

Bifurcations in liquid crystals cells

Fernando Pestana da Costa

DCeT, Universidade Aberta

CAMGSD-Instituto Superior Técnico, Universidade de Lisboa

Encontro CIÊNCIA '18
Centro de Congressos, Lisboa
July 2–4, 2018

Liquid Crystals

Generalities

Fréedericksz transition

Mathematical setting

Bifurcations in twisted cells

Collaborators and works



↑15↑13↑11↑9 8 7 6 5 4 3 2 1
16 14 12 10



Liquid crystals: uses in optical devices

Liquid Crystals

Generalities

Fréedericksz transition

Mathematical setting

Bifurcations in twisted cells

Collaborators and works





Liquid crystals: uses in optical devices

Liquid Crystals

Generalities

Fréedericksz transition

Mathematical setting

Bifurcations in twisted cells

Collaborators and works





Liquid crystals: generalities

Liquid crystals have many different occurrences in both nature and technical applications. What is the common ground?

Liquid Crystals

Generalities

Fréedericksz transition

Mathematical setting

Bifurcations in twisted
cells

Collaborators and works



Liquid crystals: generalities

Liquid crystals have many different occurrences in both nature and technical applications. What is the common ground?

WHAT CHARACTERIZES A LIQUID CRYSTAL?

Liquid Crystals

Generalities

Fréedericksz transition

Mathematical setting

Bifurcations in twisted cells

Collaborators and works



Liquid crystals: generalities

Liquid crystals have many different occurrences in both nature and technical applications. What is the common ground?

WHAT CHARACTERIZES A LIQUID CRYSTAL?

Strong molecular anisotropy leading to partially ordered
“mesophases” .

Liquid Crystals

Generalities

Fréedericksz transition

Mathematical setting

Bifurcations in twisted
cells

Collaborators and works



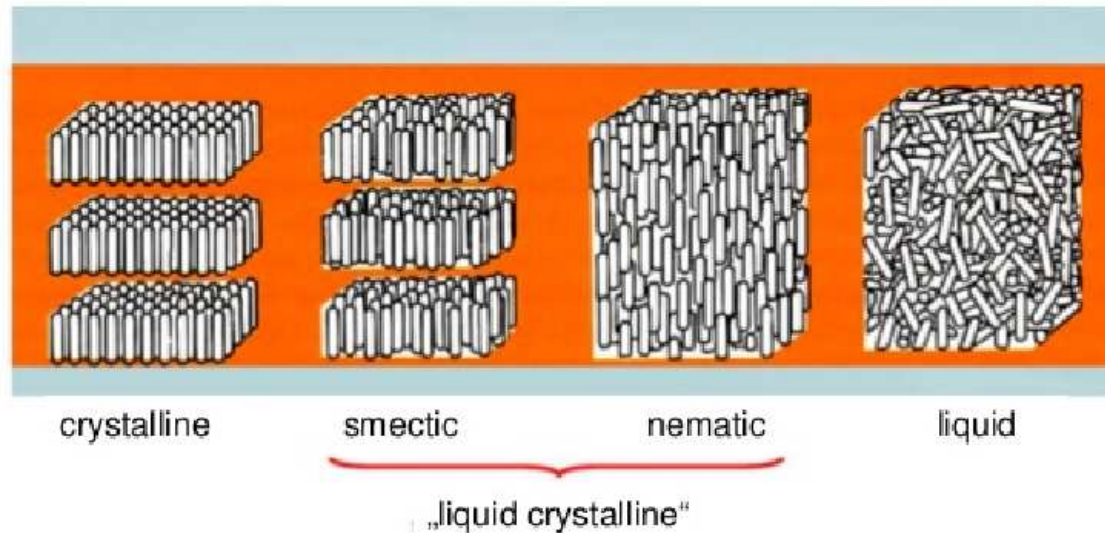
Liquid crystals: generalities

Liquid crystals have many different occurrences in both nature and technical applications. What is the common ground?

WHAT CHARACTERIZES A LIQUID CRYSTAL?

Strong molecular anisotropy leading to partially ordered “mesophases”.

crystalline phases	mesophases	amorphous phases
3D-order	2D-, 1D-order	no long-range order





Liquid crystals: generalities

Different sciences study liquid crystals differently.
How a liquid crystal molecule is seen depends on your goal.
As a **caricature** one could say that...

Liquid Crystals

Generalities

Fréedericksz transition

Mathematical setting

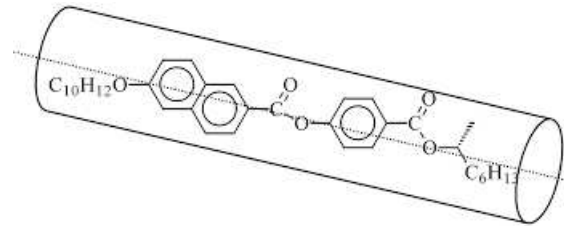
Bifurcations in twisted
cells

Collaborators and works



Liquid crystals: generalities

Different sciences study liquid crystals differently.
 How a liquid crystal molecule is seen depends on your goal.
 As a **caricature** one could say that...
 ...to a chemist:



Liquid Crystals

Generalities

Fréedericksz transition

Mathematical setting

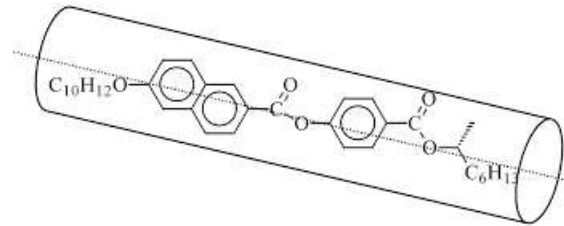
Bifurcations in twisted cells

Collaborators and works

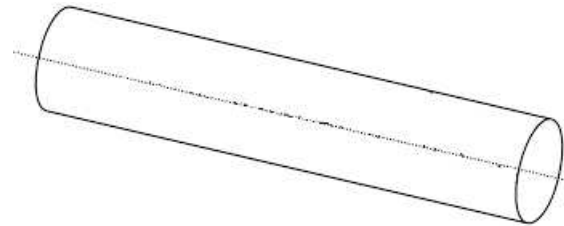


Liquid crystals: generalities

Different sciences study liquid crystals differently.
 How a liquid crystal molecule is seen depends on your goal.
 As a **caricature** one could say that...
 ...to a chemist:



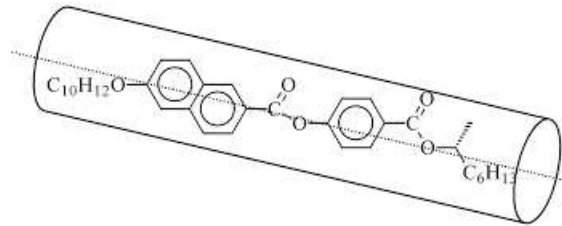
to a physicist:



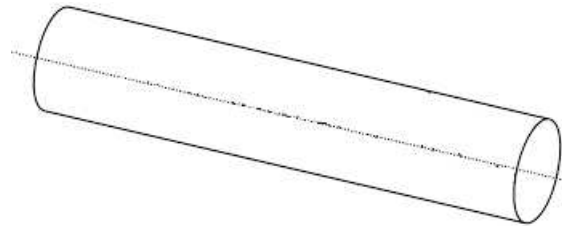


Liquid crystals: generalities

Different sciences study liquid crystals differently.
 How a liquid crystal molecule is seen depends on your goal.
 As a **caricature** one could say that...
 ...to a chemist:



to a physicist:



to a mathematician:





The liquid crystal cell

Liquid Crystals

Generalities

Fréedericksz transition

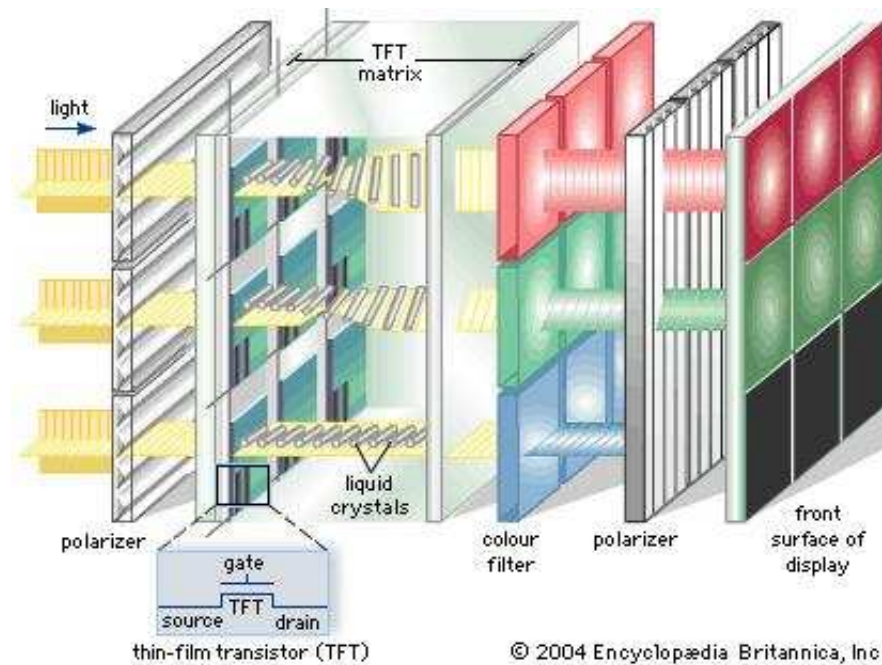
Mathematical setting

Bifurcations in twisted cells

Collaborators and works

In this talk I will deal with mathematical modelling of optical phenomena in liquid crystal cells.

These are devices of paramount technological importance.





The Fréedericksz transition

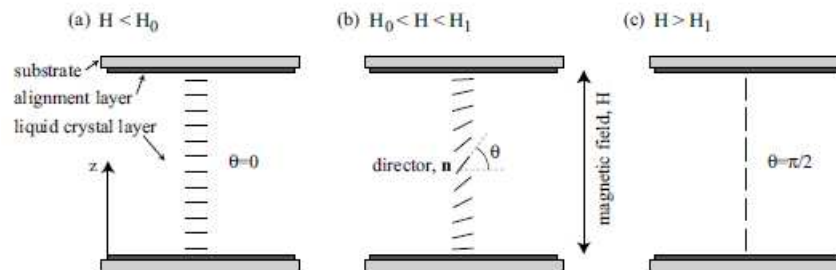
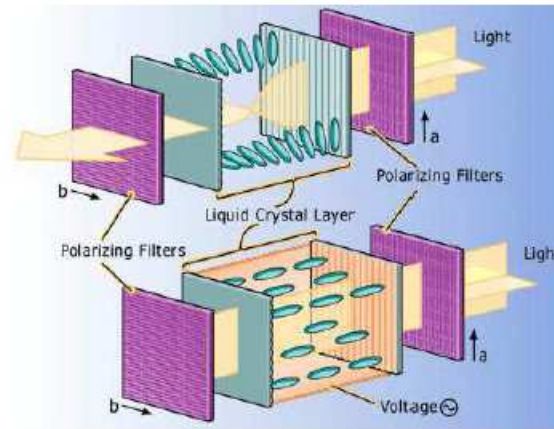
Liquid Crystals
 Generalities

Fréedericksz transition

Mathematical setting
 Bifurcations in twisted cells

Collaborators and works

The *Fréedericksz transition* is the simplest opto-electronic liquid crystal switch. It is the result of the competition between reorienting effects of an **applied electric or magnetic field**, the **bulk elastic energy** of the molecules and their **anchoring energy** to the bounding surfaces of a liquid crystal cell.





The mathematical setting

The **Helmholtz free energy functional** is given by

$$F = \int_{\Omega} (\sigma_F(\mathbf{n}, \nabla \mathbf{n}) + \sigma_H(\mathbf{n})) dV + \int_{\partial\Omega} \sigma_s(\mathbf{n}, \nabla \mathbf{n}) dS.$$

where:

σ_F is the bulk elastic Frank-Oseen energy density

σ_H is the contribution of the applied field to the free energy

σ_s is the surface contribution to the free energy, due to anchoring of the liquid crystal molecules to the liquid crystal cells

\mathbf{n} is the director vector field

$\nabla \mathbf{n}$ is the spatial gradient of the director vector field



The mathematical setting

The **Helmholtz free energy functional** is given by

$$F = \int_{\Omega} (\sigma_F(\mathbf{n}, \nabla \mathbf{n}) + \sigma_H(\mathbf{n})) dV + \int_{\partial\Omega} \sigma_s(\mathbf{n}, \nabla \mathbf{n}) dS.$$

where:

σ_F is the bulk elastic Frank-Oseen energy density

σ_H is the contribution of the applied field to the free energy

σ_s is the surface contribution to the free energy, due to anchoring of the liquid crystal molecules to the liquid crystal cells

\mathbf{n} is the director vector field

$\nabla \mathbf{n}$ is the spatial gradient of the director vector field

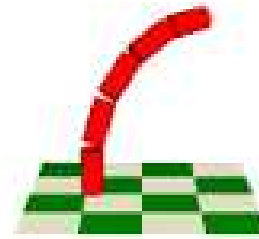
Equilibrium configurations of the LC are critical points of F .
 The dynamic behaviour is governed by the gradient flow of F .
 In this talk we shall consider only **equilibrium configurations**.

The mathematical setting

The three contributions to the Frank-Oseen elastic energy density σ_F of a *nematic* liquid crystal



Twist



Bend



Splay

$$k_3 \|\mathbf{n} \times \nabla \times \mathbf{n}\|^2, \quad k_2 (\mathbf{n} \cdot \nabla \times \mathbf{n})^2, \quad k_1 (\nabla \cdot \mathbf{n})^2$$



Bifurcations in twisted cells

Example of anchoring conditions.

Liquid Crystals

Generalities

Fréedericksz transition

Mathematical setting

Bifurcations in twisted
cells

Collaborators and works



Bifurcations in twisted cells

Example of anchoring conditions.

Strong anchoring with **twist geometry**:

Liquid Crystals

Generalities

Fréedericksz transition

Mathematical setting

Bifurcations in twisted
cells

Collaborators and works



Bifurcations in twisted cells

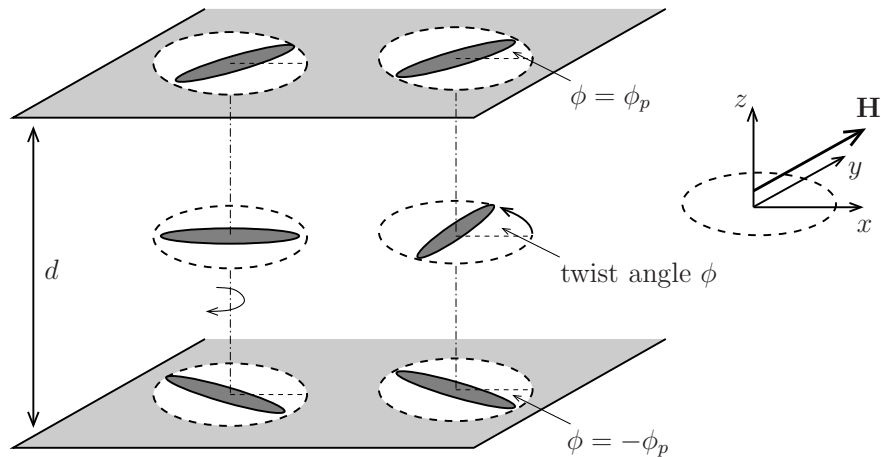
Example of anchoring conditions.

Strong anchoring with **twist geometry**:

Director $\mathbf{n} = (\cos \phi, \sin \phi, 0)$ is fixed on the cell boundary and does *not* contribute to changes in F ; e.g.: in the twist-nematic cell with pre-twist at the boundary, for fixed $0 < \phi_0, \phi_1 < \frac{\pi}{2}$, the conditions are:

$$\mathbf{n}(t, 0) = (\cos \phi_0, -\sin \phi_0, 0)$$

$$\mathbf{n}(t, d) = (\cos \phi_1, \sin \phi_1, 0)$$





Bifurcations in twisted cells

For the **strong anchoring** case just shown, the equilibrium equation in dimensionless form, together with the boundary condition, is the following boundary value problem with *non-homogeneous Dirichlet boundary condition*:

$$\begin{cases} 0 = \frac{d^2 \phi}{d\zeta^2} + \lambda \sin \phi \cos \phi, & \zeta \in (0, 1) \\ \phi(0) = -\phi_0, \quad \phi(1) = \phi_1 \end{cases}$$

where $\zeta := z/d$, $\lambda := \mu_0 \Delta \chi H^2 d^2 / k_2$.



Bifurcations in twisted cells

For the **strong anchoring** case just shown, the equilibrium equation in dimensionless form, together with the boundary condition, is the following boundary value problem with *non-homogeneous Dirichlet boundary condition*:

$$\begin{cases} 0 = \frac{d^2 \phi}{d\zeta^2} + \lambda \sin \phi \cos \phi, & \zeta \in (0, 1) \\ \phi(0) = -\phi_0, \quad \phi(1) = \phi_1 \end{cases}$$

where $\zeta := z/d$, $\lambda := \mu_0 \Delta \chi H^2 d^2 / k_2$.

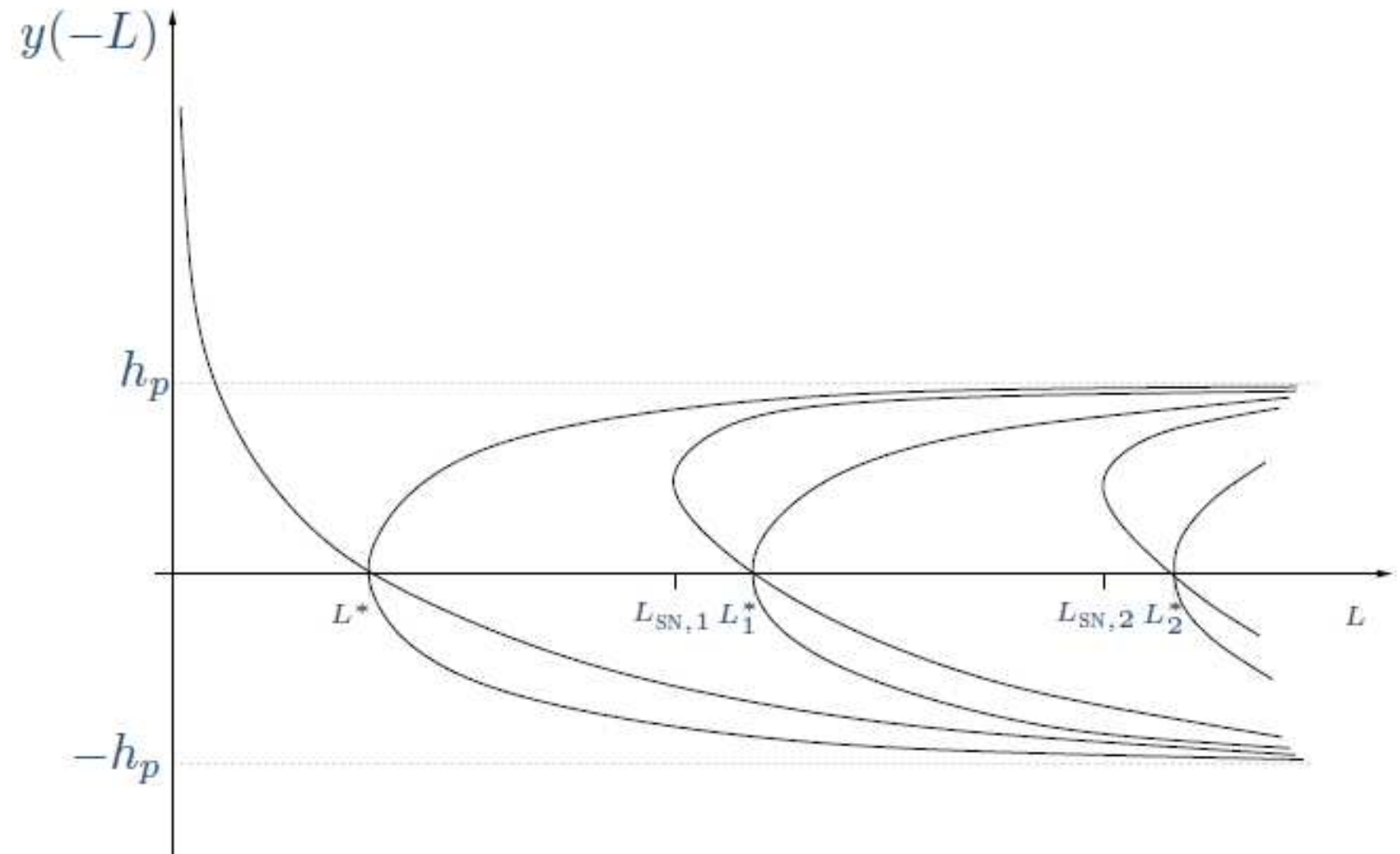
A further change of variables $\zeta \mapsto t := (\zeta - \frac{1}{2}) \sqrt{\lambda/2}$, and $L = \sqrt{\lambda/8}$, transforms it into

$$\begin{cases} x' = y, \quad y' = -\sin 2x, & t \in (-L, L) \\ x(-L) = -\phi_0, \quad x(L) = \phi_1 \end{cases} \quad (1)$$

where $x(t) = \phi(\zeta(t))$.

Bifurcations in twisted cells

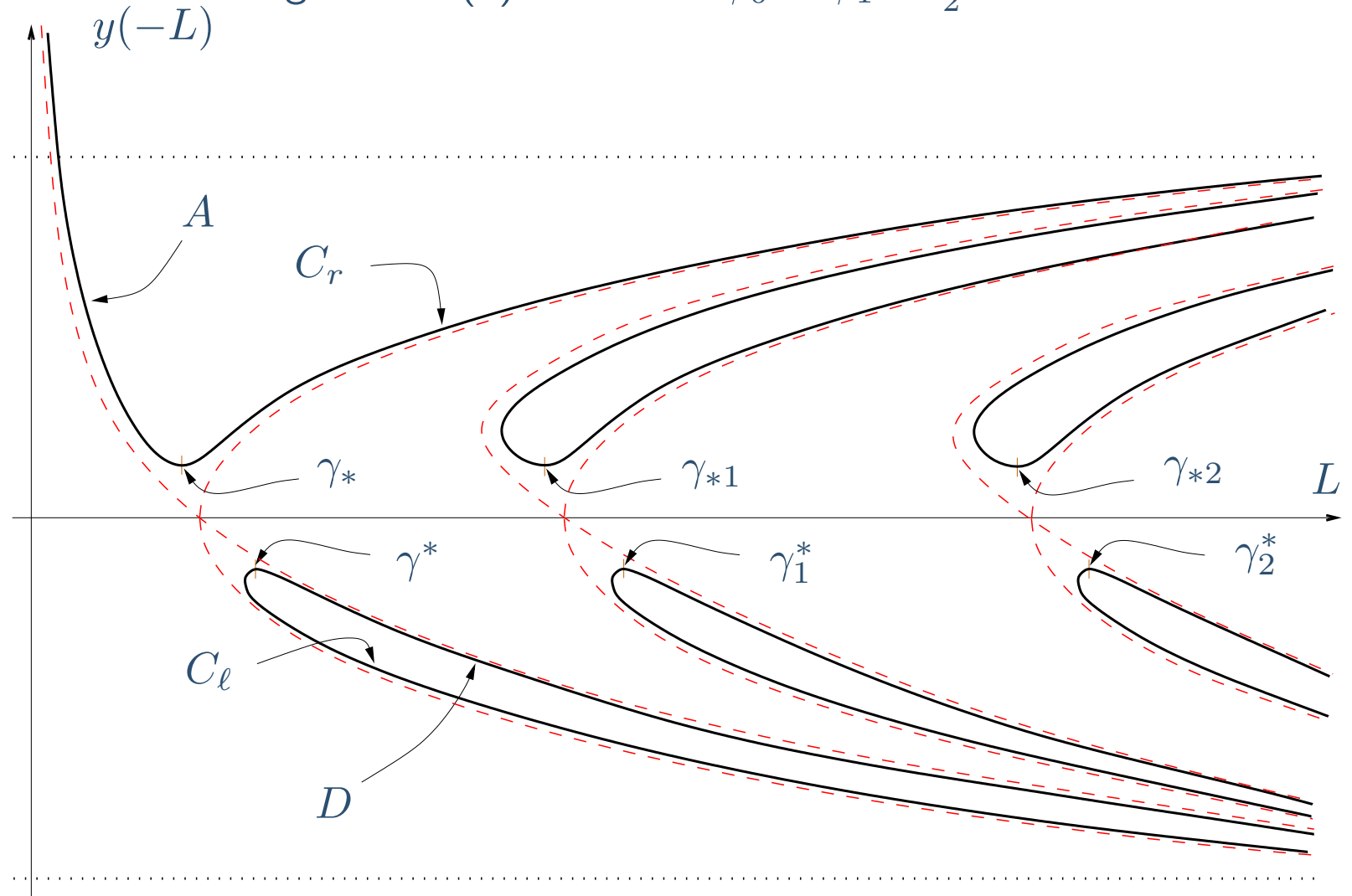
Bifurcation diagram of (1) when $\phi_0 = \phi_1 =: \phi_p \in (0, \frac{\pi}{2})$:





Bifurcations in twisted cells

Bifurcation diagram for (1) when $0 < \phi_0 < \phi_1 < \frac{\pi}{2}$:





Bifurcations in twisted cells

Tools and approach:

Time maps and phase plane analysis based on “special” solutions.

Liquid Crystals

Generalities

Fréedericksz transition

Mathematical setting

Bifurcations in twisted
cells

Collaborators and works



Bifurcations in twisted cells

Tools and approach:

Time maps and phase plane analysis based on “special” solutions.

Liquid Crystals

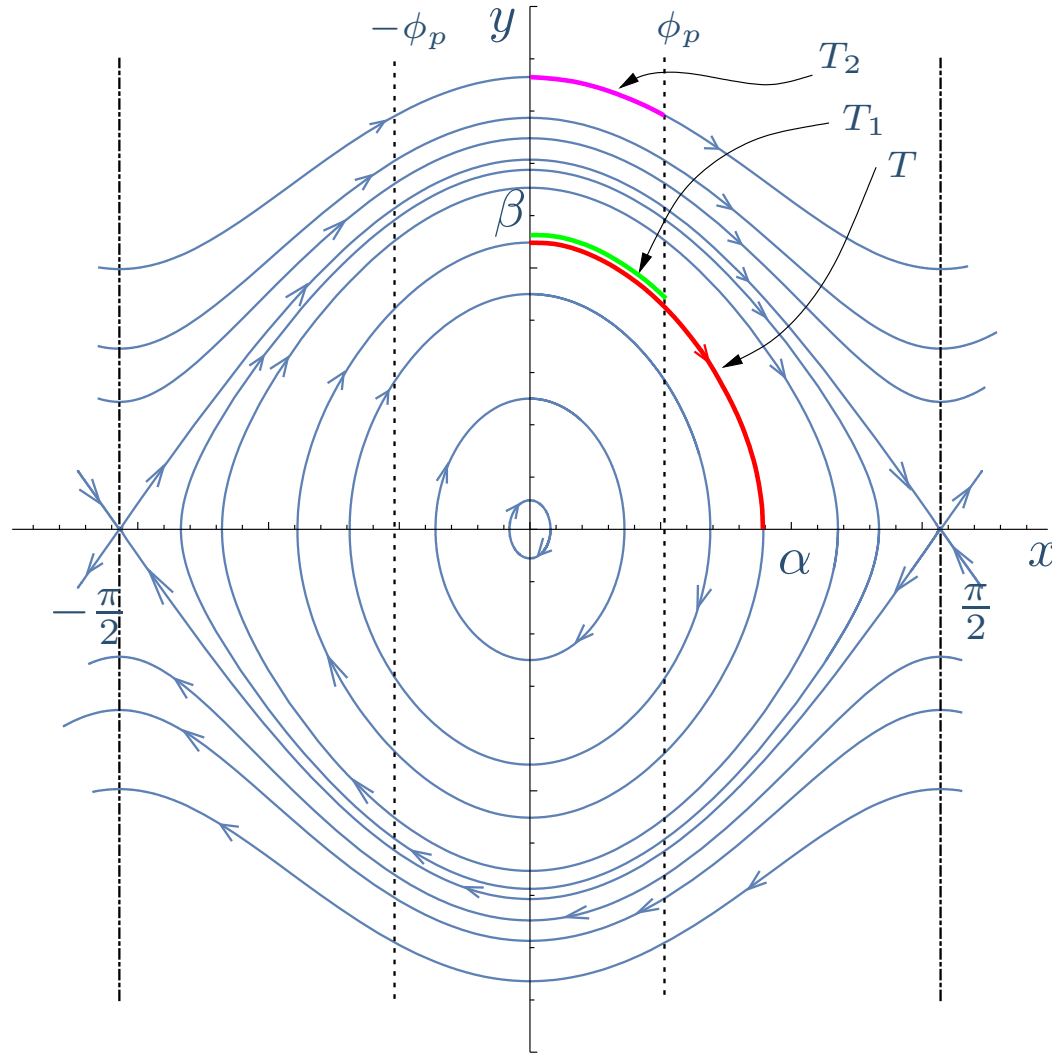
Generalities

Fréedericksz transition

Mathematical setting

Bifurcations in twisted cells

Collaborators and works





Bifurcations in twisted cells

Liquid Crystals

Generalities

Fréedericksz transition

Mathematical setting

Bifurcations in twisted
cells

Collaborators and works

We finish with a problem obtained by a minor change in the boundary condition in (1), which is possibly relevant for a cholesteric liquid crystal cell:



Bifurcations in twisted cells

We finish with a problem obtained by a minor change in the boundary condition in (1), which is possibly relevant for a cholesteric liquid crystal cell:

$$\begin{cases} x' = y \\ y' = -\sin 2x \end{cases} \quad (2)$$

$$x(-L) = -\phi, \quad y(L) = \phi^* \quad (3)$$



Bifurcations in twisted cells

We finish with a problem obtained by a minor change in the boundary condition in (1), which is possibly relevant for a cholesteric liquid crystal cell:

$$\begin{cases} x' = y \\ y' = -\sin 2x \end{cases} \quad (2)$$

$$x(-L) = -\phi, \quad y(L) = \phi^* \quad (3)$$

Some unexpected difficulties just pop up!



Bifurcations in twisted cells

We finish with a problem obtained by a minor change in the boundary condition in (1), which is possibly relevant for a cholesteric liquid crystal cell:

$$\begin{cases} x' = y \\ y' = -\sin 2x \end{cases} \quad (2)$$

$$x(-L) = -\phi, \quad y(L) = \phi^* \quad (3)$$

Some unexpected difficulties just pop up!

For a kind of “symmetric” case where $\phi^* = \sqrt{1 - \cos 2\phi}$ the following bifurcation diagram is conjectured.



Bifurcations in twisted cells

We finish with a problem obtained by a minor change in the boundary condition in (1), which is possibly relevant for a cholesteric liquid crystal cell:

$$\begin{cases} x' = y \\ y' = -\sin 2x \end{cases} \quad (2)$$

$$x(-L) = -\phi, \quad y(L) = \phi^* \quad (3)$$

Some unexpected difficulties just pop up!

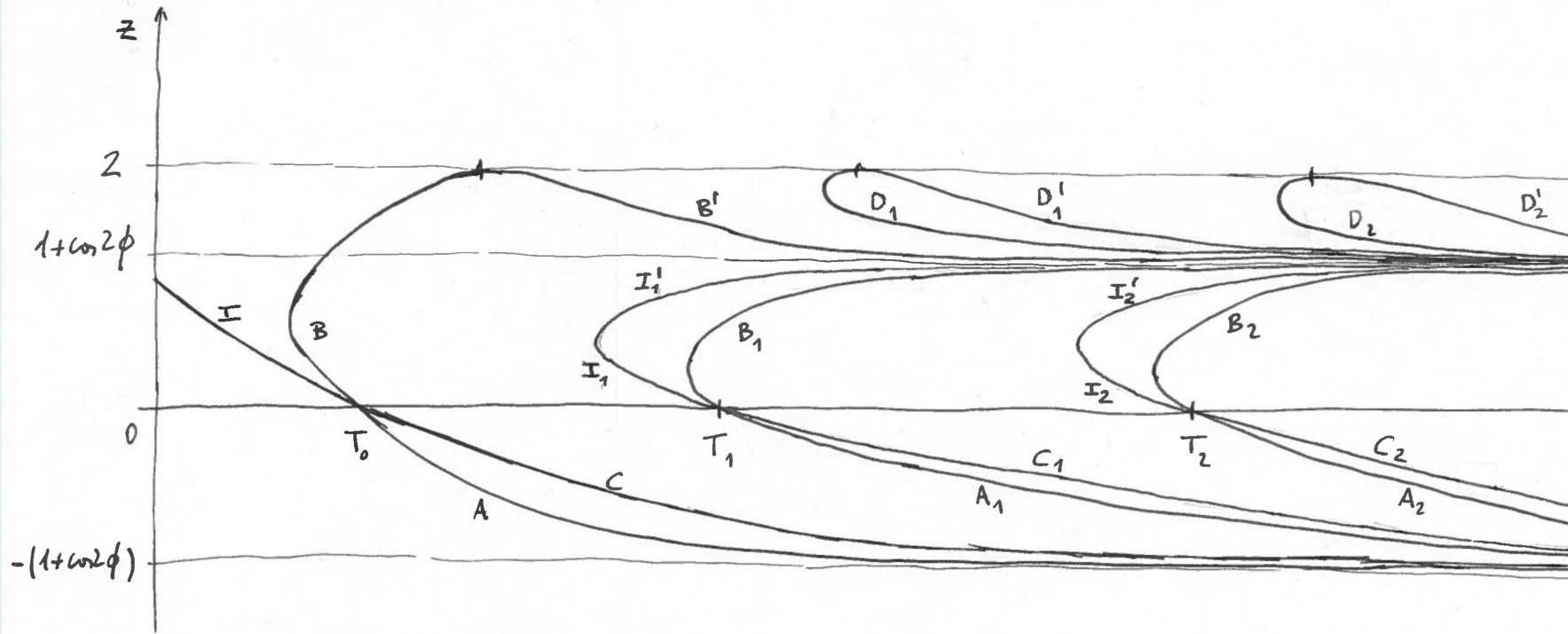
For a kind of “symmetric” case where $\phi^* = \sqrt{1 - \cos 2\phi}$ the following bifurcation diagram is conjectured.

Its proof depends on some convexity property a certain time map, that still resists current attacks.



Bifurcations in twisted cells

Liquid Crystals
 Generalities
 Fréedericksz transition
 Mathematical setting
Bifurcations in twisted cells
 Collaborators and works





From joint works with:

E.C. Gartland, Jr. (Kent State U, Kent OH)

M. Grinfeld, M. Langer, N.J. Mottram (U Strathclyde, Glasgow)

M.I. Méndez (IES Antonio López García, Madrid)

J.T. Pinto (IST, U Lisbon, Lisbon)

K. Xayxanadasy (NUOL, Vientiane)

Published in:

Math. Models Meth. Appl. Sci. (2007) **17**, 2009–2034.

J. Differ. Equ. (2009) **246**, 2590–2600.

Quart. Appl. Math. (2012) **70**, 99–110.

Eur. J. Appl. Math. (2009) **20**, 269–287; (2017) **28**, 243–260.

and work in progress.



Liquid Crystals
Generalities
Fréedericksz transition
Mathematical setting
Bifurcations in twisted
cells
Collaborators and works

Thank you!