# Coarsening (and anticoarsening) dynamics

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Encyclopedia of Complexity and Systems Science (Springer, 2009)

**Coarsening** -
The monotonic increase of the typical length scale
of a structure in time. [...]
Coarsening slows down if the length scale increases.

# Phase Transitions and Critical Phenomena

Volume 8

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## 3. The Dynamics of First-order Phase Transitions

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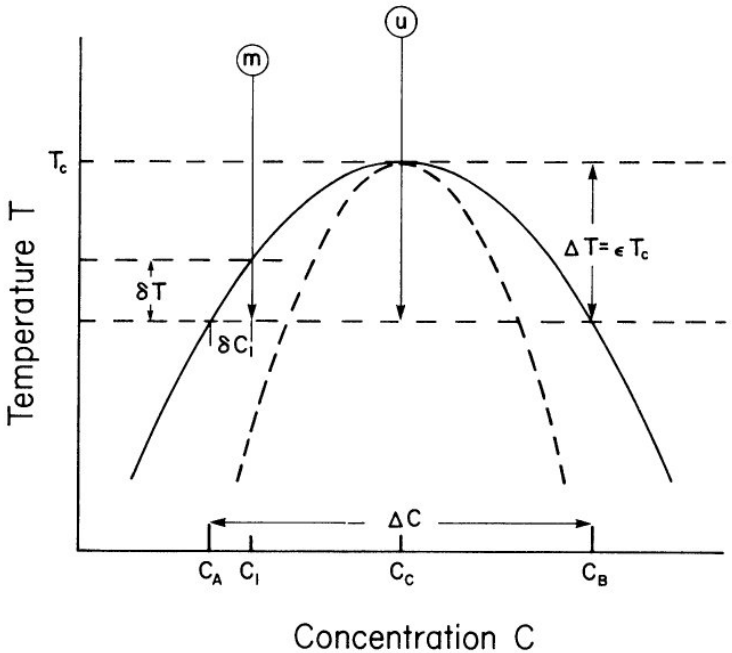


FIG. 1. The coexistence curve (solid line) and classical spinodal curve (dashed line) are shown schematically for a system such as a binary fluid or binary alloy. Typical quenches into the metastable (m) and the unstable (u) regions are also shown. In the former case the system is under-cooled by an amount $\delta T$, corresponding to an initial supersaturation $\delta c_1 = c_1 - c_A$, at a temperature $T = T_c - \Delta T$ below the critical point.

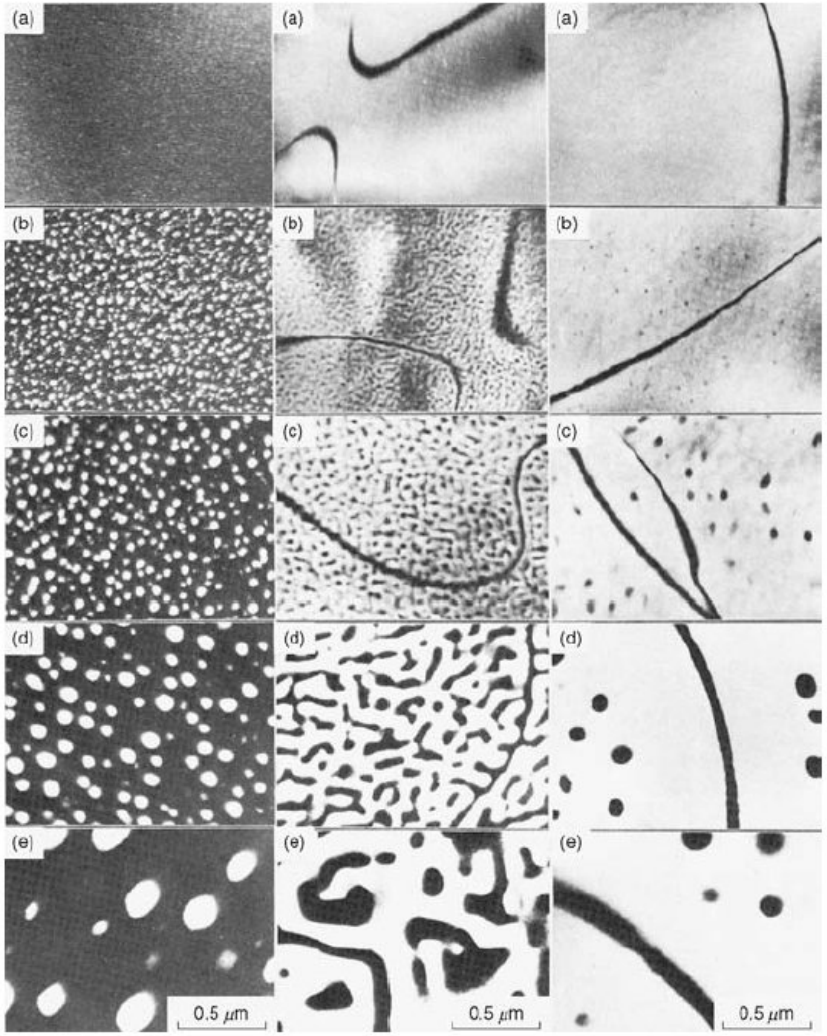


Fig. 4.2. Coarsening of domain structure following quenches from the disordered phase region at $T = 630°C$ to the region of two coexisting phases at $T = 570°C$. Two concentrations corresponding to off-critical paths (left and right panels) and a concentration corresponding to a near-critical path (center set of panels) are shown. Reprinted photo 1 with permission Oki *et al.* (1977).

# Reverse Epitaxy of Ge: Ordered and Faceted Surface Patterns

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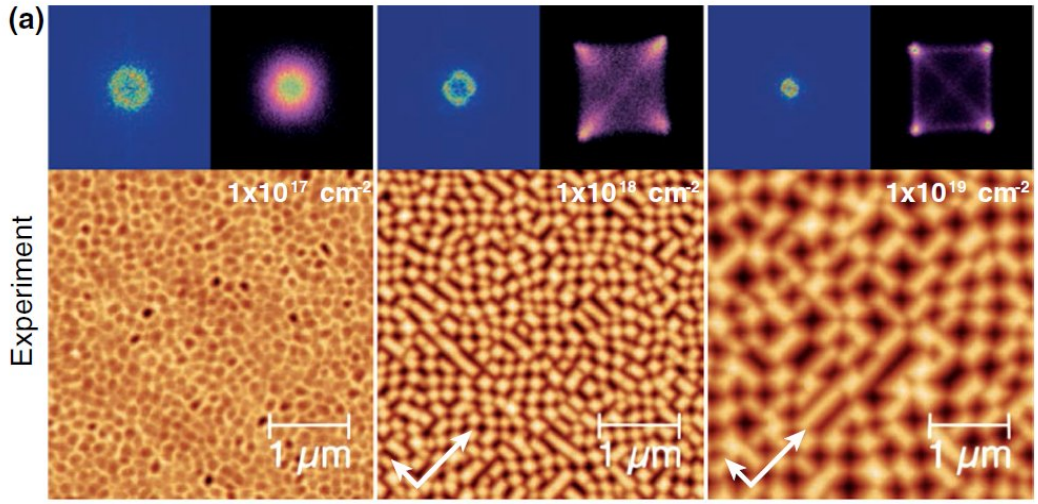
Normal incidence ion irradiation at elevated temperatures, when amorphization is prevented, induces novel nanoscale patterns of crystalline structures on elemental semiconductors by a reverse epitaxial growth mechanism: on Ge surfaces irradiation at temperatures above the recrystallization temperature of 250 °C leads to self-organized patterns of inverse pyramids. Checkerboard patterns with fourfold symmetry evolve on the Ge (100) surface, whereas on the Ge (111) surface, isotropic patterns with a sixfold symmetry emerge. After high-fluence irradiations, these patterns exhibit well-developed facets. A deterministic nonlinear continuum equation accounting for the effective surface currents due to an Ehrlich-Schwoebel barrier for diffusing vacancies reproduces remarkably well our experimental observations.








# Sand Ripples and Dunes

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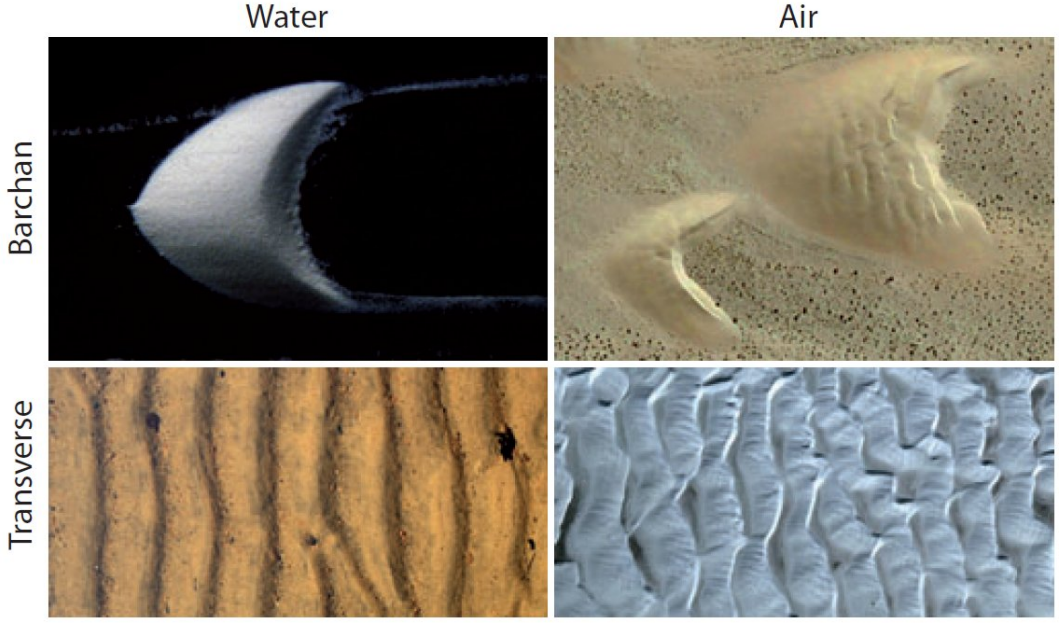

# Does Anticoarsening exist?

PHYSICAL REVIEW E **82**, 011606 (2010)

**Anticoarsening and complex dynamics of step bunches on vicinal surfaces during sublimation**

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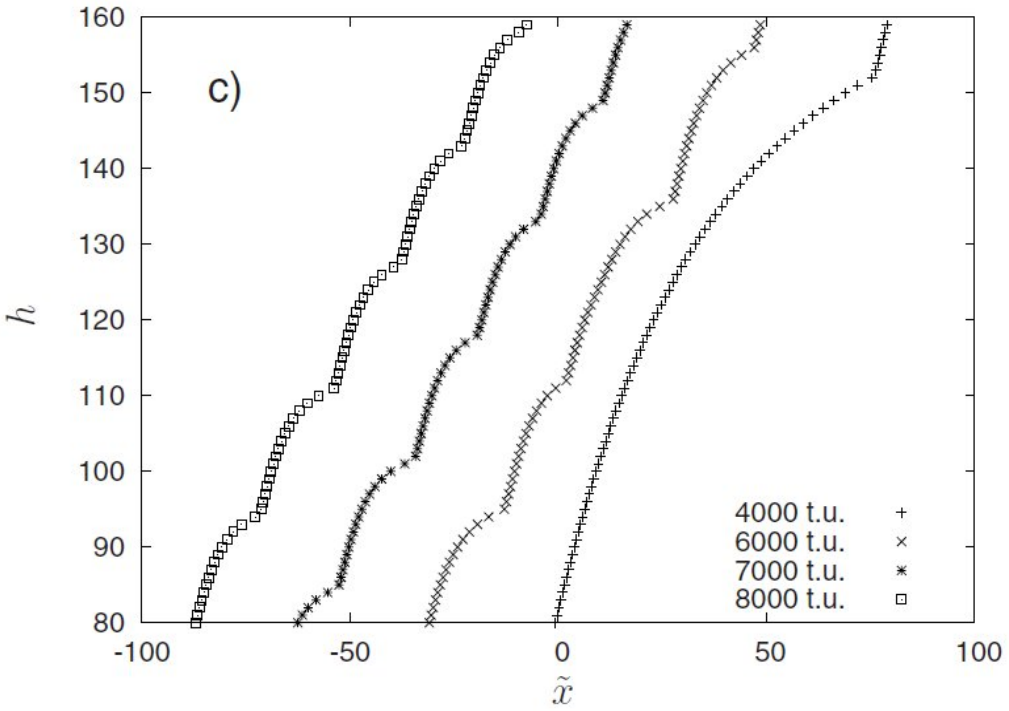


JOURNAL OF APPLIED PHYSICS **114**, 144310 (2013)

**Tuning Ag/Si(100) island size, shape, and density**

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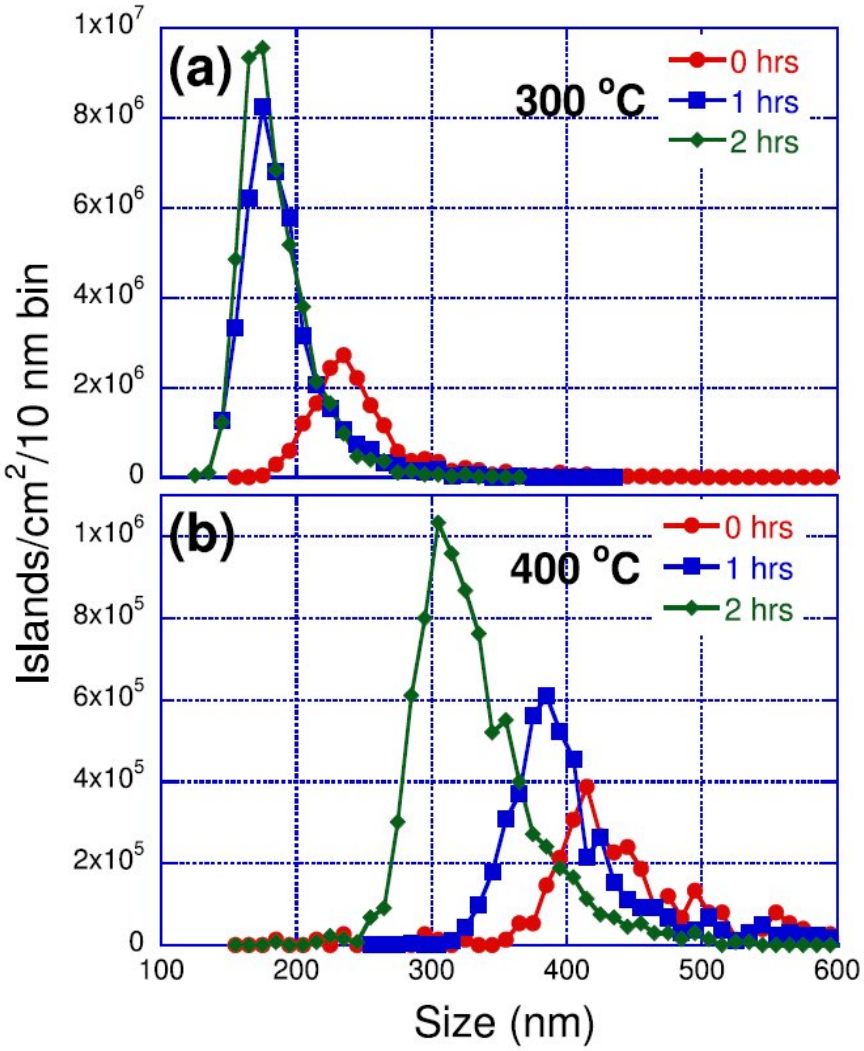


## Important questions

- When does (anti)coarsening occur?
- Why does coarsening may stop?
- What is the coarsening exponent, $L(t) \approx t^n$?

## The answers (to the third Q) highlight the importance of

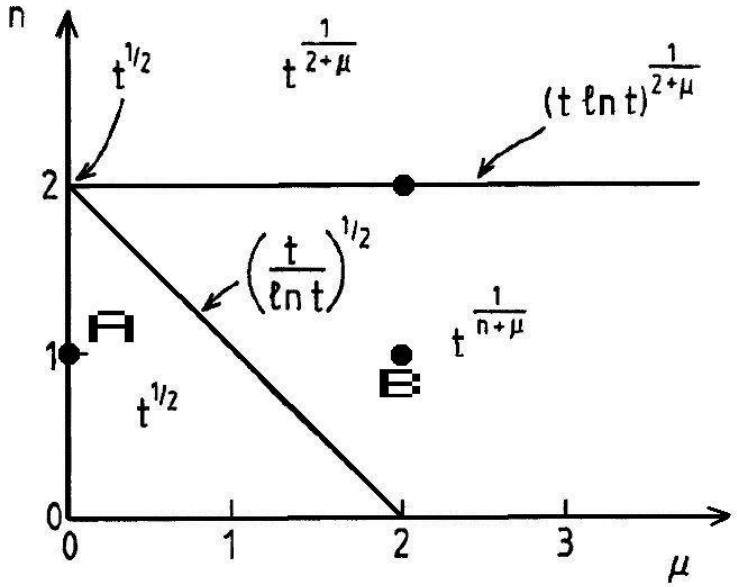
- Conservation laws
- Space dimension and order parameter dimension
- Noise

as shown (for $O(n)$ models) by Bray and Rutenberg...

## (Bray&Rutenberg)'s theory of Phase ordering [PRE **49**, R27 (1994)]

$$\partial_t \vec{\phi}_{\boldsymbol{k}} = -k^{\mu}(\partial \mathcal{H}/\partial \vec{\phi}_{-\boldsymbol{k}}) \qquad \mathcal{H}[\vec{\phi}] = \int d^d x[(\nabla\vec{\phi})^2 + (\vec{\phi}^2 - 1)^2]$$

*"We consider the time dependence of the energy as the system relaxes towards its ground state, using the dynamic scaling hypothesis. We obtain $L(t)$ consistently by comparing the global rate of energy change to the energy dissipation from the local evolution of the order parameter."*



## Beyond Bray & Ruthenberg theory:

some models { have not a Lyapunov functional
cannot be described in terms of defects
display interrupted coarsening or anticoarsening
are discrete

## Our starting point:

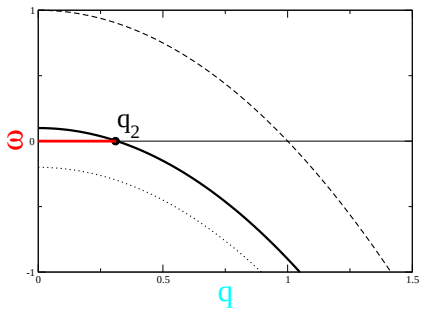
Coarsening as phase instability of periodic steady states.

## Our approach: a multiscale analysis to get a phase diffusion equation

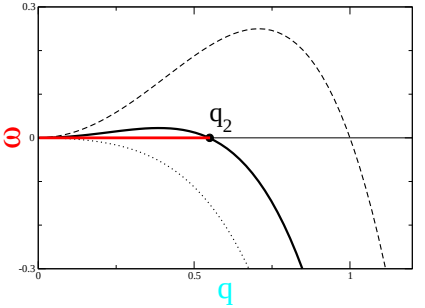
If $u_0(x)$ is a stationary solution, also $u_0(x+\psi)$ is solution.
We study phase dynamics assuming that $\psi = \psi(X,T)$.

### Highlights:

- Dynamical infos from static infos
- Systematic derivation of the coarsening exponent, $L(t) \approx t^n$
- Understanding when (and why) coarsening occurs
- Discriminate between perpetual and interrupted coarsening (and anticoarsening?)
- Applicability to non-potential equations



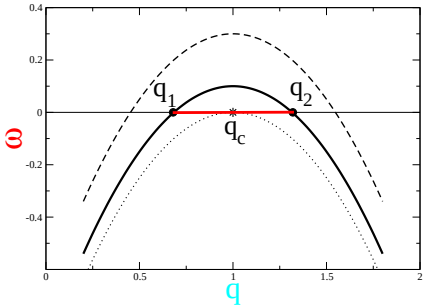

TDGL (mod A) generalized $\partial_t u = B(u) + G(u) u_{xx}$ $(d = 1, 2)$



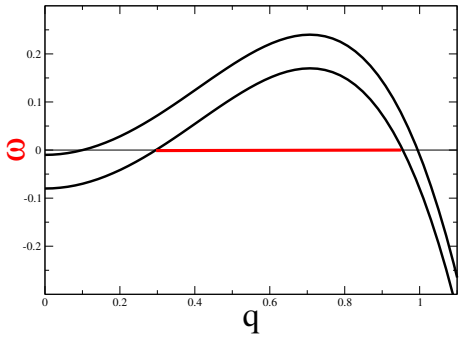

CH (mod B) generalized $\partial_t u = -C(u)\partial_{xx}[B(u)+G(u)u_{xx}]$ $(d = 1, 2)$

Crystal growth equation $\partial_t h(\mathbf{x}, t) = -\nabla \cdot \left[\mathbf{j}(\nabla h) + \nabla(\nabla^2 h)\right]$ $(d = 2)$

KS conserved $\partial_t u = -\partial_{xx}[u + u_{xx} - (u_x)^2]$




SH generalized $\partial_t u = \sum_n c_n \partial_x^{2n} u + P(u)$




Oono equation $\partial_t u = -\partial_{xx}[B(u) + u_{xx}] - \alpha u$

For all equations, we have obtained

$$\partial_T \psi = D \partial_{XX} \psi$$

where $D = D(u_\lambda(x))$ encapsulates dynamical properties:

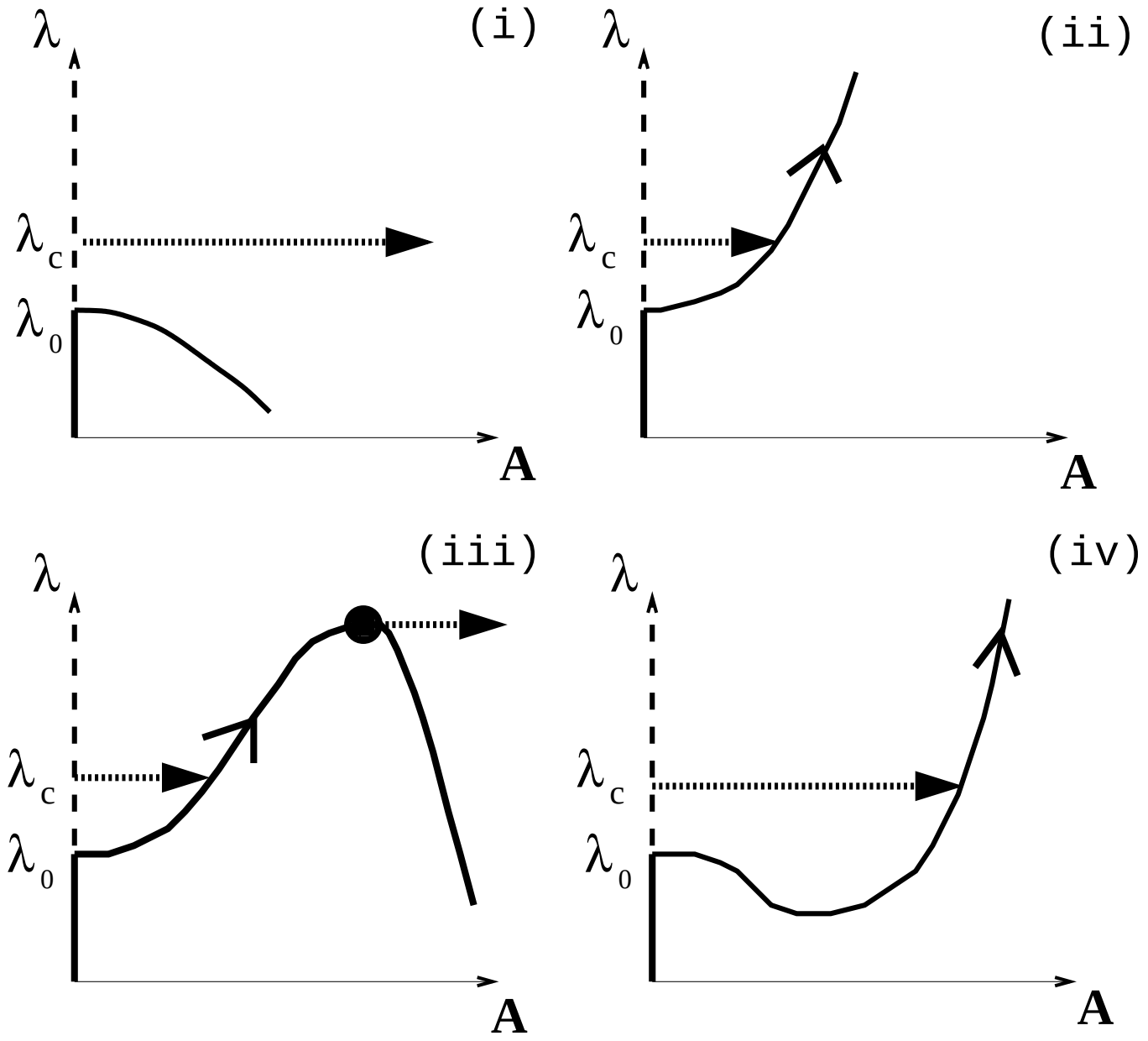
- $D = \dfrac{\partial \mathcal{A}}{\partial q} < 0 \quad \Longleftrightarrow \quad$ phase instability

- $|D(L)| \approx L^2/t \quad \Rightarrow \quad$ coarsening law $L(t)$

In some cases, we get the following criterion:

$$\text{coarsening} \Longleftrightarrow \frac{\partial \lambda}{\partial A} > 0$$

# Special dynamical scenarios in 1d (for generalized TDGL and CH)



## DNLS

$$H(n,\phi) = \sum_i n_i^2 + 2\sum_i \sqrt{n_i n_{i+1}}\cos(\phi_i - \phi_{i+1})$$

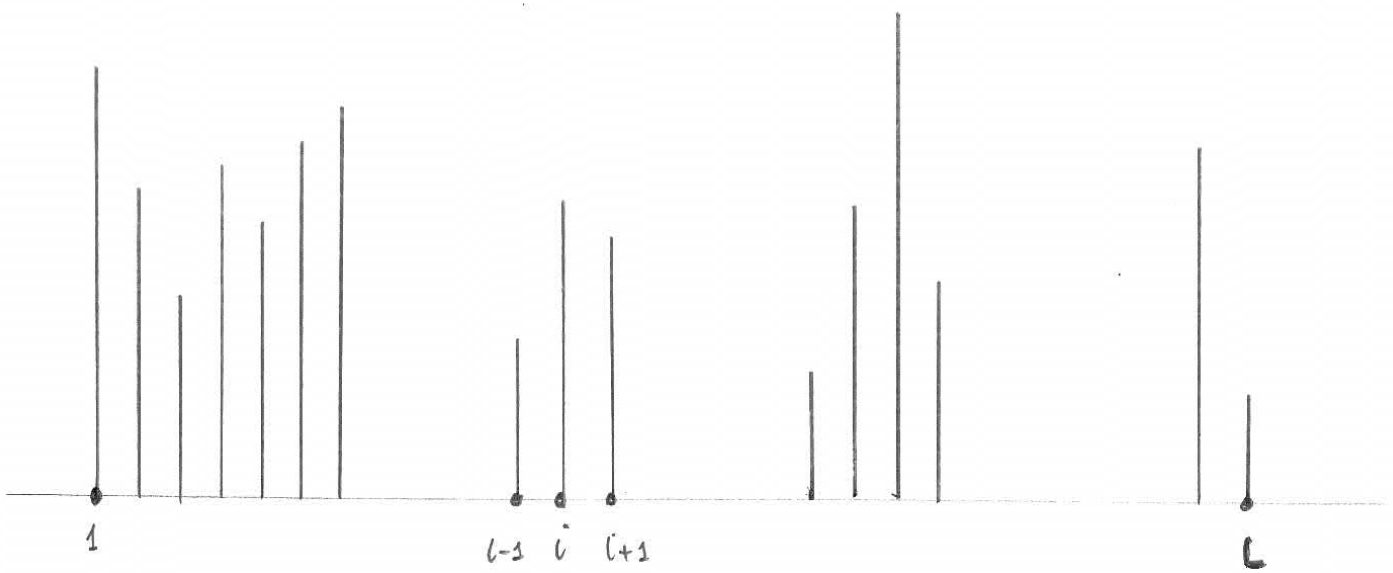
$$A(n,\phi) = \sum_i n_i$$

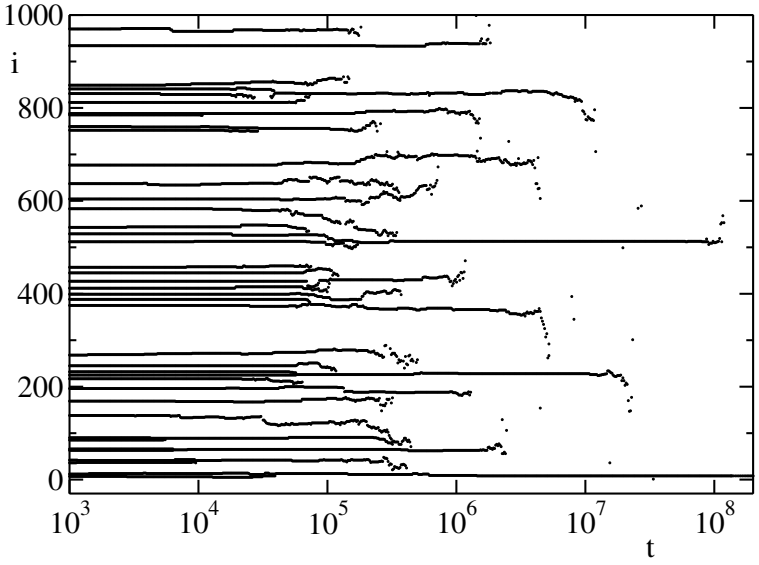
$h > 2a^2$ negative temperature region

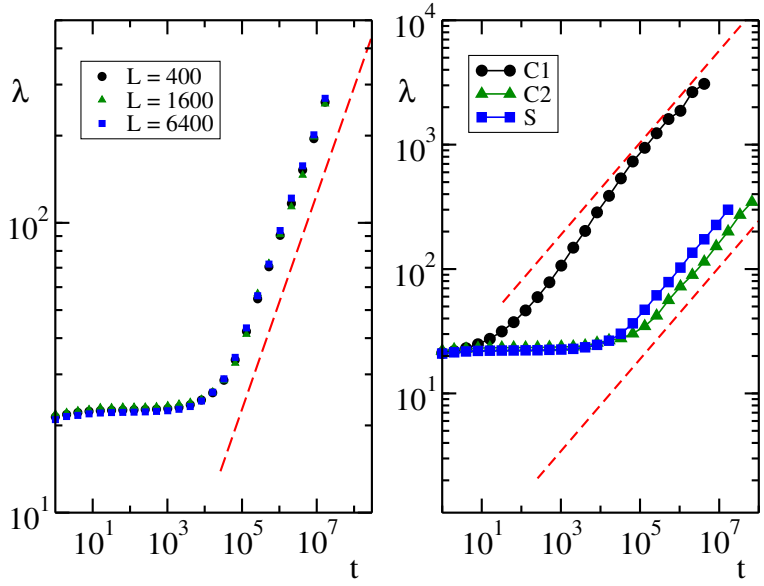
## Simplified (and purely stochastic) DNLS

$$H(n,\phi) = \sum_i n_i^2 + \cancel{2\sum_i \sqrt{n_i n_{i+1}}\cos(\phi_i - \phi_{i+1})}$$

# This model produces "breathers" which coarsen endlessly



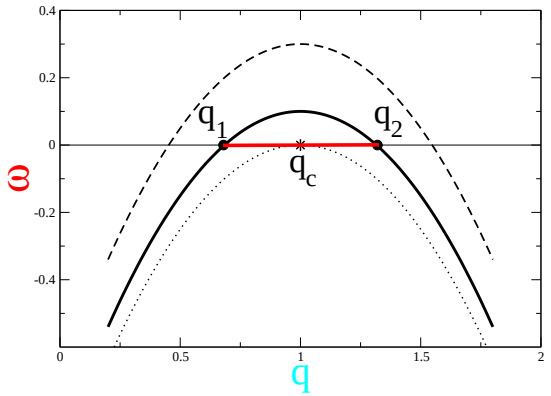
## When does coarsening stop?

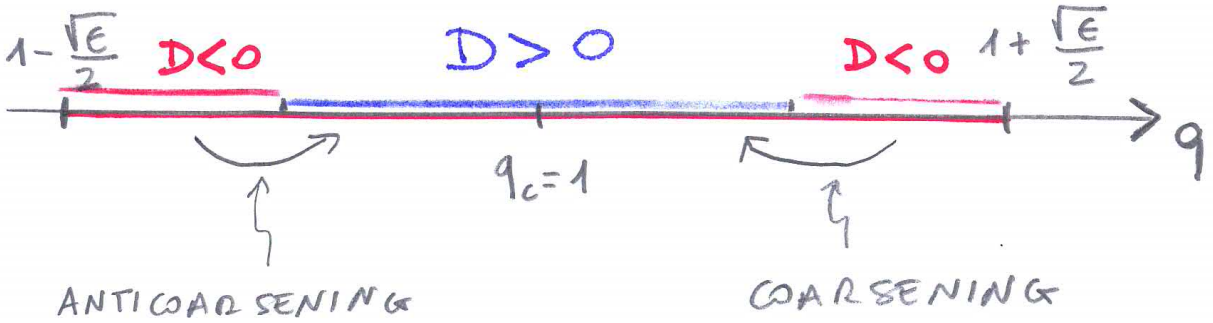
- $\frac{\partial \lambda}{\partial A} = 0 \qquad ( \ D(q) = 0 \ )$

- Coarsening is driven by a free energy, which has a minimum for a finite domain size: the 1d Ising model or the Oono equation (diblock copolymers).

- Some additional ingredient introduces a new length scale (disorder, stirring/shearing of binary fluids).
  Coarsening may stop or become extremely slow.

# Anticoarsening: the first example



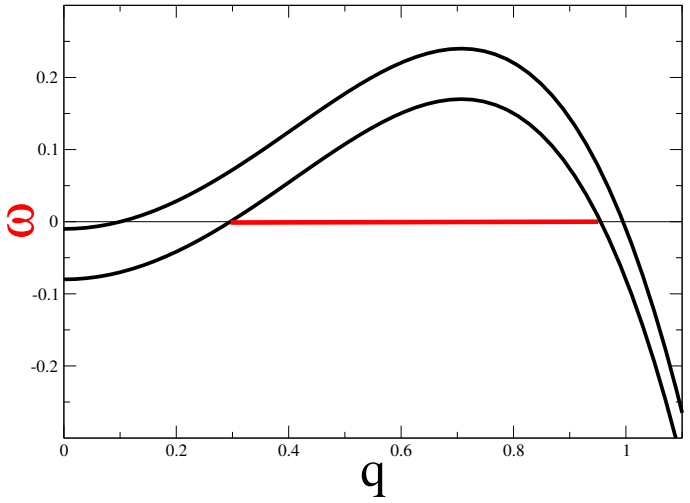

## Eckhaus instability

$$\partial_t u = \epsilon u - (1+\partial_{xx})^2 u - u^3$$

## Another (unacknowledged) example

Phase separation in diblock copolymers

$$\partial_t u = -\partial_{xx}[B(u) + u_{xx}] - \alpha u$$



## Open, general questions

- Is there coarsening outside a phase instability? (I think not)
- Is there anticoarsening outside a phase instability? (I think yes)
- How to determine $D$ for discrete models
- Is it possible to determine $D$ from a simulation?
- Is there some principle, based on $D$, driving the dynamics?

In collaboration with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Matteo Nicoli

Alessandro Torcini

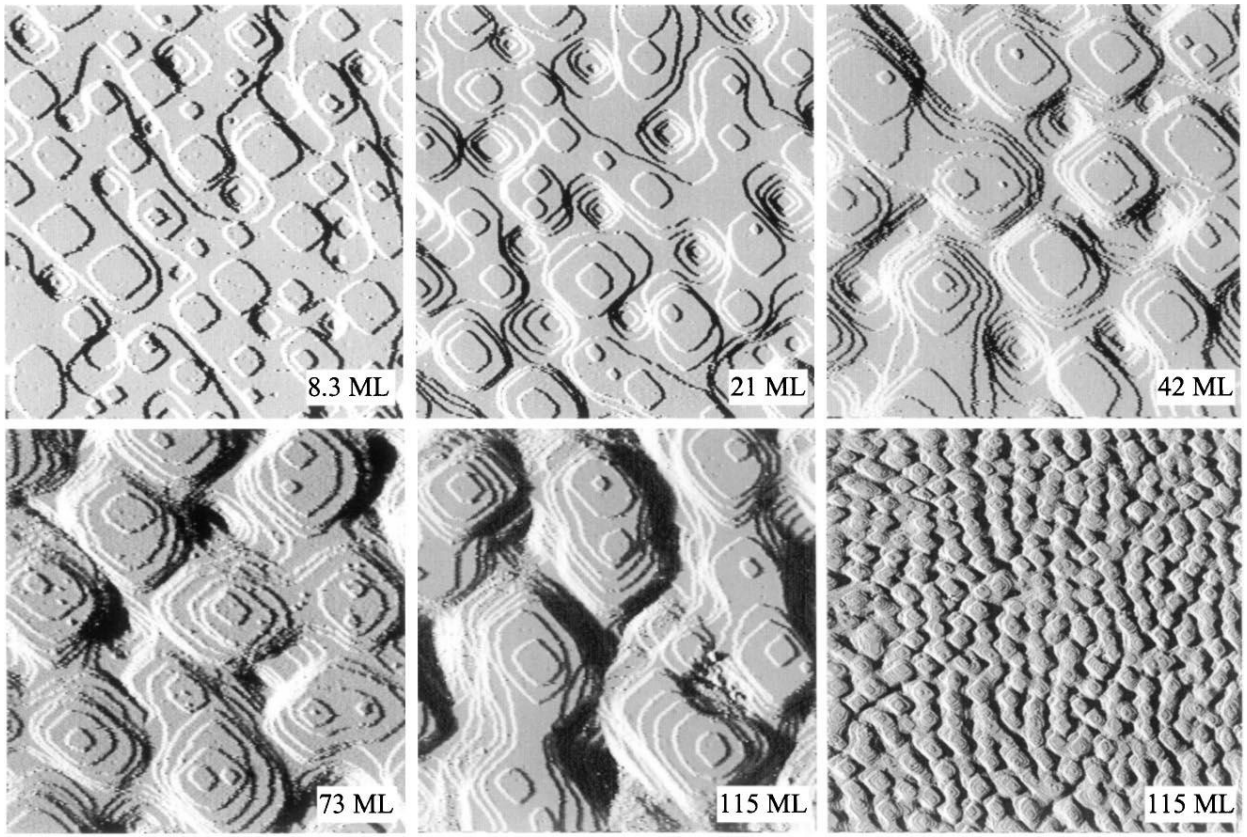

Stefano Iubini

Antonio Politi

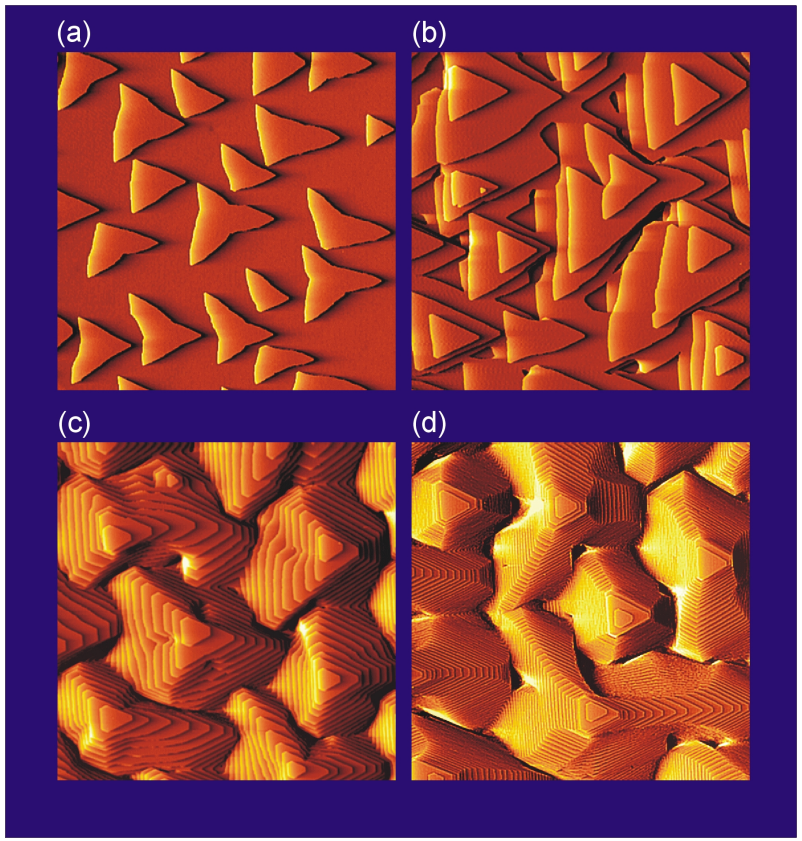
# Recent results on a growth equation in 2d

$$\partial_t h(\mathbf{x},t) = -\nabla \cdot \left[\mathbf{j}(\nabla h) + \nabla(\nabla^2 h)\right]$$

$$\mathbf{j}(\nabla h) = \nabla h + \text{nonlinear terms} \qquad \omega(\mathbf{q}) = \mathbf{q}^2 - \mathbf{q}^4$$




Cu(100)/Cu (Zuo & Wendelken, PRL 1995) [1000-5000Å]




Pt(111)/Pt (Th. Michely, Köln University)

# Multiscale approach for the growth equation

Perturbative expansion and different scales

$$h = \tilde{h}_0 + \varepsilon \tilde{h}_1 + \ldots$$

| fast scales | slow scales |
|---|---|
| $t = t$ | $T = \varepsilon^2 t$ |
| $x = x$ | $X = \varepsilon x$ |
| $y = y$ | $Y = \varepsilon y$ |
| $\varphi_i$ | $\psi_i = \varepsilon \varphi_i$ |

$$\varphi_i = \mathbf{q_i} \cdot \mathbf{x} \qquad \mathbf{q_i} = \nabla \varphi_i$$

$$\mathbf{q_i} = \mathbf{q_i}(\mathbf{X}, T) = \nabla_{\mathbf{X}} \psi_i(\mathbf{X}, T)$$

$$\partial_t = \varepsilon \left( (\partial_T \psi_1) \partial_{\varphi_1} + (\partial_T \psi_2) \partial_{\varphi_2} \right) \qquad \nabla = \nabla_0 + \varepsilon \nabla_{\mathbf{X}}$$

Phase diffusion equations

$$\begin{cases} \partial_T \psi_1 = \sum_{\alpha\beta\gamma} D^{1\alpha}_{\beta\gamma} \dfrac{\partial^2 \psi_\alpha}{\partial X_\beta \partial X_\gamma} \\ \partial_T \psi_2 = \sum_{\alpha\beta\gamma} D^{2\alpha}_{\beta\gamma} \dfrac{\partial^2 \psi_\alpha}{\partial X_\beta \partial X_\gamma} \end{cases}$$

12 diffusion coefficients $D^{i\alpha}_{\beta\gamma}$ depend on $\tilde{h}_0$ and its derivatives

For square and 6-fold patterns:

$$\partial_T \psi_1 = D_{11}\frac{\partial^2 \psi_1}{\partial X_1 \partial X_1} + D_{22}\frac{\partial^2 \psi_1}{\partial X_2 \partial X_2} + D_{12}\frac{\partial^2 \psi_2}{\partial X_1 \partial X_2}$$

$$\partial_T \psi_2 = D_{22}\frac{\partial^2 \psi_2}{\partial X_1 \partial X_1} + D_{11}\frac{\partial^2 \psi_2}{\partial X_2 \partial X_2} + D_{12}\frac{\partial^2 \psi_1}{\partial X_1 \partial X_2}$$

Their solutions $\psi_i = \psi_i^0 e^{\Omega T} e^{i\mathbf{K}\cdot\mathbf{X}}$ give the stability, through the dispersion curves: $\Omega_{1,2} = \Omega_{1,2}(\mathbf{K})$

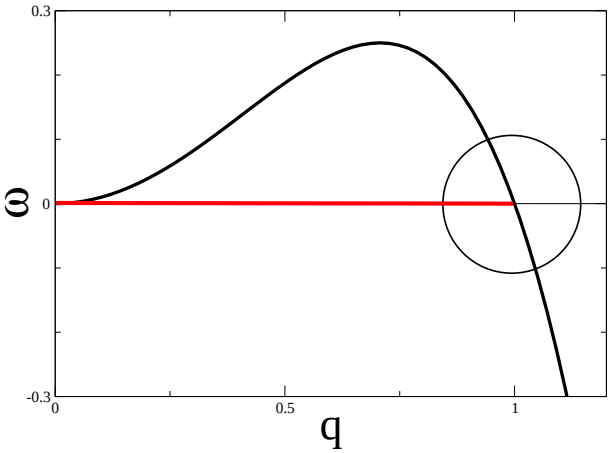
For 6-fold patterns, $D_{11} - D_{22} - D_{12} = 0$

$$\Omega_1(\mathbf{K}) < 0 \qquad \Omega_2(\mathbf{K}) = -D_{11}K^2$$

$$D_{11} = \frac{2\, q^{7/4}\partial_q \left( q^{5/4} \langle h_{11} h_{12} \rangle \right)}{\langle h^2 \rangle}$$

## Small amplitude approximation

$$h(\mathbf{x},t) = a_1(t)(e^{iq(x+y)} + e^{iq(x-y)}) + \text{c.c.}$$




We can determine the amplitude $\tilde{a}_1$ for the steady states and $D_{11}$.

We have evidence of the standard three scenarios:

- Coarsening
- No Coarsening
- Interrupted coarsening

according to the sign of $\dfrac{d\tilde{a}_1}{dq}$

## Coarsening exponents

There are two universality classes

Faceting (constant slope $\mathbf{m}$)

$$\mathbf{j} = \mathbf{m}(1 - m^2)$$

$$L(t) \approx t^{1/3}$$

No faceting (increasing slope $\mathbf{m}$)

$$\mathbf{j} = \frac{\mathbf{m}}{1 + m^2}$$

$$L(t) \approx t^{1/4}$$

| Faceting | No Faceting |
|---|---|

## Our results (until now)

| | |
|---|---|
| $\frac{1}{3}$ | $\frac{1}{4}$ |

## Exact results (specific isotropic currents)

| | | |
|---|---|---|
| | $\leq \frac{1}{3}$ [Kohn&Yan] (2003) | $\leq \frac{1}{4}$ [Bo Li] (2006) |
| *3-fold* | $\frac{1}{3}$ [Watson&Norris] (2006) | |

## Approximate results (and numerics) [Golubović]

| | | |
|---|---|---|
| *square* | $\frac{1}{3}$ or $\frac{1}{4}$ | $\frac{1}{4}$ |
| *others* | $\frac{1}{3}$ | |

## Experiments

$$\frac{1}{6} \leq n \leq \frac{1}{2}$$