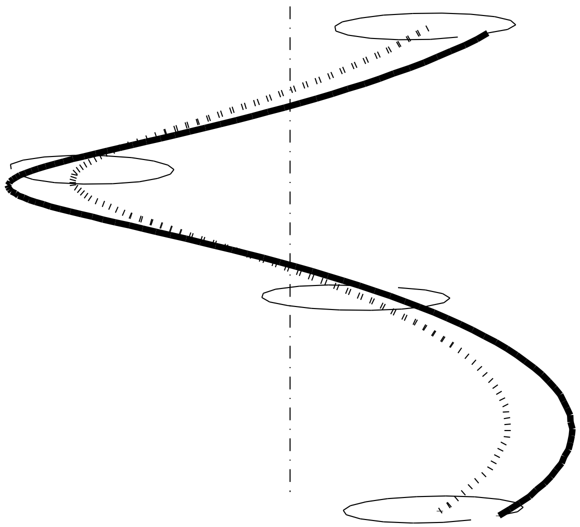
Twisted scroll waves: instabilities and a reduced model.

Blas ECHEBARRIA (Politècnica), Hervé HENRY (Polytechnique)

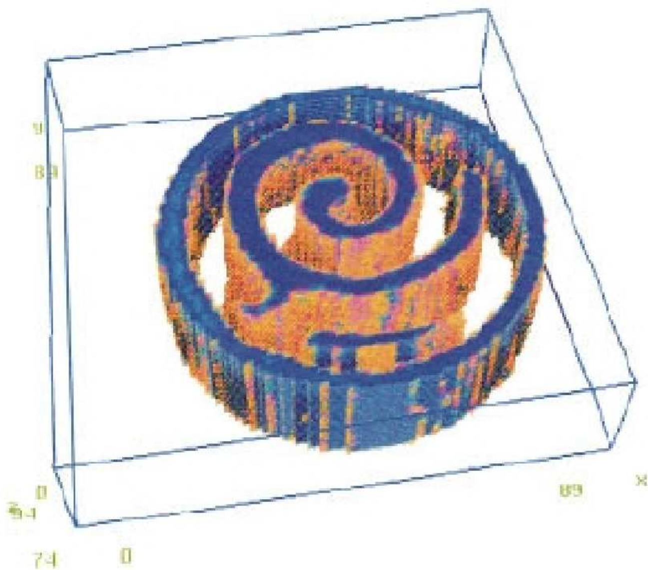
Vincent Hakim

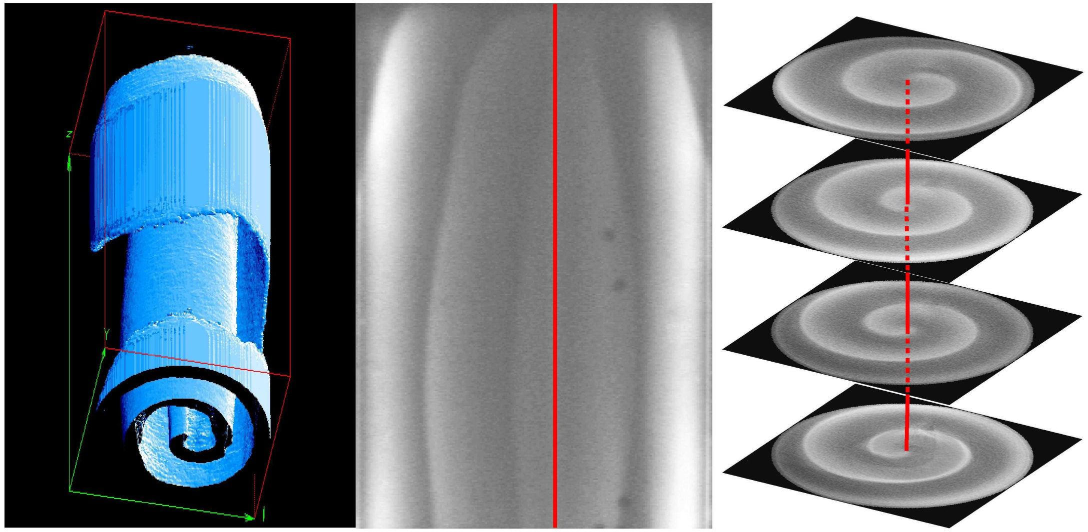
Laboratoire de Physique Statistique, Ecole Normale Supérieure, Paris



KITP, july 06

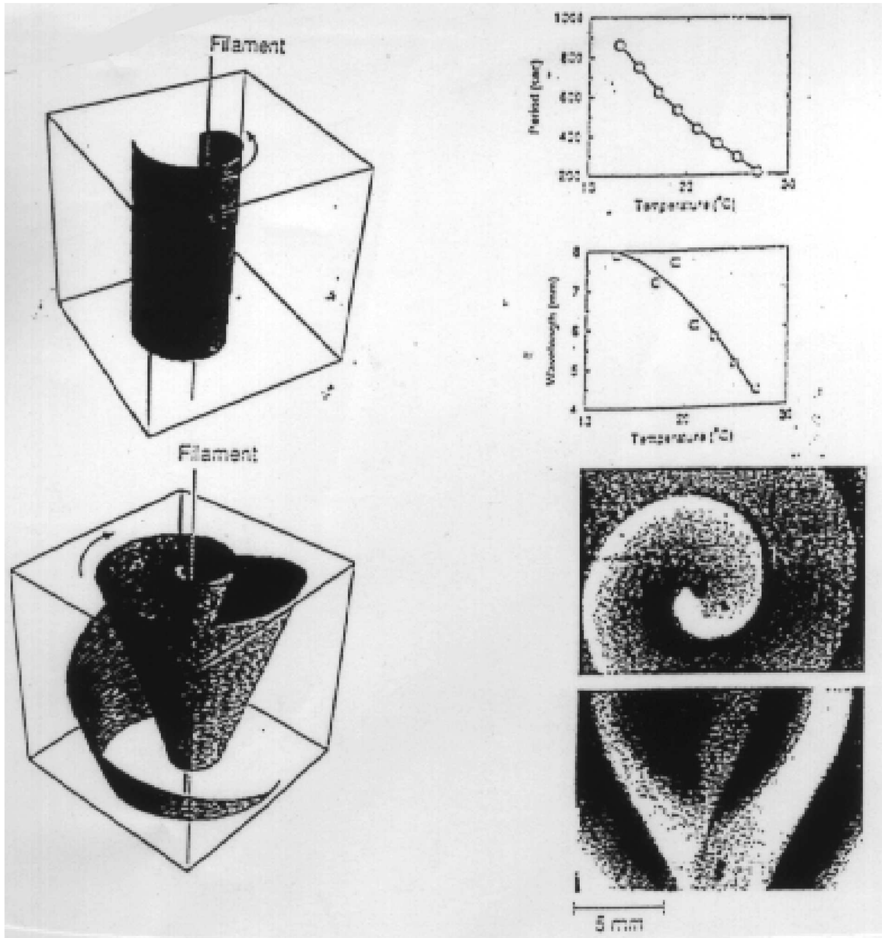
Winfree et al., Chaos **6**, 617 (1996);





U. Storb et al, PCCP **5**, 2344 (2003).

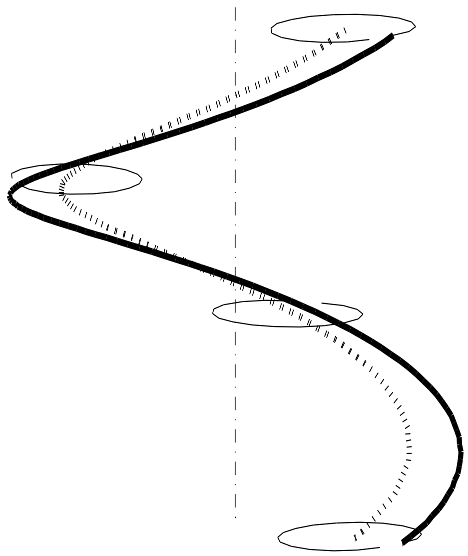
A new degree of freedom in 3D : the **twist**

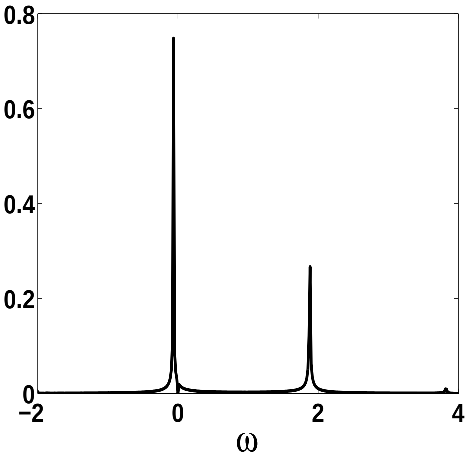


A. Pertsov et al Nature **345** 419 (1990); J. Phys.Chem. **100** 1975 (1996).

A twist induced instability : sproing

Henze, Lugosi and Winfree (1990).





- Helical deformation of the mean filament.
- Slow rotation of the center of rotation in a given plane.

A theoretical puzzle

Keener (1988): Equations for the slow motion of the core of a weakly curved (κ) and weakly twisted scroll wave in the normal plane $(\vec{\mathbf{N}}, \vec{\mathbf{B}})$, using averaging techniques,

$$\vec{\mathbf{R}}_{\mathbf{t}} \cdot \vec{\mathbf{N}} = a_1 \kappa + \cdots ,$$

$$\vec{\mathbf{R}}_{\mathbf{t}} \cdot \vec{\mathbf{B}} = a_2 \kappa + \cdots .$$

Biktashev, Holden, Zhang (1994): all the other **coefficients coupling the core motion to the twist vanish** by symmetry.

Different instabilities in different parameter regimes

- Extension of spiral instabilities:

• **3D induced meander** (Aranson et Mitkov)

...

- Instabilities specific to scrolls:

• **Negative line tension** (Panfilov and Rudenko, Brazhnik et *al*, Biktashev et *al*,...)

• **Twist-induced "sproing"** (Winfree et al.)

The **stability spectrum** of a scroll

helps to obtain a clearer view of the different instabilities

(H. Henry + V H, PRL 2000, PRE 2002).

• The excitable medium model: **two** coupled equations (FitzHugh,1961; Nagumo et al.,1962),

$$\begin{aligned} \partial_t u &= \nabla^2 u + f(u,v)/\epsilon \\ \partial_t v &= g(u,v) \end{aligned}$$

◇ Specific choice here (Barkley, 1991):

$$f(u,v) = u(1-u)[u-(v+b)/a], \;\; g(u,v) = u - v$$

The linear stability analysis

• Steadily rotating uniformly twisted straight scrolls (determined by a Newton method):

$$(u_0(r, \theta - \omega t - \tau_w z), v_0(r, \theta - \omega t - \tau_w z) \tag{1}$$

• **Computation of the linear stability spectrum**

Translation invariance along the z-direction

$\Rightarrow$ **the eigenvalues appear in bands parameterized by the wavenumber k_z along the z-direction**

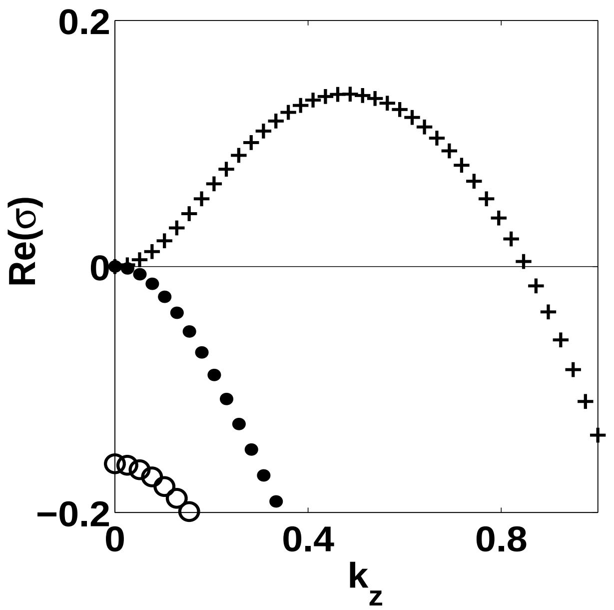
Outcome of the linear stability computation

- **Negative line tension instability** $\Rightarrow$ **small** k (**long-wavelength**) **instability of the translation bands**; directly **linked to spiral drift direction** in an electric field.

- **Twist-induced "sproing"** $\Rightarrow$ **twist-induced finite** k **instability of the translation bands.**

"Negative line tension instability" of large core non-meandering spiral

$a = .44, \ b = .01$ and $\epsilon = .025$

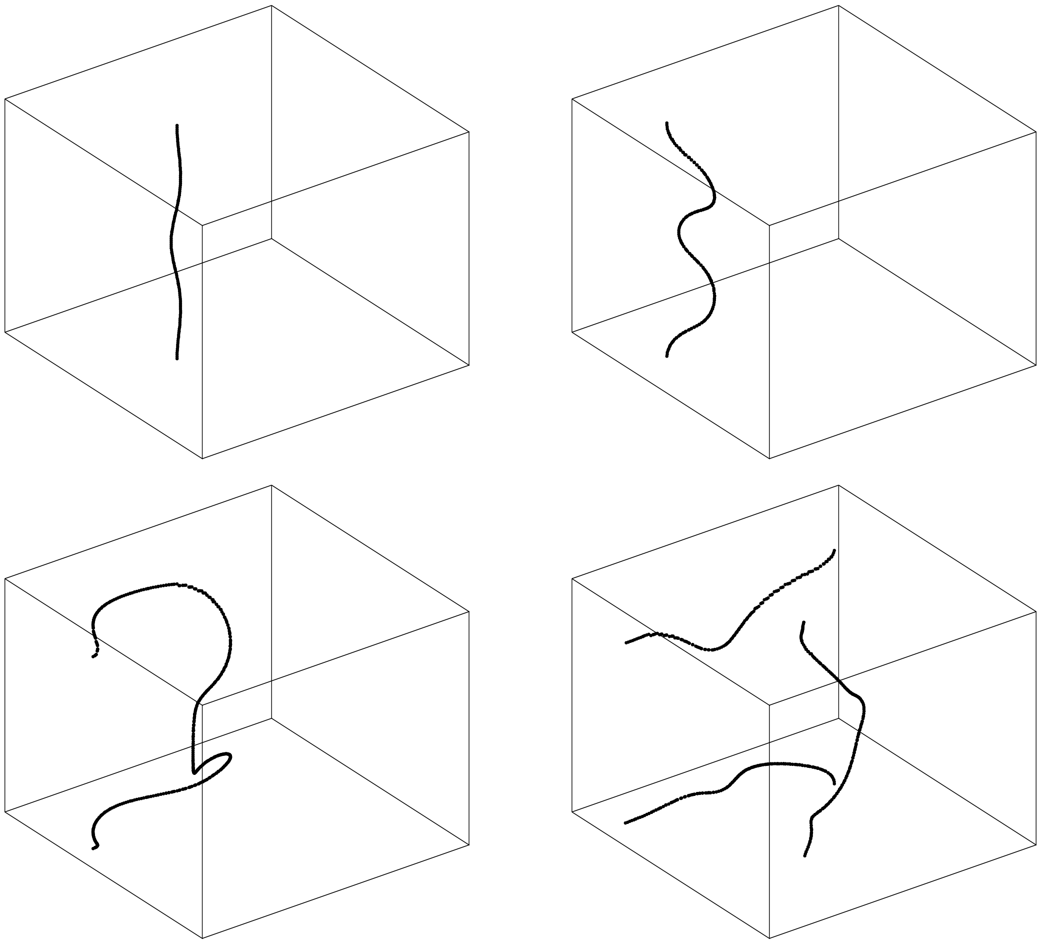


Eigenvalue bands: **(+) translation, the real part of** $\sigma(k_z)$ **is positive for small** k_z**: instability**

((•) rotation, (o) meander)

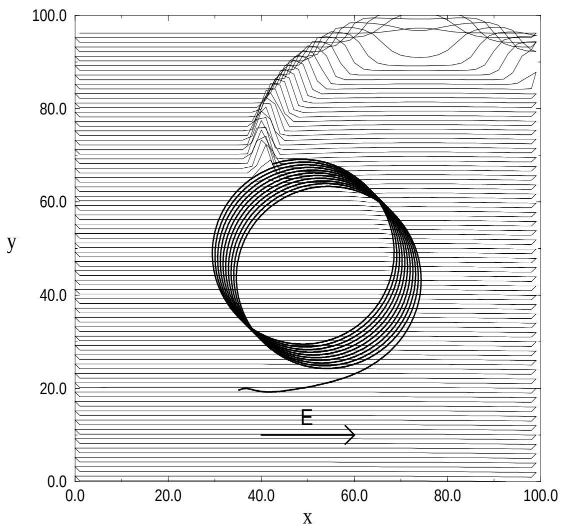
Non-linear evolution: no restabilization

$a = .44,\ b = .01$ and $\epsilon = .025$



The instability existence is determined by the direction of **spiral drift** in an external field (A Karma +VH, PRE 1999; also H. Henry, PRE 2004).

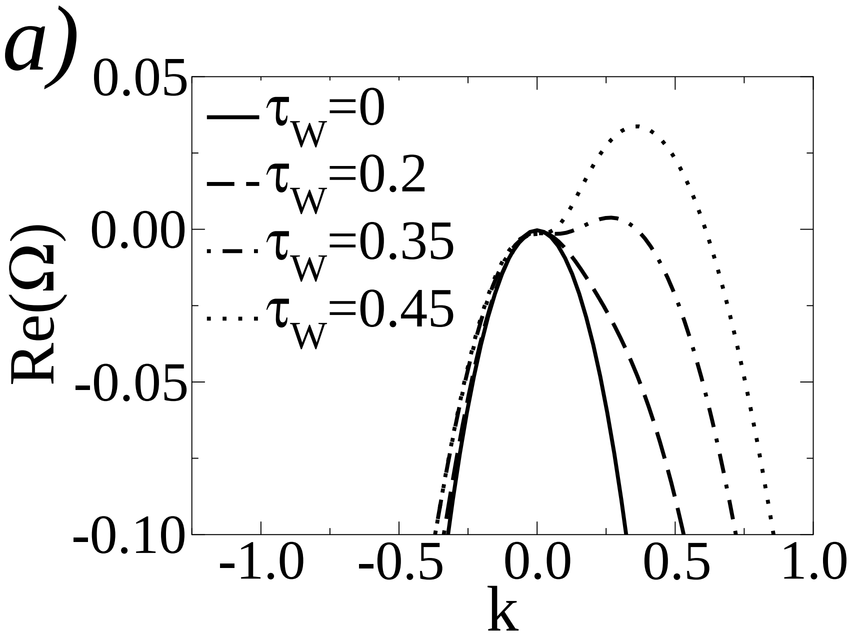
$$\sigma_{\pm}(k_z) = \pm i\omega_1 + (-\alpha_{\parallel} \pm i\alpha_{\perp})\, k_z^2 + O(k_z^4)$$



$$\partial_t u = \nabla^2 u + f(u,v)/\epsilon - E.\nabla u, \quad v_{\rm drift} = \alpha_{\parallel} E + \alpha_{\perp} \omega_1 \times E$$

Twist-induced instability of the translation bands

$(a = .8,\ b = .01,\ \epsilon = .025)$



- Instability above a threshold twist.
- The translation modes ($Re(\sigma(k_z)) = 0$) remain local extrema of $Re(\sigma(k_z))$ (consequence of 3D rotation invariance);
- The unstable modes are a finite k_z away from the translation modes.

Dynamics of twisted scrolls: difficulties for theoretical descriptions

• The instability appears above a finite threshold twist and a finite k_z away from the translation modes : it is invisible with small twist approaches (Keener; Biktashev et al).

• the twist-induced deformation of the translation modes can be analytically captured in the large core regime but untwisted scrolls are already unstable in this regime (negative line tension).

A ribbon model of twisted scroll waves

(a phenomenological extension of Keener's approach).

B. Echebarria, H. Henry and VH, PRL (2006).

The scroll is reduced to

- the line of rotation centers $\vec{\mathbf{R}}(\sigma, t)$ with tangents $\vec{\mathbf{T}}(\sigma, t)$
- the ribbon vectors in the direction of the spiral tip $\vec{\mathbf{p}}(\sigma, \mathbf{t})$

$$\text{with } \vec{\mathbf{p}} \cdot \vec{\mathbf{p}} = 1, \vec{\mathbf{T}} \cdot \vec{\mathbf{p}} = 0$$

An important quantity: the local **twist**:

$$\tau_w = (\vec{\mathbf{p}} \times \frac{\partial \vec{\mathbf{p}}}{\partial s}) \cdot \vec{\mathbf{T}}, \quad (s \text{ curvilinear abscissa}).$$

Dynamics of the mean filament

The filament velocity in the normal plane is written as a gradient expansion

$$[\vec{\mathbf{R}}_t]_\perp \quad = \quad a_1\vec{\mathbf{R}}_{ss} + a_2\vec{\mathbf{T}}\times\vec{\mathbf{R}}_{ss} + \tau_w\Big\{-d_2[\vec{\mathbf{R}}_{\mathbf{sss}}]_\perp + d_1\vec{\mathbf{T}}\times\vec{\mathbf{R}}_{sss}\Big\}$$
$$-b_1[\vec{\mathbf{R}}_{\mathbf{ssss}}]_\perp - b_2\vec{\mathbf{T}}\times\vec{\mathbf{R}}_{ssss} + \cdots$$

$$(\text{Notation:}[\vec{\mathbf{R}}_t]_\perp \equiv \vec{\mathbf{R}}_t - (\vec{\mathbf{R}}_t)\cdot\vec{\mathbf{T}})\vec{\mathbf{T}})$$

First two terms: motion induced by curvature (≡ spiral drift).

Other terms: beyond lowest order averaged equations (Keener), involve the coupling of filament motion with **twist**.

Kinematics of twist evolution

The twist characterizes the spatial rotation of $\vec{\mathbf{p}}(\sigma, t)$ around $\vec{\mathbf{T}}(\sigma, t)$. A deformation of the center line induces kinematic changes in the twist .

Global conservation

For a closed ribbon, the linking number L between the center line and the ribbon edge is conserved.

$$\mathbf{L} = \mathbf{Wr} + \int ds\, \tau_{\mathbf{w}}$$

The "writhe" **Wr** only depends on $\vec{\mathbf{R}}(\sigma, t)$. Well-studied in DNA context (White, Fuller,...))

Here, the **local form** is more useful (Klapper and Tabor,...).

Kinematics of twist evolution

The **local** twist-writhe conversion (Klapper and Tabor,...):

- **Spatial** evolution of $\vec{\mathbf{p}}(\sigma, t)$ (along the filament):

$$\frac{\partial \vec{\mathbf{p}}}{\partial \sigma} = \tau_w \frac{\partial s}{\partial \sigma} \vec{\mathbf{T}} \times \vec{\mathbf{p}} - \frac{\partial \vec{\mathbf{T}}}{\partial \sigma} \cdot \vec{\mathbf{p}}\ \vec{\mathbf{T}}$$

- **Time** evolution of $\vec{\mathbf{p}}(\sigma, t)$:

$$\frac{\partial \vec{\mathbf{p}}}{\partial t} = \alpha \vec{\mathbf{T}} \times \vec{\mathbf{p}} - \frac{\partial \vec{\mathbf{T}}}{\partial t} \cdot \vec{\mathbf{p}}\ \vec{\mathbf{T}}$$

- Comparison of cross-derivatives $\Rightarrow$ **compatibility condition**:

$$\frac{\partial}{\partial t}(\tau_w \frac{\partial s}{\partial \sigma}) = \frac{\partial \alpha}{\partial \sigma} + (\frac{\partial \vec{\mathbf{T}}}{\partial \sigma} \times \frac{\partial \vec{\mathbf{T}}}{\partial t}) \cdot \vec{\mathbf{T}}$$

A simple illustration of the kinematics

An **helical deformation** of a straight twisted filament with periodic boundary conditions. Center line : $\vec{\mathbf{R}} = (R(t)\cos(\tau z), R(t)\sin(\tau z), z)$

Local twist $\tau_w(t)$:

$$\frac{\partial}{\partial t}(\tau_w \frac{\partial s}{\partial \sigma}) = \frac{\partial \alpha}{\partial \sigma} + (\frac{\partial \vec{\mathbf{T}}}{\partial \sigma} \times \frac{\partial \vec{\mathbf{T}}}{\partial t}) \cdot \vec{\mathbf{T}} \Rightarrow$$

$$\frac{d}{dt}[\tau_w \sqrt{1+(R\tau)^2}] = -\frac{R\tau^3}{(1+(R\tau)^2)^{3/2}} \frac{dR}{dt}$$

The final twist τ_w is determined by the initial twist $\tau_w^{(0)}$ and by the geometric parameters of the final deformation

$$\tau_w = \frac{\tau_w^{(0)}}{\sqrt{1+(R\tau)^2}} - \frac{\tau}{\sqrt{1+(R\tau)^2}}[1 - \frac{1}{\sqrt{1+(R\tau)^2}}]$$

The initial twist is **decreased** both by the **length increase** and the **writhe** of the helical deformation.

Dynamics of twist evolution

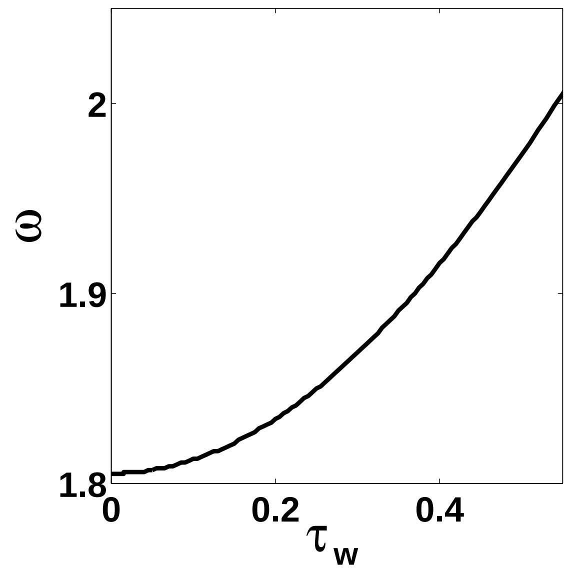
$$\frac{\partial}{\partial t}(\tau_w \frac{\partial s}{\partial \sigma}) = \frac{\partial \alpha}{\partial \sigma} + (\frac{\partial \vec{\mathbf{T}}}{\partial \sigma} \times \frac{\partial \vec{\mathbf{T}}}{\partial t}) \cdot \vec{\mathbf{T}}$$

The rotation velocity α of $\vec{\mathbf{p}}$ around $\vec{\mathbf{T}}$ entirely characterizes the twist dynamics. When

$$\alpha = \omega_1 + c\,\tau_w^2 + D\partial_s \tau_w + (\vec{\mathbf{T}} \cdot \partial_t \vec{\mathbf{R}})\tau_w$$

the twist dynamics is identical to that given by Keener's phase equation. Two effects : rotation velocity increases with τ_w^2 and with the gradient of twist. The coefficients c, D are given as scalar products with the adjoint rotation mode (Keener) and have been computed as a by-product of the linear stability analysis.

Increase of scroll frequency with twist



$$(a = 0.8,\ b = 0.01,\ \epsilon = 0.025)$$

First-order perturbation theory:

$$\omega_1(\tau_w) = \omega_1(0) - \tau_w^2 \frac{\langle \tilde{u}_\phi, \partial_{\phi\phi} u_0 \rangle}{\langle \tilde{u}_\phi, \partial_\phi u_0 \rangle + \langle \tilde{v}_\phi, \partial_\phi v_0 \rangle} + O(\tau_w^4)$$

(Full agreement with numerics : $\omega_1(\tau_w) = \omega_1(\tau_w = 0) + 0.72\tau_w^2$)

Sproing of a twisted scroll

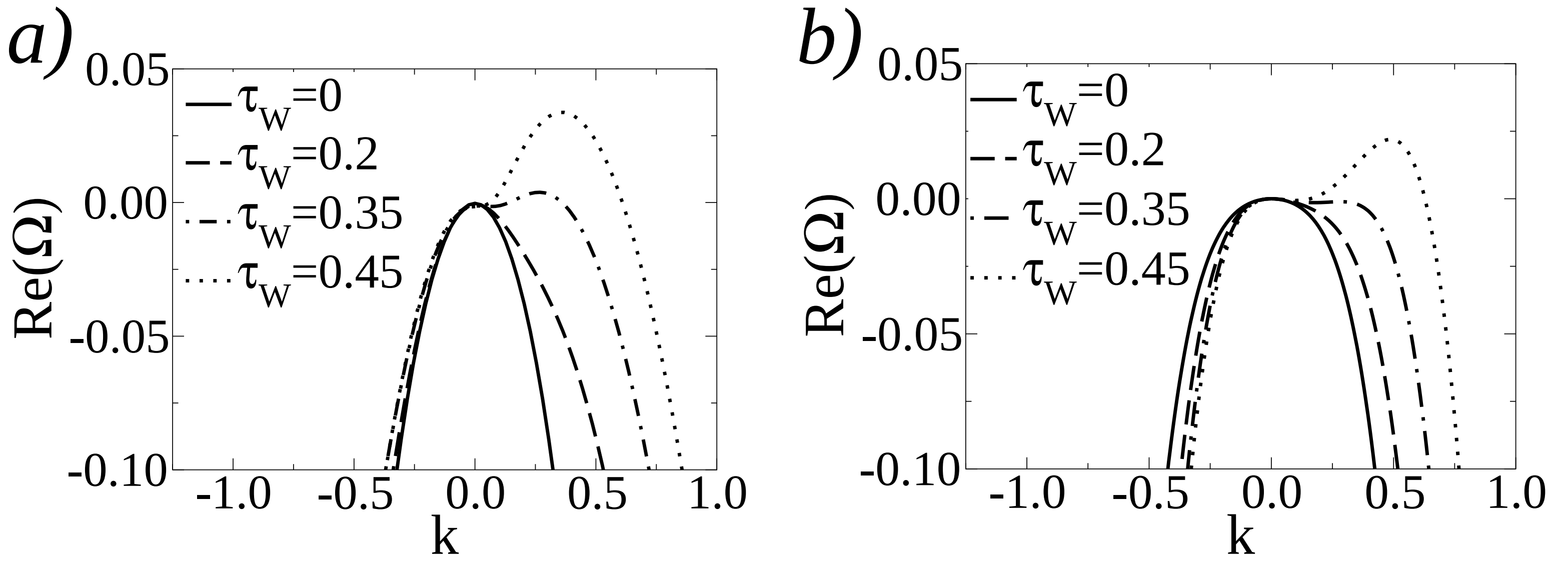
Linear stability of a twisted straight ribbon:

$$W_t = aW_{zz} + id\tau_w W_{zzz} - bW_{zzzz}, \; W = x + iy$$

and the dispersion relation ($W(t,z) = A\exp(\sigma t + ikz)$):

$$\sigma = -ak^2 + d\tau_w k^3 - bk^4$$

$a_1, b_1 > 0$, stable untwisted filament.
Threshold twist : $\tau_w^{(c)} = 2\sqrt{a_1 b_1 / d_1^2}$



Non linear evolution of a helix of pitch k:

$$R_t = d_1 k^3 [\tau_w - \tau_w^{(c)}(k)] R$$

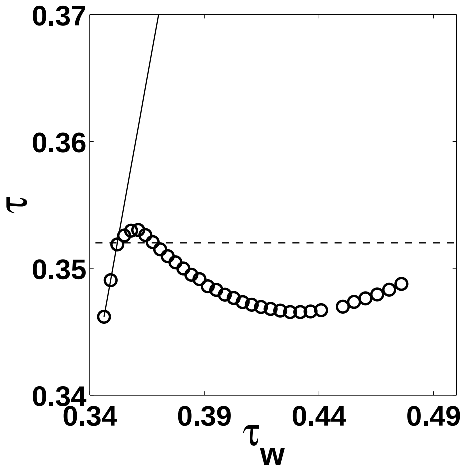
the twist decreases as the radius increases:

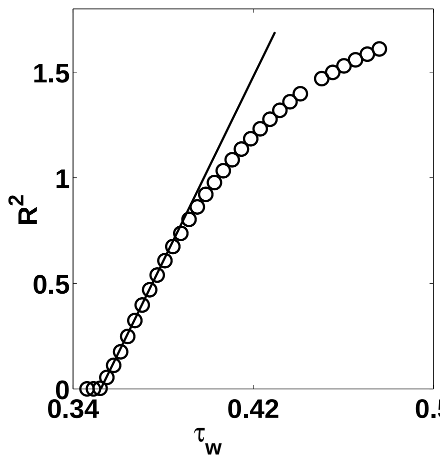
$$\frac{d}{dt}\tau_w = Re[\overline{W}_{zz}(\tau_w - i\partial_s)W_t)] \Rightarrow \tau_w(t) = \tau_w^{(0)} - \frac{1}{2}(\tau_w^{(0)} + k)k^2 R^2$$

Supercritical Hopf bifurcation;

$$R_t = d_1 k^3 \left\{ [\tau_w - \tau_w^{(c)}(k)] R - \frac{1}{2}(\tau_w^{(0)} + k) k^2 R^3 \right\}$$

R-D equations:





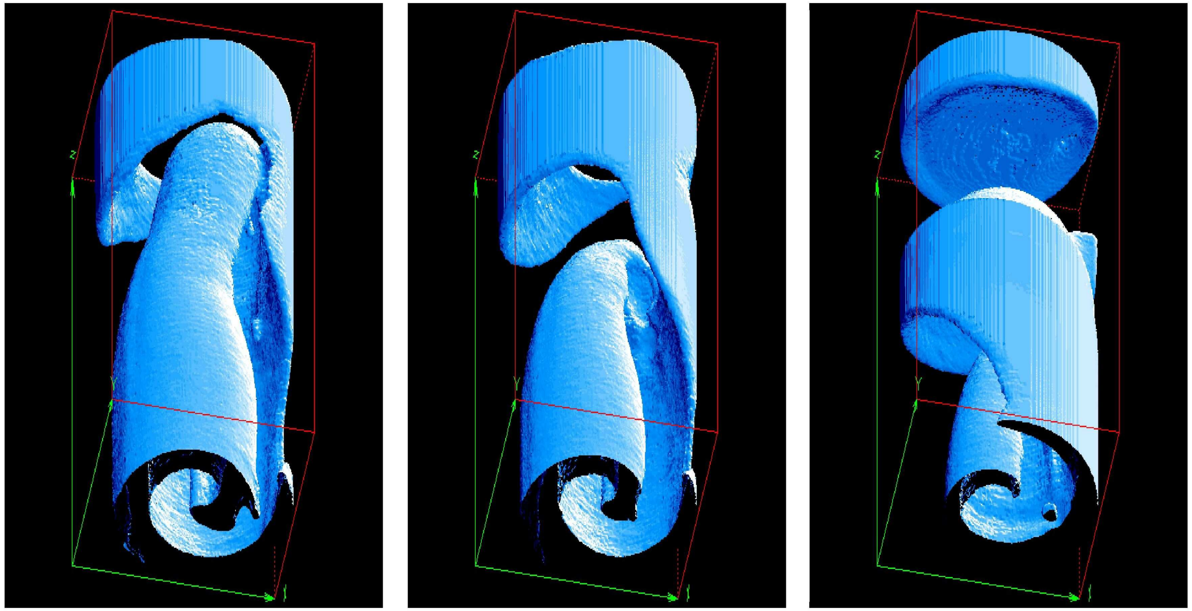
Conclusions (I)

• The ribbon model (a phenomenological extension of Keener's approach) helps to understand sproing and appears to describe well some of the essential features of twisted scroll wave dynamics.

• Is it also useful in more complicated cases? (twist has to be generated in some way for open scrolls...)

$\Rightarrow$ the case of **an excitability gradient**.

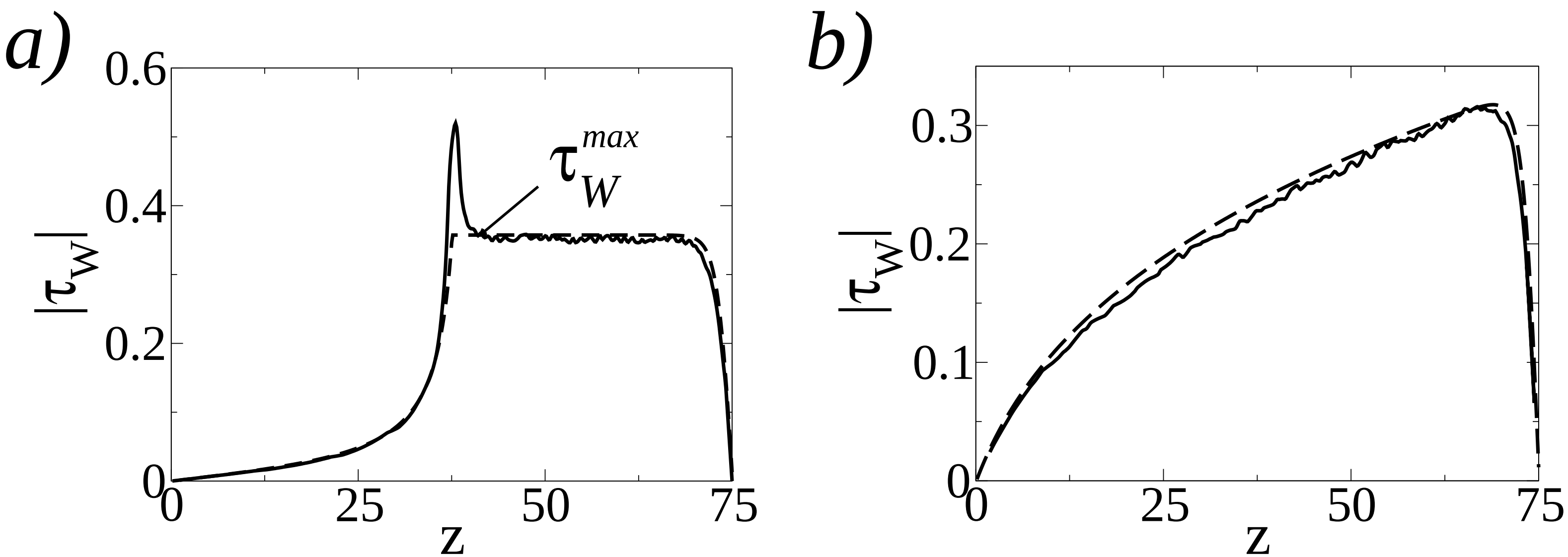
U. Storb, C. R. Neto, M. Bär and S. C. Müller, PCCP **5**, 2344 (2003).



Oxygen gradient leads to a gradient of excitability. Origin of the instability?

Twist distribution in an excitability gradient

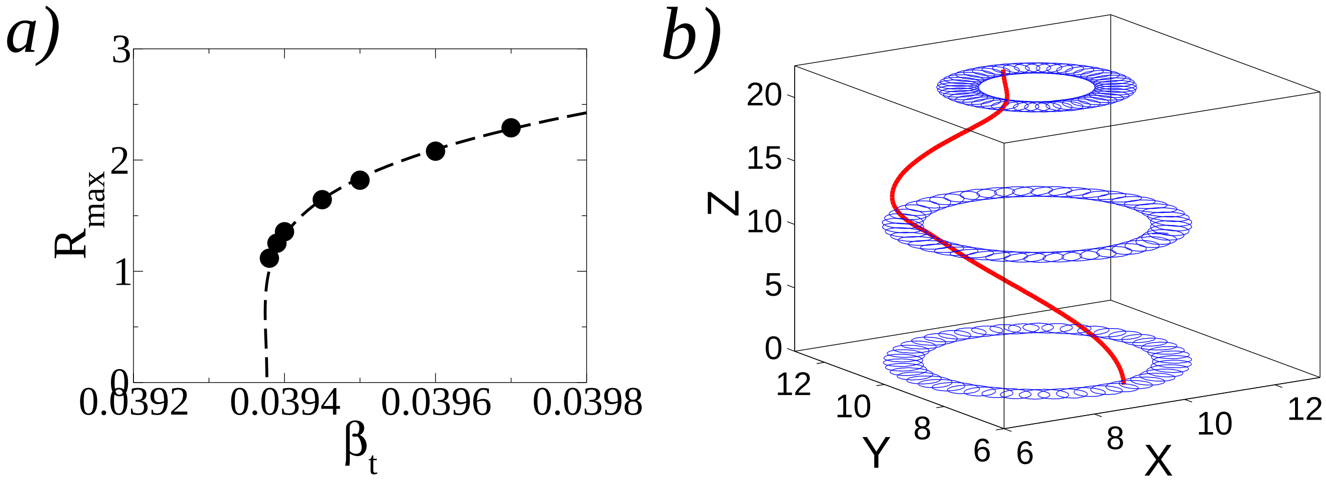
$$\partial_t \tau_w = \partial_s (D \partial_s \tau_w) + \partial_s (c\tau_w^2) + \partial_s \omega_0$$

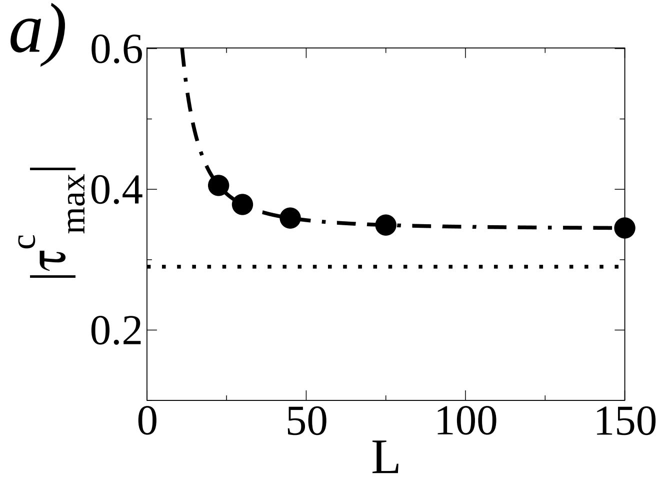


Excitability step

Linear gradient

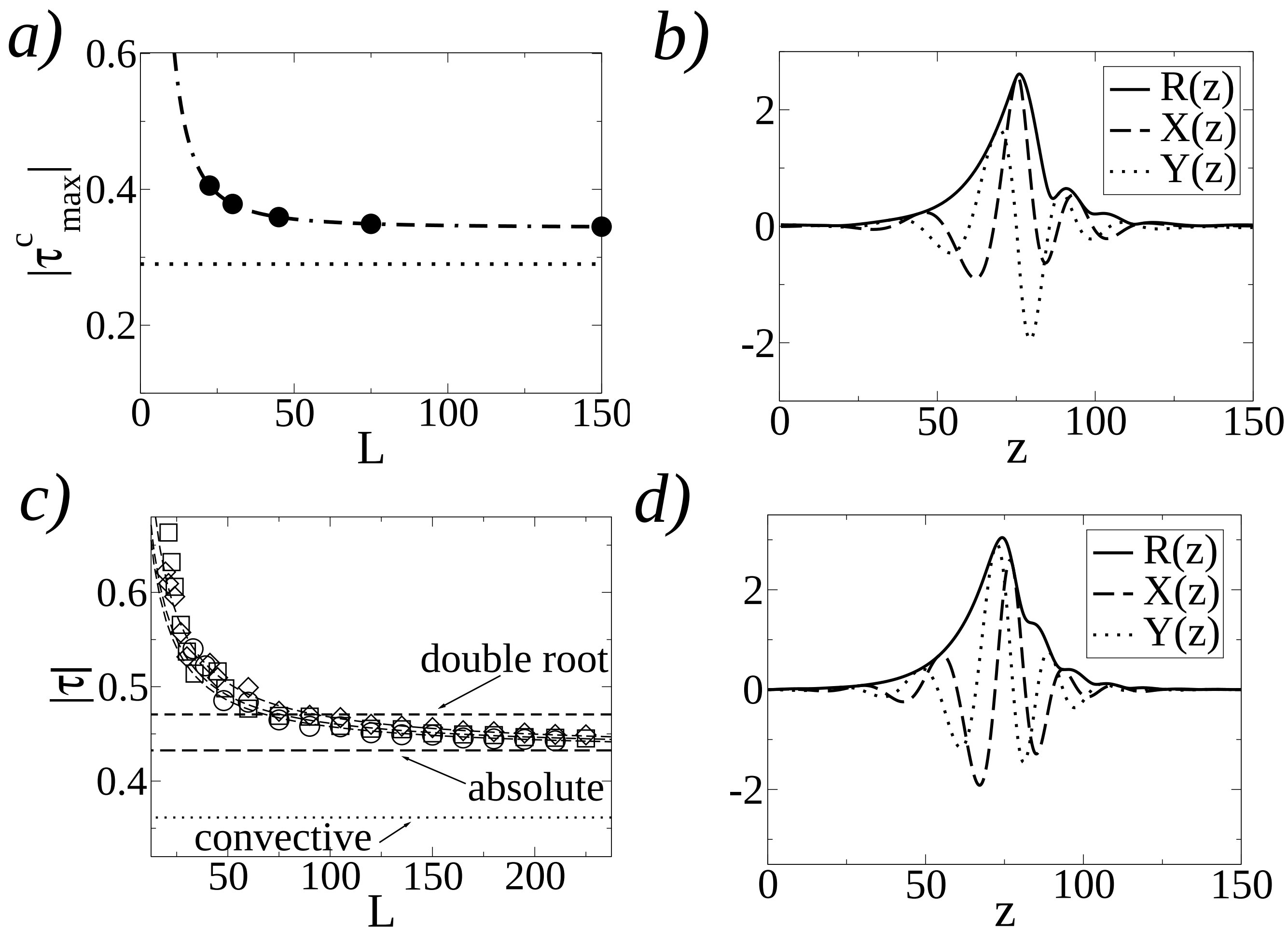
Instability for a large enough excitability step





The critical twist does **not** correspond to the previously computed sproing threshold.

RD vs. ribbon model



Very similar phenomenon in the ribbon model: different thresholds.

Linear stability: different spectra

Convective vs. absolute instability.

Simpler linear problem:

$$W_t = aW_{zz} + id\tau_w W_{zzz} - bW_{zzzz}$$

• Fourier: $\sigma = -ak^2 + dk^3 - bk^4$

$\sigma = aq^2 + idq^3 - bq^4 \Rightarrow 4$ roots $Re(q_1) \geq Re(q_2) \geq Re(q_3) \geq Re(q_4)$.

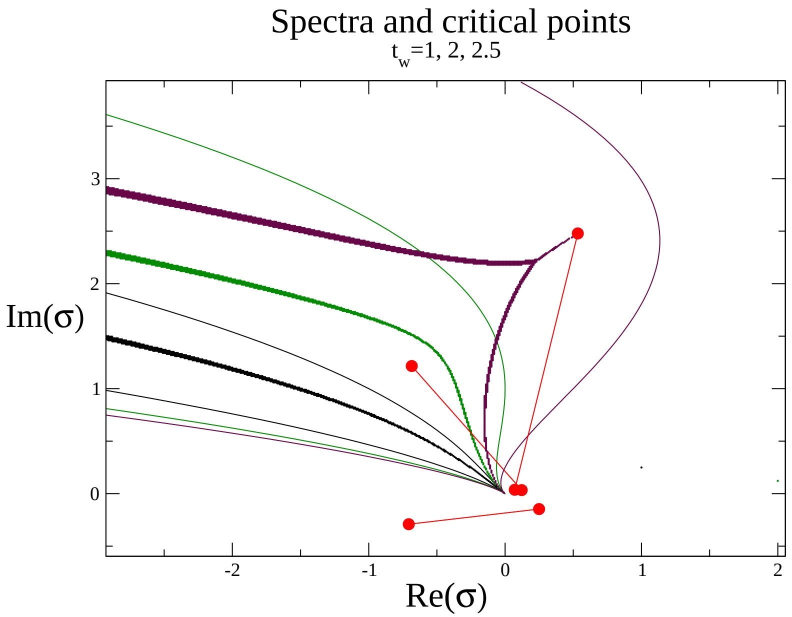
For a large domain with $W = W_z$ at $z = 0, L$,

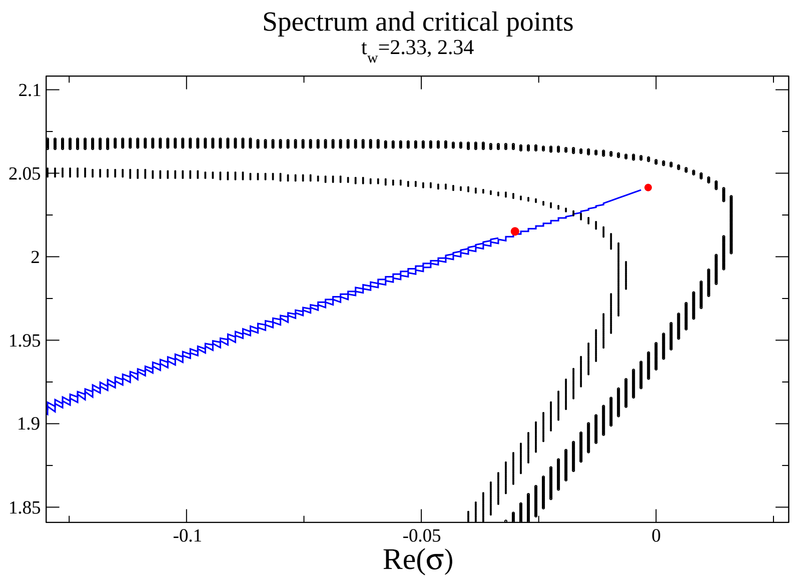
• Spectrum: σ such that $Re(q_2) = Re(q_3)$. (Kulikovskii, 1966).

• Critical points $d\sigma/dq = 0$ belong to a branch $Re(q_i) = Re(q_j)$ but not necessarily the right one.

Different spectra

- Fourier: $\sigma = -ak^2 - idk^3 - bk^4$
- Spectrum: σ such that $Re(q_2) = Re(q_3)$. (Kulikovskii, 1966).
- Critical points $d\sigma/dq = 0$





Conclusions (II)

- The reduced model seems helpful to study more complicated phenomena.
- Sproing (+ collision with the boundaries) appears to explain the instability seen in BZ reaction with an excitability gradient.
- The results highlight the influence of boundary conditions in non-potential problems even for large domains.