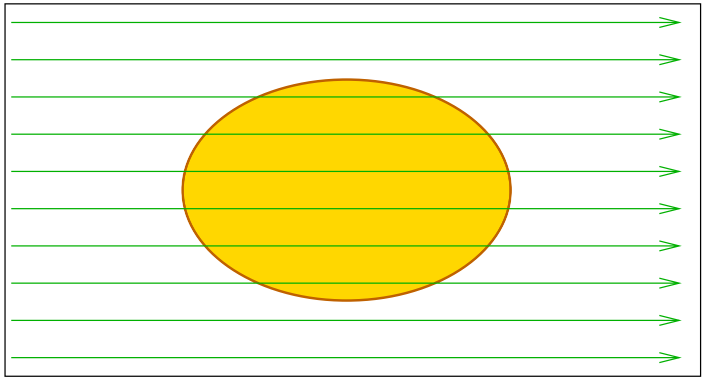
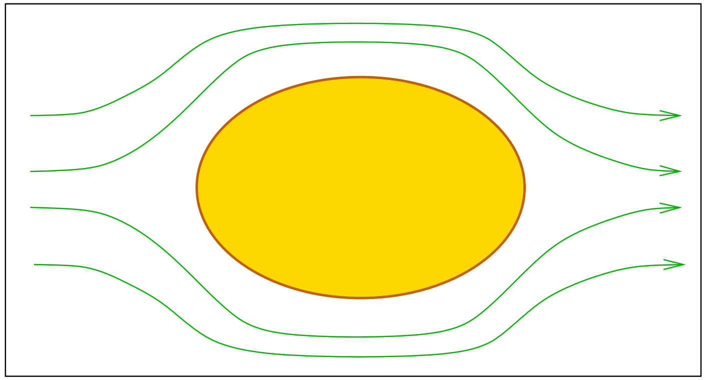
Islands in the Stream:

Complex Shape Evolution Driven by Surface Electromigration[1]





P. Kuhn, University of Duisburg-Essen

J. Krug, University of Cologne

F. Hausser and A. Voigt, research center caesar, Bonn

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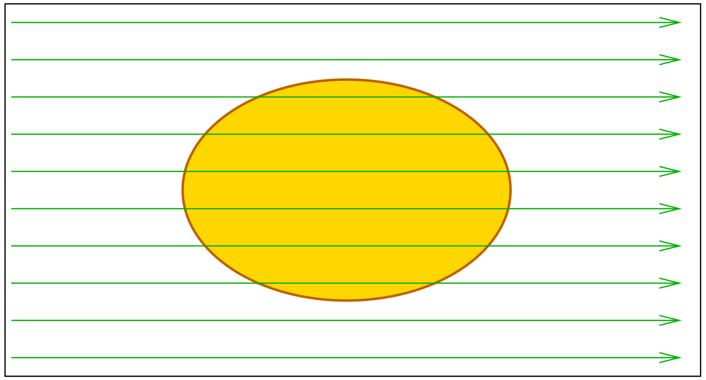
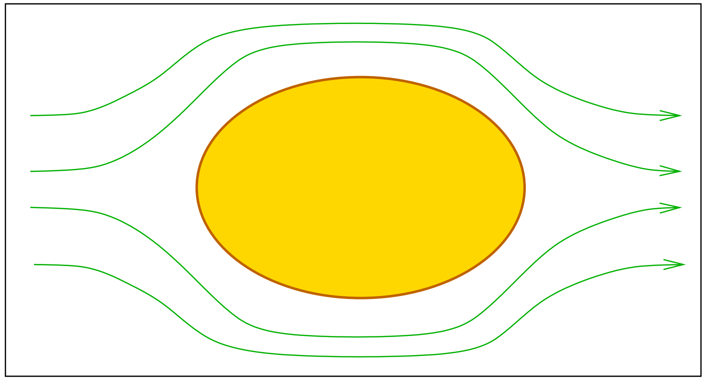
SFB 611 *Singular phenomena and scaling in mathematical models*

[1] cond-mat/0405068 & 0410745

Island in the Straits:

Complex Shape Evolution Driven by Surface Electromigration[1]





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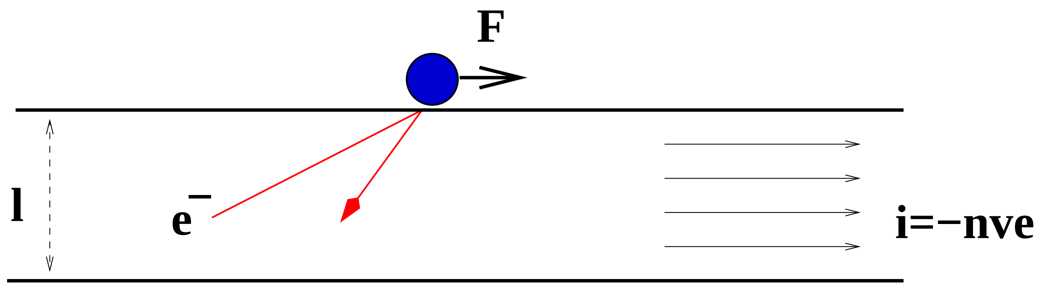
Surface Electromigration

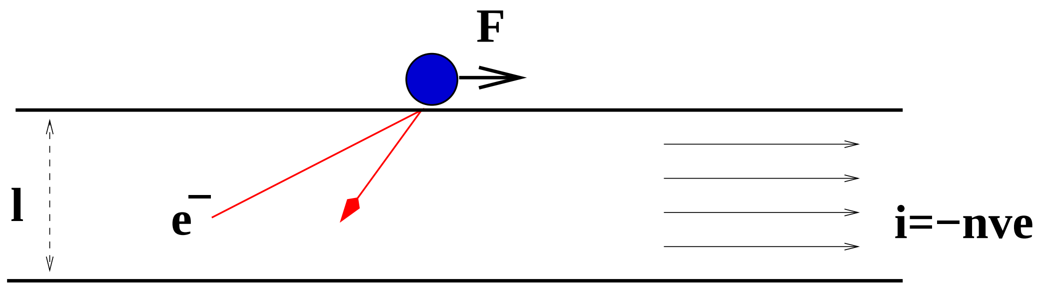


electromigration force:
$F = eZ^*E$

Z^*: effective valence

- relation to surface resistance and electronic friction
- dominant failure mechanism in integrated circuits

Surface Electromigration



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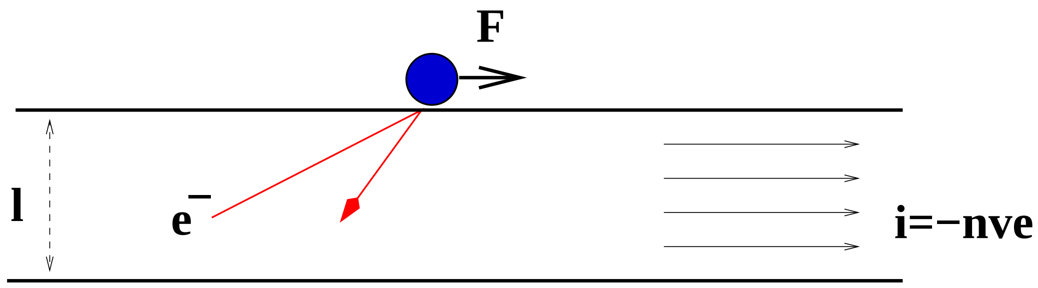
General goal: To bridge the gap between atomistic processes and large scale morphological evolution through the study of simple step and island configurations on single crystal surfaces

Surface Electromigration



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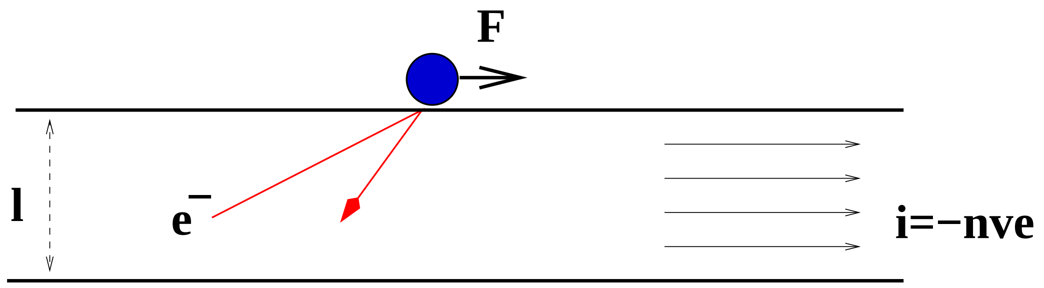
Model problems:

- electromigration-induced step bunching
- current effects on step fluctuations
- electromigration of single layer islands

Surface Electromigration



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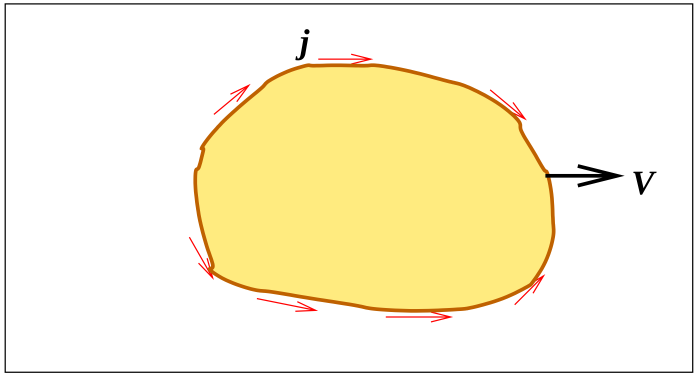
Model problems:

- electromigration-induced step bunching $\rightarrow$ M. Uwaha, J. Weeks (today)
- current effects on step fluctuations $\rightarrow$ E. Williams (yesterday)
- electromigration of single layer islands $\rightarrow$ **this talk**

Continuum Model of Shape Evolution



- mass transport restricted to the one-dimensional interface
- anisotropic mobility and stiffness

- normal edge velocity v_n satisfies

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

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 $\gg l_E = \sqrt{\tilde{\gamma}/|F|}$

- Numerical methods: Finite differences & adaptive finite elements

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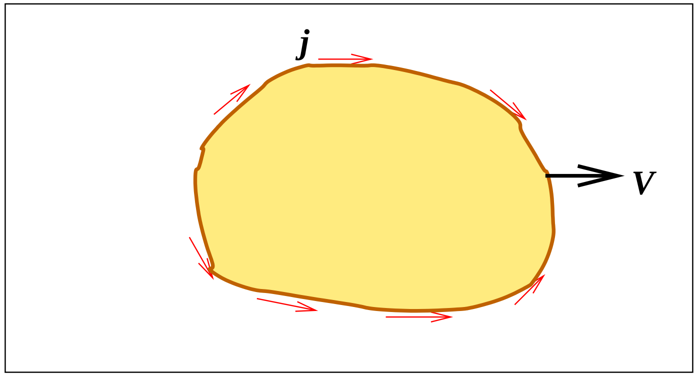

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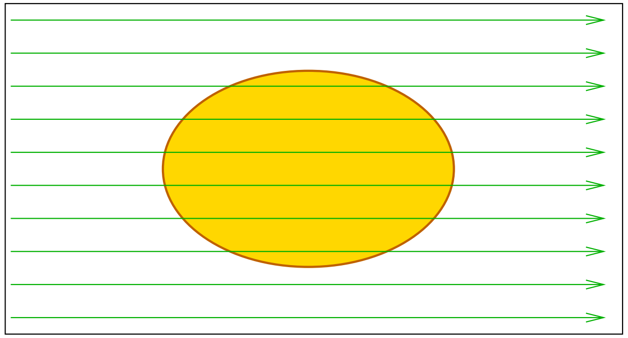
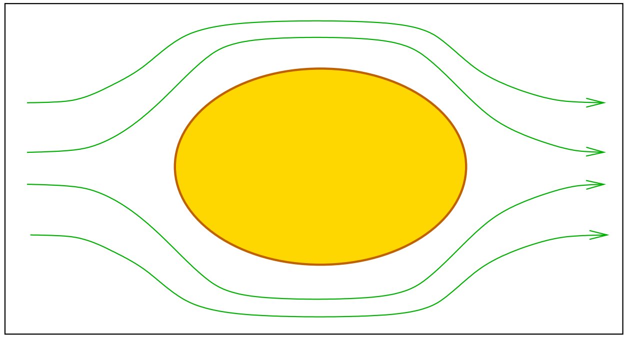
Islands vs. Voids

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...)

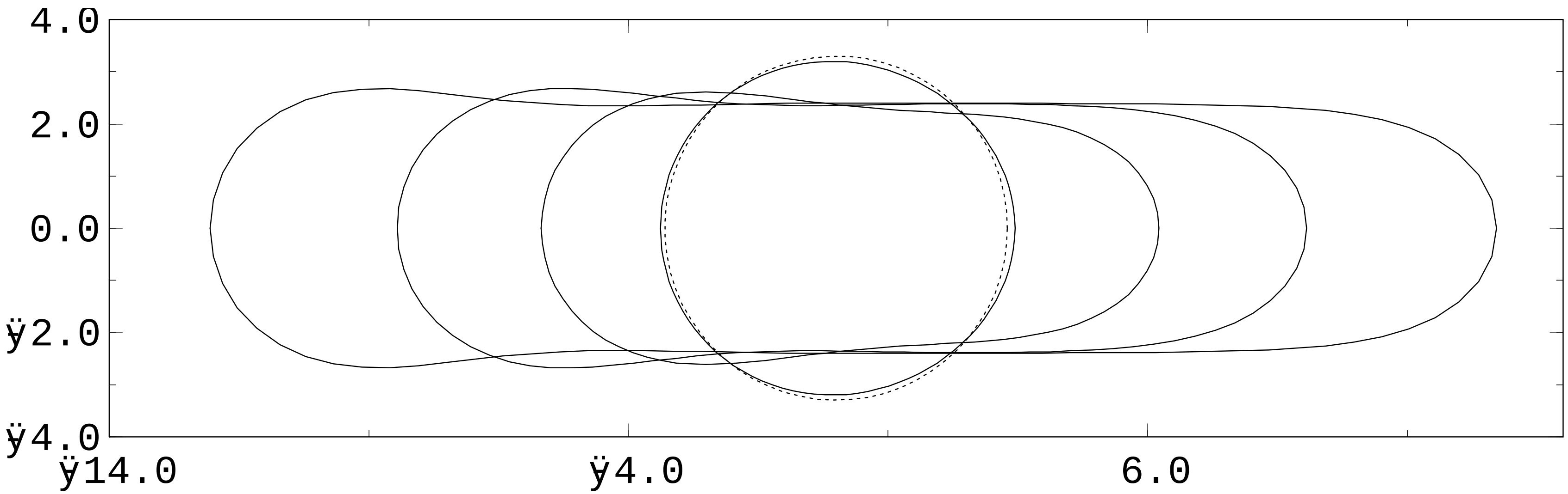
- interpolation by general conductivity ratio $\rho = \Sigma_{\text{inside}} / \Sigma_{\text{outside}} \in [0, 1]$

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)
- $\rho = 1$: Non-circular stationary shapes are stable for

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

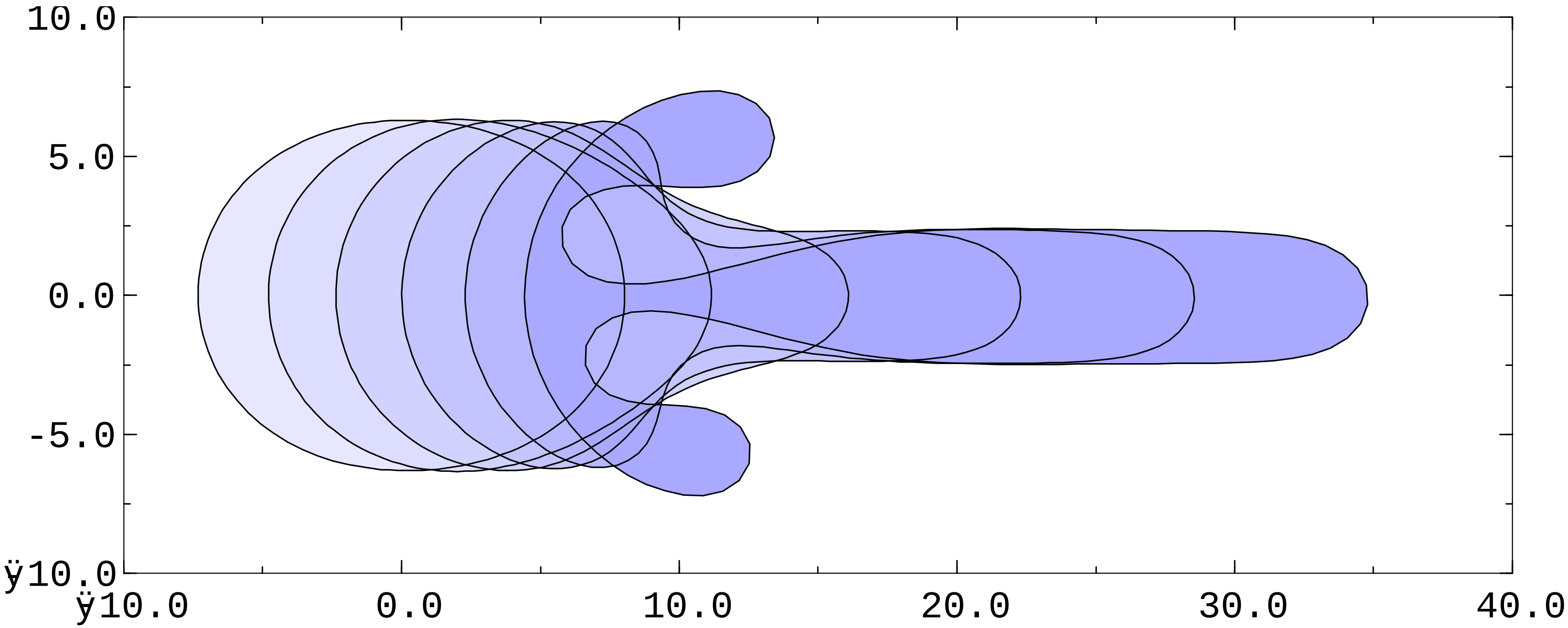
Non-circular stationary shapes



- Dimensionless initial radius $R_0 = R/l_E = 3.3, 4, 5, 6$
- Shapes approach a finger solution of width $W \approx 4.8 l_E$

(Suo, Wang, Yang 1994)

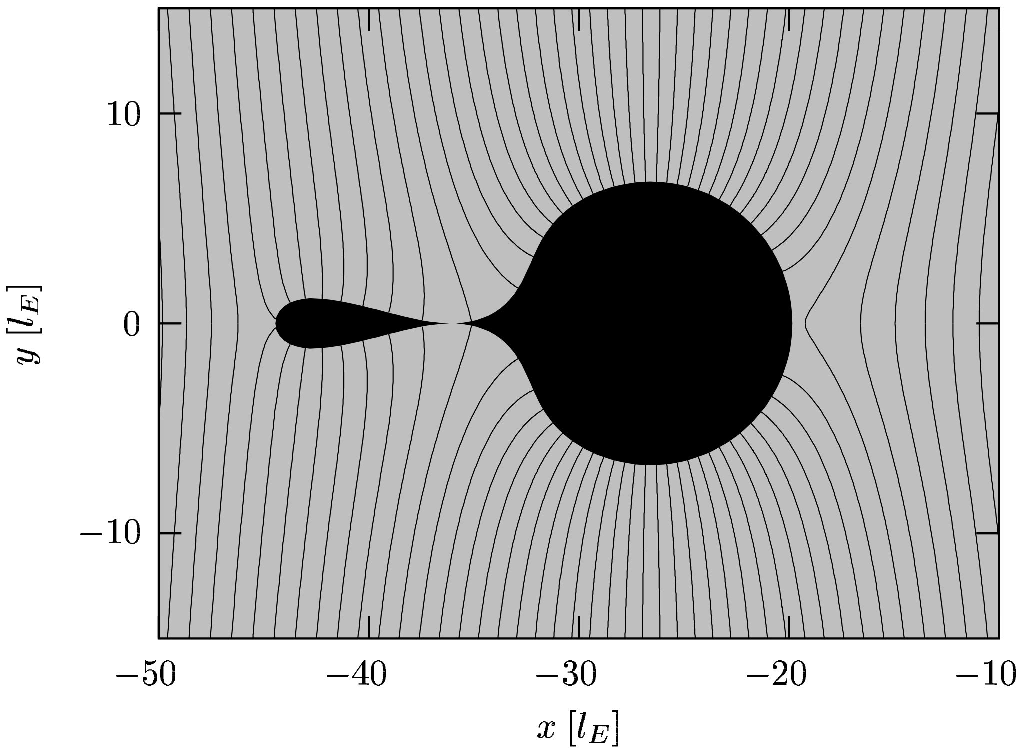
Island breakup



- Dimensionless radius $R_0 = R/l_E = 7$
- Breakup mediated by outgrowth of finger

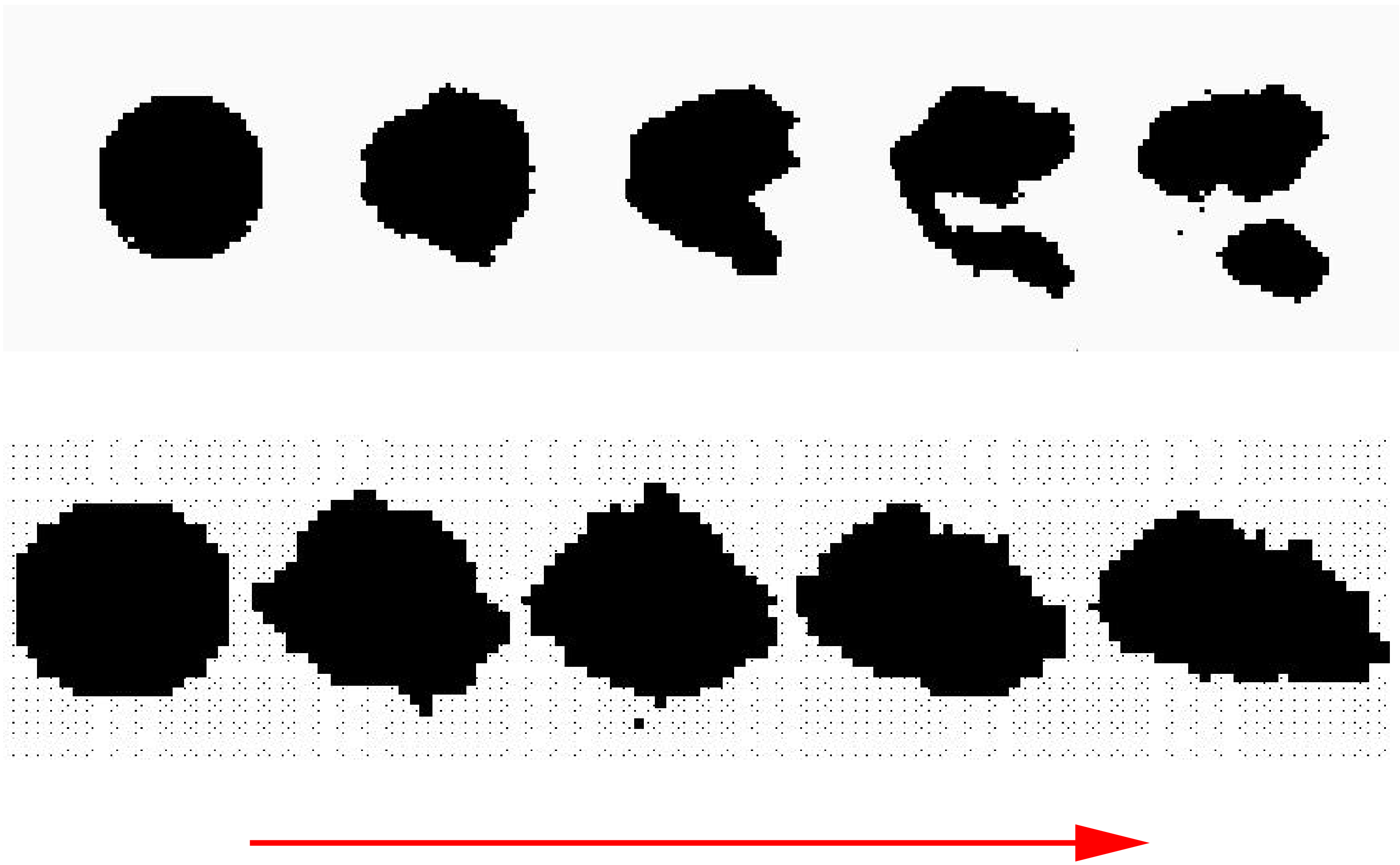
Void breakup

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



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

Island breakup in kinetic Monte Carlo simulations

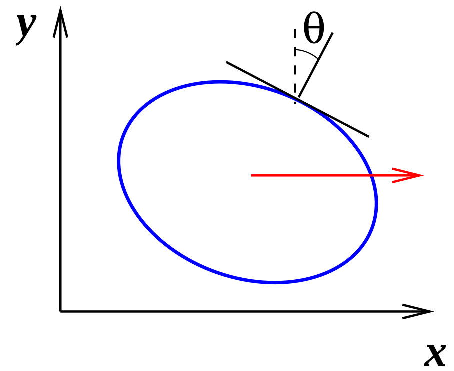


O. Pierre-Louis, T.L. Einstein, Phys. Rev. B **62**, 13697 (2000)

Anisotropic 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

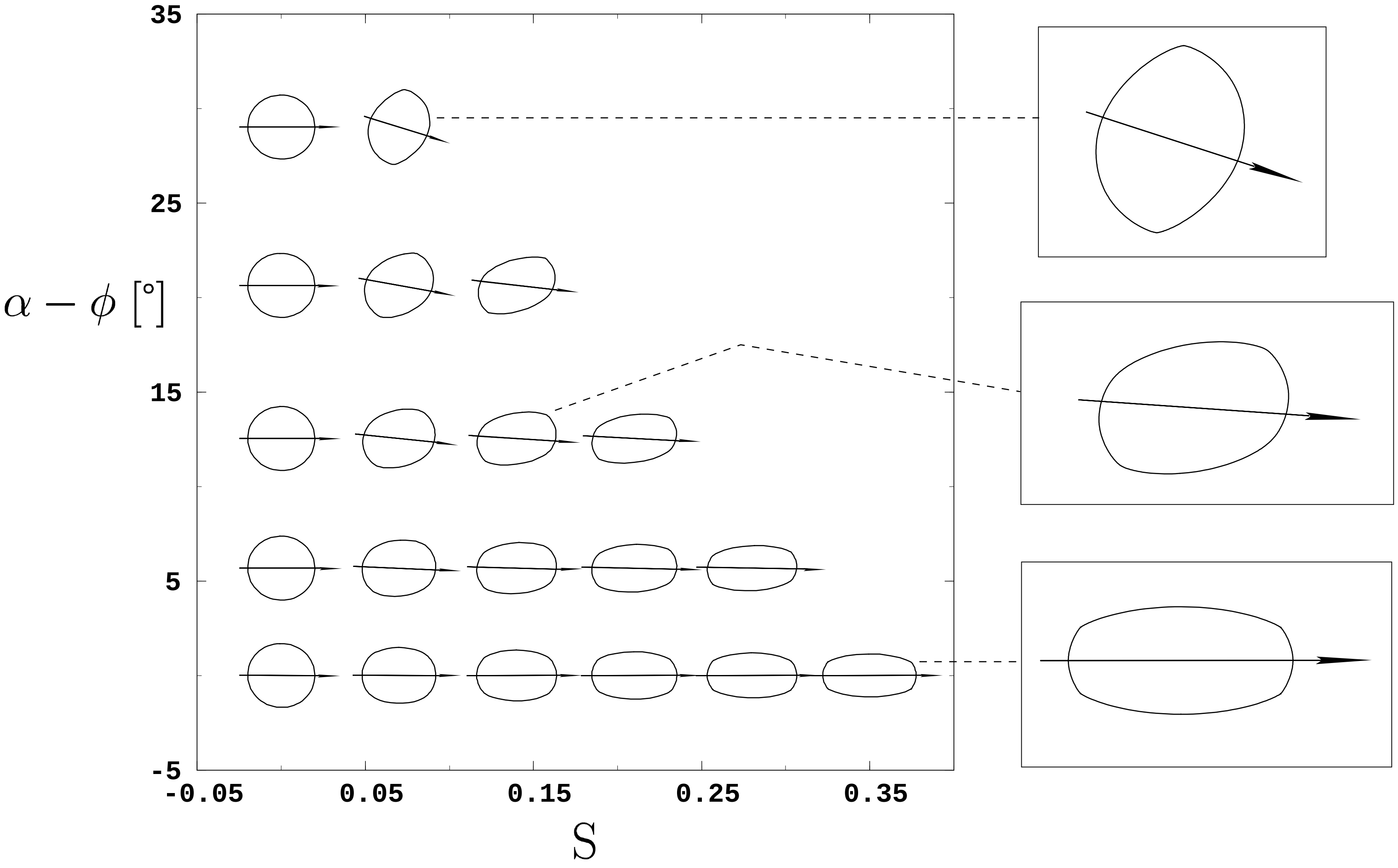
(ii) no self-intersections $\Rightarrow$ $dy/d\theta \neq 0$ for $\theta \neq 0,\ \pi$

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

Consequences:

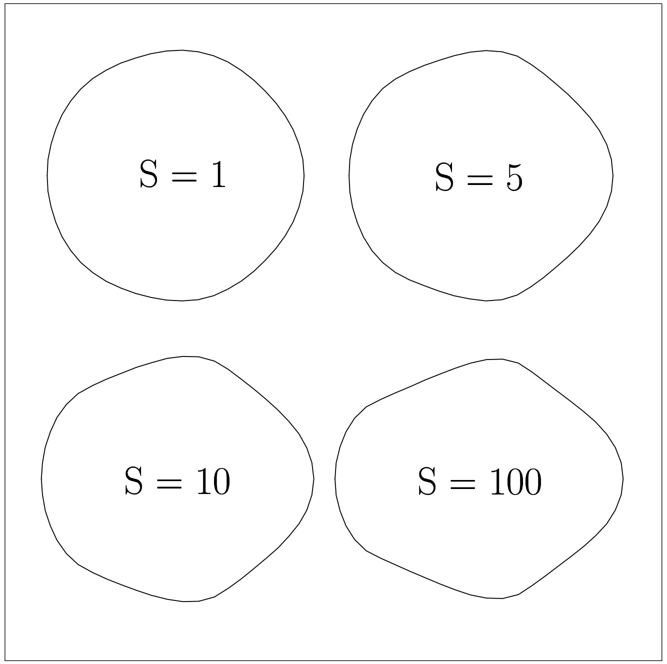
- No stationary shapes for odd n **!**
- For even n smooth stationary shapes exist in a range $0 < S < S_c$ of anisotropy strengths
- Condition (i) selects direction of island motion which is generally **different** from the direction of the field

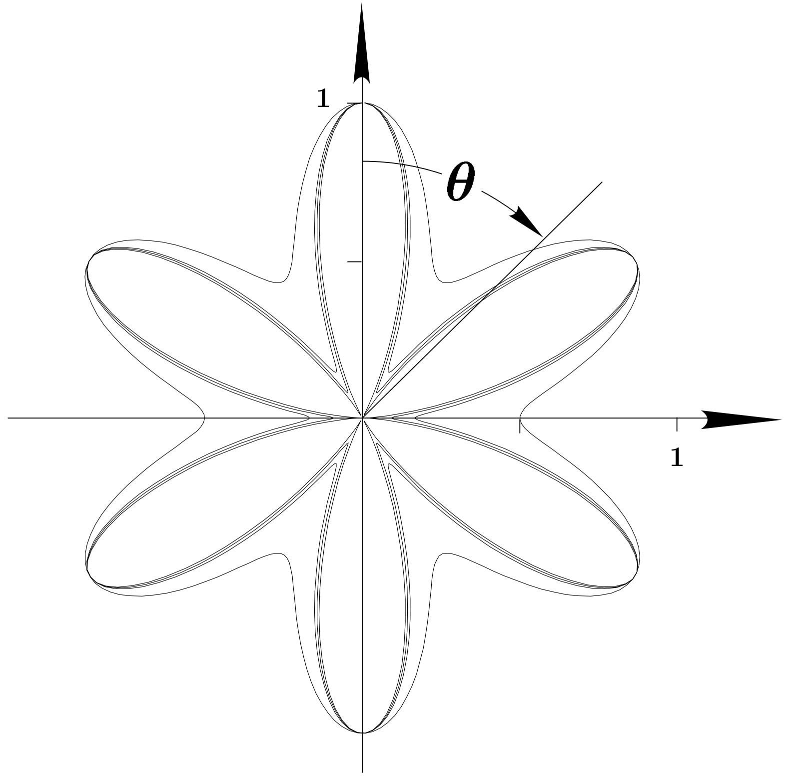
Stationary shapes without capillarity for $n = 6$



- Direction of motion may vary discontinuously with $\alpha - \phi$

Anisotropic stationary shapes with capillarity

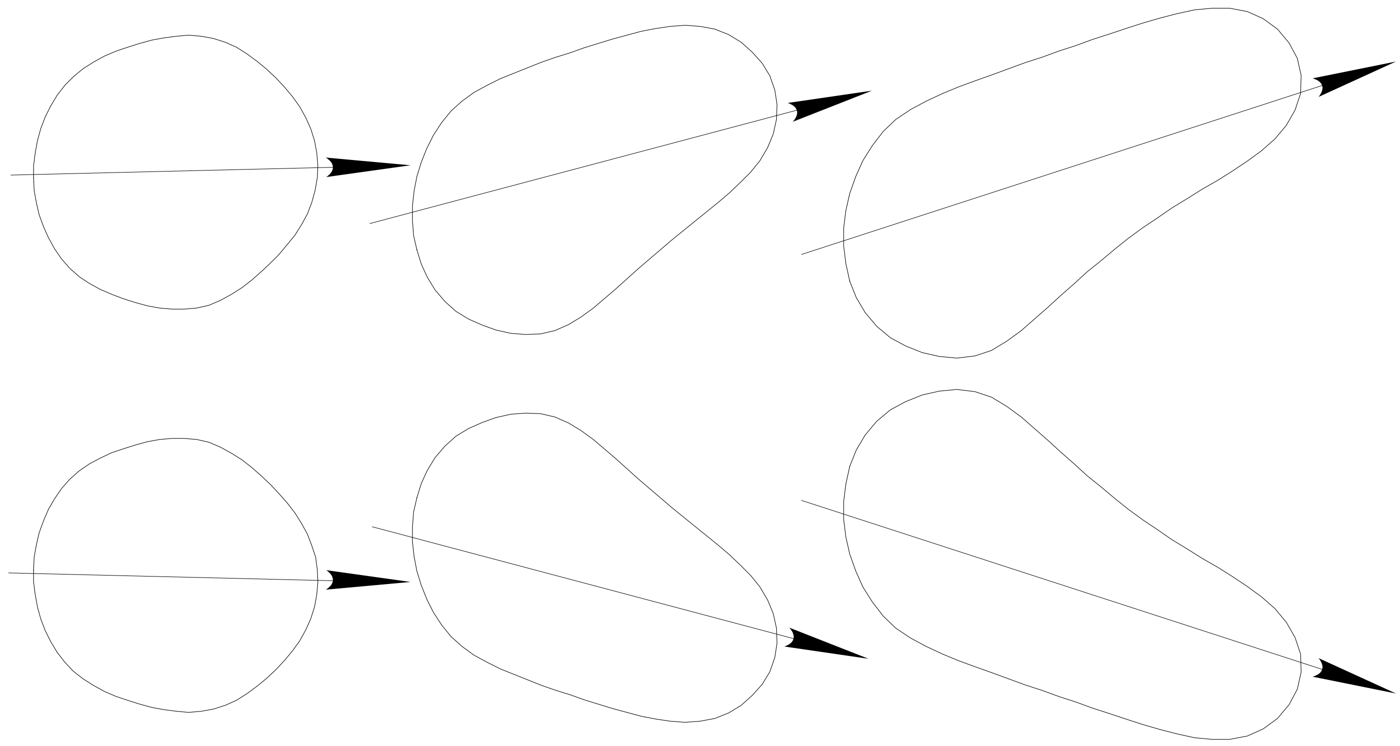




$R_0 = 2.5$ $\sigma(\theta)$ for $n = 6$

- $\sigma(\theta) = \sigma_0\{1 + S\cos^2[n\theta/2]\}$, isotropic stiffness
- R_0: Dimensionless radius of a circle of the same area

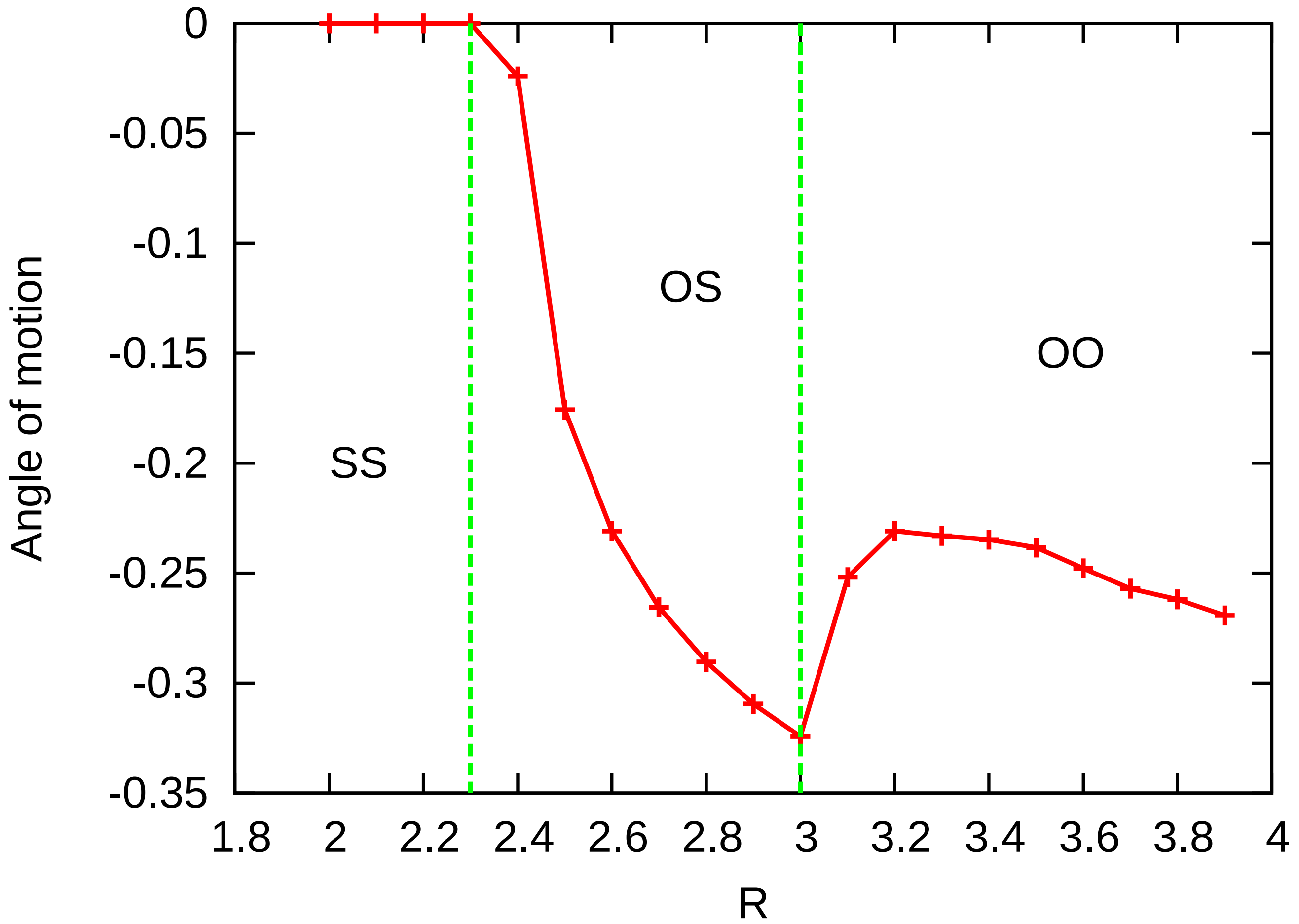
Obliquely moving stationary shapes (n=6, S=2)



$R_0 = 2.4$ $R_0 = 2.7$ $R_0 = 3.0$

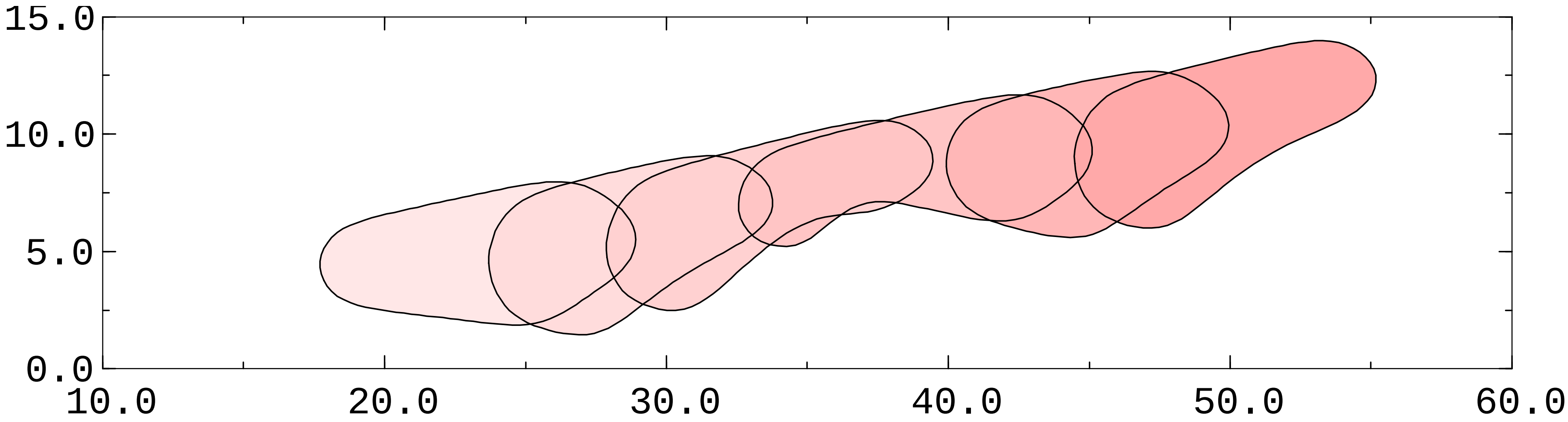
- Spontaneous breaking of symmetry w.r.t. field & anisotropy direction

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



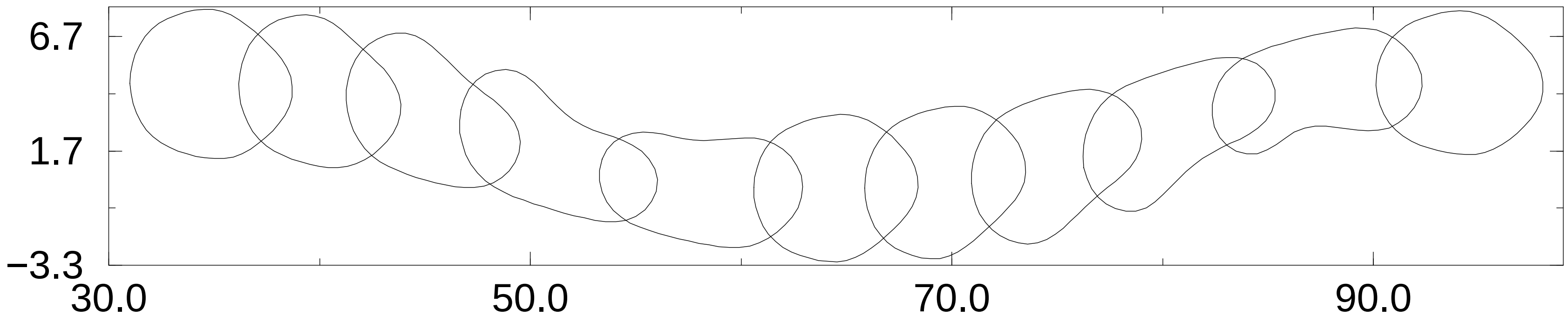
SS: straight stationary **OS**: oblique stationary **OO**: oblique oscillatory

Oblique oscillatory motion

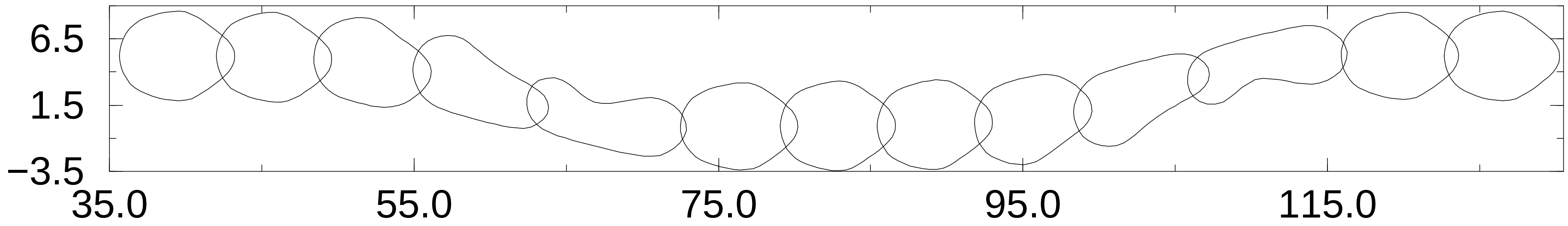


- Dimensionless radius $R_0 = 4$, anisotropy strength $S = 1$
- Upper edge is linearly stable, lower edge linearly unstable

Zig-zag motion

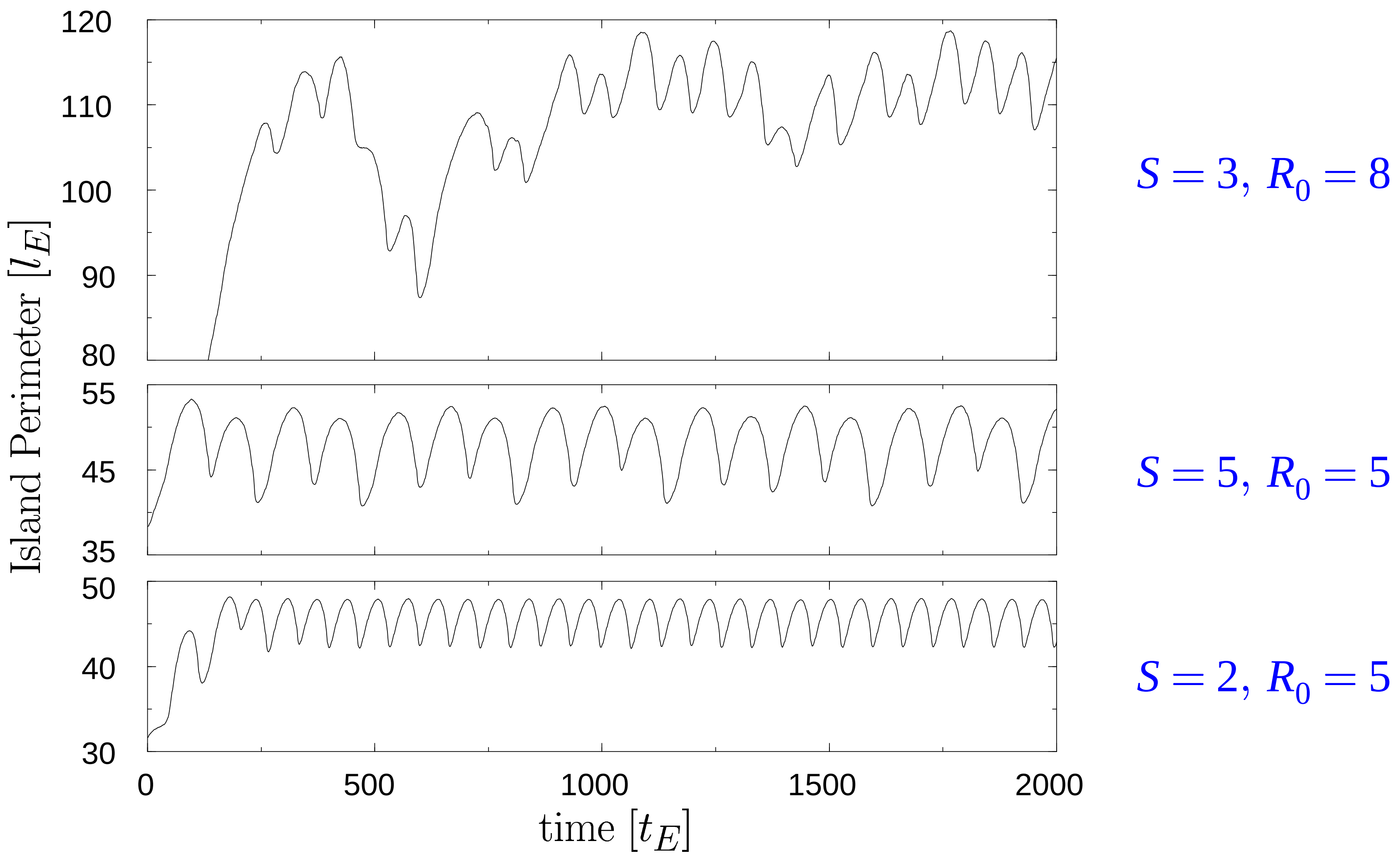


$R_0 = 3.5$, $S = 0.5$



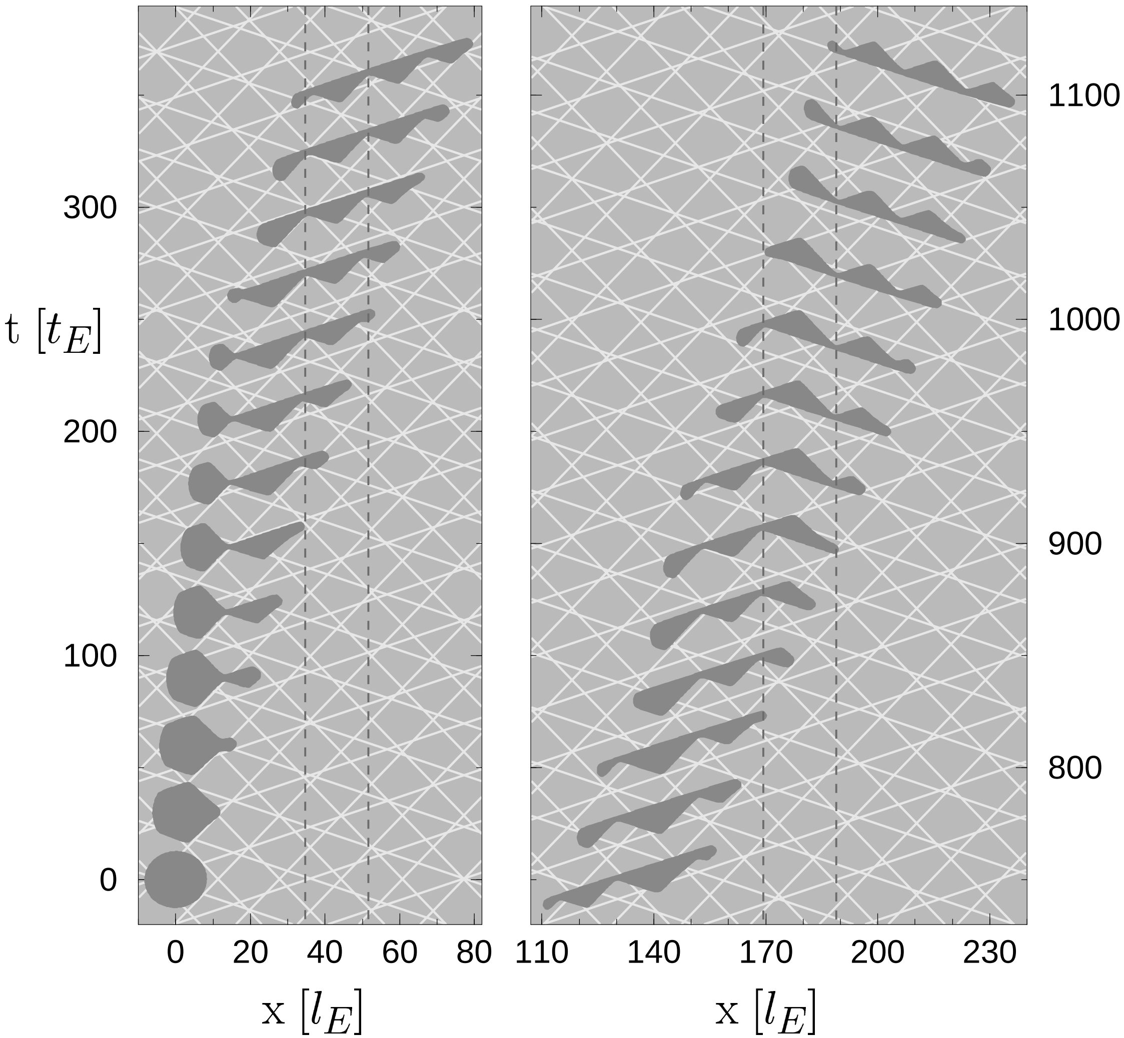
$R_0 = 3.5$, $S = 1$

Regular and irregular oscillations of the island perimeter



characteristic time scale: $t_E = l_E^4/\sigma_{\max}\tilde{\gamma}$

Complex oscillatory motion



$S = 3, R_0 = 8$

Selected facets and the origin of oscillations

- Large islands are composed of selected facets which are stationary **in the substrate frame**. Oscillations arise because islands **slide past** the static facets.

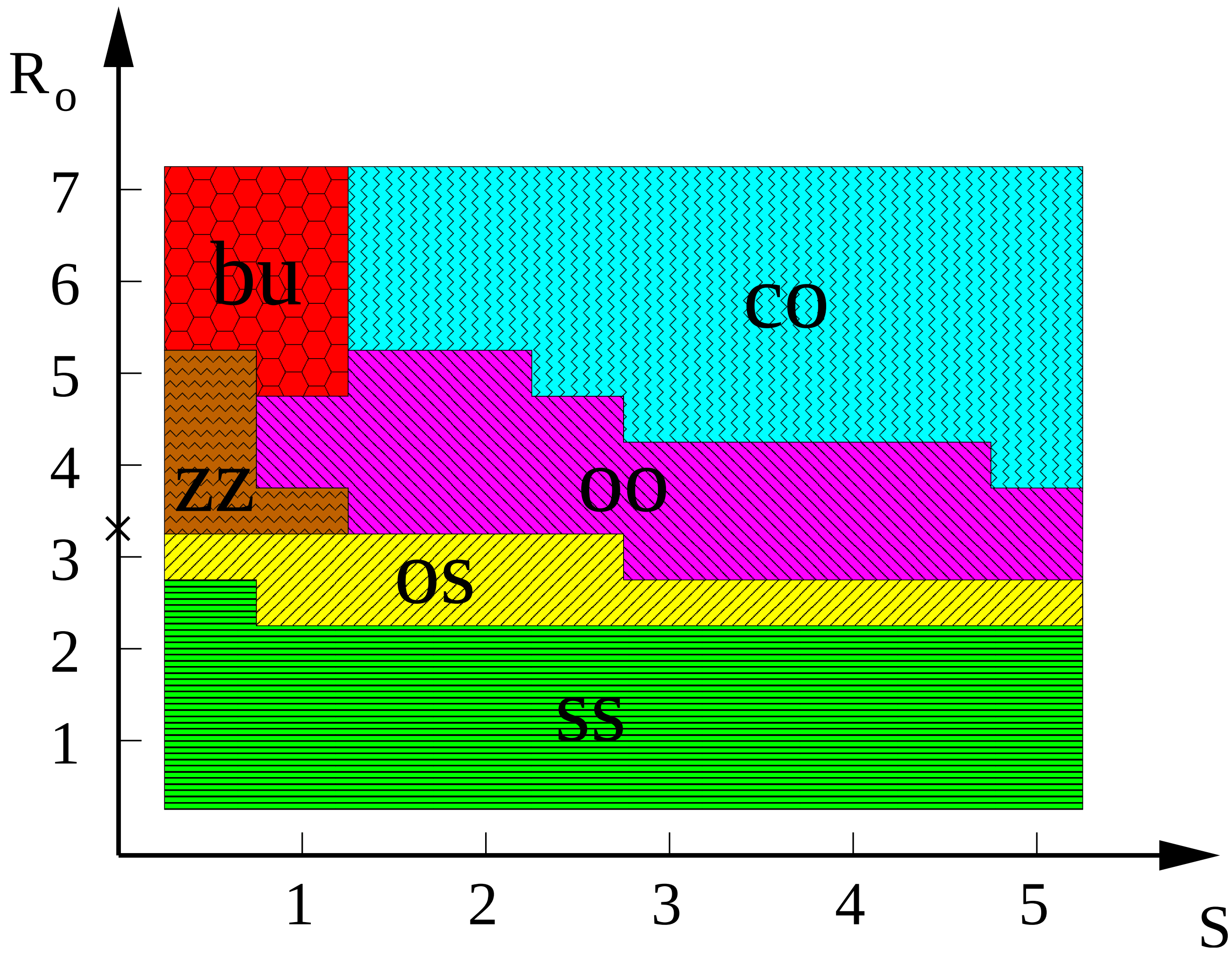
- Facets are constant current solutions of the evolution equation:

$$j = j^* \quad \Rightarrow \quad \tilde{\gamma}\frac{d^2}{ds^2}\theta(s) = -\frac{j^*}{\sigma(\theta)} + F_0\cos(\theta) \equiv -V'(\theta)$$

- Facet orientations are degenerate maxima of the "potential" $V(\theta)$

- For $n = 6,\ \alpha = 0$ there are four selected orientations, out of which three are needed to form a closed island:

A tentative phase diagram



bu: island breakup

co: complex oscillatory

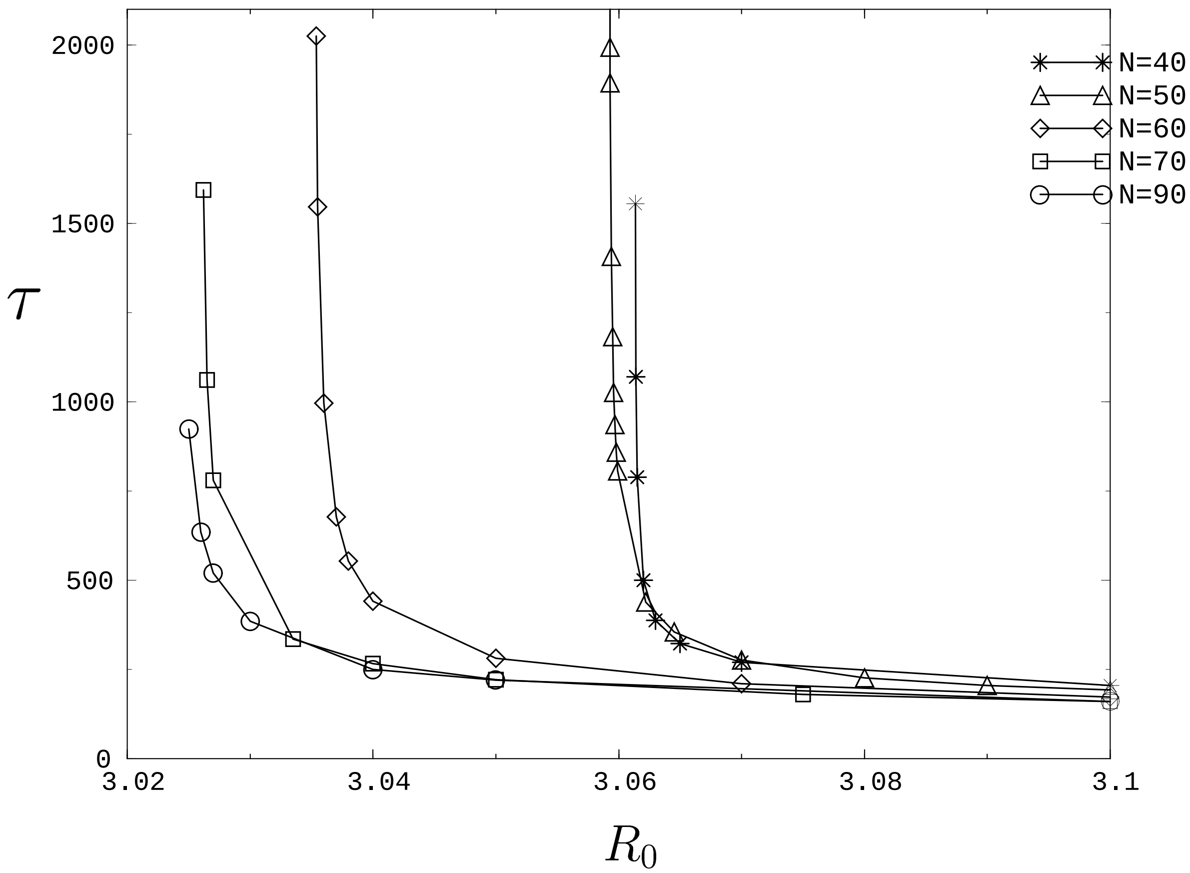
oo: oblique oscillatory

zz: zig-zag

os: oblique stationary

ss: straight stationary

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

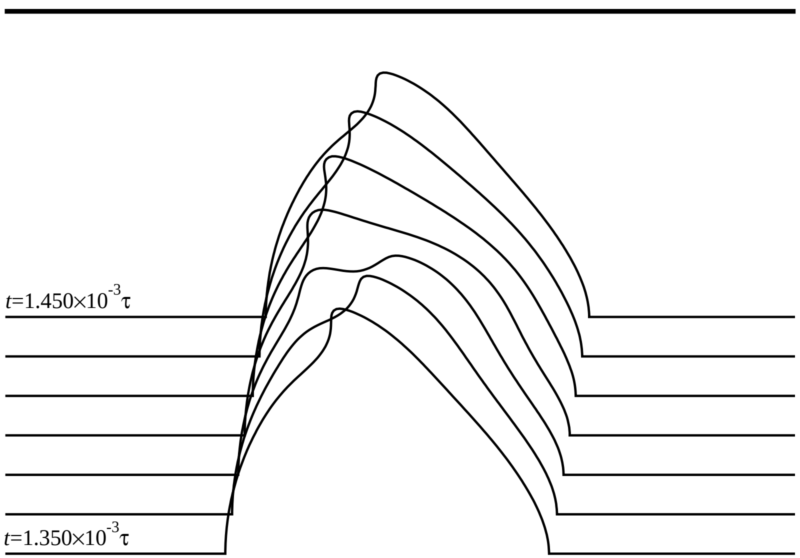


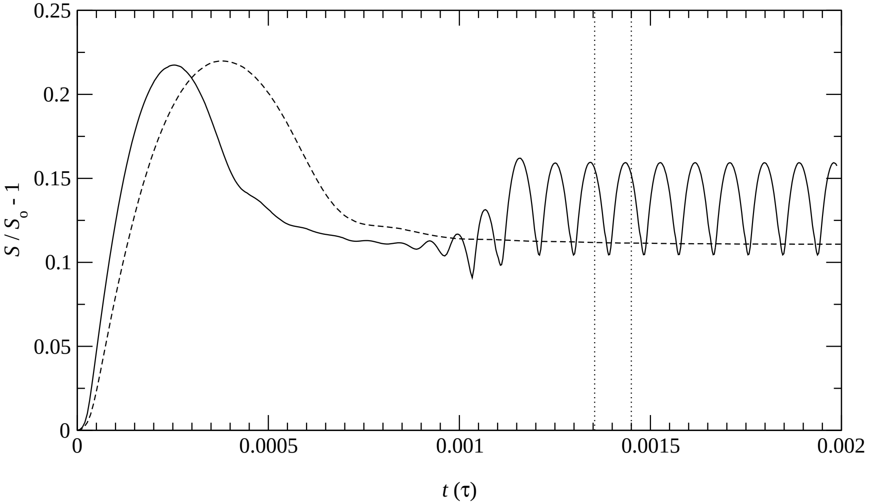
- N: Number of discretization points
- Best fit: $\tau \sim (R_0 - R_c)^{-2.5}$

Oscillatory behavior in void electromigration

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

Experimental considerations: Islands on Cu(100)

- Electromigration force on a step atom: 400 eV/cm at $i = 10^7$ A/cm^2

  H. Mehl, O. Biham, O. Millo, M. Karimi, Phys. Rev. B **61**, 4975 (2000)

- Step stiffness $\tilde{\gamma} \approx 0.13$ eV/atom for kinked steps

  S. Dieluweit, H. Ibach, M. Giesen, T.L. Einstein, Phys. Rev. B **67**, 121410 (2003)

$$\Rightarrow \quad l_E \approx 25 - 100 \text{ nm}$$

- Characteristic time scale from step fluctuation kinetics

  M. Giesen, S. Dieluweit, J. Mol. Cat. A **216**, 263 (2004)

$$\Rightarrow \quad t_E = \frac{l_E^4}{\sigma_{\max}\tilde{\gamma}} \approx 1\text{s} \;\; \text{at} \;\; 300 \text{ K}$$

Outlook

- Nature of bifurcations (low-dimensional truncation)?
- Oscillatory behavior in kinetic Monte Carlo simulations?
- Nonlinear behavior in the kinetic regimes involving mass exchange with the terrace?