Log-rolling and kayaking: periodic dynamics of a nematic liquid crystal in a shear flow

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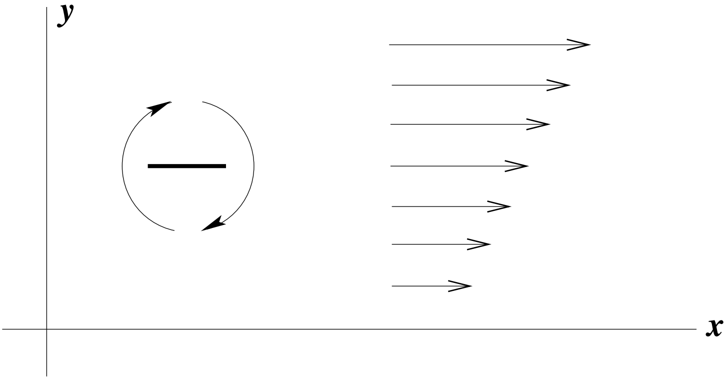
It is observed that *polymeric nematics* (large, long inflexible molecules) can exhibit prolonged unsteady response to steady simple shear flow (low shear rates).

Kiss, Gabor, and Roger S. Porter: Rheology of concentrated solutions of helical polypeptides. *J. Polymer Science: Polymer Physics Edition* 18.2 (1980): 361–388.

Tan, Zhanjie, and Guy C. Berry: Studies on the texture of nematic solutions of rodlike polymers. 3. Rheo-optical and rheological behavior in shear. *Journal of Rheology* **47** (2003): 73–104.

- **Liquid crystal** molecules like to align with each other . . .

Two dimensional shear flow



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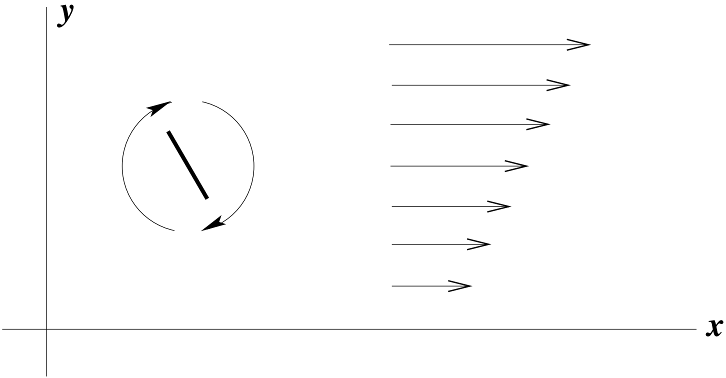

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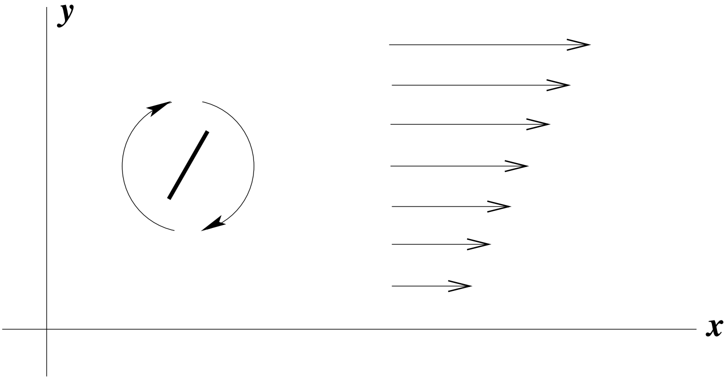

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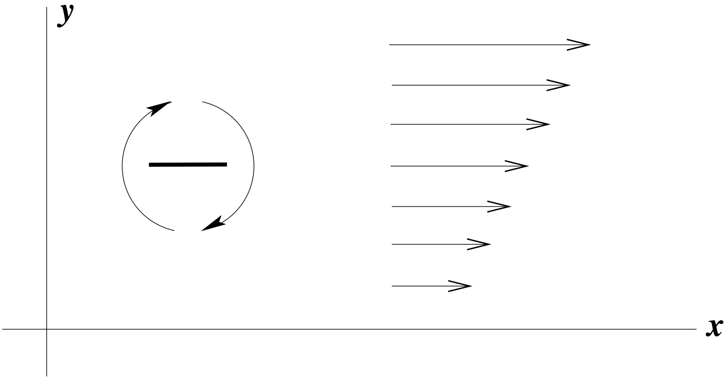

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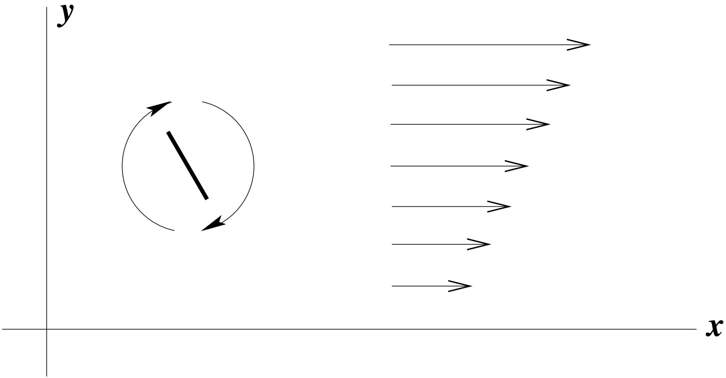

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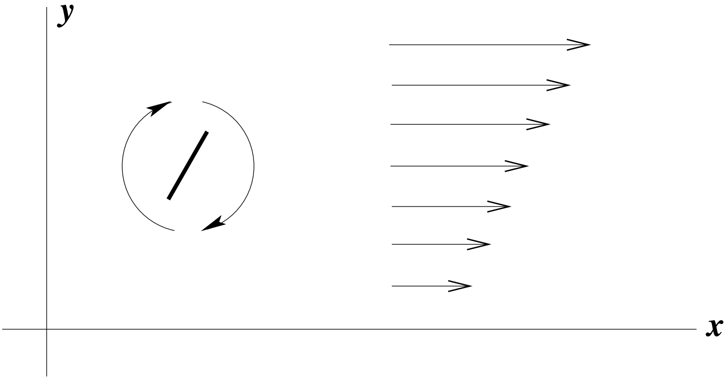

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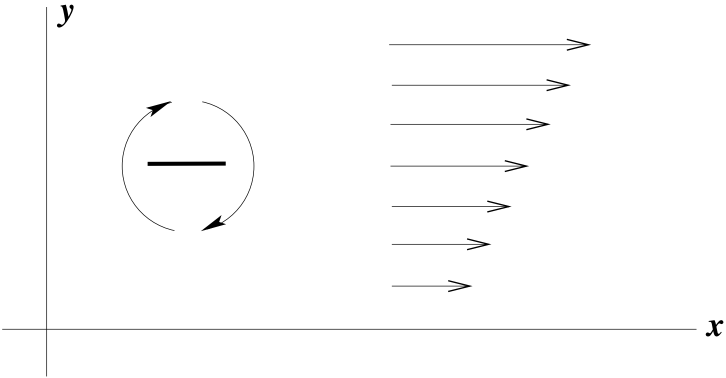

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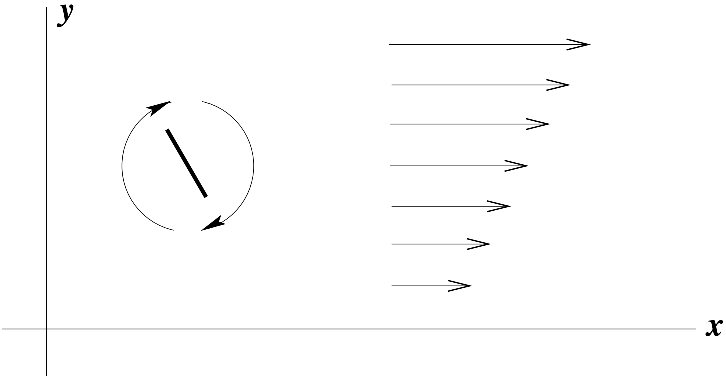

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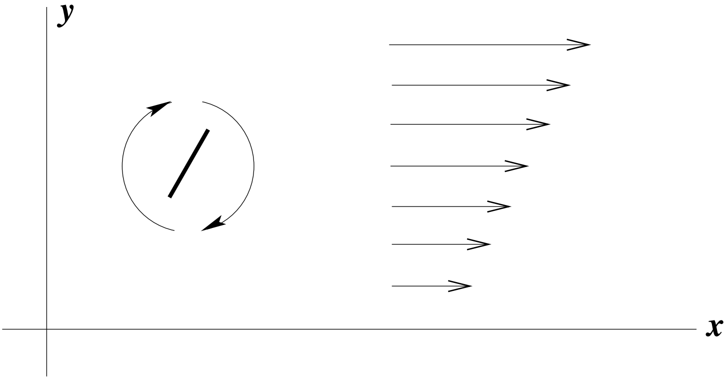

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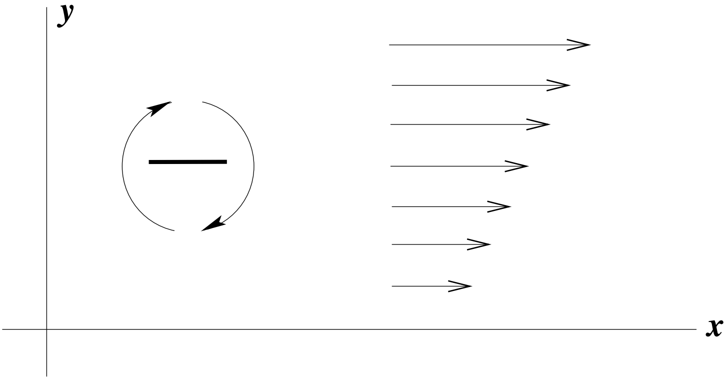
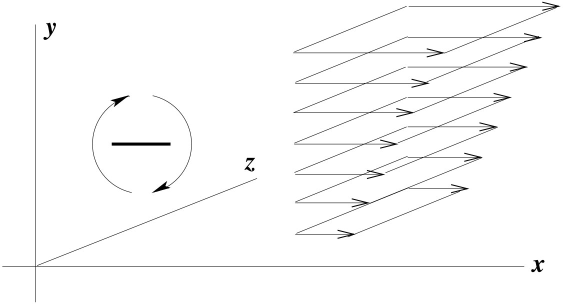


Molecular tumbling in a shear flow (2D)

What happens when we allow a third dimension? Does tumbling become unstable? If so, what stable dynamical regimes exist?



Symmetry: $z \mapsto -z$. Dynamical regimes invariant under this symmetry action of the group $\mathbf{Z}_2$ are called in-plane. For example:

Vertical: *tumbling*
Horizontal: *log-rolling*

Numerical evidence suggests many other types of (out-of-plane) periodic behaviour, in particular *kayaking* [demo].

Various mathematical models give proofs of the existence of tumbling motion; so far no full proof of kayaking.

M. Gregory Forest, Qi Wang and Ruhai Zhou: The weak shear kinetic phase diagram for nematic polymers, *Rheol. Acta* **43** (2004), 17–37 + references therein.

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The dynamical equations

Set up the dynamical equations as an ODE on the space

$$V := \{\text{symmetric, traceless } 3 \times 3 \text{ matrices}\} \cong \mathbf{R}^5.$$

Think of $Q \in V$ as the non-spherical part of the second moment of the probability that molecules will align in a given direction. Thus $0 \in V$ corresponds to the isotropic state: individual molecules will align themselves in any direction with equal probability.

If there is **no flow** then equilibrium states (phases) are taken to be critical points of a free energy function

$$\mathcal{F} : V \to \mathbf{R}$$

independent of the *choice of axes* inherent in V ...

...or, to put it another way, $\mathcal{F}$ must be invariant under the action of the group $SO(3)$ on V by conjugacy, that is

$$R : Q \mapsto RQR^T\,, \quad R \in SO(3).$$

Therefore $\mathcal{F}$ must have the form

$$\mathcal{F}(Q) = f(X, Y)$$

where

$$X = X(Q) := \mathrm{tr}\, Q^2$$
$$Y = Y(Q) := \mathrm{tr}\, Q^3.$$

Writing $\mathcal{F}_X = \frac{\partial \mathcal{F}}{\partial X}$, $\mathcal{F}_Y = \frac{\partial \mathcal{F}}{\partial Y}$ we then have

$$\nabla \mathcal{F}(Q) = \mathcal{F}_X.2Q + \mathcal{F}_Y.\big(3Q^2 - (\mathrm{tr}\, Q^2)\mathrm{I}\big)\,.$$

Decomposition of the 5-dim space V

Any space on which the group $\mathbf{Z}_2$ acts linearly can be decomposed as a direct sum of a space on which $\mathbf{Z}_2$ has *no effect* and a space on which it *changes signs*. In our case with $\mathbf{Z}_2$ generated by $z \mapsto -z$ we have

$$V = V^{in} \oplus V^{out}$$

corresponding to

$$\begin{pmatrix} p & u & t \\ u & q & s \\ t & s & r \end{pmatrix} = \begin{pmatrix} p & u & 0 \\ u & q & 0 \\ 0 & 0 & r \end{pmatrix} + \begin{pmatrix} 0 & 0 & t \\ 0 & 0 & s \\ t & s & 0 \end{pmatrix}$$

where $p + q + r = 0$. Thus

$$\dim V^{in} = 3\,, \quad \dim V^{out} = 2.$$

First, an elementary consequence of the symmetry:

Lemma

If $Q \in V^{in}$ *then* $\nabla\mathcal{F}(Q) \in V^{in}$*.*

Proof. Let $\rho : V \to V$ denote the action of the reflection $z \mapsto -z$ on V: then by definition

$$V^{in} = Fix(\rho) =: \{Q \in V : \rho Q = Q\}.$$

Differentiating $\mathcal{F}(Q) = \mathcal{F}(\rho Q)$ we have

$$\nabla\mathcal{F}(Q) = \rho\nabla\mathcal{F}(\rho Q) = \rho\nabla\mathcal{F}(Q)$$

so $\nabla\mathcal{F}(Q) \in Fix(\rho) = V^{in}$ as claimed. □

Therefore **any critical point of** $\mathcal{F}|V^{in}$ **is a critical point of** $\mathcal{F}$.

Critical points of $\mathcal{F}$

Every $Q \neq 0 \in V$ has either

- 3 distinct eigenvalues (biaxial), or
- a repeated eigenvalue (uniaxial).

Every uniaxial Q is conjugate to

$$Q^* = Q^*(a) := a\begin{pmatrix} -1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 2 \end{pmatrix}$$

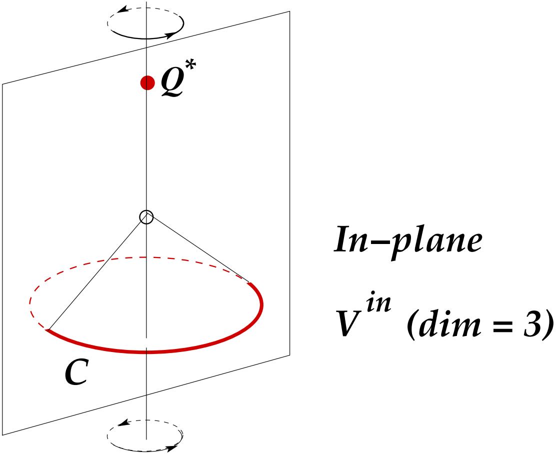
for some $a \neq 0$.

Which other matrices $Q \in V^{in}$ are conjugate to $Q^*(a)$?

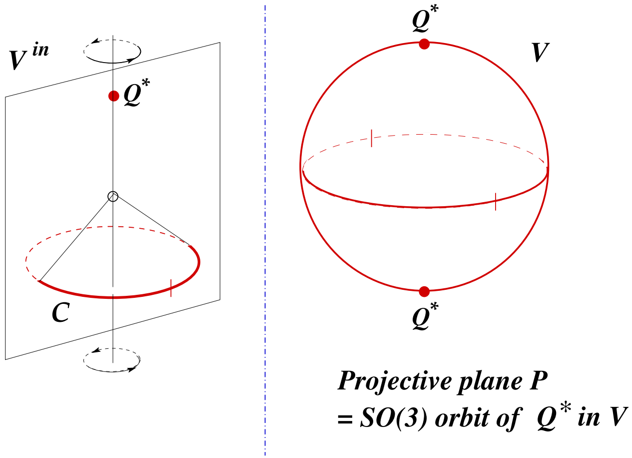
They form a circle $\mathcal{C} = \mathcal{C}(a)$ consisting of the matrices

$$\overline{Q}(\alpha) = \tfrac{1}{2}a \begin{pmatrix} 1 + 3\cos 2\alpha & 3\sin 2\alpha & 0 \\ 3\sin 2\alpha & 1 - 3\cos 2\alpha & 0 \\ 0 & 0 & -2 \end{pmatrix}$$

for $0 \leq \alpha \leq \pi$.



Q*
C
In–plane
V^in (dim = 3)



V in
Q*
C
Q*
V
Q*
Projective plane P
= SO(3) orbit of Q* in V

When is Q^* a critical point of $\mathcal{F}$?

Substituting $Q^*(a)$ into

$$\nabla \mathcal{F}(Q) = \mathcal{F}_X.2Q + \mathcal{F}_Y.\big(3Q^2 - (\operatorname{tr} Q^2)\mathrm{I}\big)$$

we find:

Lemma

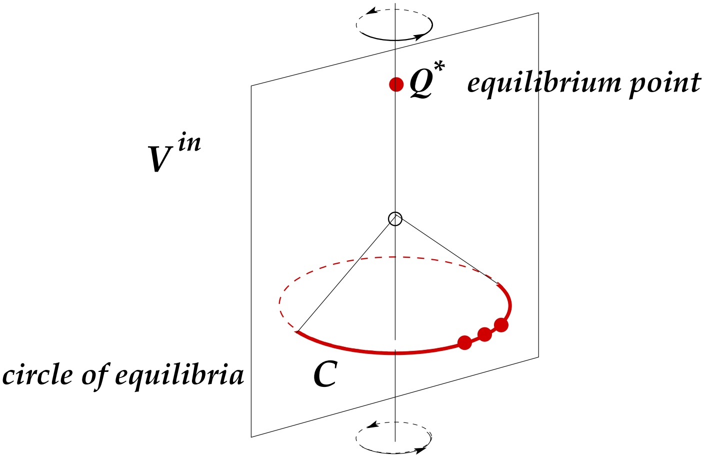
$Q = Q^*(a)$ is a critical point of $\mathcal{F}$ if and only if

$$2\mathcal{F}^*_X + 3a\mathcal{F}^*_Y = 0 \qquad (1)$$

where * denotes evaluation at Q^*.

Corollary

If (1) is satisfied, then all points of $\mathcal{C}$ are also critical points of $\mathcal{F}$.



Q^* equilibrium point
V^{in}
circle of equilibria
C

The simplest meaningful (and well-studied) case is where $\mathcal{F}$ is given by

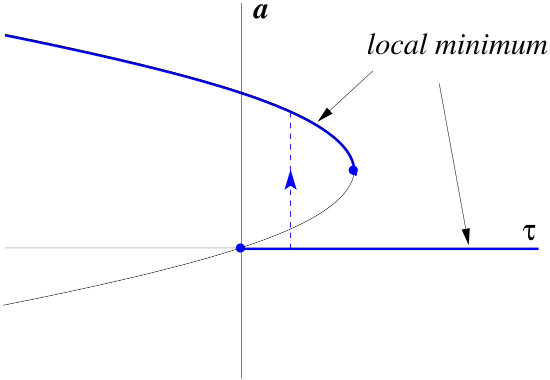
$$\begin{aligned}\mathcal{F}(Q) &:= \tfrac{1}{2}\tau\,\mathrm{tr}\,Q^2 - \tfrac{1}{3}B\,\mathrm{tr}\,Q^3 + \tfrac{1}{4}C\big(\mathrm{tr}\,Q^2\big)^2 \\ &= \tfrac{1}{2}\tau X - \tfrac{1}{3}B\,Y + \tfrac{1}{4}C\,X^2\end{aligned}$$

where we find

$$\mathcal{F}^*_X = \tfrac{1}{2} + 3Ca^2\,, \quad \mathcal{F}^*_Y = -\tfrac{1}{3}B$$

and the condition for $Q^*(a)$ to be a critical point of $\mathcal{F}$ is $a = 0$ or

$$\boxed{\tau - Ba + 6Ca^2 = 0.}$$



Branching diagram for equilibria (critical points of $\mathcal{F}$), fixed B, C.

Introducing the dynamics

The velocity field for the shear flow is

$$\begin{pmatrix} \dot{x} \\ \dot{y} \\ \dot{z} \end{pmatrix} = \begin{pmatrix} by \\ 0 \\ 0 \end{pmatrix}$$

so the fluid flow is given by

$$\mathbf{x}(t) = \begin{pmatrix} x(t) \\ y(t) \\ z(t) \end{pmatrix} = \begin{pmatrix} x(0) + b\,y(0)t \\ y(0) \\ z(0) \end{pmatrix} = \begin{pmatrix} 1 & bt & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} x(0) \\ y(0) \\ z(0) \end{pmatrix}.$$

The effect this has on the molecule represented by the quadratic form Q is given to a first approximation (allowing for different responses to rotation and compression etc.) by a differential equation of the form

$$\dot{Q} = \delta[W, Q] + \beta D(Q)$$

where $\quad [W, Q] = WQ - QW \quad$ and $\quad D(Q) = DQ + QD \quad$ with

$$W = \begin{pmatrix} 0 & -1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix} \qquad \text{and} \qquad D = \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix} \ldots$$

. . . although we may consider different expressions for the non-rotational term $D(Q)$.

Therefore the overall dynamical system that we wish to study has the form

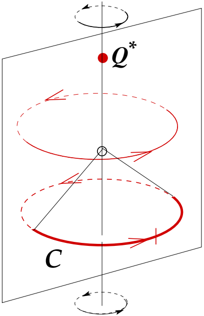
$$\dot{Q} = \mathcal{U}_{\delta,\beta}(Q) := -\nabla \mathcal{F}(Q) + \delta[W, Q] + \beta D(Q)\,.$$

We first suppose $\boxed{\beta = 0}$ and then switch it on later:

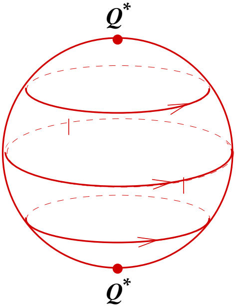
$$\dot{Q} = \mathcal{U}_{\delta,0}(Q) = -\nabla \mathcal{F}(Q) + \delta[W, Q].$$

The vector field $[W, Q]$ represents infinitesimal rotation

- about the Q^*-axis in V^{in}, and
- about the origin in V^{out}.



Action of W in V^{in}



Projective plane P
= SO(3) orbit of Q^*
in $V = V^{in} + V^{out}$

Suppose the fixed point Q^* (log-rolling) is linearly stable in V^{in}, that is the local linearization has **3 negative eigenvalues** (can show this is the case for large enough a).

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Further consequence: for sufficiently small $|\beta| > 0$ there is a normally-hyperbolic flow-invariant manifold P_β close to P in V.

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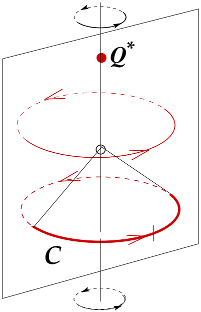
Question: What is (are?) the dynamics on P_β ?



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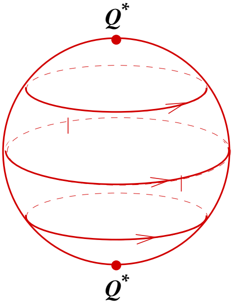

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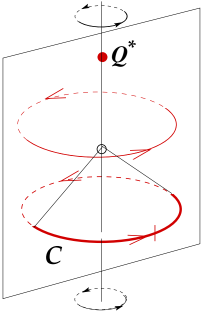

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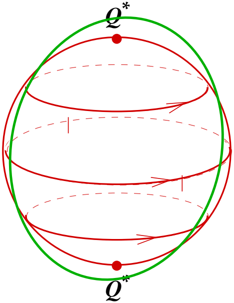

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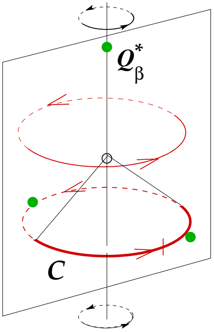

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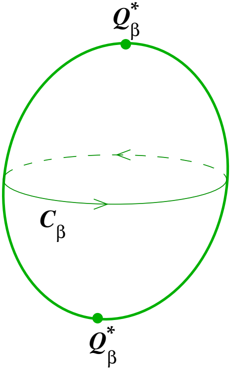
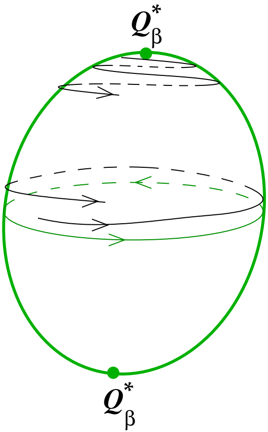


Projective plane P_β

Dynamics on P_β



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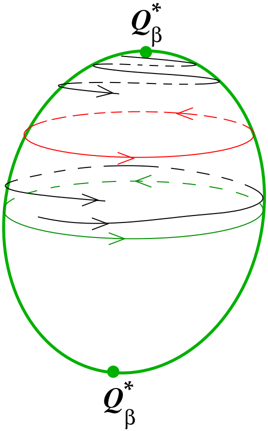

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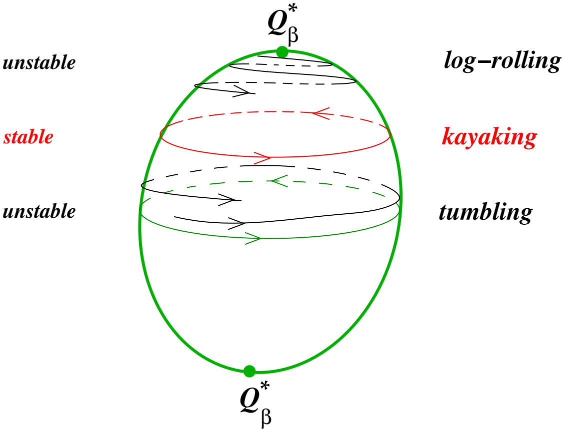

Projective plane P_β

Strategy:

Show that for $\delta > 0$ and for small $\beta > 0$ and for a suitable range of values of the parameters

- the north pole Q^*_β (fixed point) becomes repelling and
- the equator $\mathcal{C}_\beta$ (periodic orbit) becomes repelling.

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Warning: there may be more than one ...

More symmetry

Suppose $D(Q^*)$ has *zero component in the direction of* Q^* (which is certainly the case when $D(Q) = D$ or $D(Q) = DQ + QD$).

Then to first order in β the perturbing effect of the $\beta D(Q)$ term at angle α is equal and opposite to its effect at $\alpha + \frac{\pi}{2}$.

Hence the P_β-eigenvalues at Q^*_β have zero real part and we cannot decide if Q^*_β is repelling or not.

More symmetry (contd.)

Likewise suppose that to first order in β the effect of $\beta D(\overline{Q}(\alpha))$ at $\overline{Q}(\alpha)$ on $\mathcal{C}$ is equal and opposite to its effect at $\overline{Q}(\alpha + \frac{\pi}{2})$ (certainly the case when $D(Q) = D$ or $D(Q) = DQ + QD$).

Then the P_β-eigenvalue of the $\alpha = \frac{\pi}{2}$ Poincaré map for the periodic orbit $\mathcal{C}_\beta$ is -1 and we cannot decide if $\mathcal{C}_\beta$ is repelling or not.

So we are going to have to go to second order in β.

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Theorem

To second order in β the real part of the eigenvalues at Q^*_β is a positive multiple of $af_Y(Q^*)$. $\square$

In the much-studied case when

$$\mathcal{F}(Q) = f(X,Y) := \frac{1}{2}\tau X - \frac{1}{3}BY + \frac{1}{4}CX^2$$

we have simply

$$af_Y(Q^*) = -\frac{1}{3}aB$$

and so in that case

Corollary

The fixed point Q^*_β is repelling provided $a > 0$.

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which we do by integrating the *variational equation* $\dot{\xi} = D\mathcal{U}_{\delta,\beta}(Q)\xi$ along $\mathcal{C}_\beta$.

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Work in progress ...