solids. Because of these properties liquid crystals are are used in many applications including LCD televisions, thermometers, and optical imaging.

At the microscopic level liquid crystals look like small rods and at the macroscopic level these rods align themselves into locally preferred orientations modeled by a vector field, $\mathbf{n}$, called the director field, Figure 1.1.

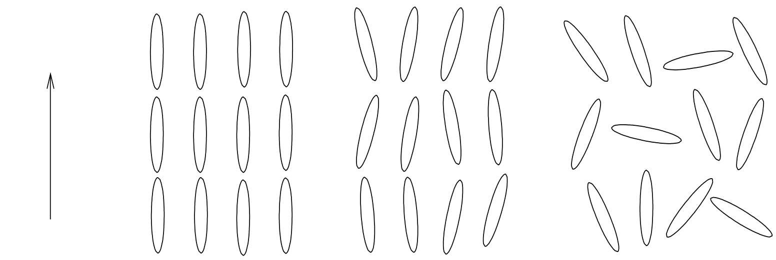

Figure 1.1: *Nematic liquid crystal phase and director unit vector describing the local orientation.*

The discovery of liquid crystals is attributed to Dr Friedrich Reinitzer in 1888, [9]. Many materials exhibit a liquid crystal phase as the the material is heated or cooled, called thermotropic liquid crystals, or by changes in concentration in a solvent, called lyotropic liquid crystals. The thermotropic liquid crystal is commonly classified into three different types:

1. **Nematic**: The molecules align on average locally into a preferred orientation.
2. **Cholesteric**: The molecules align on average locally into a preferred orientation and also longitudinally align into a preferred helical configuration.
3. **Smectic**: The molecules align on average locally into a preferred orientation and also into layers within the bulk of the material.

1.2 Classic Continuum Models for Liquid Crystals

The first static continuum theory, i.e. in the absence of positional movement, for nematic liquid crystals is due to Zocher, [48, 49], and Oseen, [35], in the 1930s and then was refined by Frank, [19], in 1958 to include cholesteric liquid crystals. The idea behind the static continuum theory is to construct an energy density functional

$$\mathscr{W}(\mathbf{n}, \nabla \mathbf{n}) \tag{1.1}$$

which measures the localized average change in energy due to a deformation from a natural undeformed state. The director field is the realization of local averaging to describe the natural state in a nematic liquid crystal, Figure 1.1. For any natural alignment of the liquid crystal, $\mathbf{n}^*$, one prescribes that $\mathscr{W}(\mathbf{n}^*, \nabla \mathbf{n}^*) = 0$.

Since the director field is used to describe the locally averaged direction of the liquid crystal it is modeled by a unit vector field

$$|\mathbf{n}| = 1, \tag{1.2}$$

and because of the rod like structure one does not differentiate between the orientations $\mathbf{n}$ and $-\mathbf{n}$. This along with the usual mechanics assumptions of frame indifference

$$\mathscr{W}(\mathbf{n}, \nabla \mathbf{n}) = \mathscr{W}(Q\mathbf{n}, Q \nabla \mathbf{n} Q^T) \tag{1.3}$$

for any orthogonal matrix Q, allowed Frank to derive the following formula for $\mathscr{W}$, commonly referred to as Frank's free energy formula.

$$\begin{aligned} \mathscr{W} = {} & K_0 \tau (\mathbf{n} \cdot \nabla \times \mathbf{n} + \tau) + K_1 (\nabla \cdot \mathbf{n})^2 + K_2 (\mathbf{n} \cdot \nabla \times \mathbf{n} + \tau)^2 \\ & + K_3 |\mathbf{n} \times \nabla \times \mathbf{n}|^2 + (K_2 + K_4)(\mathrm{tr}(\nabla \mathbf{n})^2 - (\nabla \cdot \mathbf{n})^2) \end{aligned} \tag{1.4}$$

The parameter τ is a measure of the longitudinal twist associated with a cholesteric liquid crystals with $\tau = 0$ corresponding to the nematic liquid crystal. The constants

K_1, K_2, K_3 are called *Frank's constants* and are a measure of the liquid crystal materials tendency to splay, twist, or bend respectively.

The energy density functional is defined up to a constant representing the minimal energy in the natural configuration of the liquid crystal material. By taking this constant to be zero, it is typical to assume that the energy density functional $\mathscr{W}$ is positive definite, i.e.

$$\mathscr{W}(\mathbf{n}, \mathbf{N}) \geq 0 \tag{1.5}$$

for all $\mathbf{n} \in S^2$ and $\mathbf{N} \in \mathscr{L}(\mathbf{n}, \mathbb{R}^3)$ where

$$\mathscr{L}(\mathbf{n}, \mathbb{R}^3) = \{\mathbf{N} \in \mathscr{L}(\mathbb{R}^3) \, : \, \mathbf{N}^T \mathbf{n} = 0\} \tag{1.6}$$

The space $\mathscr{L}(\mathbf{N}, \mathbb{R}^3)$ arises naturally from the restriction (1.2) since taking the derivative on both sides yields

$$(D\mathbf{n})^T \mathbf{n} = \mathbf{0}.$$

In 1966, Ericksen derived the inequalities

$$2K_1 \geq K_2 + K_4, \quad K_2 \geq |K_4|, \quad K_3 \geq 0 \tag{1.7}$$

which are necessary and sufficient conditions for (1.5) to hold.

To go from local theory to global theory one defines the energy functional

$$\mathscr{E}[n] = \int_{\mathscr{D}} \mathscr{W}(\mathbf{n}, \nabla \mathbf{n}) \, dV. \tag{1.8}$$

on a domain $\mathscr{D}$ with a smooth boundary $\partial \mathscr{D}$ and prescribed Dirichlet

$$\mathbf{n}\big|_{\partial \mathscr{D}} = 0$$

or Neumann

$$\left.\frac{\partial \mathbf{n}}{\partial \nu}\right|_{\partial \mathscr{D}} = 0$$

boundary conditions. For static configurations one looks to find minimizers of the energy functional $\mathscr{E}[n]$. Minimizers which are not smooth are of particular interest as they present defects in the alignment of the liquid crystal, [10]. Another approach is to derive a set of Euler-Lagrange equations. This variational approach is especially useful in examining special types of static director configurations, [45, 10, 44].

The dynamic continuum theory of liquid crystals was developed in series of papers by Ericksen, [18], and Leslie, [28, 27], which summarize the dynamic continuum theory. This is done via the classical approach of averaging the motion of the particles in the liquid crystal material and defining the motion by a velocity field, $\mathbf{u}(t, \mathbf{x})$. The derivation is analogous to that of the Navier-Stokes equations, [12], and we now give a brief overview of how this is done.

Consider at each point $\mathbf{x}$ in a domain $\Omega \in \mathbb{R}^3$ the motion of the liquid crystal material through that point given by the velocity field $\mathbf{u}(t, \mathbf{x})$. For a function $h : \mathbb{R} \times \mathbb{R}^3 \to \mathbb{R}^3$, we define the *material time derivative* of h by the formula

$$\frac{D}{Dt} h(t, \mathbf{x}) = \frac{\partial h}{\partial t} + (\mathbf{u} \cdot \vec{\nabla}) h.$$

The acceleration is of the liquid crystal material through the point $\mathbf{x}$ is given by

$$\mathbf{a}(t, \mathbf{x}) = \frac{D\mathbf{u}}{Dt}.$$

Following the classical approach one assumes that for every open subset $W_t \subset \Omega$, traveling along with the flow, the following conservation laws are true:

(i) **Conservation of Mass**

$$\frac{d}{dt}\int_{\Omega}\rho\, dx = 0 \tag{1.9}$$

where $\rho(t,\mathbf{x})$ is the density per unit volume.

(ii) **Conservation of Linear Momentum**

$$\frac{d}{dt}\int_{W_t}\rho\mathbf{u}\, dV = \int_{W_t}\mathbf{F}\, dV + \int_{\partial W_t}\mathbf{t}\, dS \tag{1.10}$$

where $\mathbf{F}$ is the external body force and $\mathbf{t}$ is the stress tensor with components $t_i = t_{ji}\nu_j$ where ν is the outward pointing unit normal.

(iii) **Conservation of Angular Momentum**

$$\frac{d}{dt}\int_{W_t}\rho(\mathbf{x}\times\mathbf{u}) + \rho_1(\mathbf{n}\times\dot{\mathbf{n}})\, dV = \int_{W_t}\mathbf{x}\times\mathbf{F} + \mathbf{n}\times\mathbf{G}\, dV + \int_{\partial W_t}\mathbf{x}\times\mathbf{t} + \mathbf{n}\times\mathbf{s}\, dS \tag{1.11}$$

where $\mathbf{G}$ is the external director body force, ρ_1 is a material constant, and $\mathbf{s}$ is the director stress tensor with components $s_i = s_{ji}\nu_j$.

(iv) **Conservation of Energy**

$$\frac{d}{dt}\int_{W_t}\frac{1}{2}\rho|\mathbf{u}|^2 + \frac{1}{2}\rho_1|\dot{\mathbf{n}}| + E\, dV = \int_{W_t}\mathbf{f}\cdot\mathbf{u} + \mathbf{G}\cdot\dot{\mathbf{n}}\, dV + \int_{\partial W_t}\mathbf{t}\cdot\mathbf{u} + \mathbf{s}\cdot\dot{\mathbf{n}}\, dS \tag{1.12}$$

where E is the internal energy per unit volume. Note, the left hand side constitutes the kinetic energy due to the positional movement of the material plus the kinetic energy of the liquid crystal material due to a non-natural static configuration of the director field.

By converting the surface integrals into volume integrals and enforcing that the conservation laws should hold on any arbitrary subset of Ω one obtains the differential form of the conservation laws. Yet, the the domain W_t is traveling along with the flow, thus the need for the following lemma which is proved in [12].

Lemma 1. *[Transport Theorem] Suppose that* $\varphi : \mathbb{R}\times\Omega \to \Omega$ *is the flow associated with the differential equation* $x' = u(t,\mathbf{x})$*. Then, for any function* $f \in C^1(\mathbb{R}\times\Omega,\Omega)$*,*

$$\frac{d}{dt}\int_{W_t} f(x,t)\,dV = \int_{W_t} \frac{Df}{Dt}(x,t) + f(x,t)\nabla\cdot u(x,t)\,dV$$

where $W_t = \varphi(t,W_0)$ *and* $W_0 \subset\in \Omega$ *is open. Moreover, if the vector field the u is incompressible, i.e.* $\nabla\cdot u = 0$*, then*

$$\frac{d}{dt}\int_{W_t} f(x,t)\,dV = \int_{W_t} \frac{Df}{Dt}(x,t)\,dV$$

In [28], Leslie assumes that the liquid crystal material is incompressible since a majority of applications enforce this constraint,

$$\nabla\cdot\mathbf{u} = 0. \tag{1.13}$$

The differential forms for the conservation of mass and conservation of linear momentum, using Lemma 1 are straightforward to compute and are given respectively by

$$\dot{\rho} = 0, \tag{1.14}$$

$$\rho\dot{v}_i = F_i + t_{ji.j}. \tag{1.15}$$

where $\dot{} = \frac{D}{Dt}$ and we are using the Einstein summation convention which states that one should sum over all repeated indices.

The differential form of (1.11) is more delicate. We differentiate and after eliminating the conservation of linear momentum term, (1.15), which arises we have

$$e_{ijk}(\rho_1 n_j \ddot{n}_k - n_j G_k - n_j s_{pk,p}) = e_{ijk}(t_{kj} + n_{j,p} s_{pk}). \tag{1.16}$$

The left hand side of equation is a vector orthogonal to **n** and thus so is the right hand side. There exists a vector **g** such that $\mathbf{n} \times \mathbf{g}$ is equal to the right hand side of equation (1.16) and so

$$e_{ijk} n_j g_k = e_{ijk}(t_{kj} + n_{j,p} s_{pk}), \tag{1.17}$$

where e_{ijk} is the alternating symbol. But, note that equation (1.17) doesn't completely determine the vector **g** since for any $\gamma \in \mathbb{R}$ the vector $\tilde{\mathbf{g}} \equiv \mathbf{g} + \gamma \mathbf{n}$ also satisfies equation (1.16). Equating terms in (1.16) and (1.17) we arrive at the differential form of the conservation of angular momentum

$$\rho_1 \ddot{n}_i = G_i + g_i + s_{ji,j}, \tag{1.18}$$

where g is determined only up to the addition of a constant multiple of the director **n** and satisfies equation (1.17). Finally we derive from the conservation of energy, after eliminating terms arising from (1.15) and (1.18),

$$\dot{E} = t_{ji} u_{j,i} + s_{j,i} \dot{n}_{j,i} - g_i \dot{n}_i. \tag{1.19}$$

In order to derive the constitutive relations on the the stress tensor **t** and **s** as well as the intrinsic body force **g** we define the Hemoltz free energy

$$\mathscr{H} = E - T\mathscr{S}, \tag{1.20}$$

where T is the internal temperature, which we assume to be constant, and $\mathscr{S}$ is the entropy per unit volume. By the second law of thermodynamics one has $\dot{\mathscr{S}} \geq 0$ and hence rearranging the terms in (1.20) and substituting from (1.19) gives the inequality

$$t_{ji}u_{j,i} + s_{j,i}\dot{n}_{j,i} - g_i\dot{n}_i - \dot{\mathscr{H}} \geq 0. \tag{1.21}$$

The derivation of the constitutive relations is due to Leslie [28]. The stress tensor t_{ji} is separated into an static part, t^0_{ji}, and a dynamic part, t^d_{ji},

$$t_{ji} = t^0_{ji} + t^d_{ji}, \tag{1.22}$$

with

$$t^0_{ji} = -p\delta_{ji} - \frac{\partial \mathscr{H}}{\partial n_{k,j}} n_{k,i}, \tag{1.23}$$

and

$$t^d_{ji} = \mu_1 n_k n_m d_{km} n_i n_j + \mu_2 n_j N_i + \mu_3 n_i N_j + \mu_4 d_{ji} + \mu_5 n_j n_k d_{ki} + \mu_6 n_i n_k d_{kj}, \tag{1.24}$$

where

$$N_i = \dot{n}_i - w_{ik} n_k,$$

$$2d_{ij} = v_{i,j} + v_{j,i},$$

$$2w_{ij} = v_{i.j} - v_{j,i},$$

p is an indeterminate constant, and μ_i, $i = 1\dots6$ are referred to as the Leslie coefficients of viscosity. The intrinsic director body force is also decomposed in to an static part, g^0_i, and a dynamic part, g^d_i,

$$g_i = g^0_i + g^d_i, \tag{1.25}$$

with

$$g_i^0 = \gamma n_i - \beta_j n_{i,j} - \frac{\partial \mathscr{H}}{\partial n_i}, \tag{1.26}$$

and

$$g_i^d = \lambda_1 N_i + \lambda_2 n_j d_{ji}, \tag{1.27}$$

where γ and β_j are indeterminate constants, and

$$\lambda_1 = \mu_2 - \mu_3, \qquad \lambda_2 = \mu_5 - \mu_6. \tag{1.28}$$

Also,

$$s_{ji} = \beta_j n_i + \frac{\partial \mathscr{H}}{\partial n_{i,j}}. \tag{1.29}$$

In this work we will be considering shearing flows for the nematic liquid crystal state. Thus we summarize the conservation laws for the nematic liquid crystal:

$$\rho \dot{v} = f_i + t_{ij,j}, \tag{1.30}$$

$$\rho_1 \ddot{n} = G_i + g_i + s_{ji,j}, \tag{1.31}$$

$$2\mathscr{F} = K_1(\nabla \cdot \mathbf{n})^2 + K_2(n \cdot \nabla \times \mathbf{n})^2 + K_3|\mathbf{n} \times \nabla \times \mathbf{n}|^2, \tag{1.32}$$

where t_{ji}, s_{ji}, and g_i are defined in (1.22), (1.29), and (1.25) respectively and $\mathscr{F}$ is derived from Frank's formula (1.4)

Because of the complexity inherent in the full Leslie-Ericksen continuum theory of liquid crystals only recently has global existence of weak solutions been shown, [32, 31]. There are also many other active areas of research including Poiseuille flows [7, 8], liquid crystals with variable degrees of orientation [29, 30, 6], static configurations and Fredericks transitions [7, 34].

The second portion of this work is devoted to one-dimensional shearing flows within the context of the Leslie-Ericksen continuum theory of liquid crystals. Much work has been done in the area of shearing flows of nematic liquid crystals , but there are three main drawbacks to the current analysis.

The first is a lack of analytic results concerning the multiplicity and stability of steady state solutions. Using numerical methods McIntosh et. al., [33], were able to show that only two types of solutions may be stable, which was a reduction to the number of stable candidates proposed by Currie and MacSithigh, [15].

The second is a common set of simplifying assumptions made on intrinsic parameters. More specifically the constant approximation

$$K_1 = K_2 = K_3 \tag{1.33}$$

of the Frank elasticity constants. As we will see, the constant approximation (1.33) retards the possibility of multiplicity of solutions in a one-dimensional shearing flow.

The third is a reduction in complexity made by assuming the velocity field is constant, [5]. While this is fine if one is concerned with this specific class of flows, we do not make this assumption in the following work and thus present more general results.

In the one-dimensional shearing flow regime we consider, the liquid crystal is confined between two parallel plates and a flow is induced via a shearing force applied to the upper plate. In our work we first transform the steady state equations into a Hamiltonian system and proceed to construct the Hamiltonian. We then give a complete description of the phase planes with respect to the parameter space

$$\Lambda = \{(\lambda_1, \lambda_2) \in \mathbb{R}^2\}, \tag{1.34}$$

where λ_1, λ_2 are defined through the Leslie coefficients of visocity in (1.28).

Focusing in on a particularly relevant region, in that it contains many of the commonly referenced liquid crystal materials including Isopentyl-cyanobiphenyl (5CB), we prove an existence result concerning steady state solutions subject to strong anchoring boundary conditions via time map arguments.

1.3 A Simplified Phenomenological Model

In their paper, Cheng et. al. [11], the authors consider a nematic liquid crystal fluid layer in between two parallel blocks to model frictional sliding in a geological fault. The continuum model proposed to describe this situation is

$$\mathbf{u}_t + (\mathbf{u} \cdot \nabla)\mathbf{u} = \mathrm{div}(v(\mathbf{r})\nabla \mathbf{u}) - \frac{1}{\rho}\nabla p, \quad \text{in } \Omega \tag{1.35}$$

$$\mathbf{r}_t + \nabla \mathbf{r} \cdot \mathbf{u} - \nabla \mathbf{u} \cdot \mathbf{r} = \delta \Delta \mathbf{r}, \quad \text{in } \Omega \tag{1.36}$$

where $\mathbf{u}$ is the velocity of the fluid, $\mathbf{r}$ is the director field, ρ is the density, $v(\mathbf{r})$ is the kinematic viscosity, p is the pressure, δ is a relaxation parameter, and Ω denotes the region bounded by the two solid blocks. The kinematic viscosity $v(\mathbf{r})$ is assumed to depend on the director field $\mathbf{r}$ via the model

$$v(r) = \alpha(\theta)v_1 + (1 - \alpha(\theta))v_0$$

for some decreasing function α and $0 < v_0 < v_1$, where

$$\cos\theta = \frac{|\mathbf{u} \times \mathbf{r}|}{|\mathbf{u}||\mathbf{r}|}.$$

The function $\alpha(\theta)$ determines the type of frictions modeled. In [11], the authors introduced the above model (2.1) and (2.2), and used numerical simulations to examine the behavior of solutions that allow them to compare with the empirical rate-and-state friction law. In our work we consider a more general form of the kinematic viscosity.

In order to understand the behavior in a geological fault, the authors consider a reduction to a one-dimensional shearing flow between two parallel plates. The shearing flow is assumed to be induced by a shearing velocity on the upper plate while the lower plate is held fixed. Furthermore the director is subject to a strong anchoring boundary condition, i.e. it is held in the same fixed direction on the upper and lower plate.

To begin, we completely describe the existence and multiplicity of the steady states. We are able to do so by exploiting the inherent Hamiltonian structure of the steady state equations. In the case that multiple steady-state solutions exist, it is natural to further ask which solutions are linearly (spectrally) stable. Stable solutions are ones which persist under small perturbation and hence are more physically realistic. We approach the question of spectral stability in two ways: energy methods and the Evans function [25, 24].

For small values shearing velocities we are able to show that the spectrum of the linearized operator lies in the left half complex plane, i.e. the steady state solution with small shearing velocity is spectrally stable. We are actually able to take this one step further and show that in fact for small shearing speeds the steady state solution is nonlinearly stable. Next we construct an Evans type function and show that zero is an eigenvalue of the linearized operator precisely when there is a bifurcation of the steady states.

Finally our spectral stability results suggest the possibility of an interesting hysteresis mechanism being present in this system. We use numerics to explore this subject.

For a shorter technical presentation of this work reference [11].

Chapter 2

Shearing Flows in a Liquid Crystal Model for Friction

In this section we explore a liquid-crystal type model which specifically attempts to address the issue of frictional forces in geological fault flows. Recall, the nematic liquid crystal continuum model proposed by C. H. A Cheng et. al., [11] which considers a fluid layer composed of nematic liquid crystal confined between two solid blocks:

$$\mathbf{u}_t + (\mathbf{u} \cdot \nabla)\mathbf{u} = \operatorname{div}(v(\mathbf{r})\nabla \mathbf{u}) - \frac{1}{\rho}\nabla p, \quad \text{in } \Omega \tag{2.1}$$

$$\mathbf{r}_t + \nabla \mathbf{r} \cdot \mathbf{u} - \nabla \mathbf{u} \cdot \mathbf{r} = \delta \Delta \mathbf{r}, \quad \text{in } \Omega \tag{2.2}$$

where $\mathbf{u}$ is the velocity of the fluid, $\mathbf{r}$ is the director field, ρ is the density, $v(\mathbf{r})$ is the kinematic viscosity, p is the pressure, δ is a relaxation parameter, and Ω denotes the region bounded by the two solid blocks.

To model the behavior of a fault the domain is taken to be $\Omega = (-\infty, \infty) \times (0, L)$, an infinite channel with width L, with coordinates (x, y) and is is assumed that there is no external pressure, i.e. $p \equiv 0$. Let $\mathbf{u} = (u_1(x,y), u_2(x,y))$ and $\mathbf{r} = (r_1(x,y), r_2(x,y))$ denote the velocity and director fields respectively. Under further simplifications, see

[11], these fields are assumed to take the form

$$u_1(x,y) = u(y),\ u_2 = 0; \quad r_1(x,y) = r(y),\ r_2 = 1. \tag{2.3}$$

A shearing flow is then induced by an imposed shearing velocity on the upper block, $\bar{\mathbf{u}}$, see Figure 2.1.

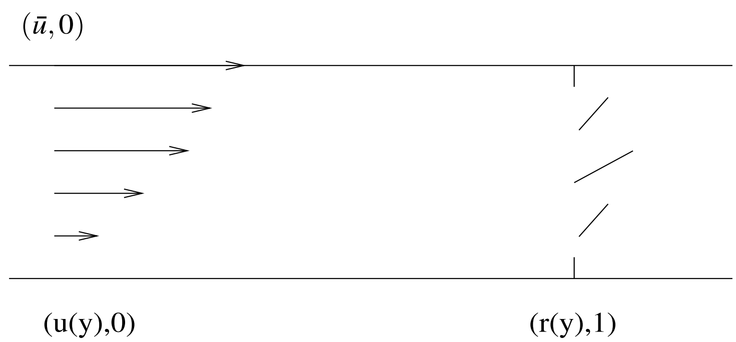

Figure 2.1: *Diagram of the shearing flow in an infinite channel*

Under these assumptions and with $v(r) = v(\mathbf{r})$, one obtains a one-dimensional version of the model:

$$u_t = (v(r)u_y)_y, \quad r_t = \delta r_{yy} + u_y, \quad \text{for } y \in (0,1), \tag{2.4}$$

with the boundary conditions

$$u(0,t) = 0, \quad u(1,t) = \bar{u}; \quad r(0,t) = r(1,t) = 0. \tag{2.5}$$

In this shearing flow, the kinematic viscosity $v(r)$ depends only on the director field r via the model

$$v(r) = \alpha(\theta)v_1 + (1 - \alpha(\theta))v_0$$

for some decreasing function α with $\alpha(0) = 1$ and $\alpha(\pi/2) = 0$ and $0 < v_0 < v_1$, where θ is the angle of $\mathbf{r}$ from the vertical.

In our analysis we consider a general $v(r)$ and assume

$$\begin{gathered} 0 < v_0 \leq v(r) \leq v_1, \quad v'(r) \leq 0 \ \text{ and} \\ \text{either } \ v'(r) = 0 \ \text{ for large } \ r \ \text{ or } \ \lim_{r\to\infty} \frac{(v'(r))^2}{v''(r)} = \mu_0. \end{gathered} \tag{2.6}$$

As it turns out the existence of the limit in the assumption (2.6) implies that $\mu_0 = 0$ (see Lemma 3).

In this chapter we give what constitutes a more or less complete study of this model. A framework for studying these types of nonlinear PDEs is well established, but this concrete model, being prescribed fully upon physical properties, presents extra difficulties which we must overcome. It is the inherent structure of the governing equations that allows us to overcome these difficulties and explicitly construct some of the important analytical tools such as the Evans function and all of its derivatives. The chapter is laid out as follows:

(i) We will first examine steady state solutions of (2.4) and (2.5). In this study we are able to give a complete characterization on the existence and multiplicity of steady states. An example with which exhibits multiple steady states is given as well.

(ii) We tackle the issue of stability of steady states. The steady states together with their stabilities play a critical role in understanding the global dynamics of general solutions. We discuss two types of stability results.

   (iia) First, using energy estimates, we prove that for small shearing speeds, $\bar{u}$, the steady state solution is linearly and nonlinearly stable.

(iib) The second result concerns the stability of steady states which bifurcate from a critical steady state. We are able to identify conditions on $\bar{u}$ which characterize this type of bifurcation as well as give stability results for the bifurcated steady states. Specifically, we show that zero is a eigenvalue of the linearization about a critical steady state and we track the bifurcation of this zero eigenvalue.

(iii) Finally, our stability result suggests that this simple model possesses hysteresis; more precisely, when one applies dynamic boundary conditions $\bar{u}(t)$ in two manners, one with slowly increasing $\bar{u}(t)$ from zero to large, and the other in the reversal way, the solution of (2.4) and (2.5) for the second setup is *not* the reverse of the first. In the last section we use numerics to explore this hysteresis phenomenon. This activity confirms a probably well-known necessary condition for hysteresis: the existence of multiple *stable* steady states.

The study outlined above is the natural approach if one considers the structure of system (2.4). The system comprises an integrable equation coupled with a Hamiltonian equation. Thus we construct a Hamiltonian function enabling us study the existence of solutions to the Hamiltonian equation. Because the linearization about a steady state is precisely the zero eigenvalue problem associated with the linearization, we are able to construct a full set of first integrals through the Hamitonian function. This allows us to explicitly construct an Evans type function for the zero eigenvalue. Having the explicit form of the Evans type function lets us freely compute the derivatives and analyze eigenvalues in a neighborhood of a zero eigenvalue.

2.1 The steady state

In this section, we will characterize the existence and multiplicity of steady-state solutions of (2.4) and (2.5) under the assumption (2.6) on the kinematic viscosity ν.

For definiteness, we assume $\bar{u} > 0$ in (2.5), i.e. the shearing on the upper plate is in the direction of the positive x-axis. We obtain the steady state problem by assuming the solution is stationary in time and setting $u_t = 0$, $r_t = 0$. After an integration of the velocity equation one obtains the steady-state problem of (2.4) and (2.5) which is for some positive constant M^2 (see (2.9)),

$$\begin{aligned} \nu(r)u' =& M^2, \quad \delta r'' + u' = 0, \quad y \in (0,1) \\ u(0) = 0, \quad & u(1) = \bar{u} > 0, \quad r(0) = r(1) = 0, \end{aligned} \tag{2.7}$$

where prime denotes the derivative with respect to y.

Upon another integration we obtain a solution of the velocity equation implicitly in terms of the director field, r. That is

$$u(y) = u(0) + M^2 \int_0^y \frac{1}{\nu(r(s))} ds. \tag{2.8}$$

In view of the boundary conditions $u(0) = 0$ and $u(1) = \bar{u} > 0$, we have

$$M^2 = \bar{u} \left\{ \int_0^1 \frac{1}{\nu(r(y))} dy \right\}^{-1} > 0. \tag{2.9}$$

2.1.1 Existence and multiplicity

In light of (2.8) a study of system (2.7) reduces to the study of the system

$$r'' + \frac{M^2}{\delta \nu(r)} = 0, \quad r(0) = r(1) = 0, \tag{2.10}$$

subject to the constraint (2.9). System (2.10) is a classical Hamiltonian system (Newtonian system) whose solutions lie on the level curves of the Hamiltonian function

$$H(r,r') = \frac{1}{2}(r')^2 + \frac{M^2}{\delta}f(r), \tag{2.11}$$

where f, called the potential function, is given by

$$f(r) = \int_0^r \frac{1}{v(\tau)}d\tau. \tag{2.12}$$

The phase portrait of system (2.10), which is obtained by plotting the level curves of (2.11), is shown in Figure 2.2.

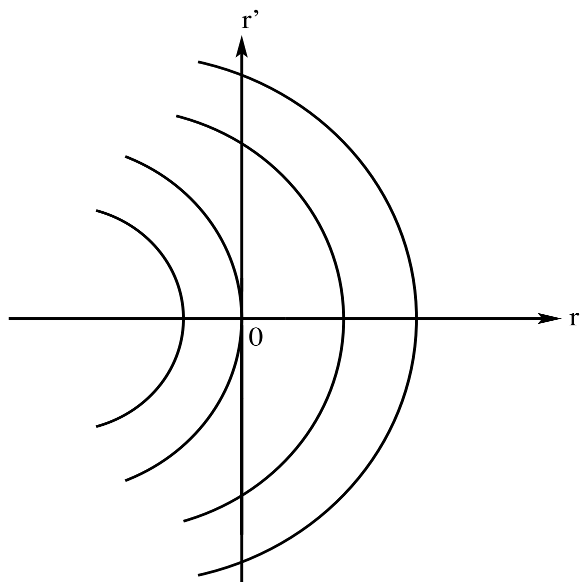

Figure 2.2: *The phase portrait of system (2.10) in the (r,r')-plane.*

It is clear that f is strictly increasing since $v(r) > 0$. Let g be the inverse function of f. The following lemma is a simple consequence of (2.6).

Lemma 2. *$f(0) = g(0) = 0$, $f(\infty) = g(\infty) = \infty$, $f'(r) = 1/v(r) > 0$, $f''(r) = -v'(r)/v^2(r) > 0$; $g'(s) = v(g(s)) \in (v_0, v_1]$, $g''(s) < 0$.*

We define the function

$$D(\beta) = \beta \int_0^1 \frac{g'(\beta t)}{\sqrt{1-t}} dt \ \text{ for } \ \beta > 0. \tag{2.13}$$

and proceed to prove the following characterization of steady state solutions.

Theorem 1. *For any $\bar{u} > 0$, the set of solutions of the boundary value problem (2.7) is in one-to-one correspondence with the set of solutions β of $\bar{u} = 4\delta D(\beta)$. In particular, there always exists at least one solution.*

Proof. We first claim that, if $r(y)$ is a solution of the boundary value problem (2.10), then $r(y) \geq 0$ for $y \in (0,1)$, $r(y)$ is symmetric about $y = 1/2$ and $r'(1/2) = 0$. In fact, it follows from the equation in (2.10) that $r(y)$ is strictly concave downward. The boundary condition $r(0) = r(1) = 0$ then implies that $r(y) > 0$ for $y \in (0,1)$ and there is a unique $y^* \in (0,1)$ so that $r'(y^*) = 0$. Set $r(y^*) = \alpha$ and $r_1(y) = r(2y^* - y)$. Then $r_1(y)$ satisfy the second-order equation in (2.10) and the initial conditions $r_1(y^*) = r(y^*) = \alpha$ and $r_1'(y^*) = -r'(y^*) = 0$. By uniqueness of initial value problems, we have $r(y) = r_1(y)$; in particular, $r_1(1) = r(2y^* - 1) = r(1) = 0$. Since $r(y) = 0$ implies $y = 0$ or $y = 1$, we have either $2y^* - 1 = 1$ or $2y^* - 1 = 0$; that is, either $y^* = 1$ or $y^* = 1/2$. We thus conclude $y^* = 1/2$ since $y^* \in (0,1)$, and hence, $r(y) = r_1(y) = r(1-y)$.

It now follows from (2.11), $r(1/2) = \alpha$ and $r'(1/2) = 0$ that

$$\frac{1}{2}(r')^2 + \frac{M^2}{\delta} f(r) = \frac{M^2}{\delta} f(\alpha),$$

and hence, for $y \in (0, 1/2)$, $r'(y) \geq 0$ and

$$r' = \sqrt{\frac{2}{\delta}} M \sqrt{f(\alpha) - f(r)} \ \text{ or } \ M dy = \sqrt{\frac{\delta}{2}} \frac{dr}{\sqrt{f(\alpha) - f(r)}}. \tag{2.14}$$

Integrate from $y = 0$ to $y = 1/2$ to get

$$M = \sqrt{2\delta} \int_0^{\alpha} \frac{dr}{\sqrt{f(\alpha) - f(r)}}.$$

Note that $r'(0) = \sqrt{2\delta^{-1}} M \sqrt{f(\alpha)}$ and

$$\begin{aligned}\int_0^1 \frac{dy}{v(r(y))} =& 2\int_0^{1/2} \frac{dy}{v(r(y))} = -\frac{2\delta}{M^2} \int_0^{1/2} r''(y) dy \\ &= -\frac{2\delta}{M^2} \left(r'(1/2) - r'(0) \right) = \frac{2\delta}{M^2} r'(0) = \frac{2\sqrt{2\delta}}{M} \sqrt{f(\alpha)}.\end{aligned}$$

The relation (2.9) then imposes that

$$\bar{u} = 2M\sqrt{2\delta}\sqrt{f(\alpha)} = 4\delta\sqrt{f(\alpha)} \int_0^{\alpha} \frac{dr}{\sqrt{f(\alpha) - f(r)}}.$$

Let $\beta = f(\alpha)$ or equivalently $\alpha = g(\beta)$. In terms of β, we have,

$$M = \sqrt{2\delta} \int_0^{\beta} \frac{g'(s)}{\sqrt{\beta - s}} ds = \sqrt{2\delta}\beta^{1/2} \int_0^1 \frac{g'(\beta t)}{\sqrt{1-t}} dt, \tag{2.15}$$

$$\bar{u} = 4\delta\beta^{1/2} \int_0^{\beta} \frac{g'(s)}{\sqrt{\beta - s}} ds = 4\delta\beta \int_0^1 \frac{g'(\beta t)}{\sqrt{1-t}} dt = 4\delta D(\beta). \tag{2.16}$$

It follows that, given any $\bar{u} > 0$, if $\beta > 0$ is a solution of (2.16), then there is a steady-state solution. It is also clear from the construction of the steady-state solution and the monotonicity of $f(r)$ that different β values provide different steady-state solutions. Therefore, the set of steady-states is in one-to-one correspondence with the set of solutions β of equation (2.16).

Since $v_0 \leq g'(s) \leq v_1$, one has that $D(\beta) \to 0$ as $\beta \to 0$ and $D(\beta) \to \infty$ as $\beta \to \infty$. Thus, for any $\bar{u} > 0$, there exists at least one $\beta > 0$ such that (2.16) is satisfied. This completes the proof. □

Next, we provide a condition on $\bar{u}$ so that the corresponding boundary value problem (2.7) has a unique solution and an example of $v(r)$ for which the boundary value problem (2.7) has multiple solutions for a range of $\bar{u}$.

Lemma 3. *Assumption (2.6) implies $\mu_0 = 0$.*

Proof. Assume, on the contrary, that $\mu_0 \neq 0$. The existence of $\lim_{r\to\infty} \frac{(v'(r))^2}{v''(r)} = \mu_0$ implicitly implies that $v''(r) \neq 0$ and $v'(r) < 0$ if $r > r_0$ for some large r_0. We claim that $v''(r) > 0$ for $r > r_1$ since, otherwise, $v'(r) \leq v'(r_0) < 0$ and hence $v(r) \leq v(r_0) + (r - r_0)v'(r_0) \to -\infty$ as $r \to \infty$ that contradicts to $v(r) \geq v_0 > 0$. Therefore, $\mu_0 > 0$. Denote, for $r > r_0$, $\frac{(v'(r))^2}{v''(r)} = \rho(r)$. Then $\rho(r) \to \mu_0$ as $r \to \infty$. Assume $\rho(r) \geq \mu_0/2$ for $r \geq r_*$ for some $r_* > r_0$. Solve the equation $\rho(r)(v')' = (v')^2$ to get, for $r \geq r_*$,

$$v'(r) = -\frac{1}{\int_{r_*}^{r} \frac{1}{\rho(\tau)} d\tau - \frac{1}{v'(r_*)}}.$$

Hence,

$$v(r) = v(r_*) - \int_{r_*}^{r} \frac{1}{\int_{r_*}^{s} \frac{1}{\rho(\tau)} d\tau - \frac{1}{v'(r_*)}} ds.$$

It follows from, for $r \geq r_*$, $\rho(r) \geq \mu_0/2$ that

$$\int_{r_*}^{r} \frac{1}{\rho(\tau)} d\tau \leq \frac{2}{\mu_0}(r - r_*).$$

Therefore,

$$v(r) \leq v(r_*) - \int_{r_*}^{r} \frac{1}{\frac{2}{\mu_0}(s - r_*) - \frac{1}{v'(r_*)}} ds \to -\infty \text{ as } r \to \infty.$$

The latter contradicts to $v_0 \leq v(r) \leq v_1$. We thus conclude $\mu_0 = 0$. $\square$

Corollary 1. *Assume (2.6). There exist* $0 < \beta_1 < \beta_2$ *such that* $D'(\beta) > 0$ *for* $0 < \beta < \beta_1$ *and for* $\beta > \beta_2$*. Hence, for* $\bar{u} \in (0, 4\delta D(\beta_1)) \cup (4\delta D(\beta_2), \infty)$*, the boundary value problem (2.7) has a unique solution.*

Proof. Note that

$$D'(\beta) = \int_0^1 \frac{g'(\beta t)}{\sqrt{1-t}} dt + \beta \int_0^1 \frac{t g''(\beta t)}{\sqrt{1-t}} dt.$$

The existence of β_1 follows from that $g' \geq v_0 > 0$ and $|g''|$ is bounded.

From $g'(s) = v(g(s))$, we have

$$\frac{dg}{v(g)} = ds \quad \text{or} \quad \int_0^{g(z)} \frac{dr}{v(r)} = z.$$

Therefore,

$$zg''(z) = zv_r(g(z))g'(z) = v_r(g(z))v(g(z)) \int_0^{g(z)} \frac{1}{v(r)} dr.$$

If $v(r) = 0$ for large r in (2.6), then $\lim_{z\to+\infty} (g'(z) + zg''(z)) = v_0 > 0$. For the other case in (2.6),

$$\begin{aligned} \lim_{z\to+\infty} \left(g'(z) + zg''(z)\right) =& v_0 + \lim_{z\to\infty} \left(v_r(g(z))v(g(z)) \int_0^{g(z)} \frac{1}{v(r)} dr \right) \\ =& v_0 - \lim_{g\to\infty} \frac{v(g)v_r^2(g)/v_{rr}(g)}{v_r^2(g)/v_{rr}(g) + v(g)} = v_0 > 0. \end{aligned}$$

One checks that, for any continuous function $q(t)$,

$$\lim_{\beta\to\infty} \int_0^1 \frac{q(\beta t)}{\sqrt{1-t}} dt = 2 \lim_{t\to\infty} q(t)$$

if the latter limit exists. Therefore,

$$\lim_{\beta\to\infty} D'(\beta) = \lim_{\beta\to\infty} \int_0^1 \frac{g'(\beta t) + \beta t g''(\beta t)}{\sqrt{1-t}} dt = 2 \lim_{z\to+\infty} \left(g'(z) + zg''(z)\right) > 0.$$

The existence of $\beta_2 > 0$ with the desired property follows directly. $\square$

Remark 1. In the proof of Corollary 1 the limit

$$\lim_{z\to+\infty}\left(g'(z)+zg''(z)\right)=\frac{\nu_0^2}{\mu_0+\nu_0}$$

Yet, one can also compute

$$\begin{aligned}\lim_{z\to+\infty}\left(g'(z)+zg''(z)\right) =& \nu_0+\lim_{z\to\infty}\left(\nu_r(g(z))\nu(g(z))\int_0^{g(z)}\frac{1}{\nu(r)}dr\right)\\ =& \nu_0-\nu_0\lim_{g\to\infty}\frac{\nu_r^2(g)/\nu_{rr}(g)}{\nu(g)}\\ =& \nu_0-\mu_0\end{aligned}$$

Thus, it must true that $\mu_0 = 0$.

2.1.2 An example of multiple steady states

We give an example of $\nu(r)$ for which $\bar{u} = 4\delta D(\beta)$ is a cubic-like function. We set $\delta = 1$ and choose a piecewise viscosity function

$$\nu(r)=\begin{cases}1, & 0\le r<1\\ (1+9(r-1)^8)^{-1}, & 1\le r<2\\ 0.1, & 2\le r.\end{cases} \tag{2.17}$$

This cubic $\bar{u}(\alpha)$ has a local maximum $\bar{u}_{\max}\approx 12.84$ and local minimum $\bar{u}_{\min}\approx 10.98$, Figure 2.3. For $\bar{u}\in(u_{\min},u_{\max})$ there are three steady-state solutions which bifurcate from a unique solution as $\bar{u}$ is varied across the local extrema.

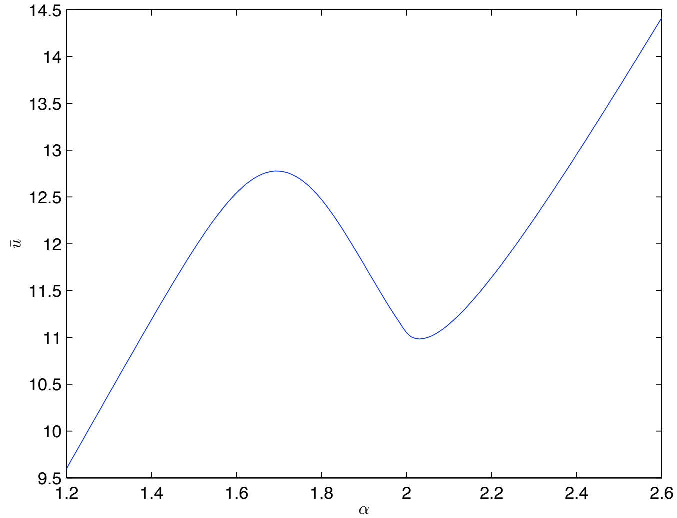

Figure 2.3: *A cubic-like $\bar{u}(\beta)$ for $v(r)$ in the example. Note that the horizontal axis is labeled by $\alpha = g(\beta)$ instead of β.*

2.2 Stability for small shearing speeds

In this section, we use energy methods to establish the nonlinear and linear stability of steady-states with small shearing speeds $\bar{u}$. In particular, this will imply the spectral stability of these steady-states, which will be relevant for the discussion of hysteresis in Section 2.4.

For fixed points of finite dimensional autonomous ODEs it is always true that spectral stability implies linear stability implies nonlinear stability. This is the result of the classical Hartman-Grobman Theorem, [38] pp. 120, which states that the flow of the nonlinear system $x' = f(x)$, $f \in C^1(\mathbb{R})$ is diffeomorphic to the flow of the linearized system $y' = Df(x_0)y$ in a neighborhood of the fixed point, x_0, $f(x_0) = 0$, provided zero is not in the spectrum of the linearized operator, i.e $0 \notin \sigma(Df(x_0))$. In this case, the fixed point is asymptotically stable is the spectrum lies in the left half complex plane, and unstable if the spectrum lies in the right half complex plane. The analogue of fixed points in finite dimensional ODEs are steady states in infinite dimensional PDEs.

For PDEs the study of stability of steady states is more complicated and it is *not* necessarily true that spectral stability implies linear stability implies nonlinear stability. Yet, this idea still permeates the analysis of steady state stability and it is often, but not always true, that spectral stability is necessary for linear stability is necessary for nonlinear stability.

2.2.1 Linear stability

Let $(u^*, r^*) = (u^*(y), r^*(y))$ be a steady-state of the problem (2.4) and (2.5) with $u^*(1) = \bar{u}$. The linearization of the problem (2.4) and (2.5) along (u^*, r^*) is

$$U_t = \left(v(r^*)U_y + u^*_y v_r(r^*)R\right)_y, \quad R_t = \delta R_{yy} + U_y, \tag{2.18}$$

with $U(t,0) = U(t,1) = R(t,0) = R(t,1) = 0$.

Our proof of stability for small shearing speeds uses Poincare's which we state here for reference, [3].

Lemma 4. *(***Poincare's Inequality***) Suppose that $y \in C^1(0,L)$ and $y(0) = 0 = y(1)$, then*

$$\int_0^1 y^2\,dx \le \frac{L^2}{\pi^2}\int_0^1 (y')^2\,dx.$$

Theorem 2. *For small $\bar{u}$, (u^*, r^*) is linearly exponentially stable in L^2; more precisely, for $K = \pi^2\delta^{-1}v_0^{-1}$, if $\bar{u}$ is small enough, then there exists $\rho > 0$ such that*

$$\int_0^1 (KU^2(t,y) + R^2(t,y))dy \le e^{-\rho t}\int_0^1 (KU^2(0,y) + R^2(0,y))dy.$$

Proof. By the Poincare inequality, we have, for R with $R(0) = R(1) = 0$,

$$\int_0^1 R^2(y)dy \leq \frac{1}{\pi^2}\int_0^1 R_y^2(y)dy.$$

It follows from (2.9) that $M^2(\beta) \leq \bar{u}v_1$ so that

$$u_y^*(y) = \frac{M^2(\beta)}{v(r^*(y))} \leq \frac{v_1}{v_0}\bar{u}, \quad |u_y^*(y)v_r(r^*(y))| \leq \frac{\bar{u}v_1\|v_r\|_\infty}{v_0}.$$

Multiply the U-equation by KU, R-equation by R, and integrate over $[0,1]$ to get

$$\begin{aligned}\frac{1}{2}\frac{d}{dt}\int_0^1 (KU^2+R^2) =& -\int_0^1 \left(Kv(r^*)U_y^2 + Ku_y^*v_r(r^*)RU_y + \delta R_y^2 - RU_y\right) dy \\ \leq& -\int_0^1 \left(Kv_0U_y^2 + \delta R_y^2\right) dy + \frac{K\bar{u}v_1\|v_r\|_\infty + v_0}{v_0}\int_0^1 |RU_y|dy.\end{aligned}$$

By Young's inequality and the Poincare inequality,

$$\begin{aligned}\int_0^1 |RU_y|dy \leq& \frac{\delta\pi^2}{2}\int_0^1 R^2dy + \frac{1}{2\pi^2\delta}\int_0^1 U_y^2dy \\ \leq& \frac{\delta}{2}\int_0^1 R_y^2dy + \frac{1}{2\pi^2\delta}\int_0^1 U_y^2dy.\end{aligned}$$

It is clear that, for small $\bar{u}$,

$$Kv_0 > \frac{K\bar{u}v_1\|v_r\|_\infty + v_0}{2\pi^2\delta v_0} \text{ and } \delta > \frac{K\bar{u}v_1\|v_r\|_\infty + v_0}{2v_0}\delta.$$

Thus, there exists $\rho > 0$ such that

$$\begin{aligned}\frac{1}{2}\frac{d}{dt}\int_0^1 (KU^2+R^2)dy \leq& -\frac{\rho}{2}\int_0^1 \frac{1}{\pi^2}(KU_y^2+R_y^2)dy \\ \leq& -\frac{\rho}{2}\int_0^1 (KU^2+R^2)dy.\end{aligned}$$

Hence, by Gronwall's inequality,

$$\int_0^1 (KU^2(t,y)+R^2(t,y))dy \le e^{-\rho t}\int_0^1 (KU^2(0,y)+R^2(0,y))dy.$$

This establishes the L^2 linear stability of steady states with small $\bar{u}$. □

2.2.2 Nonlinear stability

Theorem 2 implies that the spectrum lies in the left half complex plane, but does not necessarily prove the other direction that the steady state solution is nonlinearly stable. It turns out though that we are able to prove directly that steady states in fact are nonlinearly stable.

Theorem 3. *If $\bar{u}$ is small enough, then (u^*, r^*) is nonlinearly stable in L^2; more precisely, for $K > \delta^{-1}v_0^{-1}$, if $\bar{u}$ is small enough, then there exists $\rho > 0$ such that*

$$\begin{aligned}\int_0^1 &\left(K(u(t,y)-u^*(t,y))^2+(r(t,y)-r^*(t,y))^2\right)dy\\ &\le e^{-\rho t}\int_0^1 \left(K(u(0,y)-u^*(0,y))^2+(r(0,y)-r^*(0,y))^2\right)dy.\end{aligned}$$

Proof. Let $U = u-u^*$ and $R = r-r^*$. Then

$$\begin{aligned}U_t =&(v(r)u_y - v(r^*)u_y^*)_y = \Big(v(r)U_y + (v(r)-v(r^*))u_y^*\Big)_y,\\ R_t =&\delta R_{yy}+U_y.\end{aligned}$$

Fix $K > \delta^{-1} v_0^{-1}$. Multiply the U-equation by KU, R-equation by R, and integrate over $[0,1]$ to get

$$\begin{aligned}\frac{1}{2}\frac{d}{dt}\int_0^1 (KU^2+R^2) &= -\int_0^1 \left(Kv(r)U_y^2 + K(v(r)-v(r^*))u_y^* U_y + \delta R_y^2 - RU_y\right) dy \\ &\le -\int_0^1 \left(Kv_0 U_y^2 + \delta R_y^2 + K(v(r)-v(r^*))u_y^* U_y - RU_y\right) dy\end{aligned}$$

Now, by Young's inequality we have

$$\int_0^1 |RU_y| dy \le \frac{\delta}{2}\int_0^1 R^2 dy + \frac{1}{2\delta}\int_0^1 U_y^2 dy,$$

$$\int_0^1 |K(v(r)-v(r^*))u_y^* U_y| dy \le \int_0^1 \frac{Kv_1 \bar{u}|v_r|_0}{v_0} |RU_y| dy \le \frac{K\bar{u}v_1|v_r|_0}{2v_0}\int_0^1 (R^2+U_y^2) dy.$$

If $\bar{u}$ is small enough so that

$$\rho =: \min\left\{\frac{2\pi^2 K\delta v_0^2 - \pi^2 v_0 - \pi^2 K\delta \bar{u} v_1 |v_r|_0}{Kv_0\delta},\ \frac{v_0\delta - K\bar{u}v_1|v_r|_0}{v_0}\right\} > 0,$$

then by Poincare's inequality we have

$$\begin{aligned}\frac{1}{2}\frac{d}{dt}\int_0^1 (KU^2+R^2) &\le -\int_0^1 \Big(\frac{2K\delta v_0 - 1 - K\delta\bar{u}|v_r|_0}{2\delta} U_y^2 + \frac{\delta - K\bar{u}|v_r|_0}{2} R^2\Big) dy \\ &\le -\int_0^1 \Big(\frac{2\pi^2 K\delta v_0 - \pi^2 - \pi^2 K\delta\bar{u}|v_r|_0}{2\delta} U^2 + \frac{\delta - K\bar{u}|v_r|_0}{2} R^2\Big) dy \\ &\le -\frac{\rho}{2}\int_0^1 (KU^2+R^2).\end{aligned}$$

Hence, by Gronwall's inequality,

$$\int_0^1 (KU^2(t,y)+R^2(t,y)) dy \le e^{-\rho t}\int_0^1 (KU^2(0,y)+R^2(0,y)) dy.$$

This establishes the L^2-stability of (u^*, r^*) with small $\bar{u}$. □

2.3 Eigenvalues and bifurcations of steady-states

In view of the existence and multiplicity result (Theorem 1), steady-states of the boundary value problem (2.4) and (2.5) cannot be uniquely parameterized by $\bar{u}$ in general. We thus parameterize steady-states by the parameter β with $\bar{u}(\beta) = 4\delta D(\beta)$ and examine the spectral stability of steady-states as β varies.

It follows from the previous section that steady-states associated to small $\bar{u}$ are linearly stable. As we increase β, there are two possibilities for the steady-state to loss its stability: one is that a zero eigenvalue is created and the other is a pair of pure imaginary eigenvalues. In this section, we focus on stability changes of steady-states due to bifurcations of zero eigenvalues. The basic tool for this investigation is an Evans or a Wronskian type function.

We are concern ourselves with only the eigenvalues, or point spectrum, associated with linearized system (2.18) since its solution operator is a compact map and thus the spectrum consists only of eigenvalues, [22, 26].

2.3.1 Linearization, eigenvalues, and the Evans function

For $\beta > 0$, let $(u,r) = (u(y;\beta), r(y;\beta))$ be the steady-state with $\bar{u} = 4\delta D(\beta)$ defined in (2.16). In view of the linearized system (2.18), the eigenvalue problem associated to this steady-state is the system

$$(v(r)U_y + u_y v_r(r)R)_y = \lambda U, \quad \delta R_{yy} + U_y = \lambda R \tag{2.19}$$

with the boundary condition

$$U(0) = R(0) = 0, \quad U(1) = R(1) = 0. \tag{2.20}$$

Alternatively, we can set

$$P = v(r)U_y + u_y v_r(r)R \text{ and } Q = \delta R_y + U,$$

and rewrite system (2.19) into a system of first order equations

$$U' = \frac{1}{v(r)}P - \frac{u_y v_r(r)}{v(r)}R, \quad P' = \lambda U, \quad R' = \frac{1}{\delta}Q - \frac{1}{\delta}U, \quad Q' = \lambda R, \tag{2.21}$$

where prime denotes the derivative with respect to y. Setting $Z = (U, P, R, Q)$, system (2.21) has the compact form

$$Z' = A(y; \lambda, \beta)Z, \tag{2.22}$$

where

$$A(y;\lambda,\beta) = \begin{pmatrix} 0 & \frac{1}{v(r(y;\beta))} & -\frac{u_y(y;\beta)v_r(r(y;\beta))}{v(r(y;\beta))} & 0 \\ \lambda & 0 & 0 & 0 \\ -\frac{1}{\delta} & 0 & 0 & \frac{1}{\delta} \\ 0 & 0 & \lambda & 0 \end{pmatrix}.$$

For any given $\beta \in \mathbb{R}_+$ and $\lambda \in \mathbb{C}$, let $Z_j(y;\lambda,\beta)$ for $j = 1,2,3,4$ be the solutions of (2.21) with

$$Z_1(0;\lambda,\beta) = Z_3(1;\lambda,\beta) = e_2 = (0,1,0,0),$$

$$Z_2(0;\lambda,\beta) = Z_4(1;\lambda,\beta) = e_4 = (0,0,0,1)$$

so that Z_1 and Z_2 are linearly independent solutions and satisfy the boundary condition at $y = 0$, and Z_3 and Z_4 are linearly independent solutions and satisfy the boundary condition at $y = 1$.

Set

$$E(y;\lambda,\beta) = \det(Z_1(y;\lambda,\beta), Z_2(y;\lambda,\beta), Z_3(y;\lambda,\beta), Z_4(y;\lambda,\beta)). \tag{2.23}$$

We recall Lemma 5 which will be used to show that E is independent of y in Lemma 6.

Lemma 5. *(***Louiville's Theorem***) Suppose that $\Phi(t)$ is a fundamental matrix solution of $x' = A(t)x$. Then,*

$$\det(\Phi(t)) = \det(\Phi(0)) \exp\left\{\int_0^t tr(A(s))\right\} ds$$

Lemma 6. *The function E is independent of y and is smooth in (λ,β).*

Proof. It follows from Lemma 5 that

$$E(y;\lambda,\beta) = \exp\left\{\int_0^y \mathrm{tr}A(\tau;\lambda,\beta)d\tau\right\} E(0;\lambda,\beta).$$

Since $\mathrm{tr}A(\tau;\lambda,\beta) = 0$, then $E(y;\lambda,\beta)$ is independent of y. Smoothness of the function$E$ is a direct consequence of the smoothness of solutions of differential equations with respect to parameters and initial values, [38]. □

We thus denote $E(y;\lambda,\beta)$ by $E(\lambda,\beta) : \mathbb{C}\times\mathbb{R}_+ \to \mathbb{C}$ and refer to it as the *Evans function* of the eigenvalue problem (2.22). Evans function was widely used to study point spectrum of linearization along special solutions, such as various wave solutions, of systems of PDEs (see, for example, [23, 2, 40, 41, 20, 25, 21, 24, 37]) and the corresponding spectral problem is defined typically on the whole space. For the problem at hand, the eigenvalue problem is a boundary value problem but the idea for the construction of an Evans function is the same.

Lemma 7. *A number $\lambda \in \mathbb{C}$ is an eigenvalue if and only if $E(\lambda,\beta) = 0$.*

Proof. Suppose λ is an eigenvalue. Then there exists a nonzero solution $Z(y) = Z(y;\lambda,\beta) \neq 0$ of the boundary value problem (2.21). Let $Z(0) = (0,c_1,0,c_2)$ and $Z(1) = (0,c_3,0,c_4)$ for some c_i's, not all zeros. Since $Z(0) = c_1 Z_1(0;\lambda,\beta) + c_2 Z_2(0;\lambda,\beta)$ and $Z(1) = c_3 Z_3(1;\lambda,\beta) + c_4 Z_4(1;\lambda,\beta)$, one has

$$Z(y) = c_1 Z_1(y;\lambda,\beta) + c_2 Z_2(y;\lambda,\beta) = c_3 Z_3(y;\lambda,\beta) + c_4 Z_4(y;\lambda,\beta).$$

Therefore, $E(\lambda,\beta) = 0$. On the other hand, if $E(\lambda,\beta) = 0$, then

$$c_1 Z_1(y;\lambda,\beta) + c_2 Z_2(y;\lambda,\beta) + c_3 Z_3(y;\lambda,\beta) + c_4 Z_4(y;\lambda,\beta) = 0$$

for some c_i's, not all zeros. Since Z_1 and Z_2 are linearly independent, and Z_3 and Z_4 are linearly independent, it cannot happen that $c_1 = c_2 = 0$ or $c_3 = c_4 = 0$. Therefore,

$$Z(y) := c_1 Z_1(y;\lambda,\beta) + c_2 Z_2(y;\lambda,\beta) = -c_3 Z_3(y;\lambda,\beta) - c_4 Z_4(y;\lambda,\beta)$$

is a nonzero solution of the boundary value problem (2.21), and hence, the number λ is an eigenvalue. □

2.3.2 The Characterization of a zero eigenvalue

In the section we show that a zero is an eigenvalue of the linearization about the steady state associated with β_* if and only if β_* is a critical point of $D(\beta)$, see (2.13). In system (2.7) for the steady-states of (2.4), we introduce $p = v(r)u_y$ and $q = \delta r_y + u$. System

(2.7) becomes

$$u_y = \frac{1}{v(r)} p, \quad p_y = 0, \quad r_y = \frac{1}{\delta} q - \frac{1}{\delta} u, \quad q_y = 0. \tag{2.24}$$

It can be checked directly that

Lemma 8. *System (2.24) has three integrals given by*

$$H_1 = p, \quad H_2 = q, \quad H_3 = \frac{1}{2}(q-u)^2 + \delta f(r) p.$$

When $\lambda = 0$, system (2.21) of eigenvalue problems is reduced to

$$U' = \frac{1}{v(r)} P - \frac{u_y v_r(r)}{v(r)} R, \quad P' = 0, \quad R' = \frac{1}{\delta} Q - \frac{1}{\delta} U, \quad Q' = 0, \tag{2.25}$$

which is nothing but the linearization of system (2.24) along the solution $z = (u, p, r, q)$ of (2.24). We have

Lemma 9. *System (2.25) has three integrals $G_j = \langle \nabla H_j(z), Z \rangle$:*

$$G_1 = P,\ G_2 = Q,\ G_3 = -(q-u)U + \delta f(r) P + \frac{\delta p}{v(r)} R + (q-u) Q.$$

Proof. One can verify the statement directly. In general, if $H(z)$ is an integral for a nonlinear system $z'(t) = F(z)$, then its linearization $Z' = DF(z(t))Z$ along a solution $z(t)$ has an integral given by $G = \langle \nabla H(z(t)), Z \rangle$. □

The three integrals given in Lemma (9) constitute a full set of integrals, which allow us to explicitly construct a fundamental matrix solution of system (2.22) for $\lambda = 0$.

Lemma 10. *The principal fundamental matrix solution* $\Phi(y)$ *at* $y = 0$ *of system (2.25) is*

$$\Phi(y) = \begin{pmatrix} U_1(y) & U_2(y) & U_3(y) & U_4(y) \\ 0 & 1 & 0 & 0 \\ R_1(y) & R_2(y) & R_3(y) & R_4(y) \\ 0 & 0 & 0 & 1 \end{pmatrix}$$

where

$$\begin{aligned}
U_1(y) =& \frac{v_1}{v(r(y))} + \frac{r'(0)}{v(r(y))}\int_0^y v_r(t)dt, \\
U_2(y) =& \frac{1}{v(r(y))}\int_0^y (v_r(r(t))f(r(t)) + 1)dt, \\
U_3(y) =& -\frac{u'(0)}{v(r(y))}\int_0^y v_r(r(t))dt, \\
U_4(y) =& -\frac{1}{\delta v(r(y))}\int_0^y u(t)v_r(r(t))dt = 1 - U_1(y), \\
R_1(y) =& \frac{r'(y)}{u'(y)}U_1(y) - \frac{r'(0)}{u'(y)} = \frac{r'(y)}{u'(0)} - \frac{r'(0)}{u'(y)} + \frac{r'(0)r'(y)}{v_1u'(0)}\int_0^y v_r(r(t))dt, \\
R_2(y) =& \frac{r'(y)}{u'(y)}U_2(y) - \frac{f(r(y))}{u'(y)}, \\
R_3(y) =& \frac{r'(y)}{u'(y)}U_3(y) + \frac{u'(0)}{u'(y)}, \\
R_4(y) =& \frac{r'(y)}{u'(y)}U_4(y) + \frac{u(y)}{\delta u'(y)} = -R_1(y).
\end{aligned}$$

Proof. We construct only the second column of $\Phi(y)$ and the other columns can be found similarly. Suppose that $(U,P,R,Q)^T$ is a solution of (2.25) with with the initial condition e_2. It follows from Lemma 9 that, for all y,

$$P(y) = G_1(0) = 1,\ Q(y) = G_2(0) = 0,\ -\delta r'U + \delta f(r) + \delta u'R = G_3(0) = 0.$$

Substituting $R = \frac{r'}{u'}U - \frac{f(r)}{u'}$ into the U-equation of (2.25), we get

$$vU' + v_r r' U = v_r f(r) + 1.$$

Therefore,

$$U = \frac{1}{v}\int_0^y (v_r f(r) + 1)\, dt.$$

Hence,

$$R = \frac{r'}{u'}U - \frac{f(r)}{u'}.$$

This completes the proof. $\square$

With a fundamental matrix solution, it is possible to now explicitly construct the Evan's function for $\lambda = 0$ and all of its derivatives, most importantly at the critical values β^*.

Proposition 1. *For $\beta > 0$, $E(0,\beta) = -8\beta^2 \bar{u}'(\beta)/\bar{u}^2(\beta)$.*

Proof. Recall the definition of $Z_j(y;\lambda,\beta)$, for $j = 1,2,3,4$, given next to system (2.22). Denote $Z_j^0(y) = Z_j(y;0,\beta)$ for simplicity.

It follows from Lemmas 10 and 6, (2.14), (2.15), (2.16) and $u'(1) = M^2/v_1$ that,

$$\begin{aligned} E(0,\beta) = &\det(Z_1^0(1), Z_2^0(1), Z_3^0(1), Z_4^0(1)) = \det(\Phi(1)e_2, \Phi(1)e_4, e_2, e_4) \\ &= \frac{r'(1) - r'(0)}{u'(1)} U_2(1) = -\frac{8\beta}{\bar{u}}\left(\int_0^1 v_r(r(t))f(r(t))dt + 1\right). \end{aligned} \tag{2.26}$$

Using the symmetry of $r(y)$ with respect to $y = 1/2$ and expression (2.14) and a number of substitutions, we have

$$\begin{aligned}
\int_0^1 v_r(r(t))f(r(t))dt &= \frac{\sqrt{2\delta}}{M}\int_0^{\alpha}\frac{v_r(r)f(r)}{\sqrt{f(\alpha)-f(r)}}dr \\
&= \frac{\sqrt{2\delta}}{M}\int_0^{\beta}\frac{sv_r(g(s))g'(s)}{\sqrt{\beta-s}}ds \\
&= \frac{\sqrt{2\delta}\beta^{\frac{3}{2}}}{M}\int_0^1\frac{tv_r(g(\beta t))g'(\beta t)}{\sqrt{1-t}}dt \\
&= \frac{\sqrt{2\delta}\beta^{\frac{3}{2}}}{M}\int_0^1\frac{tg''(\beta t)}{\sqrt{1-t}}dt = \frac{4\delta\beta^2}{\bar{u}}\int_0^1\frac{tg''(\beta t)}{\sqrt{1-t}}dt.
\end{aligned} \tag{2.27}$$

In the second to last step, we have used the relation $g''(s) = v_r(g(s))g'(s)$ from $g'(s) = v(g(s))$ (see Lemma 2).

Recall that

$$\bar{u}'(\beta) = 4\delta\int_0^1\frac{g'(\beta t)}{\sqrt{1-t}}dt + 4\delta\beta\int_0^1\frac{tg''(\beta t)}{\sqrt{1-t}}dt. \tag{2.28}$$

Substitute (2.27) into (2.26) and use (2.16) and (2.28) to get

$$\begin{aligned}
E(0,\beta) &= -\frac{8\beta^2}{\bar{u}^2}\left(4\delta\beta\int_0^1\frac{tg''(\beta t)}{\sqrt{1-t}}dt + \frac{\bar{u}(\beta)}{\beta}\right) \\
&= -\frac{8\beta^2}{\bar{u}^2}\left(4\delta\beta\int_0^1\frac{tg''(\beta t)}{\sqrt{1-t}}dt + 4\delta\int_0^1\frac{g'(\beta t)}{\sqrt{1-t}}dt\right) \\
&= -\frac{8\beta^2\bar{u}'(\beta)}{\bar{u}^2(\beta)}.
\end{aligned}$$

This completes the proof. □

Our main result regarding the characterization of the zero eigenvalue is given in the next theorem and is a direct consequence of Lemma 7 and Proposition 1

Theorem 1. *The number $\lambda = 0$ is an eigenvalue associated to $\beta_* > 0$ if and only if $\bar{u}'(\beta_*) = 0$ (or equivalently, $D'(\beta_*) = 0$).*

In general

Lemma 11. *If, for some positive integer k, $\bar{u}'(\beta_*) = \cdots = \bar{u}^{(k)}(\beta_*) = 0$, then*

$$\frac{\partial^j E}{\partial \beta^j}(0,\beta_*) = 0 \;\; for \;\; j < k \;\; and \;\; \frac{\partial^k E}{\partial \beta^k}(0,\beta_*) = -\frac{8\beta_*^2}{\bar{u}^2(\beta_*)}\bar{u}^{(k+1)}(\beta_*).$$

2.3.3 Bifurcation of the zero eigenvalue

If $E(0,\beta_*) = 0$ and $E_\lambda(0,\beta_*) \neq 0$, then, by the Implicit Function Theorem, there exists an $\eta > 0$ and a unique smooth function $\lambda(\beta)$ for $\beta \in (\beta_* - \eta, \beta_* + \eta)$ such that $\lambda(\beta_*) = 0$ and $E(\lambda(\beta),\beta) = 0$ for all $\beta \in (\beta_* - \eta, \beta_* + \eta)$. Then,

$$E_\beta(\lambda(\beta),\beta) + E_\lambda(\lambda(\beta),\beta)\lambda'(\beta) = 0$$

for all $\beta \in (\beta_* - \eta, \beta_* + \eta)$. In particular,

$$\lambda'(\beta_*) = -\frac{E_\beta(0,\beta_*)}{E_\lambda(0,\beta_*)} = \frac{8\beta_*^2\bar{u}''(\beta_*)}{\bar{u}^2(\beta_*)E_\lambda(0,\beta_*)}. \tag{2.29}$$

This observation directly characterizes the type of bifurcation which occurs in a neighborhood of a zero eigenvalue when $E_\lambda(0,\beta_*) < 0$ and β_* is not a degenerate critical point of $D(\beta)$ and is summarized in the next theorem.

Theorem 2. *Assume that $E_\lambda(0,\beta_*) < 0$.*

(i) If β_* satisfies $\bar{u}'(\beta_*) = 0$ and $\bar{u}''(\beta_*) < 0$, then, for $\beta < \beta_*$ but close, there is exactly one negative eigenvalue close to zero (bifurcating from the zero eigenvalue

of β_*); for $\beta > \beta_*$ but close, there is exactly one positive eigenvalue close to zero (bifurcating from the zero eigenvalue of β_*).

(ii) If β_* satisfies $\bar{u}'(\beta_*) = 0$ and $\bar{u}''(\beta_*) > 0$, then, for $\beta < \beta_*$ but close, there is exactly one positive eigenvalue close to zero (bifurcating from the zero eigenvalue of β_*); for $\beta > \beta_*$ but close, there is exactly one negative eigenvalue close to zero (bifurcating from the zero eigenvalue of β_*).

If β_* happens to be a degenerate critical value, with $D^{(k)}$ vanishing for $k = 1 \ldots n$, then

Remark 2. In general, if $\bar{u}^{(k)}(\beta_*) = 0$ for $k = 1, \cdots, n$ and $\bar{u}^{(n+1)}(\beta_*) \neq 0$, then, from Lemma 11,

$$\lambda^{(k)}(\beta_*) = 0 \;\text{ for }\; k = 1, 2, \cdots, n-1, \quad \lambda^{(n)}(\beta_*) = \frac{8\beta^2 \bar{u}^{(n+1)}(\beta_*)}{\bar{u}^2(\beta_*) E_\lambda(0, \beta_*)}.$$

We refer the reader to Figure 2.3.3 for a graphical representation of Theorem 2.

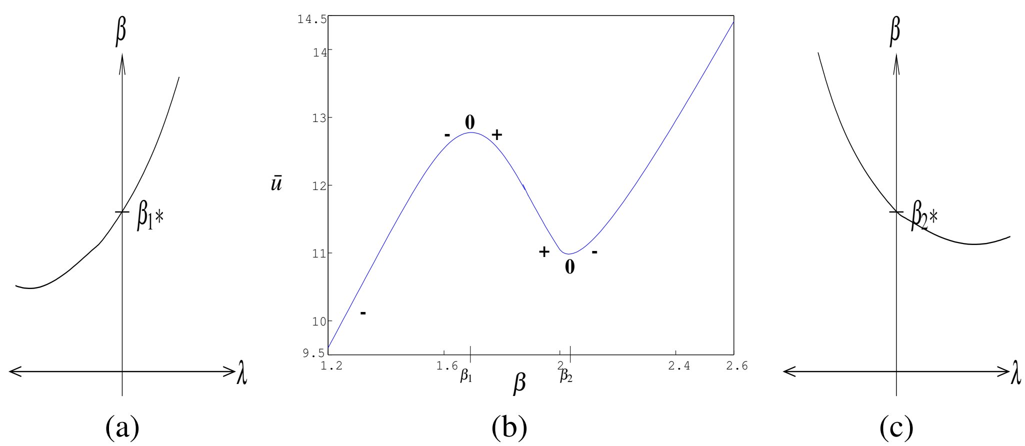

Figure 2.4: Graphs (a) and (b) show the graphs of $\lambda(\beta)$ in a neighborhood of a zero eigenvalue corresponding to local maxima and minima of $\bar{u}(\beta)$, (c), respectively.

While we are not able to prove it, we suspect that $E_\lambda(0,\beta_*)$ is always true for choices of viscosity functions $v(r)$ satisfying (2.6). This is because we are able to construct $E_\lambda(0,\beta_*)$ and after some technical manipulations we obtain a tractable form.

Proposition 2. *If β_* is a critical point of $\bar{u}(\beta)$, then*

$$E_\lambda(0,\beta_*) = \frac{16\delta\beta_*^3}{\bar{u}^3}L(\beta_*)$$

where

$$\begin{aligned} L(\beta) =& \delta\left(\int_0^1 \frac{g'(\beta\tau)}{\sqrt{1-\tau}}d\tau\right)^{-1}\Delta - \int_0^1 g'(\beta\tau)\left(1-\sqrt{1-\tau}\right)F(\tau,\beta)d\tau \\ & -\left(\int_0^1 \frac{g'(\beta\tau)}{\sqrt{1-\tau}}d\tau\right)^{-1}\int_0^1 g'(\beta\tau)\sqrt{1-\tau}G(\tau,\beta)F(\tau,\beta)d\tau, \end{aligned}$$

where

$$F(\tau,\beta) = \int_0^\tau tg'(\beta t)(1-t)^{-3/2}dt, \quad G(\tau,\beta) = \int_0^\tau g'(\beta t)(1-t)^{-3/2}dt,$$
$$\Delta = \int_0^1 \frac{g'(\beta\tau)}{\sqrt{1-\tau}}d\tau\int_0^1 \sqrt{1-\tau}F(\tau,\beta)d\tau - \int_0^1 \sqrt{1-\tau}G(\tau,\beta)F(\tau,\beta)d\tau.$$

We hold off on the proof for the moment to comment on the function Δ, which clearly plays the central role in determining the sign of $E_\lambda(0,\beta_*)$.

Corollary 2. *Fix $v(r)$ and let β_* be a critical point of $\bar{u}(\beta)$. If $\Delta < 0$ or if $\Delta > 0$ but $\delta > 0$ is small enough, then $E_\lambda(0,\beta_*) < 0$.*

We actually suspect that $\Delta < 0$, since this holds for constant, piecewise constant, and linear functions, as well as a few other special classes of functions which we have tested satisfying (2.6). On the other hand if it where the case that $\Delta > 0$ and δ sufficiently large, then this would imply that the negative eigenvalue associated to a steady state with small shearing velocity must split into a pair of complex conjugate eigenvalues passing through the imaginary axis and then returning to the positive real axis before approaching the zero eigenvalue.

We now proceed to prove Proposition (2), but first we will need some preparatory observations.

Lemma 12. *$R_2(0) = R_2(1) = 0$ and $R_2(y) < 0$ for $y \in (0,1)$ and $R_2(y)$ is monotone for $y \in [0,1/2)$.*

Proof. Note that $r_\beta(y;\beta_*) = p_\beta(\beta_*)R_2(y)$. Recall from (2.14) that, for $y \in (0,1/2)$,

$$r'(y;\beta) = \sqrt{2\delta^{-1}}M(\beta)\,(\beta - f(r(y;\beta))^{1/2},$$

and hence,

$$r'_\beta = a(y;\beta)r_\beta + \sqrt{\frac{2}{\delta(\beta - f(r))}}\left(\frac{M(\beta)}{2} + M_\beta(\beta)\,(\beta - f(r))\right),$$

where

$$a(y;\beta) = -\frac{M(\beta)}{v(r)\sqrt{2\delta(\beta - f(r))}}.$$

Denote $\Psi(y)$ the principal fundamental matrix solution with system matrix $a(y;\beta)$. Then, noting that $r_\beta(0;\beta^*) = 0$,

$$r_\beta(y;\beta_*) = \int_0^y \Psi(y)\Psi^{-1}(t)\sqrt{\frac{2}{\delta(\beta_* - f(r))}}\left(\frac{M(\beta_*)}{2} + M_\beta(\beta_*)\,(\beta_* - f(r))\right)dt.$$

It follows from

$$M(\beta) = \frac{\bar{u}(\beta)\beta^{-1/2}}{\sqrt{8\delta}} \text{ and } M_\beta(\beta_*) = -\frac{\bar{u}(\beta_*)\beta_*^{-3/2}}{2\sqrt{8\delta}}$$

that, for $y \in (0, 1/2)$,

$$\frac{M(\beta_*)}{2} + M_\beta(\beta_*)\,(\beta_* - f(r)) = \beta_*^{-3/2} f(r(y)) > 0.$$

Therefore, $r_\beta(y;\beta_*) > 0$ for $y \in (0, 1/2)$. The statement for $R_2(y)$ follows. □

Lemma 13. *If β_* is a critical value of $\bar{u}(\beta)$, then*

$$\int_0^1 \frac{g''(\beta_* t)}{\sqrt{1-t}} dt = \frac{\bar{u}(\beta_*)}{8\delta\beta_*^2} - \frac{v_1}{\beta_*} - \frac{\bar{u}(\beta_*)}{4\delta\beta_*^2} = -\frac{\bar{u}(\beta_*)}{8\delta\beta_*^2} - \frac{v_1}{\beta_*},$$

$$\int_0^1 v_r(r(t;\beta_*))dt = -\frac{1}{2\beta_*} - \frac{4\delta v_1}{\bar{u}(\beta_*)}, \quad U_1(1) = -1 - \frac{\bar{u}(\beta_*)}{4\delta\beta_* v_1}, \quad R_1(1) = \frac{1}{\delta}.$$

Proof. It follows from the same line in (2.27) that, for any β,

$$\int_0^1 v_r(r(t;\beta))dt = \frac{4\delta\beta}{\bar{u}(\beta)} \int_0^1 \frac{g''(\beta t)}{\sqrt{1-t}} dt.$$

If β_* is a critical value of $\bar{u}(\beta)$, then, from (2.16) and (2.28),

$$\frac{4\delta\beta_*^2}{\bar{u}(\beta_*)} \int_0^1 \frac{t g''(\beta_* t)}{\sqrt{1-t}} dt = -1 \ \text{ or } \ \int_0^1 \frac{t g''(\beta_* t)}{\sqrt{1-t}} dt = -\frac{\bar{u}(\beta_*)}{4\delta\beta_*^2}.$$

Now,

$$\begin{aligned}\int_0^1 \frac{(1-t)g''(\beta_* t)}{\sqrt{1-t}} dt &= \int_0^1 \sqrt{1-t}\, g''(\beta_* t)dt = \int_0^1 \sqrt{1-t} \left(\frac{1}{\beta_*} g'(\beta_* t)\right)' dt \\ &= -\frac{g'(0)}{\beta_*} + \frac{1}{2\beta_*} \int_0^t \frac{g'(\beta_* t)}{\sqrt{1-t}} dt = \frac{\bar{u}(\beta_*)}{8\delta\beta_*^2} - \frac{v_1}{\beta_*}.\end{aligned}$$

Thus,

$$\int_0^1 \frac{g''(\beta_* t)}{\sqrt{1-t}} dt = \frac{\bar{u}(\beta_*)}{8\delta\beta_*^2} - \frac{v_1}{\beta_*} - \frac{\bar{u}(\beta_*)}{4\delta\beta_*^2} = -\frac{\bar{u}(\beta_*)}{8\delta\beta_*^2} - \frac{v_1}{\beta_*}.$$

Other statements follow immediately. □

Lemma 14. *If β_* is a critical value of $\bar{u}(\beta)$, then $U_2(y)$ is odd and $R_2(y)$ is even with respect to $y = 1/2$.*

Proof. We will show that $U_2(y)$ is odd with respect to $y = 1/2$ from which it follows by the relation in Lemma (10) that $R_2(y)$ is even. Fix $y \in [0,1]$. Note that from the symmetry of $r(y)$ we have

$$\int_y^1 v_r(r(t))f(r(t))\,dt = \int_0^{1-y} v_r(r(t))f(r(t))\,dt.$$

Lemma (1) and the above give

$$\begin{aligned} 0 &= \int_0^1 \big(v_r(r(t))f(r(t)) + 1\big)\,dt \\ &= \int_0^y \big(v_r(r(t))f(r(t)) + 1\big)\,dt + \int_0^{1-y} \big(v_r(r(t))f(r(t)) + 1\big)\,dt. \end{aligned}$$

This implies $-U(y) = U(1-y)$ proving the result. □

It follows from (2.23) and Lemma 6 that

$$\begin{aligned} E(\lambda,\beta) &= \det(Z_1(1;\lambda,\beta), Z_2(1;\lambda,\beta), Z_3(1;\lambda,\beta), Z_4(1;\lambda,\beta)) \\ &= \det(Z_1(1;\lambda,\beta), Z_2(1;\lambda,\beta), e_2, e_4). \end{aligned}$$

Hence,

$$\begin{aligned} E_\lambda(0,\beta_*) &= \det(Z_{1,\lambda}(1;0,\beta_*), Z_2(1;0,\beta_*), e_2, e_4) \\ &\quad + \det(Z_1(1;0,\beta_*), Z_{2,\lambda}(1;0,\beta_*), e_2, e_4). \end{aligned}$$

At $\lambda = 0$, $Z_1(1;0,\beta_*) = e_2$ and hence,

$$E_\lambda(0,\beta_*) = \det(Z_{1,\lambda}(1;0,\beta_*), Z_2(1;0,\beta_*), e_2, e_4).$$

If we denote $Z_{1,\lambda}(1;0,\beta_*) = (E_1,E_2,E_3,E_4)^T$, noting that

$$Z_2(1;0,\beta_*) = (U_4(1), 0, R_4(1), 1)^T,$$

then

$$E_\lambda(0,\beta_*) = U_4(1)E_3 - R_4(1)E_1 = \frac{U_4(1)}{u'(1)}(u'(1)E_3 - r'(1)E_1) - \frac{\bar{u}}{\delta u'(1)}E_1. \quad (2.30)$$

It is known that $Z_{1,\lambda}(y) = Z_{1,\lambda}(y;0,\beta_*)$ is the solution of

$$Z' = A(y;0,\beta_*)Z + A_\lambda(y;0,\beta_*)Z_1(y;0,\beta_*) \quad (2.31)$$

with initial condition $Z(0) = 0$. Hence,

$$Z_{1,\lambda}(y) = \Phi(y)\int_0^y \Phi^{-1}(t)A_\lambda(t;0,\beta_*)Z_1(t;0,\beta_*)dt. \quad (2.32)$$

Using Lemma 10, one has

$$\Phi(1) = \begin{pmatrix} U_1(1) & 0 & U_3(1) & U_4(1) \\ 0 & 1 & 0 & 0 \\ R_1(1) & 0 & R_3(1) & R_4(1) \\ 0 & 0 & 0 & 1 \end{pmatrix}$$

and

$$\Phi^{-1}(y) = \begin{pmatrix} R_3 & U_3R_2 - U_2R_3 & -U_3 & U_3R_4 - U_4R_3 \\ 0 & 1 & 0 & 0 \\ -R_1 & U_2R_1 - U_1R_2 & U_1 & U_4R_1 - U_1R_4 \\ 0 & 0 & 0 & 1 \end{pmatrix}.$$

Also,

$$A_\lambda(y;0,\beta_*) = \begin{pmatrix} 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \end{pmatrix}.$$

If we denote

$$\int_0^1 \Phi^{-1}(t)A_\lambda(t;0,\beta_*)Z_1(t;0,\beta_*)dt = (S_1,S_2,S_3,S_4)^T,$$

then

$$S_1 = \int_0^1 (U_2(U_3R_2 - U_2R_3) + R_2(U_3R_4 - U_4R_3))\,dt,\ S_2 = \int_0^1 U_2dt,$$
$$S_3 = \int_0^1 (U_2(U_2R_1 - U_1R_2) + R_2(U_4R_1 - U_1R_4))\,dt,\ S_4 = \int_0^1 R_2dt.$$

It then follows from (2.32) that

$$E_1 = U_1(1)S_1 + U_3(1)S_3 + U_4(1)S_4 \text{ and } E_3 = R_1(1)S_1 + R_3(1)S_3 + R_4(1)S_4.$$

Using the fact that $r'(0) = -r'(1) = \bar{u}/2\delta$, $u'(0) = u'(1)$, and the relations in Lemma (10) it is easy to show that

$$E_\lambda(0,\beta_*) = (r'(0)\delta)^{-1}\left(r'(0)S_1 - u'(0)S_3\right) - 2S_3.$$

For convenience we consider the integrands L_1 and L_3 of S_1 and S_3 respectivly. It follows from Lemma 10 that

$$U_4R_1 - U_1R_4 = R_1,$$

which gives

$$L_3 = U_2^2R_1 - U_1U_2R_2 + R_1R_2$$

The expanded terms in L_1 are

$$\begin{aligned} U_3R_2 - U_2R_3 &= \frac{u'(0)}{r'(0)}\left(\frac{v_1}{v} - U_1\right)R_2 - U_2\left(\frac{r'}{r'(0)} - \frac{u'(0)}{r'(0)}R_1\right) \\ &= \frac{u'(0)v_1}{r'(0)v}R_2 - \frac{u'(0)}{r'(0)}U_1R_2 - \frac{r'}{r'(0)}U_2 + \frac{u'(0)}{r'(0)}R_1U_2 \end{aligned}$$

and

$$\begin{aligned} U_3R_4 - U_4R_3 &= \frac{u'(0)}{r'(0)}\left(\frac{v_1}{v} - U_1\right)(-R_1) - (1-U_1)\left(\frac{r'}{r'(0)} - \frac{u'(0)}{r'(0)}R_1\right) \\ &= -\frac{u'(0)}{r'(0)}\frac{v_1}{v}R_1 + \frac{u'(0)}{r'(0)}R_1 + \frac{r'}{r'(0)}U_1 - \frac{r'}{r'(0)} \end{aligned}$$

Hence,

$$\begin{aligned} \frac{r'(0)}{u'(0)}L_1 =& \frac{v_1}{v}U_2R_2 - U_1U_2R_2 - \frac{r'}{u'(0)}U_2^2 + U_2^2R_1 - \frac{v_1}{v}R_1R_2 \\ &+ R_1R_2 + \frac{r'}{u'(0)}U_1R_2 - \frac{r'}{u'(0)}R_2 \\ =& \frac{v_1}{v}U_2R_2 - \frac{r'}{u'(0)}U_2^2 - \frac{v_1}{v}R_1R_2 + \frac{r'}{u'(0)}U_1R_2 - \frac{r'}{u'(0)}R_2 + L_3. \end{aligned}$$

As a consequence of Lemma 14, after integration over the interval $[0,1]$, the first two terms $\frac{v_1}{v}U_2R_2$ and $u'(0)r'U_2^2$ will vanish. Thus, we drop these terms. It follows from

Lemma 9 that $-r'(0) = -r'U_1 + u'R_1$, which gives the reduction

$$r'(0)L_1 = \left(r'(0) - r'\right) R_2 + u'(0)L_3$$

Again we drop the term $r'R_2$, as it will vanish after integration, to obtain

$$r'(0)L_1 - u'(0)L_3 = r'(0)R_2 \tag{2.33}$$

Turning our attention back to L_3, since

$$\begin{aligned}
\int_0^y r'(t)U_1(t)\,dt =& \int_0^y r'(0)\frac{d}{dt}\big(f(r(t))\big)\int_0^t v_r(r(s))\,ds + v_1\frac{d}{dt}[f(r(t))]\,dt \\
=& f(r(y))\left(r'(0)\int_0^y v_r(r(t))\,dt + v_1\right) \\
&- r'(0)\left(\int_0^y f(r(t))v_r(r(t)) + 1\,dt\right) + r'(0)y \\
=& v(r(y))f(r(y))U_1(y) - v(r(y))r'(0)U_2(y) + r'(0)y,
\end{aligned}$$

after expanding $U_2R_1 - U_1R_2$ we have

$$\int_0^1 U_2^2R_1 - U_1U_2R_2\,dt = \int_0^1 U_2\int_0^t \frac{1}{v(r(s))}R_1(s)\,ds\,dt. \tag{2.34}$$

Finally, noting that $-\delta R_2(y) = \int_0^y U_2(t)\,dt$, we integrate the above expression by parts and combine with (2.33) to obtain

$$E_\lambda(0,\beta_*) = \frac{1}{\delta}\int_0^1 R_2(t)\,dt - 2\int_0^1 R_1(t)R_2(t)\,dt - 2\int_0^1 \frac{\delta}{v(r(t))}R_1(t)R_2(t)\,dt.$$

It is easy to check that, for any function $\phi(v)$ and $\psi(v) = v\phi(v)$,

$$\begin{aligned}\int_0^1 \phi(v(r))R_2 dy =& 2\int_0^{1/2} \phi(v(r))R_2 dy \\ =& \frac{2}{M^2}\int_0^{1/2} \phi(v(r))r' \int_0^y (v_r f + 1) dt dy - \frac{2}{M^2}\int_0^{1/2} f(r)\psi(v(r)) dy.\end{aligned}$$

We have

$$\begin{aligned}&\int_0^{1/2} \phi(v(r(y)))r'(y) \int_0^y (v_r f + 1) dt dy \\ &= \int_0^{\alpha} \phi(v(p)) \int_0^{r^{-1}(p)} (v_r f + 1) dt dp \\ &= \frac{\sqrt{\delta}}{\sqrt{2}M}\int_0^{\alpha} \phi(v(p)) \int_0^{p} \frac{v_r(z)f(z)+1}{\sqrt{f(\alpha)-f(z)}} dz dp \\ &= \frac{\sqrt{\delta}}{\sqrt{2}M}\int_0^{\alpha} \phi(v(p)) \int_0^{f(p)} \frac{sg''(s)+g'(s)}{\sqrt{\beta - s}} ds dp \\ &= \frac{\sqrt{\delta}}{\sqrt{2}M}\int_0^{\beta_*} \psi(g'(w)) \int_0^{w} \frac{sg''(s)+g'(s)}{\sqrt{\beta_* - s}} ds dw \\ &= \frac{\sqrt{\delta}\beta_*^{3/2}}{\sqrt{2}M}\int_0^{1} \psi(g'(\beta_*\tau)) \int_0^{\tau} \frac{\beta_* t g''(\beta_* t)+g'(\beta_* t)}{\sqrt{1-t}} dt d\tau \\ &= \frac{\sqrt{\delta}\beta_*^{3/2}}{\sqrt{2}M}\int_0^{1} \psi(g'(\beta_*\tau)) \int_0^{\tau} \frac{(tg'(\beta_* t))_t}{\sqrt{1-t}} dt d\tau,\end{aligned}$$

and

$$\begin{aligned}\int_0^{1/2} f(r)\psi(v(r)) dy =& \frac{\sqrt{\delta}}{\sqrt{2}M}\int_0^{\alpha} \frac{f(p)\psi(v(p))}{\sqrt{f(\alpha)-f(z)}} dp \\ =& \frac{\sqrt{\delta}}{\sqrt{2}M}\int_0^{\beta_*} \frac{sg'(s)\psi(g'(s))}{\sqrt{\beta_* - s}} ds \\ =& \frac{\sqrt{\delta}\beta_*^{3/2}}{\sqrt{2}M}\int_0^{1} \frac{\tau g'(\beta_*\tau)\psi(g'(\beta_*\tau))}{\sqrt{1-\tau}} d\tau.\end{aligned}$$

Also,

$$\begin{aligned}\int_0^\tau \frac{(tg'(\beta_* t))_t}{\sqrt{1-t}}dt =& tg'(\beta_* t)(1-t)^{-1/2}|_0^\tau - \frac{1}{2}\int_0^\tau tg'(\beta_* t)(1-t)^{-3/2}dt\\ =& \frac{\tau g'(\beta_*\tau)}{\sqrt{1-\tau}} - \frac{1}{2}\int_0^\tau tg'(\beta_* t)(1-t)^{-3/2}dt.\end{aligned}$$

Therefore,

$$\int_0^1 \phi(v(r(y)))R_2(y)dy = -\frac{\sqrt{\delta}\beta_*^{3/2}}{\sqrt{2}M^3}\int_0^1 \psi(g'(\beta_*\tau))\int_0^\tau tg'(\beta_* t)(1-t)^{-3/2}dt\,d\tau.$$

Note that

$$\begin{aligned}&\int_0^1 \frac{v+\delta}{v}R_1(y)R_2(y)dy\\ &= \int_0^1 \left(\frac{r'}{u'(0)} - \frac{r'(0)}{u'} + \frac{r'(0)r'}{M^2}\int_0^y v_r dt\right)\frac{v+\delta}{v}R_2 dy\\ &= -\int_0^1 \frac{r'(0)}{u'}\frac{v+\delta}{v}R_2 dy + \frac{r'(0)}{M^2}\int_0^1 r'\int_0^y v_r dt\frac{v+\delta}{v}R_2 dy\\ &= -\frac{2r'(0)}{M^2}\int_0^{1/2}(v+\delta)R_2 dy + \frac{r'(0)}{M^2}\int_0^{1/2} r'\int_0^y v_r dt\frac{v+\delta}{v}R_2 dy\\ &\quad + \frac{r'(0)}{M^2}\int_{1/2}^1 r'\int_0^y v_r dt\frac{v+\delta}{v}R_2 dy\\ &= -\frac{r'(0)}{M^2}\int_0^1 (v+\delta)R_2 dy - \frac{2r'(0)}{M^2}\int_0^{1/2} r'\int_y^{1/2} v_r dt\frac{v+\delta}{v}R_2 dy,\end{aligned}$$

and

$$\int_0^{1/2} r' \int_y^{1/2} v_r dt \frac{v+\delta}{v} R_2(y) dy = \frac{1}{M^2} \int_0^{1/2} \frac{v+\delta}{v} r' r' \int_0^y (v_r f + 1) dt \int_y^{1/2} v_r dt dy$$
$$- \frac{1}{M^2} \int_0^{1/2} (v+\delta) f r' \int_y^{1/2} v_r dt dy$$
$$=: \frac{1}{M^2}(I_1 - I_2).$$

Now,

$$\begin{aligned}
I_1 =& \frac{\sqrt{2}M}{\sqrt{\delta}} \int_0^\alpha \frac{v(p)+\delta}{v(p)} \sqrt{f(\alpha)-f(p)} \int_0^{r^{-1}(p)} (v_r f + 1) dt \int_{r^{-1}(p)}^{1/2} v_r dt dp \\
=& \frac{\sqrt{\delta}}{\sqrt{2}M} \int_0^\alpha \frac{v(p)+\delta}{v(p)} \sqrt{\beta_* - f(p)} \int_0^p \frac{v_r(z) f(z) + 1}{\sqrt{\beta_* - f(z)}} dz \int_p^\alpha \frac{v_r(z)}{\sqrt{\beta_* - f(z)}} dz dp \\
=& \frac{\sqrt{\delta}}{\sqrt{2}M} \int_0^\alpha \frac{v(p)+\delta}{v(p)} \sqrt{\beta_* - f(p)} \int_0^{f(p)} \frac{s g''(s) + g'(s)}{\sqrt{\beta_* - s}} ds \int_{f(p)}^{\beta_*} \frac{g''(s)}{\sqrt{\beta_* - s}} ds dp \\
=& \frac{\sqrt{\delta}}{\sqrt{2}M} \int_0^{\beta_*} (g'(q)+\delta) \sqrt{\beta_* - q} \int_0^q \frac{s g''(s) + g'(s)}{\sqrt{\beta_* - s}} ds \int_q^{\beta_*} \frac{g''(s)}{\sqrt{\beta_* - s}} ds dq,
\end{aligned}$$

and

$$\begin{aligned}
I_2 =& \int_0^\alpha (v(p)+\delta) f(p) \int_{r^{-1}(p)}^{1/2} v_r dt\, dp \\
=& \frac{\sqrt{\delta}}{\sqrt{2}M} \int_0^\alpha (v(p)+\delta) f(p) \int_p^\alpha \frac{v_r(z)}{\sqrt{\beta_* - f(z)}} dz dp \\
=& \frac{\sqrt{\delta}}{\sqrt{2}M} \int_0^\alpha (v(p)+\delta) f(p) \int_{f(p)}^{\beta_*} \frac{g''(s)}{\sqrt{\beta_* - s}} ds dp \\
=& \frac{\sqrt{\delta}}{\sqrt{2}M} \int_0^{\beta_*} (g'(q)+\delta) g'(q) q \int_q^{\beta_*} \frac{g''(s)}{\sqrt{\beta_* - s}} ds dq.
\end{aligned}$$

Therefore,

$$
\begin{aligned}
I_1 - I_2 &= -\frac{\sqrt{\delta}}{2\sqrt{2}M} \int_0^{\beta_*} (g'(q)+\delta)\sqrt{\beta_* - q} \int_0^q \frac{sg'(s)}{(\beta_* - s)^{3/2}} ds \int_q^{\beta_*} \frac{g''(s)}{\sqrt{\beta_* - s}} ds\, dq \\
&= -\frac{\sqrt{\delta}\beta_*^{5/2}}{2\sqrt{2}M} \int_0^1 (g'(\beta_*\tau)+\delta)\sqrt{1-\tau} \int_0^\tau \frac{tg'(\beta_* t)}{(1-t)^{3/2}} dt \int_\tau^1 \frac{g''(\beta_* t)}{\sqrt{1-t}} dt\, d\tau.
\end{aligned}
$$

Set, as introduced in the statement of Proposition 2,

$$
F(\tau, \beta_*) = \int_0^\tau \frac{tg'(\beta_* t)}{(1-t)^{3/2}} dt.
$$

Then,

$$
\begin{aligned}
-\frac{\sqrt{2}M^3 \bar{u}}{8\sqrt{\delta}\beta_*^{5/2}} E_\lambda(0, \beta_*) = &\int_0^1 \left(\frac{\bar{u}}{8\beta_*\delta} + g'(\beta_*\tau) + \delta \right) g'(\beta_*\tau) F(\tau, \beta_*) d\tau \\
&+ \beta_* \int_0^1 (g'(\beta_*\tau)+\delta)\sqrt{1-\tau} F(\tau, \beta_*) \int_\tau^1 \frac{g''(\beta_* t)}{\sqrt{1-t}} dt\, d\tau.
\end{aligned}
$$

It follows from Lemma 13 that

$$
\begin{aligned}
\beta_*(g'(\beta_*\tau)+\delta)\sqrt{1-\tau} \int_\tau^1 \frac{g''(\beta_* t)}{\sqrt{1-t}} dt = &-(g'(\beta_*\tau)+\delta)\sqrt{1-\tau} \left(\frac{\bar{u}}{8\beta_*\delta} + v_1 \right) \\
&- \beta_*(g'(\beta_*\tau)+\delta)\sqrt{1-\tau} \int_0^\tau \frac{g''(\beta_* t)}{\sqrt{1-t}} dt,
\end{aligned}
$$

and

$$
\begin{aligned}
&-\beta_*(g'(\beta_*\tau)+\delta)\sqrt{1-\tau}\int_0^\tau \frac{g''(\beta_* t)}{\sqrt{1-t}}dt = -(g'(\beta_*\tau)+\delta)\sqrt{1-\tau}\int_0^\tau \frac{(g'(\beta_* t))_t}{\sqrt{1-t}}dt \\
&= -\,(g'(\beta_*\tau)+\delta)\sqrt{1-\tau}\left(\frac{g'(\beta_*\tau)}{\sqrt{1-\tau}} - v_1 - \frac{1}{2}\int_0^\tau g'(\beta_* t)(1-t)^{-3/2}dt\right) \\
&= -\,(g'(\beta_*\tau)+\delta)g'(\beta_*\tau) + v_1(g'(\beta_*\tau)+\delta)\sqrt{1-\tau} \\
&\quad + \frac{1}{2}(g'(\beta_*\tau)+\delta)\sqrt{1-\tau}\int_0^\tau g'(\beta_* t)(1-t)^{-3/2}dt.
\end{aligned}
$$

If we set

$$
\begin{aligned}
G(\tau,\beta_*) &= \int_0^\tau g'(\beta_* t)(1-t)^{-3/2}dt, \\
L(\beta_*) &= \frac{8\beta_*\delta}{\bar{u}}\frac{\sqrt{2}M^3\bar{u}}{8\sqrt{\delta}\beta_*^{5/2}}E_\lambda(0,\beta_*) = \frac{\sqrt{2\delta}M^3}{\beta_*^{3/2}}E_\lambda(0,\beta_*),
\end{aligned}
$$

Then,

$$
\begin{aligned}
L(\beta) = &\int_0^1 (g'(\beta\tau)+\delta)\sqrt{1-\tau}F(\tau,\beta)d\tau - \int_0^1 g'(\beta\tau)F(\tau,\beta)d\tau \\
&- \frac{4\beta\delta}{\bar{u}}\int_0^1 (g'(\beta\tau)+\delta)\sqrt{1-\tau}G(\tau,\beta)F(\tau,\beta)d\tau \\
=&\delta\left(\int_0^1 \frac{g'(\beta\tau)}{\sqrt{1-\tau}}d\tau\right)^{-1}\Delta - \int_0^1 g'(\beta\tau)\left(1-\sqrt{1-\tau}\right)F(\tau,\beta)d\tau \\
&- \left(\int_0^1 \frac{g'(\beta\tau)}{\sqrt{1-\tau}}d\tau\right)^{-1}\int_0^1 g'(\beta\tau)\sqrt{1-\tau}G(\tau,\beta)F(\tau,\beta)d\tau,
\end{aligned}
$$

where

$$
\Delta = \int_0^1 \frac{g'(\beta\tau)}{\sqrt{1-\tau}}d\tau\int_0^1 \sqrt{1-\tau}F(\tau,\beta)d\tau - \int_0^1 \sqrt{1-\tau}G(\tau,\beta)F(\tau,\beta)d\tau.
$$

This then completes the proof of Proposition 2.

2.4 Hysteresis: a numerical simulation of dynamic boundary conditions

Our bifurcation analysis of the zero eigenvalue shows the stability change of the steady-state when β crosses critical points of $\bar{u}(\beta)$. For a certain potential functions $v(r)$ (see the example in Chapter 2.1.2), the function $\bar{u} = 4\delta D(\beta)$ is cubic-like and the condition in Corollary 2 holds. Assume we are in this case. Let $\bar{u}_1$ be the local maximum value and let $\bar{u}_2$ be the local minimum value. The stability result suggests the following scenario for a hysteresis: if we consider the dynamic boundary condition by letting $\bar{u}(t)$ increase in t slowly from small value to large value, then, for $t < t_1$ so that $\bar{u}(t_1) = \bar{u}_1$, the solution $(u(y,t), r(y,t))$ of (2.4) and (2.5) with $\bar{u} = \bar{u}(t)$ will behave closely to the left-branch of steady-states associated to $\bar{u} = \bar{u}(t)$ and, for $t > t_1$, the solution $(u(y,t), r(y,t))$ will behave closely to the steady-state associated to $\bar{u} = \bar{u}(t) > \bar{u}_1$ on the right-branch; if we now reverse the dynamic boundary condition by letting $\bar{u}(t)$ decreases slowly from large value to small value, then, for $t < t_2$ where t_2 is the first time so that $\bar{u}(t_2) = \bar{u}_2$, the solution $(u(y,t), r(y,t))$ will behave closely to the right-branch of steady-states associated to $\bar{u} = \bar{u}(t)$ and, for $t > t_2$, the solution $(u(y,t), r(y,t))$ will behave closely to the steady-state associated to $\bar{u} = \bar{u}(t) < \bar{u}_2$ on the left-branch. In particular, the two processes are not reversible to each other over the range $(\bar{u}_2, \bar{u}_1)$ of $\bar{u}$; that is, this problem possesses a hysteresis phenomenon. Although we could not justify this hysteresis rigorously, a numerical simulation provides a strong support.

Remark 3. The hysteresis phenomenon is exhibited in other simplified continuum theories of liquid crystal,[17], and in the Leslie-Ericksen continuum theory as well as in other interesting models such as climate change models, [1].

For the numerical simulation, we consider two 'opposite' dynamic boundary conditions for (2.4) and (2.5) with

$$\bar{u} = \bar{u}_+(t) = \begin{cases} L, & t \in [0, T_1] \\ h(t), & t \in [T_1, T_2] \\ R, & t \in [T_2, T] \end{cases}$$

and its 'reverse'

$$\bar{u} = \bar{u}_-(t) = \begin{cases} R, & t \in [0, T_1] \\ h(T_1 + T_2 - t), & t \in [T_1, T_2] \\ L, & t \in [T_2, \infty) \end{cases}$$

where $L < \bar{u}_2 < \bar{u}_1 < R$, $T_2 \gg T_1 \gg 1$, and $h(t)$ is increasing with $h(T_1) = L$ and $h(T_2) = R$. So the first dynamic boundary condition $\bar{u} = \bar{u}_+(t)$ is slowly increasing in t and the other $\bar{u} = \bar{u}_-(t)$ slowly decreasing. For the first boundary condition $\bar{u} = \bar{u}_+(t)$, we choose the steady-state associated to boundary condition $\bar{u} = L$ as the initial condition and for the second the steady-state associated to boundary condition $\bar{u} = R$ as the initial condition. Snaps shots of the numerical simulation (u-component only) are provided in Figure 2.4 with the left set for $\bar{u} = \bar{u}_+(t)$ and the right for $\bar{u} = \bar{u}_-(t)$. It shows clearly that the two sets of figures are not 'reverse' to each other.

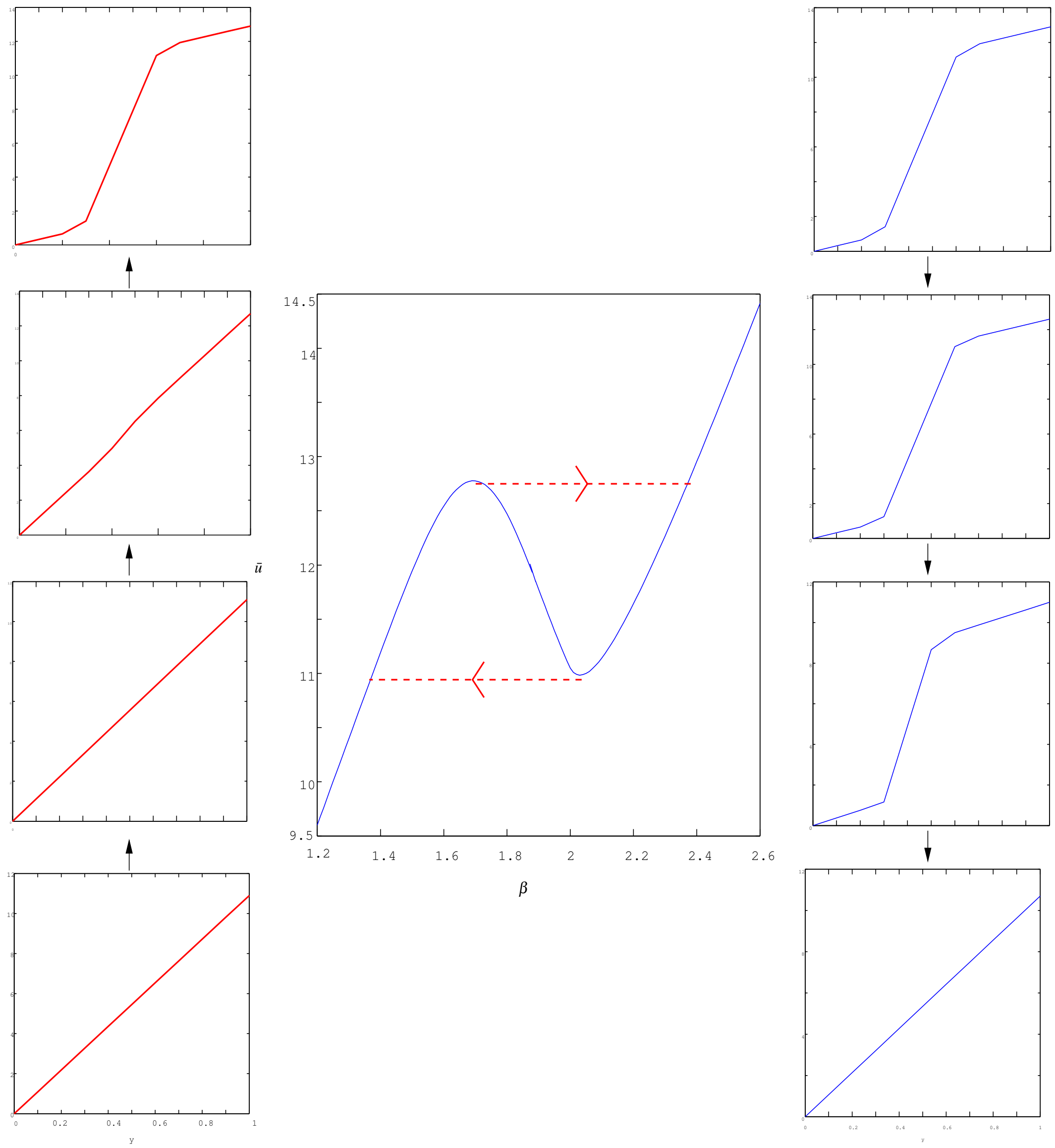

Figure 2.5: *On the left, beginning at the bottom, the right boundary condition $\bar{u}$ is slowly increased. When a value of $\bar{u}$ is near a critical point $\bar{u}_1 \approx 10.98$ or $\bar{u}_2 \approx 12.78$, we pause the boundary condition in order to converge to a steady state. The left hand side pauses at the values $u_L^1(1) = 10.6, u_L^2(1) = 11.1, u_L^3(1) = 12.7$, and $u_L^4(1) = 12.9$ and the bottom, beginning from the right, pauses at the values $u_R^1(1) = 12.9, u_R^2(1) = 12.6, u_R^3(1) = 11$, and $u_R^4(1) = 10.7$.*

Chapter 3

Shearing Flows in the Leslie-Ericksen Continuum Theory of Nematic Liquid Crystals

In this chapter we consider a one-dimensional shearing flow within the context of the Leslie-Ericksen continuum theory of liquid crystals. In this shearing flow, a nematic liquid crystal layer is confined between two parallel plates a distance $2h$ apart with the velocity field parallel to the plates and the velocity gradient perpendicular to the plates. We assume the velocity and director fields are of the form

$$\mathbf{v}(t,y) = \langle v(t,y), 0, 0 \rangle, \tag{3.1}$$

$$\mathbf{n}(t,y) = \langle \cos(\theta(t,y)), \sin(\theta(t,y)), 0 \rangle \tag{3.2}$$

where θ is the angle between the x-axis and the director field. Notice, that $|\mathbf{n}| = 1$.

We now reformulate the governing equations (1.22)- (1.32) for this shearing flow. We compute

$$\nabla \cdot n = n_{2,2},$$

$$\nabla \times n = \langle 0, 0, n_{1,2} \rangle,$$

$$n \cdot \nabla \times n = 0,$$

$$n \times \text{curl}(n) = \langle -n_2 n_{1,2}, n_1 n_{1,2}, 0 \rangle,$$

$$\mathbf{N} = \frac{1}{2}\frac{\partial v}{\partial y}\langle -n_2, n_1, 0\rangle + \theta_t \langle -\sin(\theta(t,y)), \cos(\theta(t,y)), 0\rangle. \tag{3.3}$$

The stress tensor terms are

$$t^o_{j1,j} = -\frac{\partial p}{\partial x} - \sum_{j=1}^{3}\sum_{k=1}^{3} \frac{\partial}{\partial x_j}\frac{\partial F}{\partial n_{k,j}} n_{k,1} = -\frac{\partial p}{\partial x},$$

$$\begin{aligned} t^o_{j2,j} &= -\frac{\partial p}{\partial y} - \sum_{j=1}^{3}\sum_{k=1}^{3} \frac{\partial}{\partial x_j}\frac{\partial F}{\partial n_{k,j}} n_{k,2} \\ &= -\frac{\partial p}{\partial y} - \frac{d}{dy}[\frac{\partial F}{\partial n_{1,2}} n_{1,2} + \frac{\partial F}{\partial n_{2,2}} n_{2,2}] \\ &= -\frac{\partial p}{\partial y} - \frac{d}{dy}[K_3 n_{1,2}^2 + K_1 n_{2,2}^2], \end{aligned}$$

$$t^o_{j3,j} = -\frac{\partial p}{\partial z} - \sum_{j=1}^{3}\sum_{k=1}^{3} \frac{\partial}{\partial x_j}\frac{\partial F}{\partial n_{k,j}} n_{k,3} = -\frac{\partial p}{\partial z},$$

since $n_{k,1} = n_{k,3} = 0$ for all k, and

$$t^d_{j1,j} = \sum_{j=1}^{3} \frac{\partial}{\partial x_j} t^d_{j1} = \frac{\partial}{\partial y} t'_{21}(y),$$

$$t^d_{j2,j} = \sum_{j=1}^{3} \frac{\partial}{\partial x_j} t^d_{j2} = \frac{\partial}{\partial y} \tilde{t}_{22}(y),$$

$$t^d_{j3,j} = \sum_{j=1}^{3} \frac{\partial}{\partial x_j} t^d_{j3} = 0,$$

where

$$t^d_{21} = g(\theta)\frac{dv}{dy} + h(\theta)\theta_t,$$

$$\tilde{t}_{22} = -2f(\theta) + \frac{1}{4}\sin(2\theta)[2\mu_1 \sin^2(\theta) + \mu_2 + \mu_3 + \mu_4 + \mu_5]v_y - 1/2h_\theta(\theta)\theta_t,$$

$$h(\theta) = \mu_3 \cos^2(\theta) - \mu_2 \sin^2(\theta),$$

$$g(\theta) = \mu_1 \cos^2(\theta)\sin^2(\theta) + 1/2[\mu_5 - \mu_2]\sin^2(\theta) + 1/2[\mu_3 + \mu_6]\cos^2(\theta) + 1/2\mu_4,$$

$$f(\theta) = K_1 \cos^2(\theta) + K_3 \sin^2(\theta).$$

In the construction of the dynamic theory, [28], Leslie shows that $g > 0$, which we will assume from here on. Additionally, to simplify our analysis, we assume that $f > 0$.

Given the Onsager-Parodi relation, [14, 36],

$$\mu_2 + \mu_3 = \mu_6 - \mu_5, \tag{3.4}$$

we express g by the formula

$$\begin{aligned} 2g(\theta) &= 2\mu_1 \cos^2(\theta)\sin^2(\theta) + \mu_5 + \mu_4 + \mu_3 + [\mu_3 + \mu_2]\cos(2\theta) \\ &= 2\mu_1 \cos^2(\theta)\sin^2(\theta) + \mu_5 + \mu_4 + \mu_3 - \lambda_2 \cos(2\theta) \end{aligned}$$

The condition $g > 0$ leads to the inequality

$$|\lambda_2| < \mu_3 + \mu_4 + \mu_5. \tag{3.5}$$

Frank's free energy formula, (1.4), reduces to

$$\mathscr{F} = K_1 n_{2,2}^2 + 0 + K_3 n_{1,2}^2 (n_2^2 + n_1^2) = K_1 n_{2,2}^2 + K_3 n_{1,2}^2. \tag{3.6}$$

Using the derived formulas of the stress tensors the component form of (1.30) is

$$\begin{aligned} \rho v_t &= f_1 - \frac{\partial p}{\partial x} + \frac{\partial}{\partial y} t_{21}^d(t,y), \\ 0 &= f_2 - \frac{\partial p}{\partial y} + \frac{\partial}{\partial y} t_{22}^d(t,y), \\ 0 &= f_3 - \frac{\partial p}{\partial z}. \end{aligned}$$

At this point we assume that the external director body force is conservative. That is

$$\langle f_1, f_2, f_3 \rangle = -\nabla(\chi)$$

for some real valued scalar potential function χ. An electromagnetic field is an example of a conservative director body force and is used in determining Frank's constants by measuring the the strength of magnetic field needed to induce a Freédericksz effect, [10, 16].

Taking the derivative of the first equation with respect to x, then substituting in the second equation and noticing from the third equation that $\chi + p$ is independent of z gives

$$\frac{\partial}{\partial y} t_{21}^d(t,y) + A = \rho v_t,$$

and

$$(\chi + p) = Ax + \tilde{t}_{22}(t,y) + d,$$

where

$$A = -\frac{\partial}{\partial x}(\chi + p).$$

Finally from the first of these equations we obtain

$$\frac{d}{dy}[g(\theta)\frac{dv}{dy} + (\mu_3 \cos^2(\theta(t,y)) - \mu_2 \sin^2(\theta(t,y)))\theta_t] + A = \rho v_t. \tag{3.7}$$

To derive an equation for θ, be begin by setting $\rho_1 = 0$; that is we assume that the contribution of the positional movement of the director is negligible when compared to the alignment energy, E, see equation (1.12). We also assume that there are no external body forces, i.e. $G_i = 0$, $i = 1,2,3$. Then the component form of (1.31) is

$$0 = g_i + s_{ji,j},$$

with

$$\begin{aligned} g_1 &= \gamma n_1 - \beta_2 n_{1,2} - 1/2\lambda_1 \frac{dv}{dy} n_2 + 1/2\lambda_2 n_2 \frac{dv}{dy} - \lambda_1 \sin(\theta)\theta_t \\ &= \gamma \cos(\theta) + \beta_2 \sin(\theta)\theta' + 1/2(\lambda_2 - \lambda_1)\sin(\theta)v' - \lambda_1 \sin(\theta)\theta_t, \end{aligned}$$

$$\begin{aligned} g_2 &= \gamma n_2 - \beta_2 n_{2,2} + 1/2\lambda_1 \frac{dv}{dy} n_1 + 1/2\lambda_2 n_1 \frac{dv}{dy} + \lambda_1 \cos(\theta)\theta_t \\ &= \gamma \sin(\theta) - \beta_2 \cos(\theta)\theta' + 1/2(\lambda_1 + \lambda_2)\cos(\theta)v' + \lambda_1 \cos(\theta)\theta_t, \end{aligned}$$

$$g_3 = 0,$$

$$s_{j1,j} = \beta_2 n_{1,2} + K_3 \frac{d}{dy} n_1, 2$$
$$= -\beta_2 \sin(\theta)\theta' - K_3 \cos(\theta(y))(\theta'(y))^2 - K_3 \sin(\theta(y))\theta''(y),$$

$$s_{j2,j} = \beta_2 n_{2,2} + K_1 \frac{d}{dy} n_2, 2$$
$$= \beta_2 \cos(\theta)\theta' - K_1 \sin(\theta(y))(\theta'(y))^2 + K_1 \cos(\theta(y))\theta''(y),$$

$$s_{j3,j} = 0,$$

where $\prime = d/dy$. Solving for the indeterminate γ in the first equation and substituting back into the second equation gives

$$0 = \sin(\theta)(1/2\lambda_1 v' \sin(\theta) - 1/2\lambda_2 v' \sin(\theta) + K_3 \cos(\theta)(\theta')^2 + K_3 \sin(\theta)\theta'' + \lambda_1 \sin(\theta)\theta_t)$$
$$+ \cos(\theta)(1/2\lambda_1 v' \cos(\theta) + 1/2\lambda_2 v' \cos(\theta) - K_1 \sin(\theta)(\theta')^2 + K_1 \cos(\theta)\theta'' + \lambda_1 \cos(\theta)\theta_t)$$
$$= (K_3 \sin^2(\theta) + K_1 \cos^2(\theta))\theta'' + (K_3 \cos(\theta)\sin(\theta) - K_1 \cos(\theta)\sin(\theta))(\theta')^2$$
$$+ 1/2(\lambda_1 + \lambda_2 \cos(2\theta))v' + \lambda_1 \theta_t,$$

which we express as the second order nonlinear partial differential equation

$$2f(\theta)\theta'' + f_\theta(\theta)(\theta')^2 + v'(\lambda_1 + \lambda_2 \cos(2\theta)) + 2\lambda_1 \theta_t = 0. \tag{3.8}$$

We obtain from (3.7) and (3.8) the governing system of pdes of the nematic liquid-crystal in shear flow

$$\rho v_t = \frac{\partial}{\partial y}[g(\theta)v' + h(\theta)\theta_t] + A, \tag{3.9}$$

$$-2\lambda_1\theta_t = 2f(\theta)\theta'' + f_\theta(\theta)(\theta')^2 + v'(\lambda_1 + \lambda_2\cos(2\theta)). \tag{3.10}$$

The shearing flow is completely described once we stipulate that the flow is induced by a shearing force applied to the upper plate and that the director has a fixed orientation on the upper and lower plate. These are the boundary conditions for (3.9) and (3.10)

$$v(t,-h) = 0, \qquad v(t,h) = \bar{v}, \tag{3.11}$$

$$\theta(t,-h) = \phi = \theta(t,h). \tag{3.12}$$

where $2h$ is the distance between the two plates and $\phi \in [0,\pi)$ since one does not distinguish between $\mathbf{n}$ and $-\mathbf{n}$.

With the shearing flow fully prescribed we begin an exploration of the existence, dynamics, and stability of steady state solutions. As in Chapter 2, it is the underlying structure in the governing equations which allows us move forward through difficulties. The general plan of study will be as follows:

(i) Steady states: existence and uniqueness.

(ii) Stability of steady states.

(iii) Semi-global and global dynamics.

We begin the plan of study by exploring the existence of steady states. This is made more complicated by the shear number of parameters, the Leslie coefficients and Frank constants, as well as their interdependencies. In what follows we set up the steady state problem and using a clever change of variables transform the system into a Hamiltonian system. Then, we give a complete description of phase plane configurations on a subset of the Leslie coefficients. Focusing in on one region in particular we then give a necessary condition for the existence of a steady state solution. Even with this extensive work we have only begun to explore the tip of the iceberg and thus end the chapter by with a discussion of what may lie below the surface.

3.1 The steady state system

In the steady state, $\theta_t = 0, v_t = 0$, equations (3.9) and (3.10) reduce to the system of nonlinear ordinary differential equations

$$M = g(\theta)v' + Ay \tag{3.13}$$

$$0 = 2f(\theta)\theta'' + f_\theta(\theta)(\theta')^2 + v'(\lambda_1 + \lambda_2 \cos(2\theta)) \tag{3.14}$$

where $M = t_{21}^d(h)$ and subject to the boundary conditions

$$v(-h) = 0, \qquad v(h) = \bar{v}, \quad \theta(-h) = \phi = \theta(h). \tag{3.15}$$

Assuming the absence of external director body forces, i.e. $A = 0$, equation (3.13) is integrable. Thus the velocity is given by

$$v(t) = \int_{-h}^{t} \frac{M}{g(\theta(\tau))}\, d\tau.$$

From this we see that the study of system (3.13),(3.14) reduces to the study of equation (3.14).

Set

$$\theta' = \frac{\eta}{f(\theta)}.$$

Under this transformation (3.14) can be written as the system of odes

$$\begin{aligned} \theta' &= \frac{1}{f(\theta)}\eta \\ \eta' &= \frac{f_\theta(\theta)}{2f(\theta)^2}\eta^2 - \frac{v'}{2}(\lambda_1 + \lambda_2\cos(2\theta)) \end{aligned} \tag{3.16}$$

Theorem 3. *The system (3.16) is a Hamiltonian system with a Hamiltonian function given by*

$$H(\theta,\eta) = \frac{1}{2f(\theta)}\eta^2 + MG(\theta) \tag{3.17}$$

where $G(\theta) = \int \frac{\lambda_1 + \lambda_2\cos(2\theta)}{4g(\theta)}d\theta$ *is an antiderivative.*

3.2 Phase plane configurations

In this section we analyze the phase plane associated with system (3.16) and give a complete characterization with respect to the parameter space $\Lambda = \{(\lambda_1,\lambda_2) \in \mathbb{R}^2\}$, where λ_1, λ_2 are defined in (1.28)

If $|\lambda_2| < |\lambda_1|$ the system contains no equilibrium on the η-axis. It is in this region, $\{(\lambda_1,\lambda_2) : |\lambda_2| < |\lambda_1|\}$, that solutions of (3.16) cannot undergo multiple twists within the channel. Yet, there is still the possibility for a multiplicity of solutions, which is a topic for further research.

Now suppose that either $|\lambda_1| < |\lambda_2|$ or $|\lambda_1| = |\lambda_2|$ and let θ_0 be the unique value $[0,\pi/2)$ such that $\cos(2\theta_0) = -\frac{\lambda_1}{\lambda_2}$. System (3.16) possess fixed points with $\eta = 0$ and

$$\theta = \theta_0 \pm k\pi$$

or

$$\theta = -\theta_0 \pm k\pi,$$

for all $k \in \mathbb{Z}$. The linearization about the fixed points $(\theta_0 + k\pi, 0)$ is

$$\mathbf{x}' = \begin{pmatrix} 0 & [f(\theta_0)]^{-1} \\ \frac{M\lambda_2}{g(\theta_0)} \sin(2\theta_0) & 0 \end{pmatrix} \mathbf{x}, \tag{3.18}$$

which has eigenvalues

$$\mu = \pm\sqrt{\frac{c\lambda_2 \sin(2\theta_0)}{f(\theta_0)g(\theta_0)}}$$

and the eigenvalues of the linearization about the fixed points $(-\theta_0 + k\pi, 0)$ are

$$\mu = \pm\sqrt{\frac{-c\lambda_2 \sin(2\theta_0)}{f(\theta_0)g(\theta_0)}}.$$

We see that the eigenvalues of the linearizations are independent of λ_1 allowing us to give a complete characterization of fixed points based upon the sign of λ_2. The fixed points $(\theta_0 + k\pi, 0)$ are hyperbolic if $\lambda_2 > 0$ and are centers if $\lambda_2 < 0$. The fixed points $(-\theta_0 + k\pi, 0)$ are centers if $\lambda_2 < 0$ and hyperbolic if $\lambda_2 > 0$.

In order to analyze the phase plane on the region $\Lambda_>$, defined by

$$\Lambda_> = \{(\lambda_1, \lambda_2) \in \mathbb{R}^2 : 0 < |\lambda_1| < |\lambda_2|\}, \tag{3.19}$$

we introduce the function $F : \Lambda_> \to \mathbb{R}$ given by the formula

$$F(\lambda_1, \lambda_2) = \int_0^{\pi} \frac{\lambda_1 + \lambda_2 \cos(2t)}{2g(t)}\, dt. \tag{3.20}$$

By symmetry and π-periodicity of the functions $g(t)$ and $\cos(2t)$, we compute an alternate form

$$F(\lambda_1, \lambda_2) = 2\int_0^{\frac{\pi}{4}} \frac{\lambda_1(2\mu_1 \cos^2(t)\sin^2(t) + \mu_{3,4,5}) + \lambda_2^2 \cos^2(2t)}{g(t)g_+(t)}\, dt, \tag{3.21}$$

where $\mu_{3,4,5} = \mu_3 + \mu_4 + \mu_5$ and $g_+(t) = g(t + \pi/2)$.

Without loss of generality we take $G(\theta)$ in Theorem 3 to be

$$G(\theta) \equiv G(\theta, \lambda_1, \lambda_2) = \int_{\theta_0 - \pi}^{\theta} \frac{\lambda_1 + \lambda_2 \cos(2t)}{4g(t)}\, dt. \tag{3.22}$$

Then, by construction

$$F(\lambda_1, \lambda_2) = 2G(\theta_0). \tag{3.23}$$

Now, fix $\lambda_2 > 0$, then

$$G'(\theta) = \frac{\lambda_1 + \lambda_2 \cos(2t)}{4g(t)} \begin{cases} < 0, & \text{if } \theta_0 - \pi < \theta < -\theta_0 \\ = 0, & \text{if } \theta = -\theta_0 \\ > 0, \text{ if} & -\theta_0 < \theta < \theta_0 \end{cases} \tag{3.24}$$

for all $(\lambda_1, \lambda_2) \in \Lambda_>$.

The saddle point $(\theta_0 - \pi, 0)$ lies on the level curve with $H(\theta_0 - \pi, 0) = G(\theta_0 - \pi, \lambda_1, \lambda_2) = 0$, Theorem 3. Thus, if $0 = F(\lambda_1, \lambda_2)$, then equations (3.24), (3.23), and Theorem 3 together imply that there exists a herteroclinic orbit from the point $(\theta_0 - \pi, 0)$ to the point $(\theta_0, 0)$, and by symmetry a heteroclinic orbit from the point $(\theta_0, 0)$ to the point $(\theta_0 - \pi, 0)$. Furthermore, since $\lambda_2 > 0$, then $\theta_0 \in (0, \pi/4)$ and so

$$\theta_0 - \pi < 0 < \theta_0.$$

If $F(\lambda_1, \lambda_2) > 0$, then by the same arguments used above there exists a unique value $\theta_h \in (-\theta_0, \theta_0)$ such that $G(\theta_h) = 0$, Figure 3.1 (a). Hence $H(\theta_h, 0) = 0$, which proves the existence of a homoclinic orbit to $(\theta_0 - \pi, 0)$ containing the point $(\theta_h, 0)$.

On the other hand, if $F(\lambda_1,\lambda_2) < 0$, then there exists a unique value $\theta_h \in (\theta_0 - \pi, -\theta_0)$ such that $G(\theta_h) = G(\theta_0)$, Figure 3.1(b). Hence $H(\theta_0,0) = H(\theta_h,0)$, which proves the existence of a homoclinic orbit to $(\theta_0,0)$ containing the point $(\theta_h,0)$.

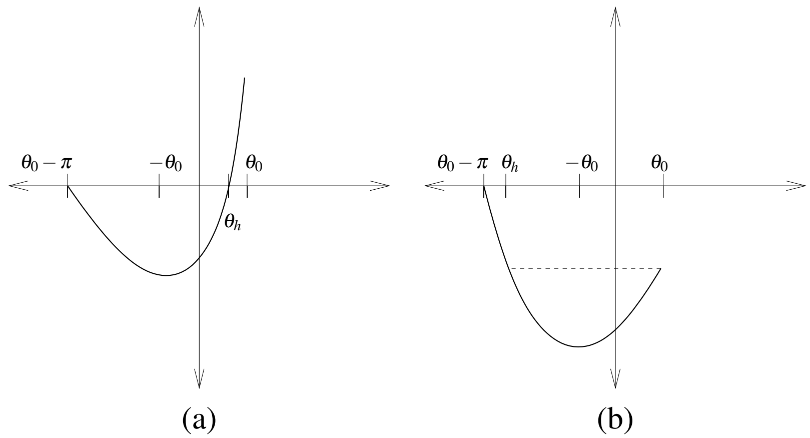

Figure 3.1: Graphs of $G(\theta)$ with (a) $F(\lambda_1,\lambda_2) > 0$ and (b) $F(\lambda_1,\lambda_2) < 0$.

We now show that each of these cases can be realized in $\Lambda_>$.

Lemma 15. *With F defined above, there exists a C^1 curve $h : \mathbb{R}_+ \to \mathbb{R}$ such that $(h(\lambda_2),\lambda_2) \in \Lambda_>$ and*

$$F(h(\lambda_2),\lambda_2) = 0$$

for all $\lambda_2 \in (0,\infty)$. Furthermore, for all $(\lambda_1,\lambda_2) \in \Lambda_> 0$,

$$F(\lambda_1,\lambda_2) > 0 \textit{ if } \lambda_1 > h(\lambda_2)$$

and

$$F(\lambda_1,\lambda_2) < 0 \textit{ if } \lambda_1 < h(\lambda_2).$$

Proof. Fix $\lambda_2 > 0$ and set $\lambda_1 = -\lambda_2$. Then using formula 3.20,

$$F(-\lambda_2,\lambda_2) = \lambda_2 \int_0^{\pi} \frac{-1+\cos(2t)}{2g(t)}\, dt < 0,$$

and by continuity $F(\lambda_1,\lambda_2) < 0$ for $\lambda_1 \approx -\lambda_2$. Similarly $F(\lambda_1,\lambda_2) > 0$ for $\lambda_1 \approx \lambda_2$.

By the Intermediate Value Theorem there exists a λ_1^* such that $-\lambda_2 < \lambda_1^* < \lambda_2$ and

$$F(\lambda_1^*,\lambda_2) = 0.$$

Now,

$$F_{\lambda_1} = \int_0^{\pi} \frac{1}{2g(t)}\,dt > 0,$$

and thus by the implicit function theorem there exists an $\varepsilon > 0$ and a C^1 function $h : (\lambda_2-\varepsilon,\lambda_2+\varepsilon) \to \mathbb{R}$ such that $h(\lambda_2) = \lambda_1^*$ and $F(h(\tau),\tau) = 0$ for all $\tau \in (\lambda_2-\varepsilon,\lambda_2+\varepsilon)$. Since λ_2 was fixed arbitrarily, then the function h can be smoothly extended to all of $\mathbb{R}_+$. □

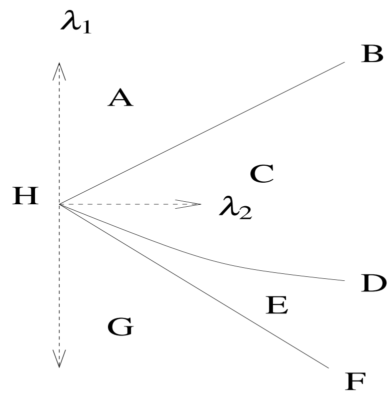

Figure 3.2: *Bifurcation of phase portraits of system (3.16) on regions of the parameter space* Λ*. The Region D is defined by the function h in Lemma 15 and is characterized by the existence of a pair of heteroclinic orbits* $(\theta_0-\pi,0)$ *to* $(\theta_0,0)$

Using Lemma 15 we obtain the bifurcation diagram, Figure 3.2, of the phase portraits of system (3.16) with respect to the parameter space Λ. We only show detail in the right half plane $\lambda_2 > 0$, but the left half plane $\lambda_2 < 0$ is similar. Detail of the specific regions are shown in Figure 3.3 and Figure 3.4 in Figures section.

Notice that for λ_2 fixed, as we vary the value of λ_1, the value of θ_0 varies as well. More specifically $\theta_0 \to \pi/4^-$ as $\lambda_1 \to -\lambda_2^+$ and $\theta_0 \to 0^+$ as $\lambda_1 \to 0^-$.

3.3 Existence in the region containing 5CB

Two of the most well studied nematic liquid crystals 4-mthoxybenzylidene-4'-butylaniline (MBBA) and 4-pentyl-4'cyanobiphenyl (5CB) have parameter sets which lie in the the region E shown in Figure 3.2; the values of the Leslie coefficients and Franks constants for 5CB and MBBA can be found in [44] Appendix D. Thus we study the region E as a jumping off point of in our study of steady state solutions subject to to the strong anchoring boundary condition

$$\theta(-h) = 0 = \theta(h). \tag{3.25}$$

Physically the boundary condition (3.25) is such that the liquid crystal lies on the upper and lower plate in a direction parallel to the plates. We rely on the time map method for our analysis and so before continuing we give a brief overview of this now.

3.3.1 The time map technique

The time map technique developed in a series of papers by Smoller and Wasserman, [42, 43, 13], as well as Brunovsky and Chow, [4], is a method for characterizing the existence and bifurcation of steady state solutions of the reaction-difusion equation

$$u_t = u_{xx} + f(u), \tag{3.26}$$

subject to Dirichlet,

$$u(t,-L) = 0 = u(t,L), \tag{3.27}$$

or Neumann,

$$u_x(t,-L) = 0 = u_x(t,L), \tag{3.28}$$

boundary conditions. Reaction-diffusion systems arises naturally as a models of chemical reactions and biological processes. It is well known that every solution of (3.26),(3.27), which does not blow up in finite time, approaches a steady state solution as $t \to \pm\infty$, [4]. Thus, it is of importance to understand the existence and multiplicity of solutions of the steady state equation

$$u_{xx} + f(u) = 0, \tag{3.29}$$

subject to boundary conditions

$$u(-L) = 0 = u(L). \tag{3.30}$$

This is exactly what the time map technique aims to accomplish by exploiting the Hamiltonian structure of system (3.29).

We make the change of variables $x \equiv Lx$ and set $v = u'$, so that we can rewrite system (3.26) as the equivalent two dimensional linear system

$$u' = v, \qquad v' = -L^2 f(u). \tag{3.31}$$

The system (3.31) is called a classical Hamiltonian (Newtonian) system and the solutions lie on the level curves of the Hamiltonian function

$$H(u,v) = \frac{v^2}{2} + L^2 F(u), \tag{3.32}$$

where $F(u)$ is an antiderivative of $f(u)$ and without loss of generality we assume $F(0) = 0$. Now suppose that $(u(x), v(x))$ is a solution of (3.31) lying on the level curve $H(u,v) = \xi$, $\xi > 0$, with initial condition $(u(0), v(0)) = (0, \sqrt{2\xi})$. Suppose this solution intersects the positive x-axis at a point $(\alpha, 0)$, $\alpha > 0$. Then the *time map* is defined by

$$T(\alpha) = \inf \{t > 0 : u(t) = \alpha, v(t) = 0\}, \tag{3.33}$$

and is such that $(u(T(\alpha)), v(T(\alpha))) = (\alpha, 0)$ and for $0 < x < T(\alpha)$, $v(x) > 0$. Furthermore, by symmetry it is also true that $(u(2T(\alpha)), v(2T(\alpha))) = (0, -\sqrt{2\xi})$. The existence of a solution to (3.29),(3.30) boils down to showing that there exists and α in the domain of T such that $T(\alpha) = 2L$.

The characterization of multiplicity of steady state solutions is done through analyzing the derivatives of the time map. Examples of this can be found in the works of SH Wang and Kazarinoff, [46], in the case of the classic Kolmogorov equation

$$u_t = \frac{1}{2} u_{xx} + f(u), \tag{3.34}$$

where $f \in C^2([0,1])$ satisfies $f(x) > 0$ on $(0,1)$, $f(1) = 0$, and there exists a small $\delta > 0$ such that $f'(u) \leq 0$ in $(1-\delta, 1)$. More recent work via time map techniques by Qian, [39], concerns L-periodic solutions of (3.29) and work by Z. Wang, [47], concerns L-periodic solutions of the nonlinear equation

$$x'' + f(x)x' + g(x) = e(t), \tag{3.35}$$

where $f, g, e \in C([0, \infty))$ and $e(t)$ is an L-periodic forcing term.

The last few examples show that the time map technique is highly dependent of the form of $f(u)$ and as such work is done on a case by case basis.

3.3.2 Existence of single twist solutions

We proceed to set up the time map for our problem to prove the existence of a singly twisted solution; i.e. the liquid crystal undergoes a single twist in the channel. Suppose that $(\theta(y), \eta(y))$ is a solution of (3.16) satisfying the boundary condition

$$\theta(-h) = \phi = \theta(h) \tag{3.36}$$

for fixed $\phi \in [-\theta_0, \theta_0)$. Without loss of generality we take G in Theorem 3 to be

$$G(\theta) = \int_{-\theta_0}^{\theta} \frac{\lambda_1 + \lambda_2 \cos(2s)}{4g(s)}\, ds. \tag{3.37}$$

Now suppose that the solution $(\theta(y), \eta(y))$ with initial condition $(\theta(0), \eta(0)) = (\phi, \xi)$, $\xi > 0$, traversing in a clockwise manner, intersects the θ-axis for the first time at a point $(\alpha, 0)$. In region E, these types of solutions always exist and lie inside the homoclinic orbit to $(\theta_0, 0)$, see Figure 3.4 in Figures section.

By our choice of G, this solution lies on the level set $H(\alpha, 0)$, given by

$$MG(\alpha) = \frac{1}{2f(\theta)}\eta^2 + MG(\theta). \tag{3.38}$$

Since $\eta = \theta' f(\theta)$ then using separation of variables in (3.38) we have

$$y = \frac{2}{\sqrt{M}} \int_{\phi}^{\theta(y)} \frac{\sqrt{f(t)}}{\sqrt{G(\alpha) - G(t)}}\, dt,$$

from which we are able to derive the explicit form of the time map given by

$$T(\alpha) = \frac{2}{\sqrt{M}} \int_{\phi}^{\alpha} \frac{\sqrt{f(t)}}{\sqrt{G(\alpha) - G(t)}}\, dt. \tag{3.39}$$

By construction the time map is such that $(\theta(T(\alpha)),\eta(T(\alpha))) = (\alpha,0)$ and by symmetry $(\theta(2T(\alpha)),\eta(2T(\alpha))) = (\phi,-\xi)$.

Making the linear change of variables $t \equiv l(u,\alpha) = \alpha u + (1-u)\phi$ we have

$$\frac{\sqrt{M}}{2}T(\alpha) = (\alpha-\phi)\int_0^1 \frac{\sqrt{f(l(u,\alpha))}}{\sqrt{G(\alpha)-G(l(u,\alpha))}}du, \tag{3.40}$$

and

$$\begin{aligned}\frac{\sqrt{M}}{2}T'(\alpha) &= \int_0^1 \frac{f(l(u,\alpha))(G(\alpha)-G(l(u,\alpha)))}{\sqrt{f(l(u,\alpha))}(G(\alpha)-G(l(u,\alpha))^{3/2}}du \\ &\quad + \frac{\alpha-\phi}{2}\int_0^1 \frac{uf'(l(u,\alpha))(G(\alpha)-G(l(u,\alpha))-f(l(u,\alpha))(G'(\alpha)-uG'(l(u,\alpha))}{\sqrt{f(l(u,\alpha))}(G(\alpha)-G(l(u,\alpha))^{3/2}}du \\ &= \int_0^1 \frac{f(l(u,\alpha))[\varphi(\alpha)-\varphi(l(u,\alpha))]+\frac{\alpha-\phi}{2}uf'(l(u,\alpha))(G(\alpha)-G(l(u,\alpha))}{\sqrt{f(l(u,\alpha))}(G(\alpha)-G(l(u,\alpha))^{3/2}}du,\end{aligned}$$

where

$$\varphi(t) = G(t) - \frac{t}{2}G'(t),$$

and

$$f'(t) = 2(K_3-K_1)\cos(t)\sin(t) = (K_3-K_1)\sin(2t).$$

The time map we constructed is generic for solutions inside the homoclinic orbit, but properties of the time map, T, depend on the choice of boundary conditions ϕ. We show the existence of a single twist solution for $\phi \geq -\theta_0$,

Lemma 16. *Suppose that $K_3 > K_1$, $\mu_1 > 0$, and λ_1, λ_1 lie in region E. If $\phi > -\theta_0$, then the minimum time, h, it takes for a solution $(\theta(y),\eta(y))$ satisfying $0 \leq \eta(0) < \sqrt{2Mf(\theta_0)G(\theta_0)}$ and $(\theta(h),\eta(h)) = (\alpha,0)$ is given by$T(\alpha)$ which satisfies*

(i) $T'(\alpha) > 0$ *for* $\alpha \in (\phi,\theta_0)$

(ii) $\lim_{\alpha \to \phi^+} T_1(\alpha) = 0$

(iii) $\lim_{\alpha \to \theta_0^-} T_1(\alpha) = \infty$

Proof. Since we are in region E, $\theta_0 \in (0, \pi/4)$. The condition $0 \leq \eta(0) < \sqrt{2Mf(\theta_0)G(\theta_0)}$ guarantees that the solution is periodic lying inside the homoclinic orbit to $(\theta_0, 0)$. To prove the first part of the lemma is suffices to show that $\varphi'(t) > 0$ for $t \in (-\theta_0, \theta_0)$ since $K_3 > K_1$ and $G(\alpha) - G(l(u,\alpha)) > 0$. We compute

$$\begin{aligned} 2g'(t) &= 4\mu_1 \cos^3(t)\sin(t) - 4\mu_1 \cos(t)\sin^3(t) + 2\lambda_2 \sin(2t) \\ &= 2\mu_1 \sin(2t)\cos(2t) + 2\lambda_2 \sin(2t) \\ &= 2\sin(2t)[\mu_1 \cos(2t) + \lambda_2], \end{aligned}$$

and so

$$\begin{aligned} 2\varphi'(t) &= G'(t) - tG''(t) \\ &= \frac{2g(t)(\lambda_1 + \lambda_2\cos(2t)) + 4\lambda_2 t g(t)\sin(2t) + 2tg'(t)(\lambda_1 + \lambda_2\cos(2t))}{(2g(t))^2} \\ &= \frac{2g(t)(\lambda_1 + \lambda_2\cos(2t)) + t\sin(2t)[4\lambda_2 g(t) + 2(\mu_1\cos(2t) + \lambda_2)(\lambda_1 + \lambda_2\cos(2t))]}{(2g(t))^2}. \end{aligned}$$

We see that each term in the numerator is positive and hence $\varphi'(t) > 0$.

The asymptotic behavior can be proved using the fact that the solution $(\theta(y), \eta(y))$ approaches the stable branch of the hyperbolic fixed point $(\theta_0, 0)$ as $\alpha \to \theta_0^-$. On the other side, near ϕ, the denominator is bounded below, and hence the term $\sqrt{\alpha - \phi}$ governs the asymptotic behavior. □

Lemma 17. *Suppose that $K_3 > K_1$, $\mu_1 > 0$, and λ_1, λ_2 lie in region E. If $\phi = -\theta_0$, then the minimum time, h, it takes for a solution $(\theta(y), \eta(y))$ satisfying $0 \leq \eta(0) < \sqrt{2Mf(\theta_0)G(\theta_0)}$ and $(\theta(h), \eta(h)) = (\alpha, 0)$ is given by $T(\alpha)$ which satisfies* *(i)* $T'(\alpha) > 0$ *for* $\alpha \in (-\theta_0, \theta_0)$

(ii) $\lim_{\alpha \to -\theta_0^+} T_1(\alpha) = \pi \sqrt{\frac{f(\theta_0)g(\theta_0)}{M\lambda_2 \sin(2\theta_0)}}$

(iii) $\lim_{\alpha \to \theta_0^-} T_1(\alpha) = \infty$

Proof. The proof of $T' > 0$ carries over from Lemma 16. The asymptotic behavior is proved using the fact that the solution $(\theta(y), \eta(y))$ approaches the stable branch of the fixed point $(\theta_0, 0)$ as $\alpha \to \theta_0^-$. On the other side, as $\alpha \to -\theta_0^+$ the system is approximated by the linearization (3.18) and hence the time it takes is one half π the frequency which is given by the eigenvalue of the linearization at $(-\theta_0, 0)$. Note one may also directly perform an asymptotic expansion of the integrand to prove this fact. □

We define

$$h_e = \pi \sqrt{\frac{f(\theta_0)g(\theta_0)}{M\lambda_2 \sin(2\theta_0)}}. \tag{3.41}$$

In order to prove the existence of a solution for the full system (3.16) with boundary conditions (3.15) it is necessary to show that a solution of (3.14) with boundary condition (3.36) exists.

Theorem 4. *Suppose the hypothesis of Lemma 16, then there exists a solution of (3.14) subject to the boundary conditions*

$$\theta(-h) = \phi = \theta(h)$$

with $-\theta_0 < \phi < \theta_0$ *which undergoes a single twist within the channel. If* $\phi = -\theta_0$*, then there exists a singly twisted solution if and only if* $h > h_e$.

Proof. If $\phi = -\theta_0$, then the result follows immediately from the definition of h_e together with Lemma 17. If $\theta_0 - \pi < \phi < \theta_0$ then the result follows immediately from Lemma 16. □

3.4 Further Research

There are many interesting dynamics exhibited by nematic liquid crystals in shearing flow and we have simply scratched the surface in this chapter. A quick glance at Figure 3.2 shows that there are many types of steady state solutions which may exist satisfying the strong anchoring boundary condition $\theta(-h) = \phi = \theta(h)$. These include symmetric, asymmetric, and super twisted solutions, although certain regions of the parameter space Λ and choices of Frank constants place a restriction on their existence. Thus a more thorough analysis on the different regions of phase space configurations is needed.

In the region E, see Figure 3.2, we will focus first on the critical periodic solution $(\theta(y), \eta(y))$ which satisfies the boundary condition $\theta(-h) = 0 = \theta(h)$ and $\theta'(-h) = 0 = \theta'(h)$. This is the solution which wraps once and touches the η-axis. Treating the length of the channel,h, as a bifurcation parameter we see that this symmetric steady state solution has the possibility to bifurcate two asymmetric solutions. A more rigorous analysis of the time map is needed to determine if this is a possible.

Region A is also interesting and more directly analogous to our previous work in Chapter 2 in that on this parameter region system (3.16) contains no equilibrium points. Moreover, while there is the possibility of multiple singly twisted steady state solutions, there cannot exist super twisted solutions.

Similar to the study done in Chapter 2, an inspection of bifurcations of the zero eigenvalue can be carried out by noting that the zero eigenvalue problem associated with the linearization about a steady state is precisely the linearization about a steady state. Thus we will be able to exploit the Hamiltonian structure of the steady state system in order to better understand the spectrum in a neighborhood of the zero eigenvalue. For the bifurcation of a critical periodic solution mentioned above, the condition $\theta'(-h) = 0 = \theta'(h)$ implies that $\theta'(y)$ is a solution of the zero eigenvalue problem. This is important because it shows that the zero eigenvalue may have multiplicity greater than one, which allows for the possibility of more complex types of bifurcations.

Figures

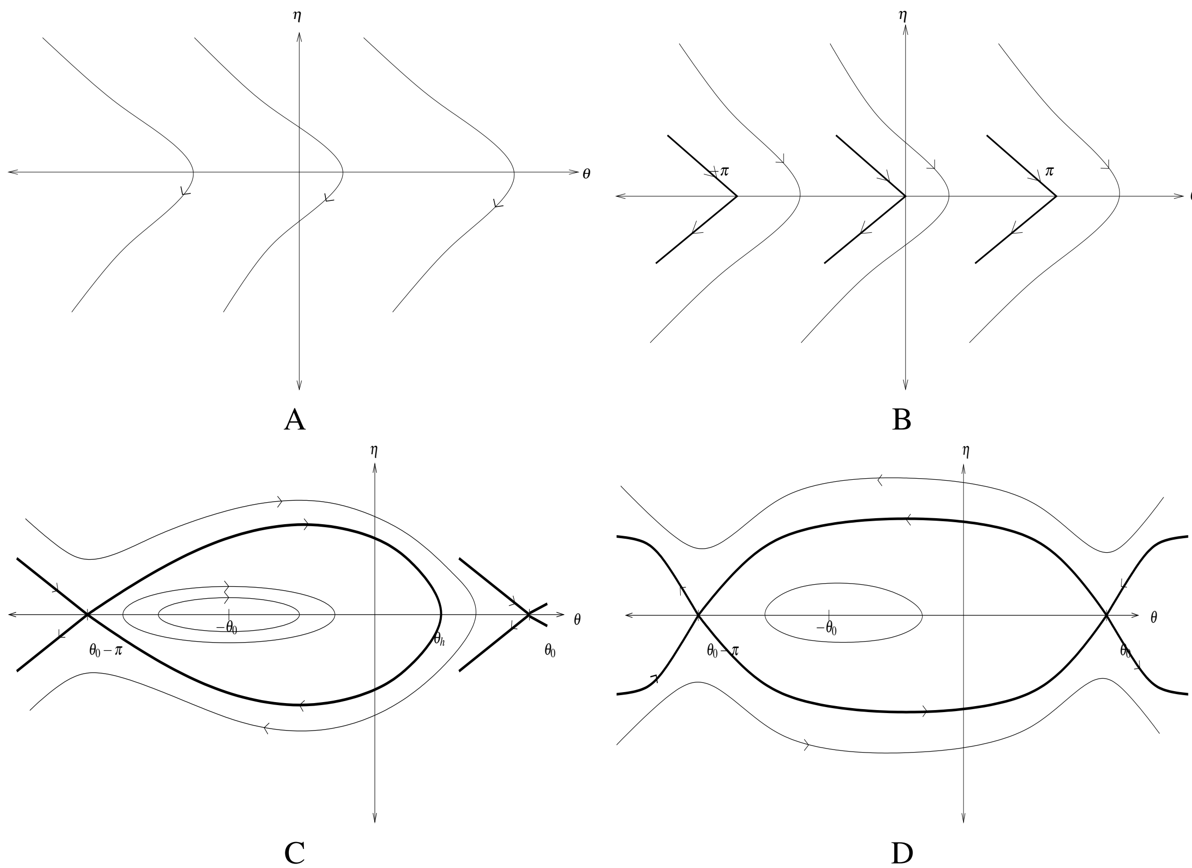

Figure 3.3: Phase portraits of system (3.16) on Regions A-D of Λ, see Figure 3.2

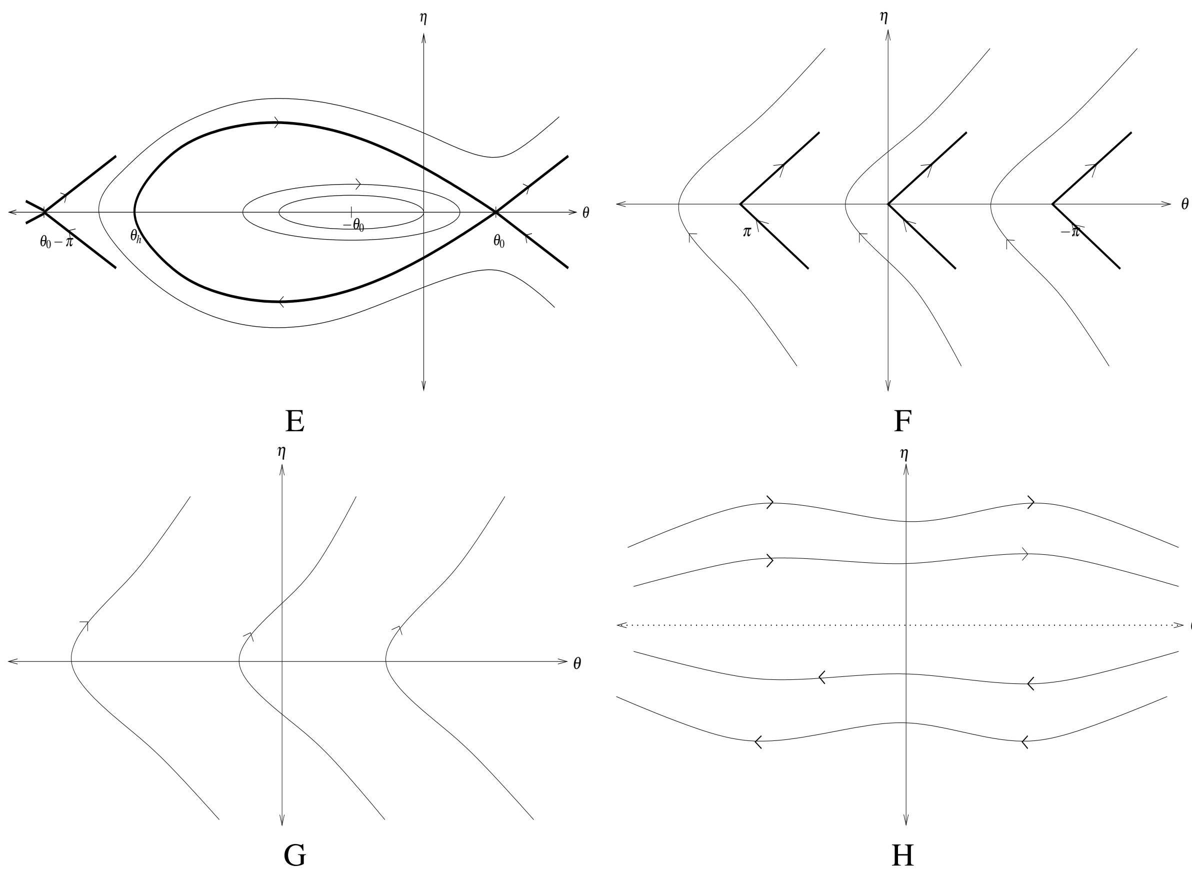

Figure 3.4: Phase portraits of system (3.16) on Regions E-H of Λ, see Figure 3.2

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