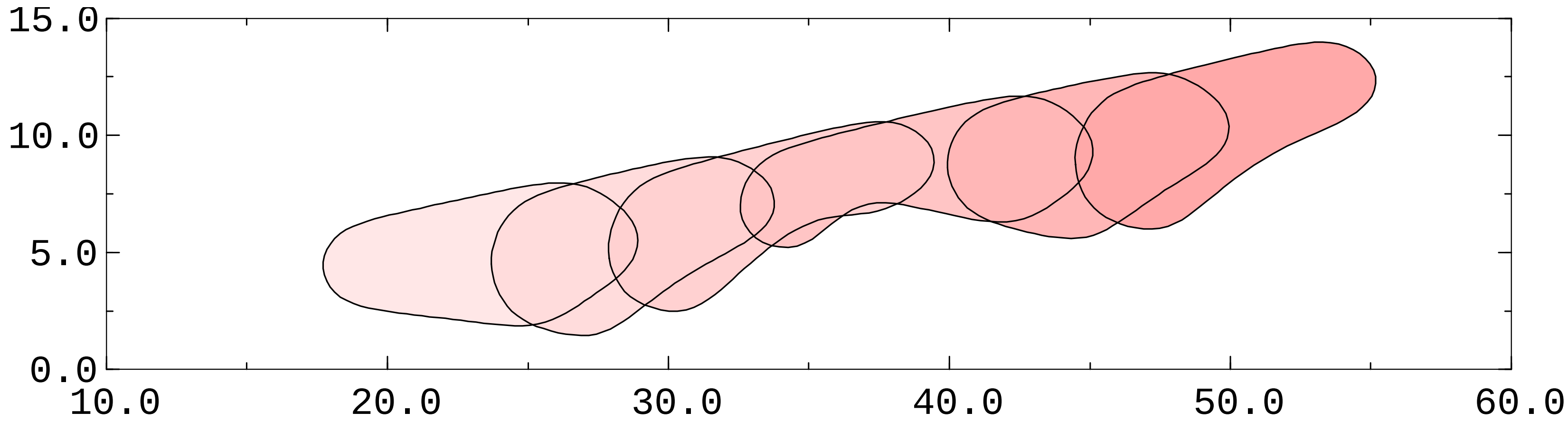
Islands in the Stream:

Electromigration-Driven Shape Evolution with Crystal Anisotropy[1]



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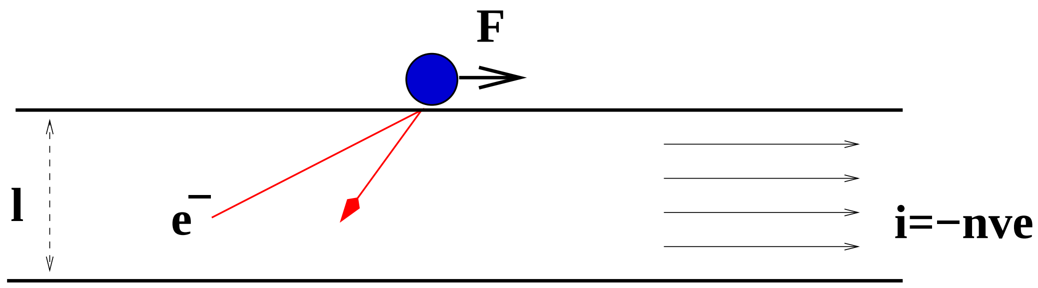
Supported by DFG within SFB 616 *Energy Dissipation at Surfaces*

[1]cond-mat/0405068

Surface Electromigration



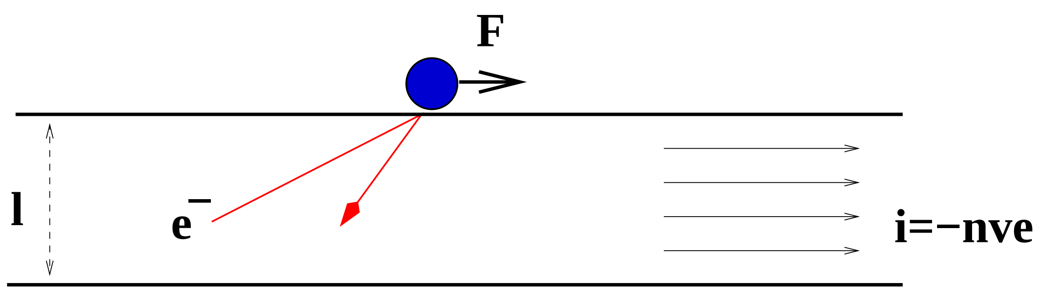
electromigration force:

$F = eZ^{*}E$

Z^{*}: effective valence

- relation to surface resistance and electronic friction
- relevance for reliability of integrated circuits

Surface Electromigration



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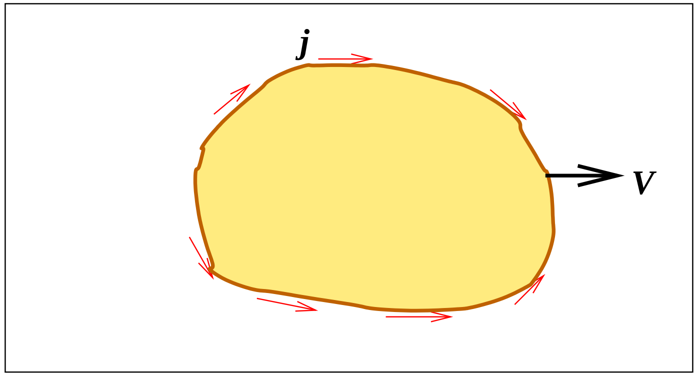
General goal: To bridge the gap between atomistic processes and large scale morphological evolution through the study of simple step and island configurations on single crystal surfaces

Continuum Model of Shape Evolution



- mass transport along island edges
- anisotropic mobility and stiffness

- normal edge velocity v_n satisfies

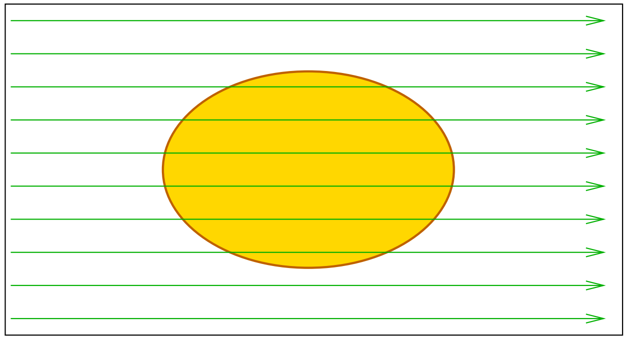
$$v_n + \partial j/\partial s = 0, \quad j = \sigma(\theta)\left[F_t - \frac{\partial}{\partial s}\tilde{\gamma}(\theta)\kappa\right]$$

s: arc length	θ: edge orientation	κ: edge curvature
$\sigma(\theta)$: adatom mobility	$\tilde{\gamma}(\theta)$: step stiffness	F_t: tangential force

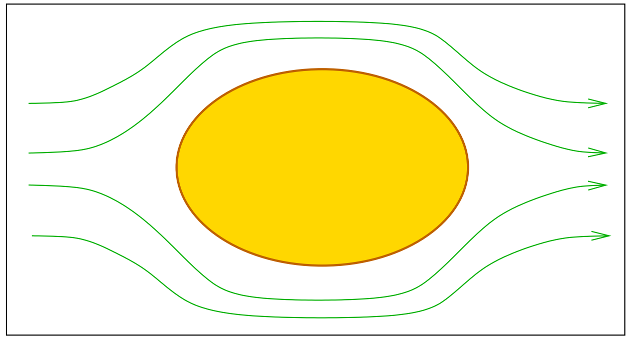
- electromigration dominates on length scales $\gg l_E = \sqrt{\tilde{\gamma}/|F|}$

Local vs. Nonlocal Evolution

local



nonlocal



- **local model**: $F_t = F_0 \cos(\theta + \phi)$ ϕ: field direction
  single layer islands (Pierre-Louis & Einstein 2000)
  dislocation loops (Suo 1994)

- **nonlocal model**: $F_t = -\partial U / \partial s$ with $\nabla^2 U_{\text{outside}} = U_{\text{inside}} = 0$
  insulating voids in metallic thin films
  (Kraft & Arzt, Gungor & Maroudas, Mahadevan & Bradley, Schimschak & JK...)

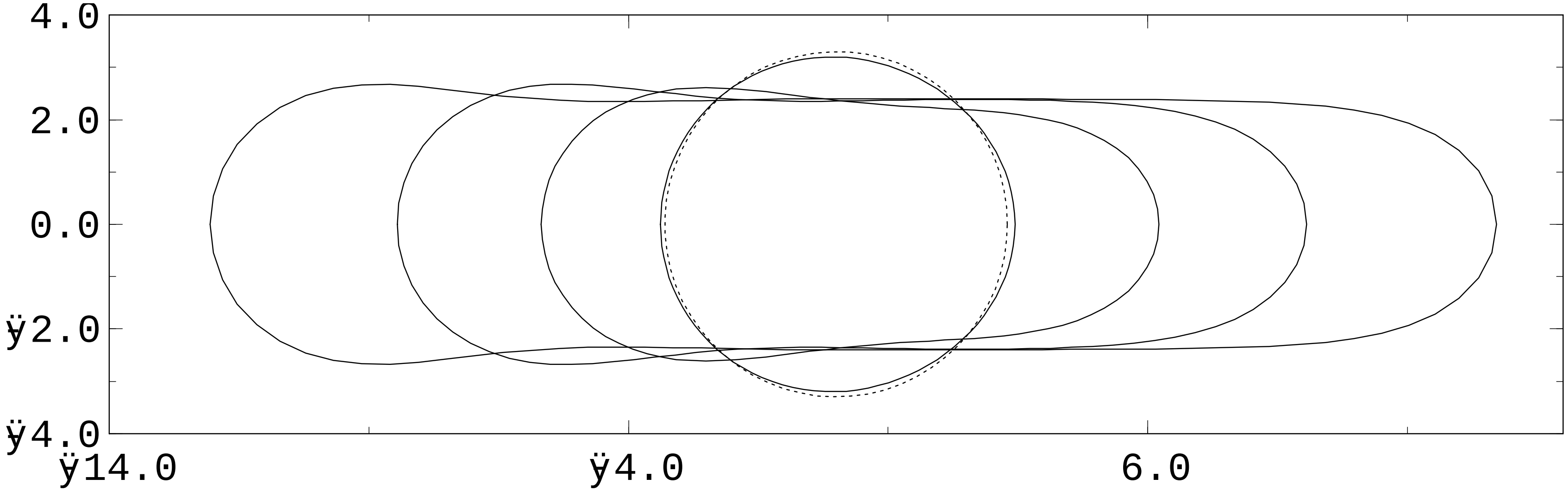
- interpolation by general conductivity ratio $\rho = \Sigma_{\text{inside}} / \Sigma_{\text{outside}} \in [0, 1]$

Results for the isotropic case

- The circle is a stationary solution for any ρ (Ho, 1970)
- Linear instability at critical radius $R_c^{(1)} = \hat{R}_c^{(1)} l_E$ for $\rho > 0$ (Wang, Suo, Hao 1996)
- Nonlinear instability for $\rho = 0$ (Schimschak & JK, 1998)
- No non-circular stationary shapes for $\rho = 0$ (Cummings, Richardson, Ben Amar 2001)
- $\rho = 1$: Slightly distorted circles approach non-circular stationary shapes for

$$\hat{R}_c^{(1)} \approx 3.26 < R/l_E < \hat{R}_c^{(2)} \approx 6.2$$

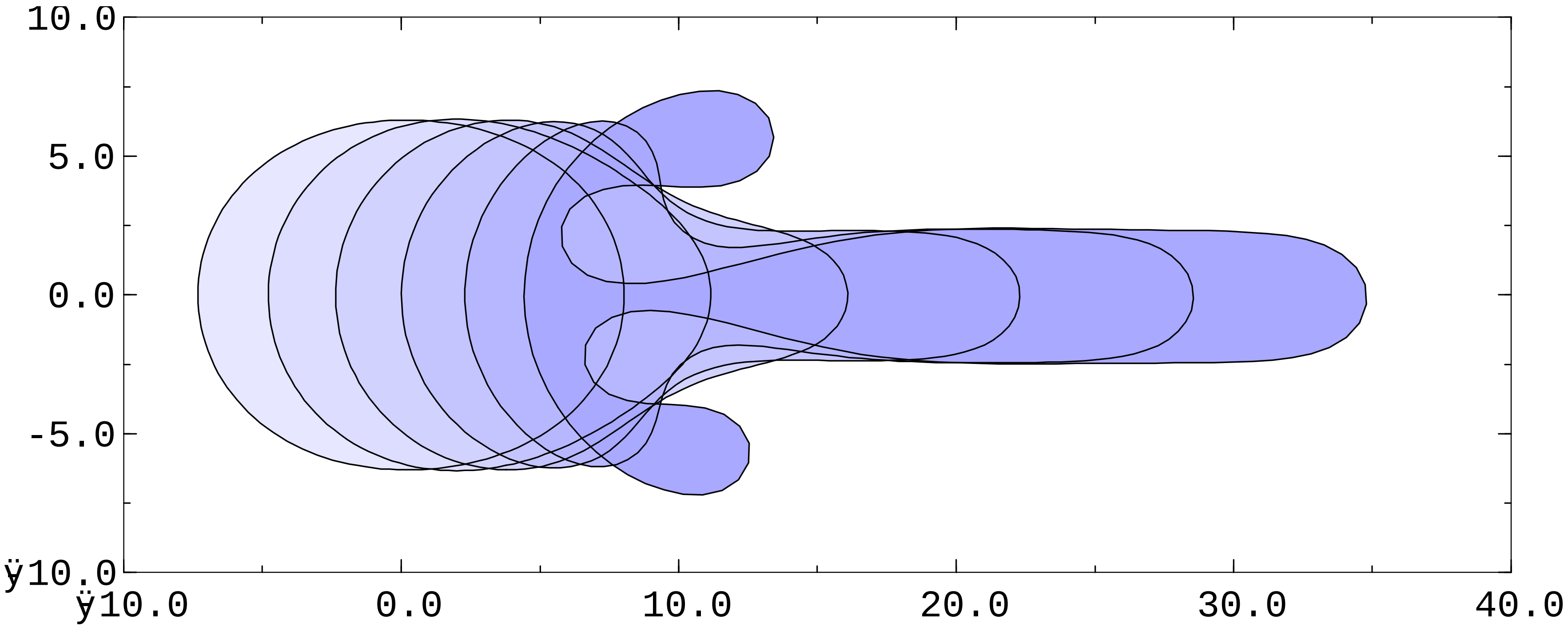
Non-circular stationary shapes



- Effective radius $R/l_E = 3.3, 4, 5, 6$
- Shapes approach finger solution of width $W \approx 4.8 l_E$

  (Suo, Wang, Yang 1994)

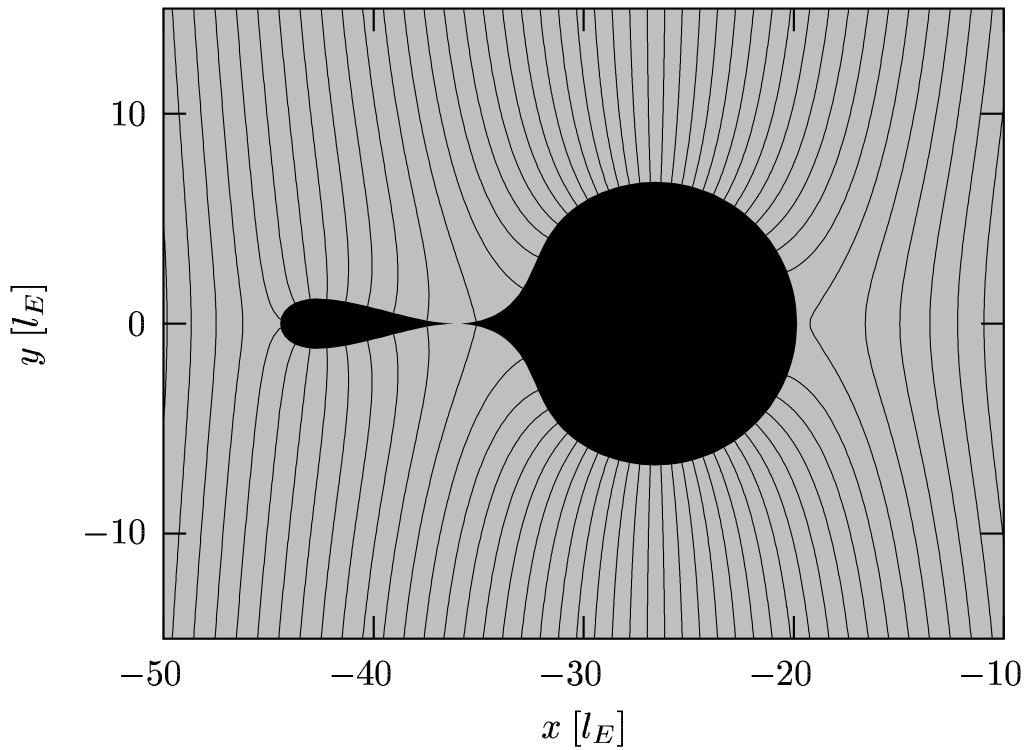
Island breakup



- Effective radius $R/l_E = 7$
- Breakup mediated by outgrowth of finger

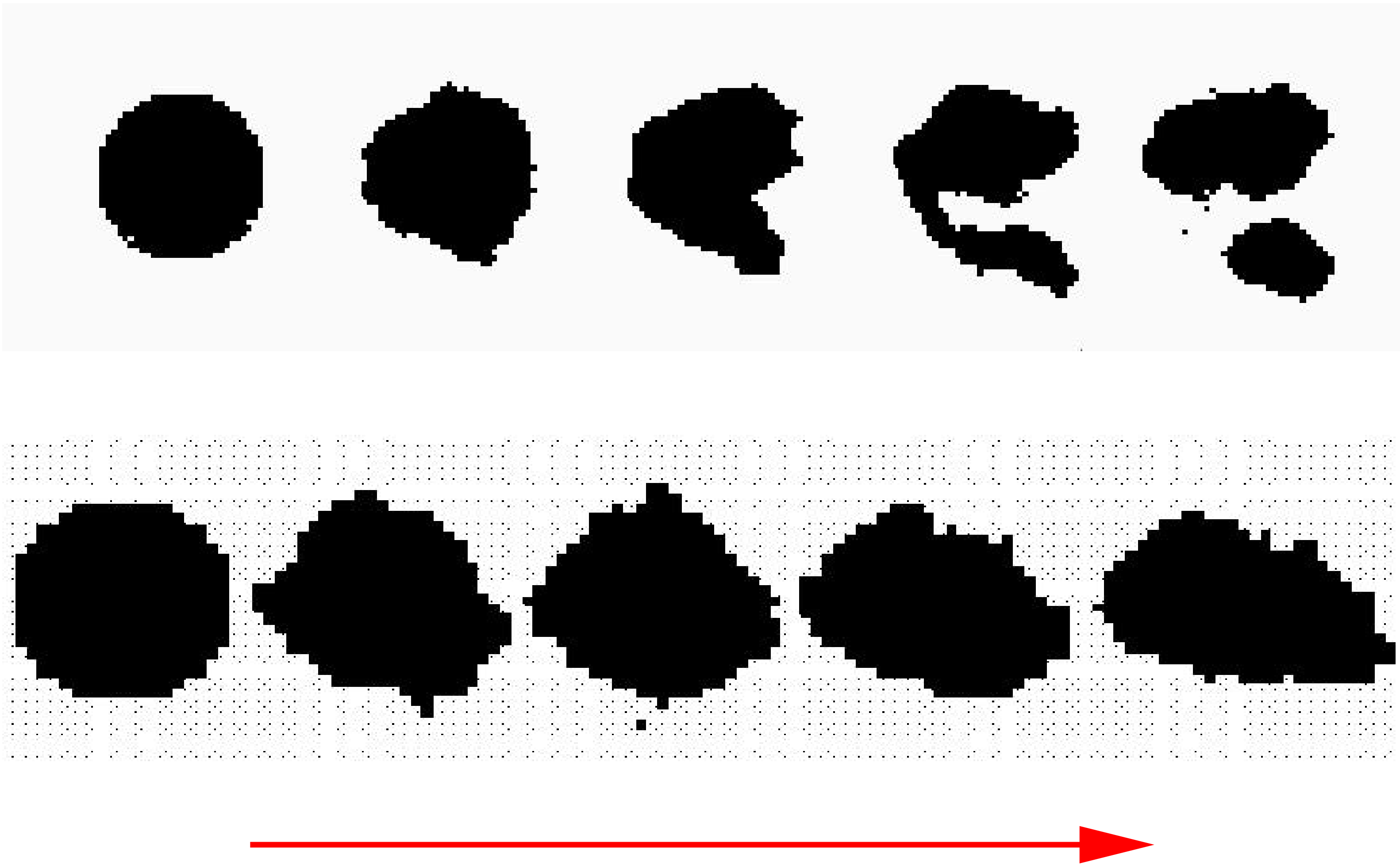
Void breakup in the nonlocal model

M. Schimschak, J.K., J. Appl. Phys. **87**, 695 (2000)



- Splitoff of **circular** void, no finger solution

Island breakup in kinetic Monte Carlo simulations

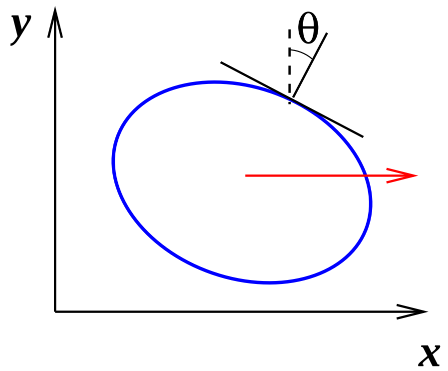


O. Pierre-Louis, T.L. Einstein, Phys. Rev. B **62**, 13697 (2000)

Stationary shapes without capillarity

- Island moves along x-axis

- Parametrization: $x = x(\theta),\ y = y(\theta)$
  $dy/dx = -\tan(\theta)$



- Stationarity condition: $v_n = V \sin(\theta) \Rightarrow Vy = j + \text{const.}$ (Suo 1994)

- In the absence of capillarity $(\tilde{\gamma} = 0)$ this implies

$$y(\theta) = \frac{F}{V}\sigma(\theta)\cos(\theta + \phi), \quad x(\theta) = -\int_0^\theta d\theta' \, \frac{dy}{d\theta'} \cot(\theta')$$

- Mobility model: $\sigma(\theta) = \sigma_0\{1 + S\cos^2[n(\theta + \alpha)/2]\}$

S: Anisotropy strength
n: Number of symmetry axes
α: Orientation of symmetry axes

Conditions on physical shapes:

(i) $x(\theta)$ finite $\Rightarrow$ $dy/d\theta = 0$ at $\theta = 0$ and π

(ii) no self-intersections $\Rightarrow$ $dy/d\theta \neq 0$ for $\theta \neq 0,\ \pi$

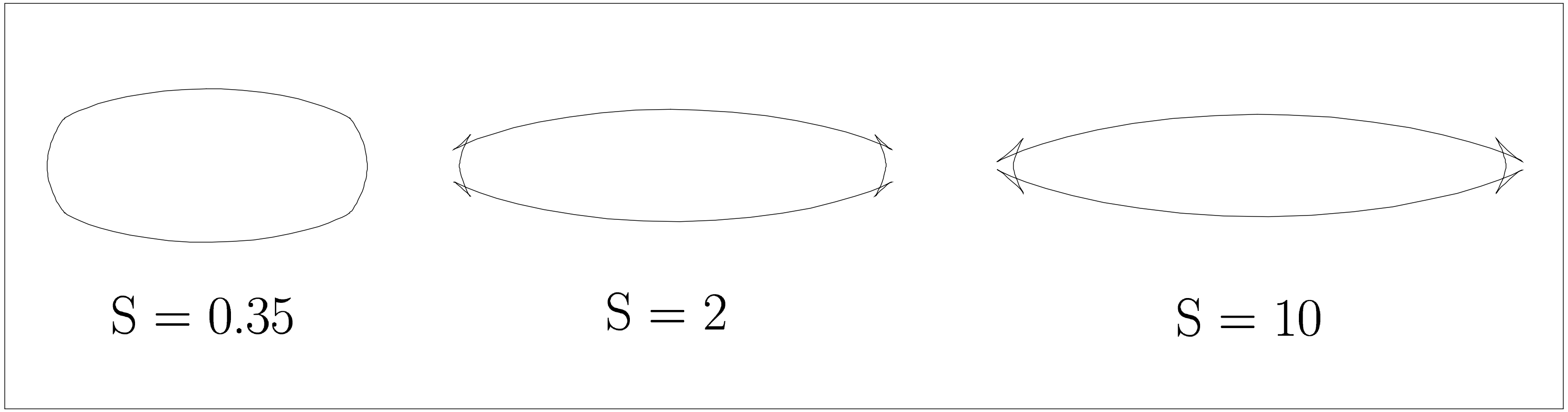
(iii) closed contour: $x(\theta + 2\pi) = x(\theta)$ $\Rightarrow$ $\tan(n\alpha)\tan(\phi) = n$ for odd n

Consequences:

- No stationary shapes for odd n **!**
- For even n smooth stationary shapes exist in a range $0 < S < S_c$ of anisotropy strengths
- Condition (i) selects direction of island motion which is generally **different** from the direction of the field

Formation of self-intersections

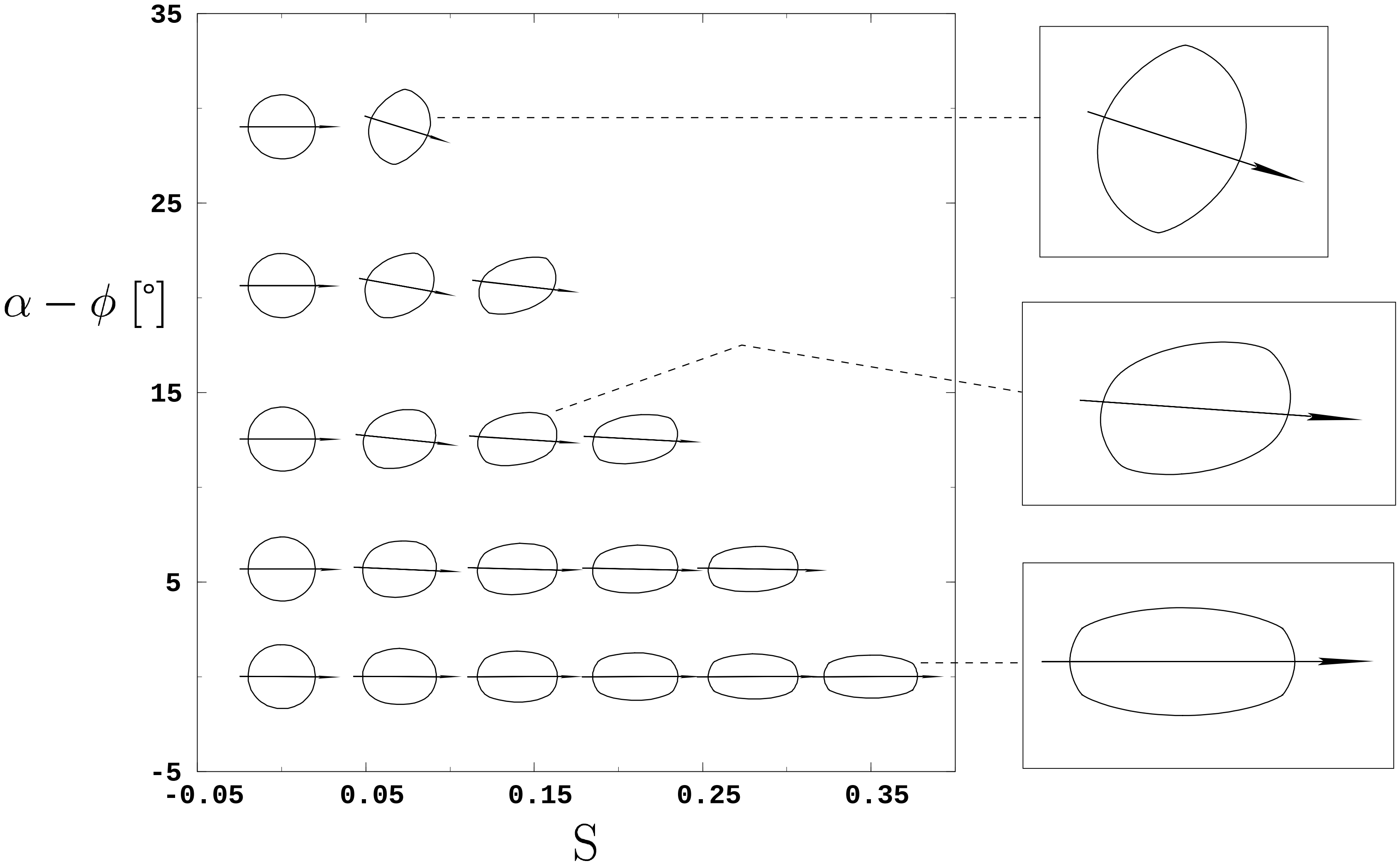
- $n = 6$, $\alpha - \phi = 0$, $S_c \approx 0.35$:



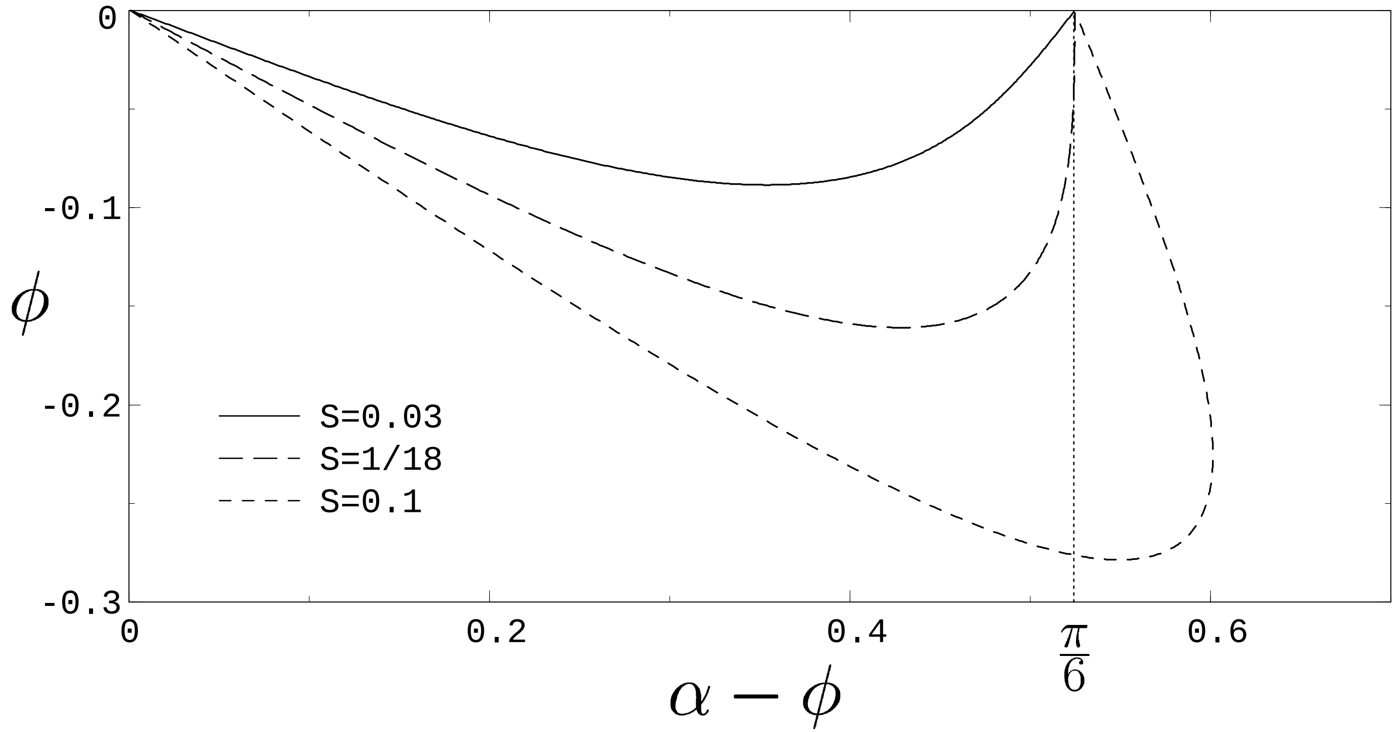
- For $\alpha = \pi/n$ and $\phi = 0$ self-intersections appear at $\theta = 0$ and π with

$$S_c = \frac{1}{n^2/2 - 1}$$

Stationary shapes for sixfold anisotropy

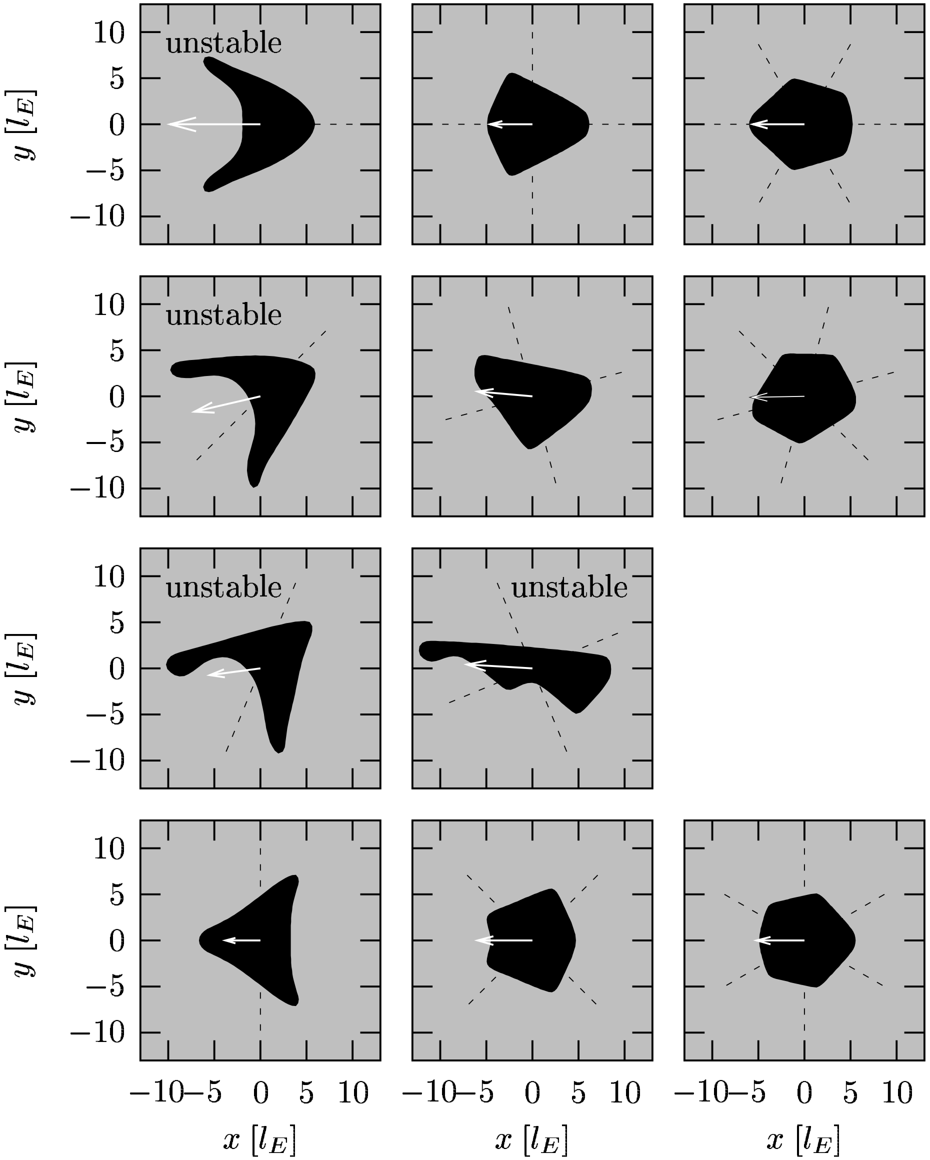


Direction of island motion



For $S > \tilde{S}_c = 2/n^2$ the direction of motion changes **discontinuously** at the angle $\alpha - \phi = \pi/n$ of minimal mobility

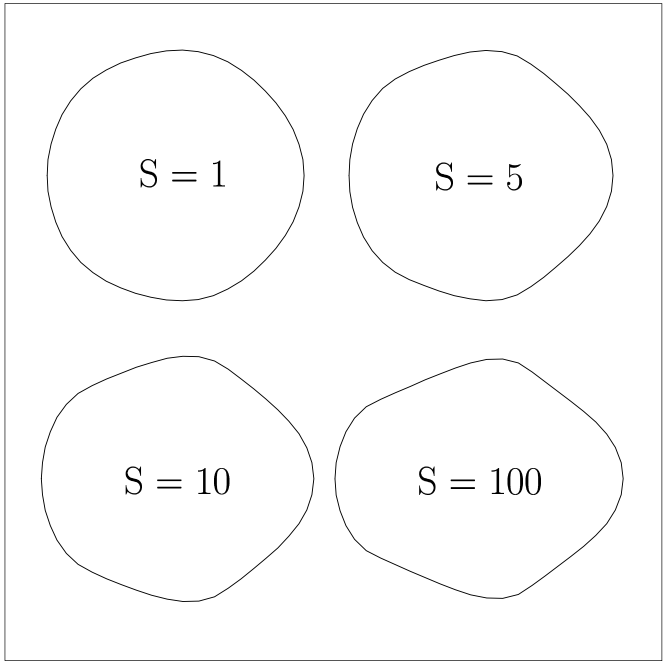
Anisotropic stationary shapes for the nonlocal model



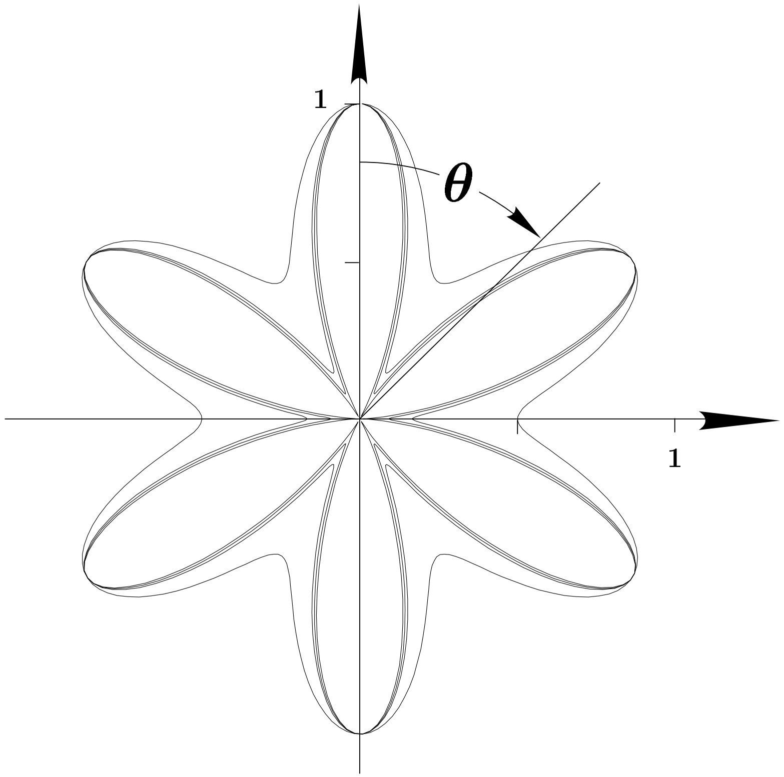
M. Schimschak, J.K.

J. Appl. Phys. **87**, 695 (2000)

Anisotropic stationary shapes for the local model

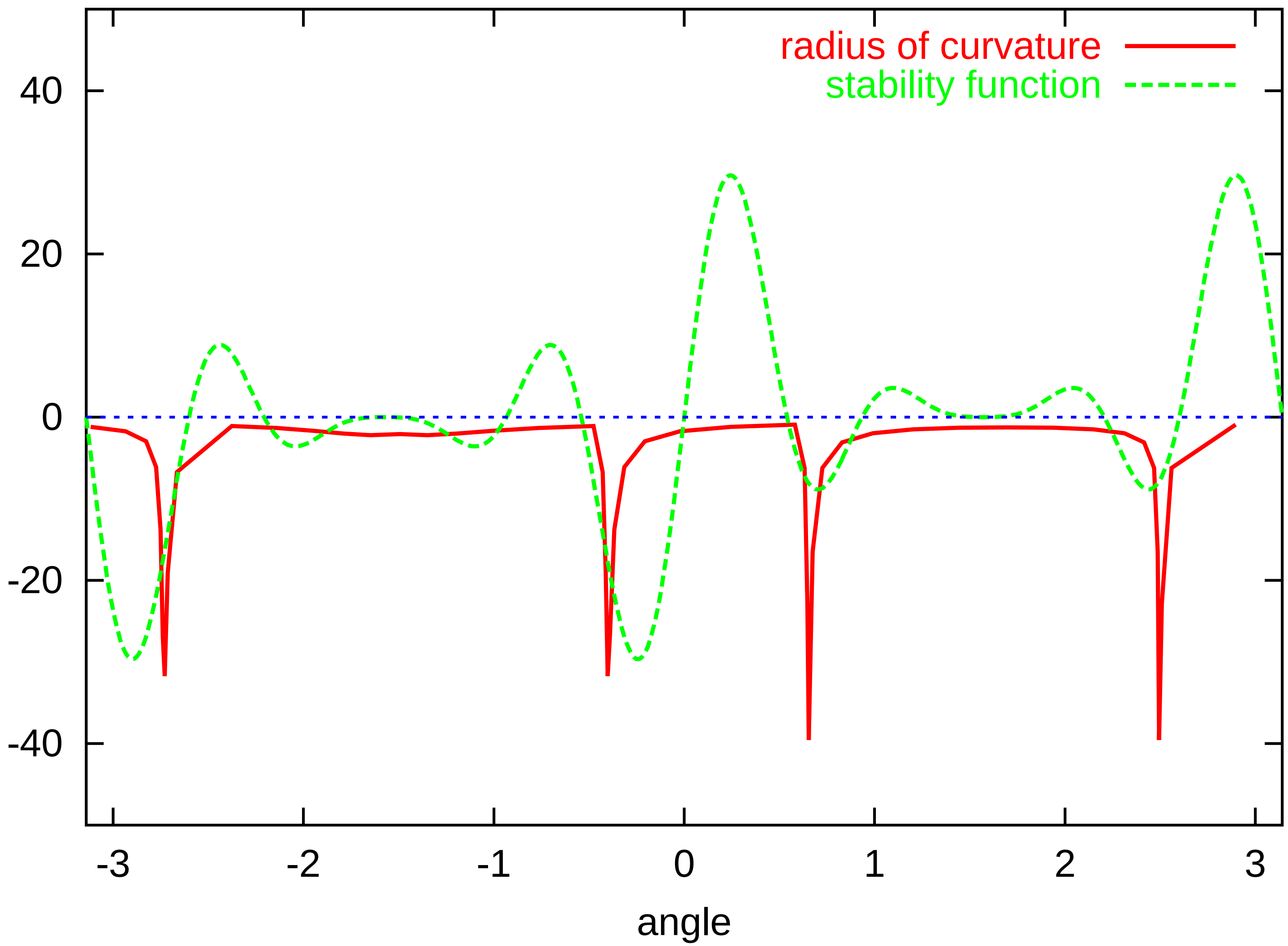


$\hat{R} = 2.5$



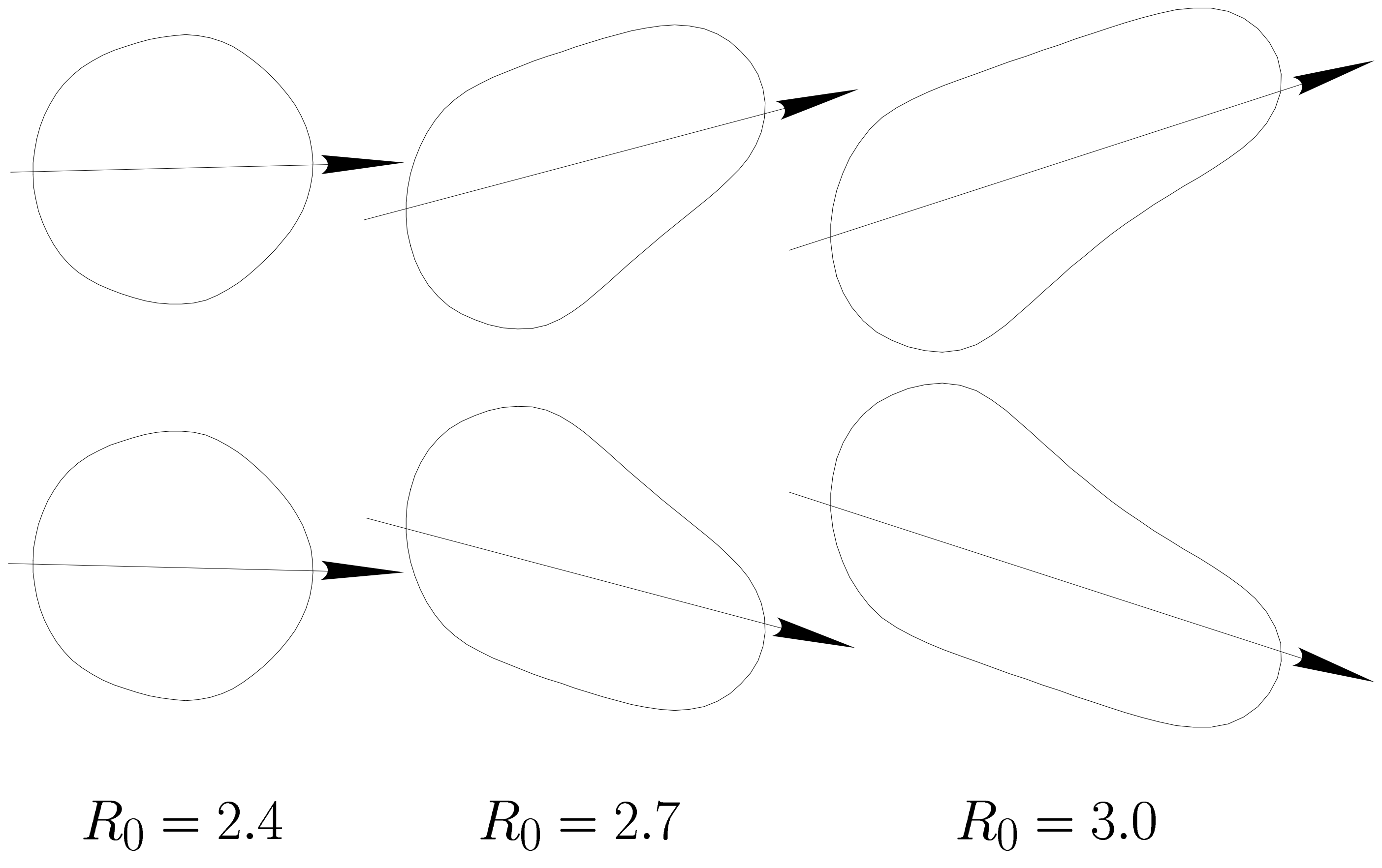
$\sigma(\theta)$ for $n = 6$

- “Facet” orientations are close to orientations of maximal linear stability:



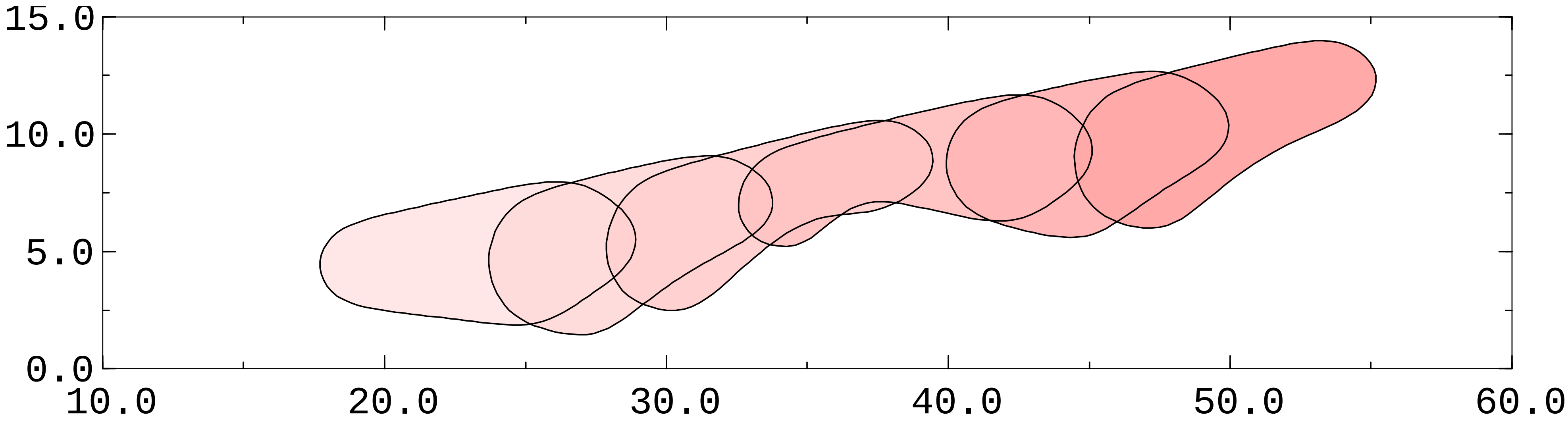
$\hat{R} = 2.5$, $S = 100$

Obliquely moving stationary shapes (n=6, S=2)



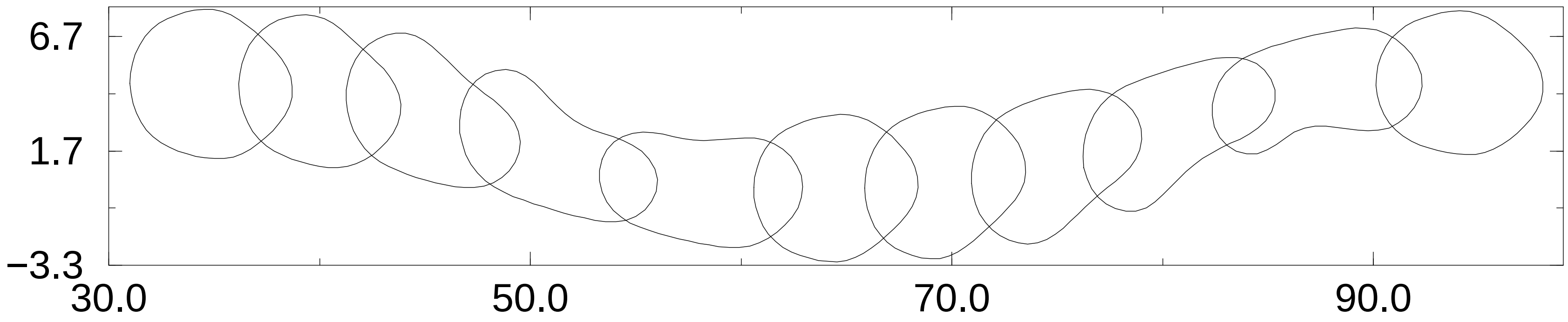
- "Spontaneous" breaking of symmetry w.r.t. field & anisotropy direction

Oblique oscillatory motion

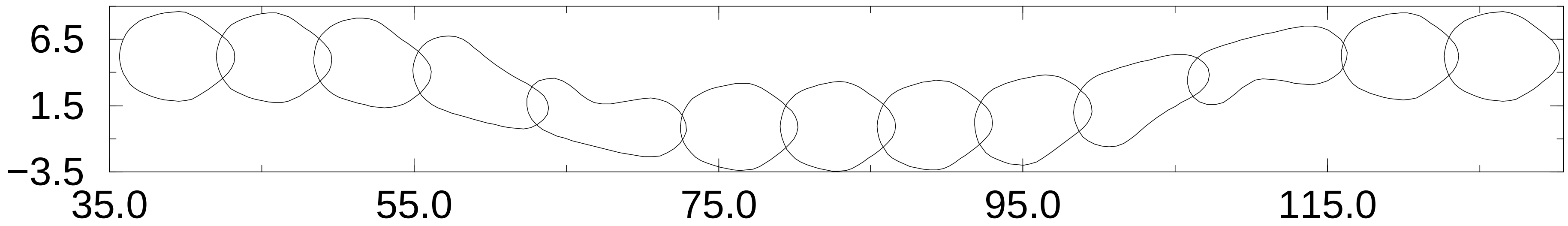


- Initial radius $\hat{R} = 4$, anisotropy strength $S = 1$, maximal mobility at $\theta = 0$
- Upper edge is linearly stable, lower edge linearly unstable

Zig-zag motion



$\hat{R} = 3.5$, $S = 0.5$

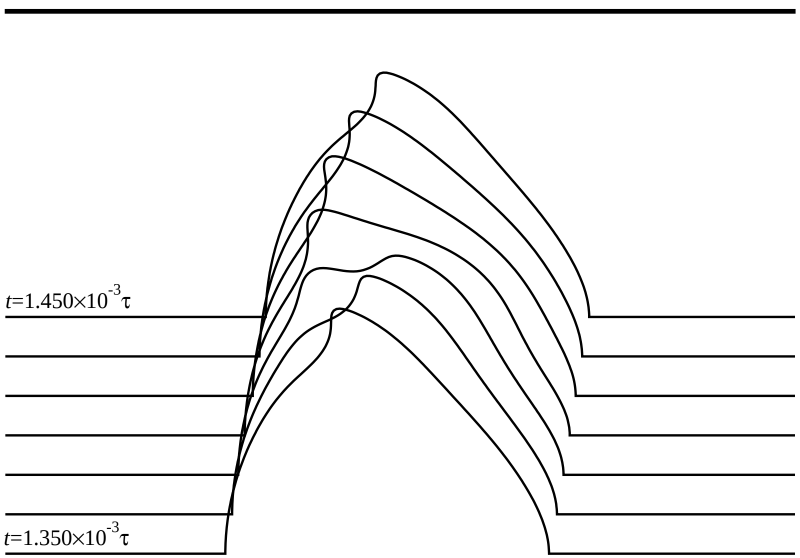


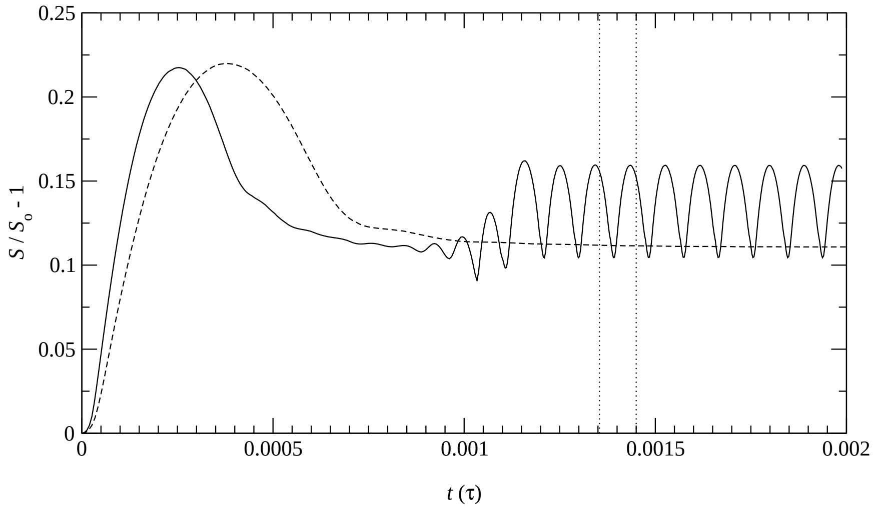
$\hat{R} = 3.5$, $S = 1$

Oscillatory behavior in the nonlocal model

M.R. Gungor, D. Maroudas, Surf. Sci. **461** (2000), L550

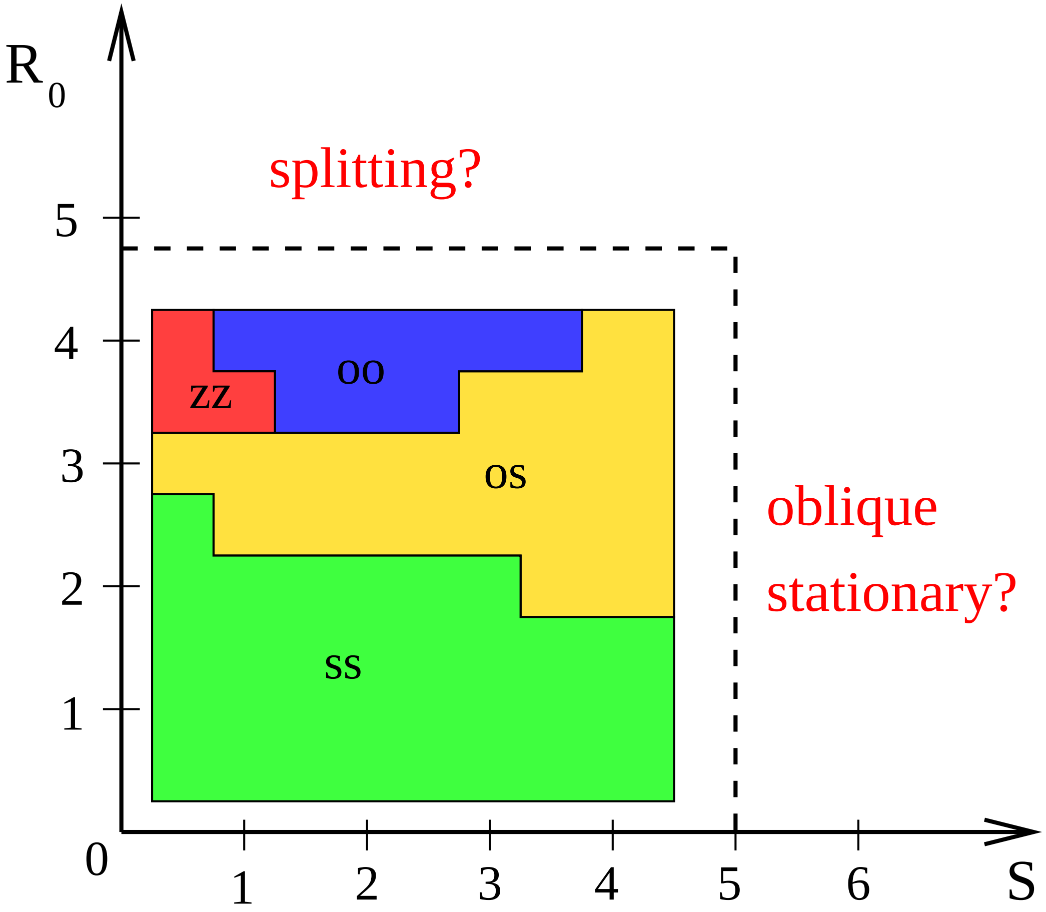
- Propagation of edge voids with crystal anisotropy





- Onset of oscillations at a critical void size
- Divergence of oscillation period at onset

Tentative phase diagram for $n = 6$, $\alpha = 0$



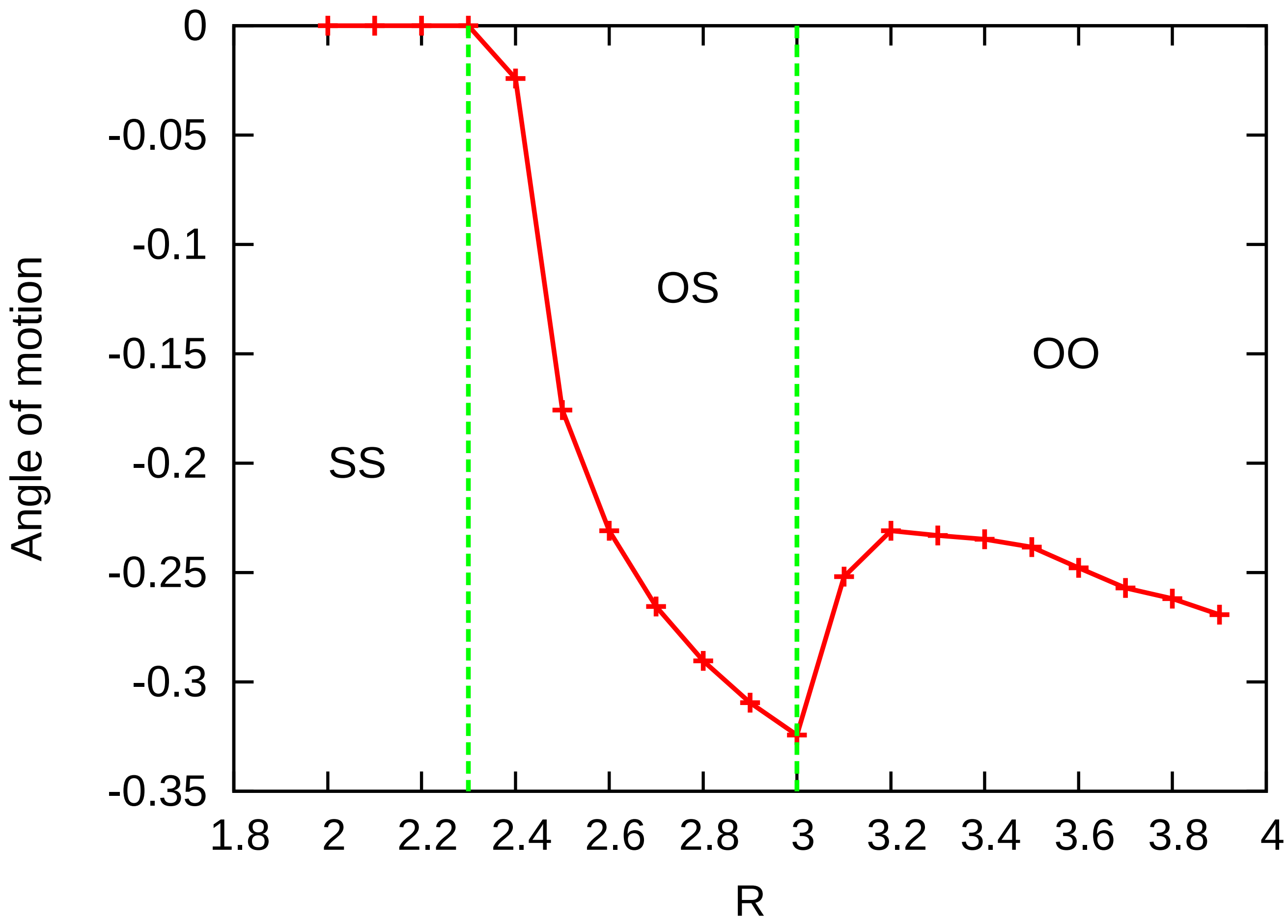
zz = zig zag

oo = oblique oscillatory

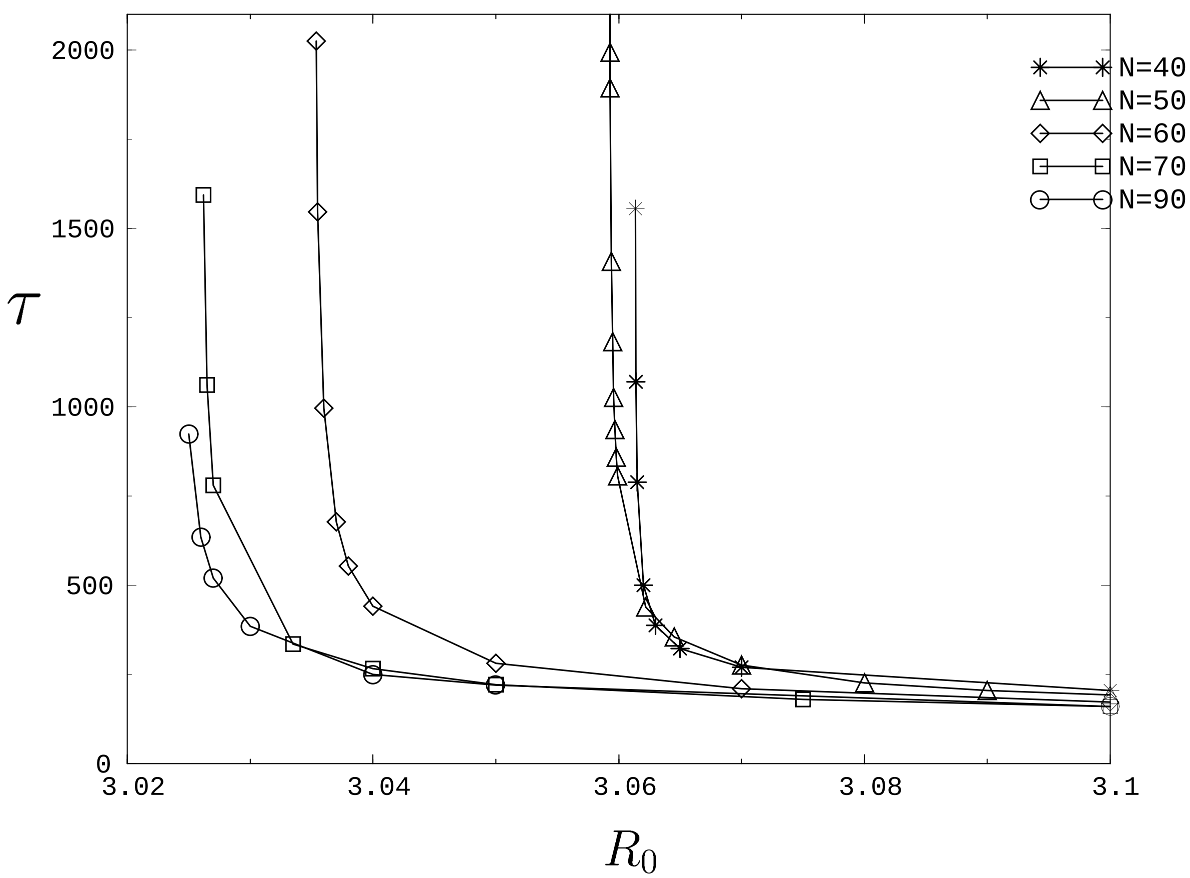
os = oblique stationary

ss = straight stationary

Angle of motion as an order parameter ($S = 2$)



Divergence of the oscillation period at the oo $\rightarrow$ os transition



- N: Number of discretization points
- Best fit: $\tau \sim (R_0 - R_c)^{-2.5}$

Outlook

- Nature of bifurcations (low-dimensional truncation)?
- Oscillatory behavior in kinetic Monte Carlo simulations?
- Different kinetic regimes of Pierre-Louis & Einstein?
  (with F. Hausser & A. Voigt, *caesar*)