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Executive Summary of the Thesis

Bifurcation analysis of spontaneous flows in active nematic fluids

Laurea Magistrale in Mathematical Engineering

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1. Introduction

The large spectrum of active matter, from molecular scale with colonies of bacteria to macroscopic scale with bird flocks has attracted the interest of several researchers coming from different scientific fields. In an active system, a collection of self-driven units is able to continuously exchange energy with the environment and create a collective behavior.

It is difficult to model this phenomenon, because of the numerous degrees of freedom, the lack of reversibility and the fact that molecules are out of the thermodynamic equilibrium. For many active systems, there are similarities with nematic liquid crystals whose dynamic is described by the Eriksen-Leslie theory [2]. Classic theories of active matter are based on this model, with the addition of term to the stress tensor. However, this choice is not universally accepted due to some problems with a clear interpretation in terms of irreversible thermodynamics.

In this thesis, we study an alternative model presented in[4]. We focus on the fluid approximation in a two-dimensional channel. Indeed, the spontaneous flow presents a two-fold degeneracy which is not usually observed in other theories or can only be found under very specific conditions.

By contrast, we show that this two-fold bifurcation is a generic feature and it is due to symmetry. To this end, we first present the model and the bifurcation in §2. Then in §3, we study the robustness of the instability to changes in the model parameters. To have a complete picture of the bifurcation diagram, we perform a Lyapunov-Schmidt reduction §4. Finally, we show using symmetry arguments that the bifurcation is general in §5.

2. Alternative model and bifurcation

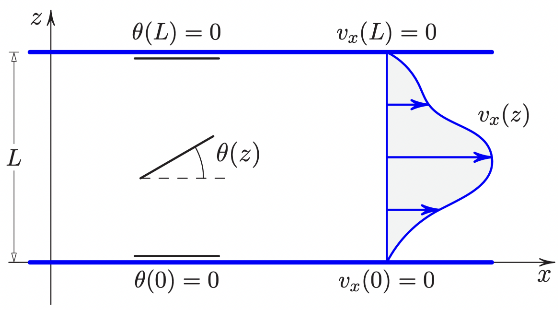

Figure 1: Scheme of the studied channel geometry (*source: "Active nematic gels as active relaxing solids" [4]*).

In classic theories, the consideration of the active term leads to some incoherences with respect to the irreversibility of active systems and the active effects are difficult to differentiate from the passive effects. The model presented in [4] is developed in order to avoid these incoherences. The existence of the spontaneous flow in a two-dimensional channel (*see* Figure 1) is a characteristic behavior of active nematics. Here we consider no-slip boundary condition for the velocity and horizontal orientation of the particles at the confining walls.

Two important equations have to be recalled to understand the model. First the model is based on an energy which is derived from nematic elastomer theory. The free-energy density per unit of mass is

$$\sigma(\rho,\mathbf{B}_e,\mathbf{n},\nabla\mathbf{n}) = \frac{1}{2}\mu[\mathrm{tr}(\mathbf{\Psi}^{-1}\mathbf{B}_e-\mathbf{I}) - \log(\det(\mathbf{\Psi}^{-1}\mathbf{B}_e))] + \frac{1}{2}k|\nabla\mathbf{n}|^2, \tag{1}$$

where $\mathbf{n}$ is the director or preferred orientation of the molecules, $\mathbf{\Psi}$ is the shape tensor representing the volume-preserving uniaxial stretch along the director, measured by a shape parameter a_0, k is the Frank constant, $\rho\mu$ is the shear modulus, and $\mathbf{B}_e$ is the effective left-Cauchy-Green deformation tensor.

A second key equation describes the microscopic remodeling,

$$\mathbb{D}(\mathbf{B}_e^{\nabla}) + \rho\frac{\partial\sigma}{\partial\mathbf{B}_e} = \mathbf{T}_a, \tag{2}$$

where $\mathbb{D}$ is the dissipation tensor, containing information about the relaxation times and viscosity coefficients, $\mathbf{B}_e^{\nabla}$ is the codeformational derivative of the effective left-Cauchy-Green deformation tensor, and finally, $\mathbf{T}_a$ is the active tensor , proportional to an activity coefficient ζ.

We consider the governing equations within the active fluid approximation. Furthermore, we make the following nondimensionalization,

$$z = L\xi,\ v_x(z) = \frac{LV(\xi)}{\tau},\ \theta(z) = q(\xi), \tag{3}$$

and we introduce a dimensionless ratio between the length of the channel and the "elastic length"

$$r = \frac{\mu L^2}{k} = (\frac{L}{L_e})^2. \tag{4}$$

After this transformation, the new equations depend only on three key parameters, the anisotropic ratio a_0, r and the activity ζ

$$\begin{aligned}&4(a_0^3-1)q'(\xi)\Big\{2V'(\xi)\sin(2q(\xi))\\ &[(a_0^3-1)\cos(2q(\xi)) - 2a_0\zeta\cos(2q(\xi))]\Big\}\\ &-V''(\xi)\Big\{4(a_0^6-1)\cos(2q(\xi)) - 5a_0^6\\ &+(a_0^3-1)^2\cos(4q(\xi)) + 2a_0^3 - 5\Big\} = 0,\end{aligned} \tag{5a}$$

$$\begin{aligned}&(a_0^3-1)rV'(\xi)\Big\{(a_0^3+1)\cos(2q(\xi))\\ &-a_0^3+1\Big\} + 2a_0^2q'' = 0.\end{aligned} \tag{5b}$$

By defining an operator $F(V,q,\zeta)$, our problem (5a) and (5b) is equivalent to

$$F(V,q,\zeta) = 0. \tag{6}$$

The linearized equations in the neighborhood of the trivial solution $(V,q) = (0,0)$ is

$$8V'' - 8a_0(a_0^3-1)\zeta q' = 0, \tag{7a}$$

$$2(a_0^3-1)rV' + 2a_0^2 q'' = 0. \tag{7b}$$

We call the corresponding linear operator L and its adjoint L*. The kernel of the linear operator is two dimensional when ζ takes the critical value.

$$\zeta_c = \frac{4a_0\pi^2}{(a_0^3-1)^2 r}. \tag{8}$$

The kernel of L is generated by the vectors $\mathbf{u}_1$ and $\mathbf{u}_2$

$$V(\xi) = \alpha(1-\cos(2\pi\xi)) + \beta(\sin(2\pi\xi)), \tag{9a}$$

$$q(\xi) = \frac{r(a_0^3-1)}{2\pi a_0^2}(\alpha\sin(2\pi\xi) + \beta(\cos(2\pi\xi)-1), \tag{9b}$$

$$(V,q) = \alpha\mathbf{u}_1 + \beta\mathbf{u}_2. \tag{9c}$$

The adjoint kernel has the same structure but the amplitudes are rescaled with a ration depending on a_0, r and ζ. Let us call its generating vectors, $\mathbf{u}_{a,1}$ and $\mathbf{u}_{a,2}$. The basis vectors of ker(L) and ker(L*) are orthogonal.

$$\langle\mathbf{u_1},\mathbf{u_2}\rangle = \langle\mathbf{u_{a,1}},\mathbf{u_{a,2}}\rangle = 0. \tag{10}$$

As it can be noticed with the previous results, the linear kernel presents a bifurcation with a two-fold degeneracy. The work of the thesis is to analyze the reasons of this bifurcation and try to formulate the more general results about its existence.

3. Test of the instability robustness

The first step is to test whether the linear bifurcation analysis is robust to the parameter changes. We consider three changes in the model:

- The active tensor, $\mathbf{T}_a$ is no longer $\mathbf{T}_a \propto -\zeta\mathbf{I}$ but it is now taken to be proportional to the shape tensor, $\mathbf{T}_a \propto -\zeta\mathbf{\Psi}$.
- New boundary conditions, the no-slip boundary conditions are changed, we now assume $v_x'(L) = 0$.
- Considering more than one relaxation time, this change implies a larger class of possible viscosity coefficients: $\mathbb{D} = (\mathbf{\Psi}^{-1}\otimes\mathbf{\Psi}^{-1})\mathbb{T}$, where $\mathbb{T}$ contains the different relaxation times [3].

We re-derive the equations (5a)and (5b) with these modifications. Then we perform an equivalent linear analysis. We compare our results with the original case in terms of the form of the equations, the critical value, the dimension of the kernel and the form of its vectors. In the following table we summarize the different results.(see the thesis for the details)

Change	(eq)	ζ_c	dim ker(L)	eigen-vectors
$\mathbf{T}_a \propto \mathbf{\Psi}$	c	r	2	r
Boundary conditions ($v'_x(L) = 0$)	u	r	1	r
More relaxation times	c	u	2	r

(c:changed, u:unchanged, r:rescaled)

These comparisons show that the linear bifurcation analysis is robust to parameter changes. Indeed, the two-fold degeneracy is still present, we only observe a rescaling of the equations, of the critical value and of the amplitudes of the vectors.
However, using the new boundary condition $v'_x(L) = 0$, we lose one of the two modes. We will show that the reason behind this is the breaking of the symmetries in the system.

4. Lyapunov-Schmidt reduction and bifurcation diagram

Because the degeneracy is robust, it is pertinent to look for a complete information about this instability and draw a complete bifurcation diagram. We reduce the problem to finite dimensional in order to obtain the diagram of bifurcations. To this end, we perform a Lyapunov-Schmidt reduction. The method consists in projecting the general equation to the range of the linear operator, range(L). By definition of the adjoint operator, this space is equivalent to the orthogonal complement of the adjoint kernel

$$\text{range(L)} = \ker(\text{L}^*)^\perp. \tag{11}$$

To perform the Lyapunov-Schmidt reduction, we look for a solution of the form

$$\big(V(\xi), q(\xi)\big) = \alpha\mathbf{u_1}(\xi) + \beta\mathbf{u_2}(\xi) + \big(w_v(\xi), w_q(\xi)\big). \tag{12}$$

such that

$$\langle\big(w_v(\xi), w_q(\xi)\big), \mathbf{u_1}\rangle = \langle\big(w_v(\xi), w_q(\xi)\big), \mathbf{u_2}\rangle = 0. \tag{13}$$

In other words, the solution is a linear combination of the linear kernel vectors and a unknown function which is orthogonal to the linear kernel.

We can define the projector to the range of the linear operator as the projector to the orthogonal complement of the adjoint kernel, by definition of the adjoint operator

$$QF(V,q,\zeta) = F(V,q,\zeta) - \frac{\langle F(V,q,\zeta), \mathbf{u_{a,1}}\rangle}{||\mathbf{u_{a,1}}||^2}\,\mathbf{u_{a,1}} - \frac{\langle F(V,q,\zeta), \mathbf{u_{a,2}}\rangle}{||\mathbf{u_{a,2}}||^2}\,\mathbf{u_{a,2}}. \tag{14}$$

Imposing $QF = 0$, we obtain a unique solution $\big(w_v(\xi), w_q(\xi)\big)$ as a function of α, $\mathbf{u_1}(\xi)$, β, $\mathbf{u_2}(\xi)$ and ζ.
Substituting the obtained relation into (6), we find the bifurcation equation by solving $(\mathbf{I} - Q)F = 0$ since the vectors, generating the adjoint kernel, are orthogonal (10), this is equivalent to impose:

$$\langle F(V,q,\zeta), \mathbf{u_{a,1}}\rangle = 0, \quad \langle F(V,q,\zeta), \mathbf{u_{a,2}}\rangle = 0. \tag{15}$$

For simplification in the computations, we replace $\zeta = \zeta_c(1+\lambda)$.
Finally, the bifurcation equations are the following

$$\beta\Big\{(a_0^3-1)^2r^2\Big((13+5a_0^3+6a_0^6)\alpha^2 + (25+a_0^3+14a_0^6)\beta^2\Big) - 16a_0^4\pi^2\lambda\Big\} = 0, \tag{16a}$$

$$\alpha\Big((a_0^3-1)^2r^2(5-3a_0^3+6a_0^6)\alpha^2 + (17-7a_0^3+14a_0^6)\beta^2 - 16a_0^4\pi^2\lambda\Big) = 0. \tag{16b}$$

The solutions of the system composed by (16a) and (16b) are of the form

$$(\alpha,\beta) \in \big\{(0,0),\ (\pm\alpha(\lambda),0),\ (0,\pm\beta(\lambda))\big\}, \tag{17a}$$

$$\alpha(\lambda) = \frac{4a_0^2\pi\sqrt{\lambda}}{r\sqrt{6a_0^{12}-15a_0^9+17a_0^6-13a_0^3+5}}, \tag{17b}$$

$$\beta(\lambda) = \frac{4a_0^2\pi\sqrt{\lambda}}{r\sqrt{14a_0^{12}-27a_0^9+37a_0^6-49a_0^3+25}}. \tag{17c}$$

We obtain the two modes, they exist for all the values of the parameters when $\lambda > 0$. Indeed, the parameters only rescale the amplitudes of the solutions. However, there is no possible mixing of the modes. Indeed, if we plot the contourlines (Figure 2), the only intersection point is at the critical activity, ζ_c ($\lambda = 0$).

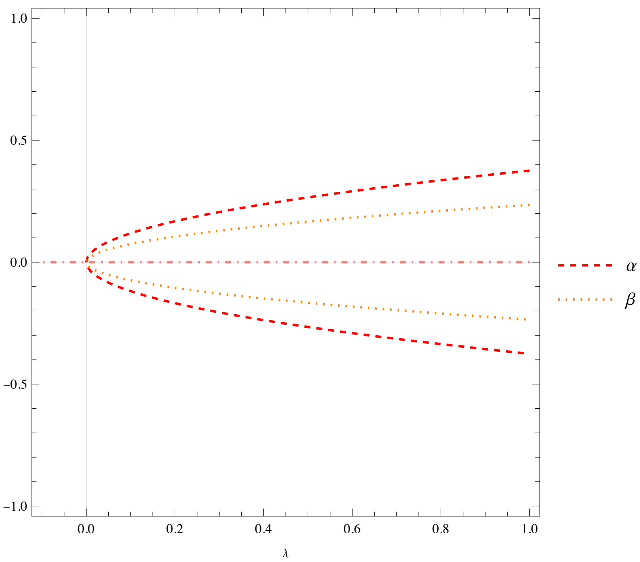

Figure 2: Bifurcation diagram, as given in (16a) and (16b) with $a_0 = 2$ and $r = 1$.

5. Symmetries and generalized branching lemma

We can notice three symmetries of the system.
(i)The nematic symmetry, $\mathbf{n} \mapsto -\mathbf{n}$ does not influence our problem. Our model automatically satisfies by construction the head-tail symmetry of the molecules.
(ii) The symmetry with respect to the $\mathbf{e}_x$ axis, thanks to the homogeneous boundary conditions, the bottom and the top of the channel cannot be distinguished.
(iii) The symmetry with respect to the $\mathbf{e}_z$ axis, thanks to the transversal invariance along the $\mathbf{e}_x$ axis, left and right cannot be distinguished.
In the following table we show the transformation on the dimensionless space variable ξ, the dimensionless variables V and q, the amplitudes, and the corresponding action $\mathbf{T}_g$:

Sym	$\hat{\xi}$	$\hat{V}$	$\hat{q}$	$\hat{\alpha}$	$\hat{\beta}$	$\mathbf{T}_g$
(i)	ξ	V	$q+\pi$	α	β	$\begin{pmatrix}1 & 0\\ 0 & 1\end{pmatrix}$
(ii)	$1-\xi$	V	$-q$	α	$-\beta$	$\begin{pmatrix}1 & 0\\ 0 & -1\end{pmatrix}$
(iii)	ξ	$-V$	$\pi-q$	$-\alpha$	$-\beta$	$\begin{pmatrix}-1 & 0\\ 0 & -1\end{pmatrix}$
(iv)	$1-\xi$	$-V$	$\pi+q$	$-\alpha$	β	$\begin{pmatrix}-1 & 0\\ 0 & 1\end{pmatrix}$

The fourth symmetry is obtained by the composition of the symmetries (ii) and (iii). It can be easily demonstrated that the four symmetries form an abelian group which can be identified as the Klein four-group $K_4 \cong \mathbb{Z}_2 \times \mathbb{Z}_2$.
In addition, it can be checked that (5a) and (5b), (16a) and (16b) are K_4-equivariant. This means for the system defined by (5a) and (5b),

$$\forall \mathbf{T}_g \in K_4,\ \mathbf{T}_g F(V,q,\zeta) = F(\mathbf{T}_g(V,q),\zeta) = 0. \quad (18)$$

A key notion in this analysis is that of fixed-point space, for a subgroup Σ of K_4,

$$\mathrm{Fix}(\Sigma) = \{\mathbf{x} \in \mathbb{V},\ \mathbf{T}_g\mathbf{x} = \mathbf{x},\ \forall\ \mathbf{T}_g \in \Sigma\}. \quad (19)$$

And the equivalent notion of a stabilizer subgroup for a vector $\mathbf{x} \in V$.

$$\mathrm{Stab}(\mathbf{x}) = \big\{\mathbf{T}_g \in K_4,\ \mathbf{T}_g\mathbf{x} = \mathbf{x}\big\}. \quad (20)$$

Because $F(\cdot,\zeta)$ is K_4-equivariant, it maps $\mathrm{Fix}(\Sigma)$ to $\mathrm{Fix}(\Sigma)$, and the bifurcation analysis can be restricted to $\mathrm{Fix}(\Sigma)$ space.
For our problem, we have the following fixed-point spaces in the plane (α,β):
(i)All points are fixed by $\Sigma_0 = \{\mathbf{T}_{(i)}\} = \{\mathbf{I}\}$. So $\mathrm{Fix}(\Sigma_0) = \mathrm{Span}\big\{\mathbf{e}_1,\mathbf{e}_2\big\} \cong \mathbb{R}^2$.
(ii)All points of the form $(\alpha,\beta) = (1,0)$ are fixed by $\Sigma_1 = \{\mathbf{I},\mathbf{T}_{(ii)}\}$. So $\mathrm{Stab}\big((1,0)\big) = \Sigma_1$ and$\mathrm{Fix}(\Sigma_1) = \mathrm{Span}\big\{\mathbf{e}_1\big\} \cong \mathbb{R}$.
(iii)No point is fixed by $\Sigma_2 = \{\mathbf{I},\mathbf{T}_{(iii)}\}$. So $\mathrm{Fix}(\Sigma_2) = \big\{\mathbf{0}\big\}$.
(iv)All points of the form $(\alpha,\beta) = (0,1)$ is fixed by $\Sigma_3 = \{\mathbf{I},\mathbf{T}_{(iv)}\}$. So $\mathrm{Stab}\big((0,1)\big) = \Sigma_3$ and $\mathrm{Fix}(\Sigma_3) = \mathrm{Span}\big\{\mathbf{e}_2\big\} \cong \mathbb{R}$.
(v)Only the origin is fixed by K_4. We have only two proper subgroups of K_4 of dimension 1, Σ_1 and Σ_3. We can now use the following theorem[1].

Theorem 5.1 (Generalized equivariant branching lemma). *Let Γ be a finite group or a compact Lie group acting on a real vector space, $\mathbb{V}$, with $\mathrm{Fix}(\Gamma) = \{\mathbf{0}\}$.*
Let

$$F(\mathbf{U},\lambda) = 0, \quad (21)$$

be a Γ-equivariant bifurcation problem with $DF|_{(\mathbf{0},\lambda_c)}\mathbf{W} = 0$ and $DF_\lambda|_{(\mathbf{0},\lambda_c)}\mathbf{W} \neq 0$ for nonzero $\mathbf{W} \in \mathrm{Fix}(\Sigma)$, where Σ is a stabilizer subgroup of Γ. Then, if Σ satisfies:

$$\dim(\mathrm{Fix}(\Sigma)) = 1, \quad (22)$$

there is a smooth solution branch $\mathbf{U} = s\mathbf{W},\ \lambda = \lambda(s)$ to $F(\mathbf{U},\lambda) = 0$.

Since we only have two one-dimensional fixed-point subspaces, our model has two independent branches and this is a general results for any system which has the K_4-symmetries.

6. Conclusions

In this thesis, we studied the spontaneous flows arising in an alternative model for active nematics in the existence of a spontaneous flow. As it has been noticed in [4], the system has a two-fold degeneracy. We tested the robustness of this instability and showed that it is robust to material changes but not to new boundary condition which break the $\mathbb{Z}_2 \times \mathbb{Z}_2$ symmetry
Applying the Lyapunov-Schmidt reduction to make the study bifurcation, a finite-dimensional problem, we were able to draw the bifurcation diagram. This allowed us to see that the existence of the two modes does not depend on the material parameters which only rescale their amplitudes. In addition, we saw that no mixing of the mode is possible in a stationary state.
Finally, with the generalized equivariant branching lemma we explained the presence of the two-fold degeneracy by the fact that the system is equivariant under the transformations of the Klein four-group. When the boundary conditions are changed, the symmetries are broken, leading to the lost of the degeneracy.

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