Coarsening dynamics during the growth of one-dimensional interfaces

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Outline

One dimensional interfaces

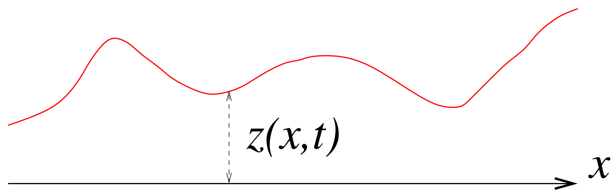
- Growth equations in crystal growth (MBE)
- Rigorous formulation of the problem:
  generalized Ginzburg-Landau (nonconserved) and Cahn-Hilliard (conserved) equations

Stationary configurations and dynamical properties:

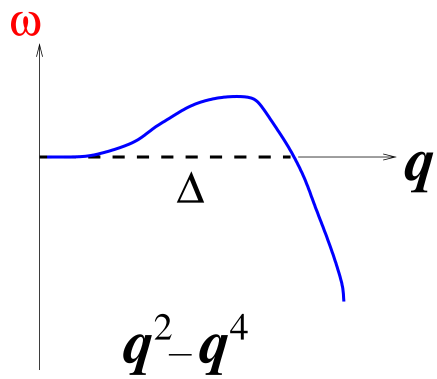
coarsening $\Longleftrightarrow \partial_A \lambda > 0$

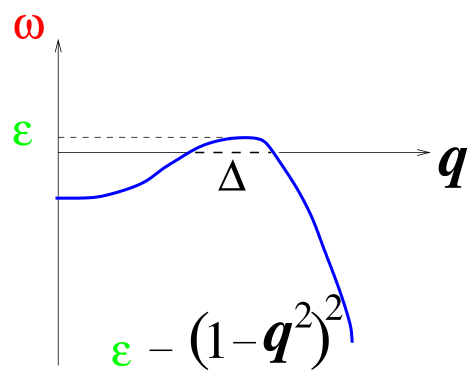
- The pseudo free energy $\mathcal{F}$
- The phase diffusion equation

Time dependence of coarsening



$$\partial_t z(x,t) = \mathcal{A}(\{z(x,t)\})$$
$$z(x,t) = z_0 + \delta z \exp(iqx + \omega t)$$





- Perpetual coarsening: $\lambda(t) \to \infty$

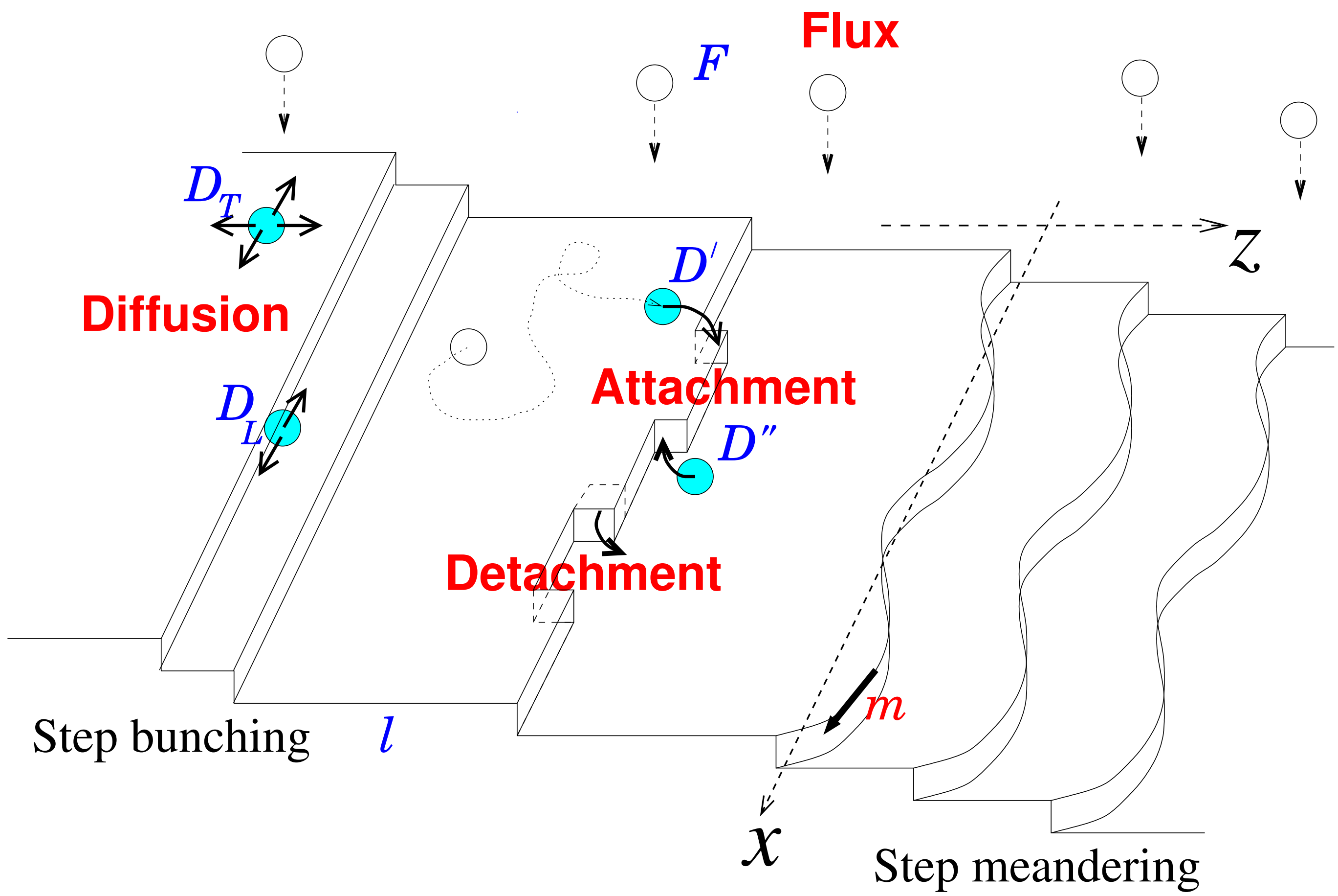
- Fixed wavelength: $\lambda(t) \sim \lambda_c$

  - Diverging amplitude: $A(t) \to \infty$

  - Oscillating/Chaotic amplitude

- Interrupted coarsening: $\lambda(t) \nearrow$ up to λ^*

Is it possible to establish
a priori criteria for coarsening ?



$$\partial_t z(x,t) = -\partial_x j = -\partial_x \{B(m) + G(m)\partial_x[C(m)\partial_x m]\}$$

In the limit of small slopes ($m \equiv \partial_x z \ll 1$):

$$\partial_t z = -B'(0)\,\partial_x^2 z - G(0)C(0)\,\partial_x^4 z$$

$$z(x,t) = \exp(\omega t + iqx) \qquad \omega(q) = B'(0)q^2 - G(0)C(0)q^4$$

Stationary configurations: $j = 0$

$$M(m) = \int^m ds C(s) \Longrightarrow B(M) + G(M)\partial_{xx}M = 0$$

$$V(M) = \int dM \frac{B(M)}{G(M)}$$

[F. Gillet, Ph.D. Thesis (2000)]

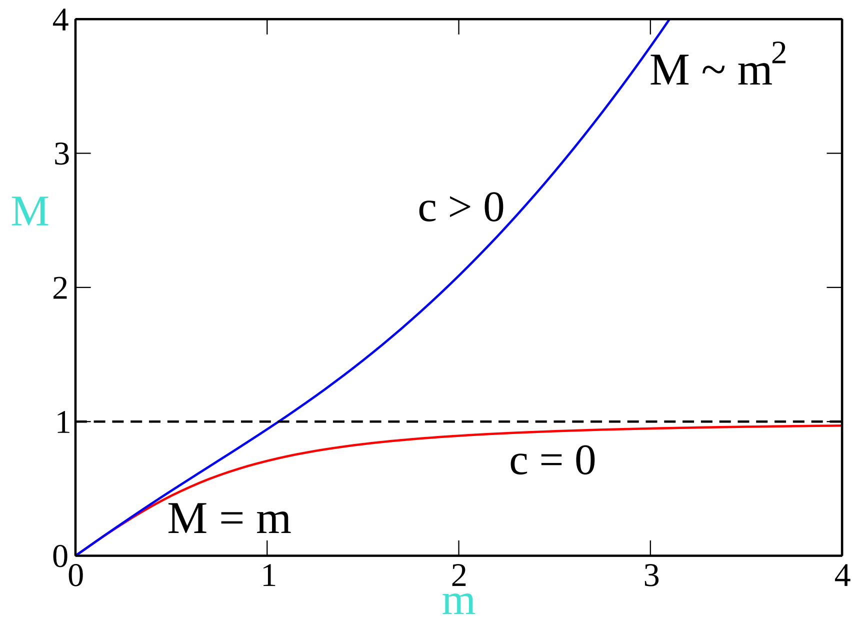
$$B(m) = \frac{m}{1+m^2} \qquad G(m) = \frac{1+\beta\sqrt{1+m^2}}{(1+\beta)(1+m^2)}$$

$$C(m) = \frac{1+c(1+m^2)(1+2m^2)}{(1+c)(1+m^2)^{3/2}}$$

$$\beta = \frac{D_{\mathsf{L}} a}{D_{\mathsf{T}} \ell} \equiv \frac{\texttt{line diffusion}}{\texttt{terrace diffusion}}$$

$$c \sim \frac{Ea^4}{\tilde{\gamma}\ell^2} \equiv \frac{\texttt{step-step elastic interaction}}{\texttt{step stiffness}}$$

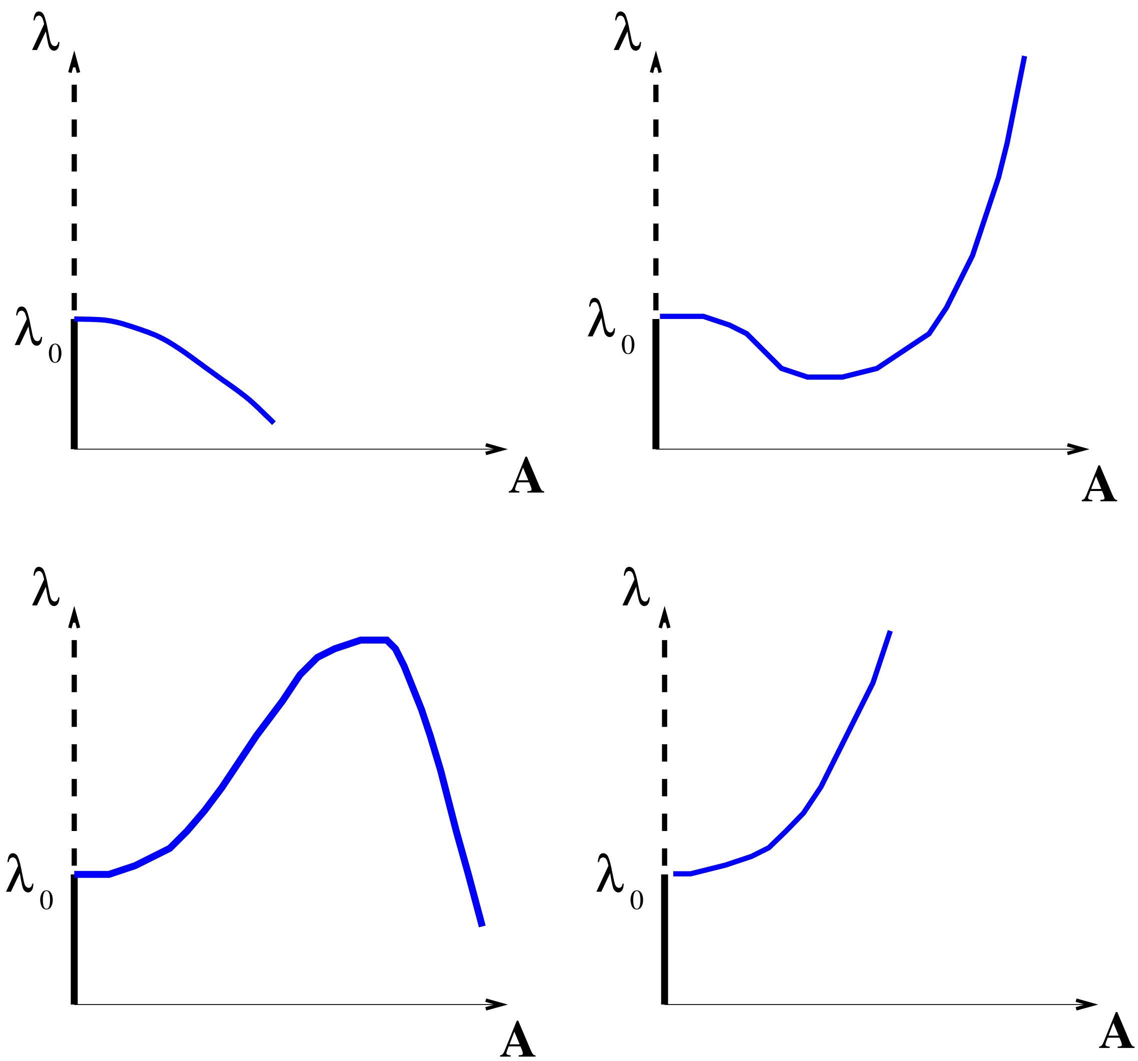
$$M(m) = \frac{m}{1+c} \frac{1+c(1+m^2)}{(1+m^2)^{1/2}}$$



- A particle oscillating in the potential $V(M)$

What about $\lambda(A)$?

$c = 0$ $\qquad$ $0 < c < 1/(1+2\beta)$



Anisotropy effects $\qquad$ $c > 1/(1+2\beta)$

[Danker et al., PRE 68, 020601 (2003)]

The generalized models ...

$$\partial_t u = \partial_x^2 u - F(u) \equiv L[u]$$

nonconserved (generalized GL eq.)

$$\partial_t u = -\partial_x^2 [\partial_x^2 u - F(u)] \equiv -\partial_x^2 L[u]$$

conserved (generalized CH eq.)

Mechanical analogy:

Steady states satisfy the relation $\partial_x^2 u - F(u) = 0$

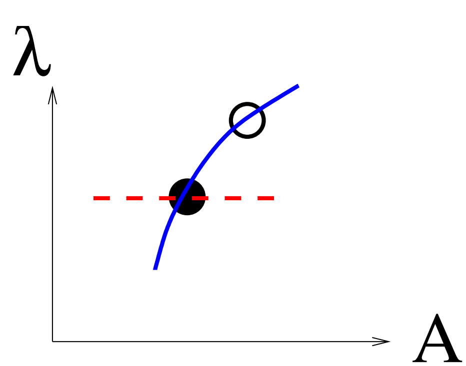
... and the pseudo free energy

$$\partial_x^2 u - F(u) = -\delta \mathcal{F}/\delta u$$
$$\mathcal{F}[u(x,t)] = \int dx \left[\frac{1}{2}(\partial_x u)^2 - V(u) \right] \quad , \; F(u) = -V'(u)$$

$d\mathcal{F}/dt \leq 0$ for GL & CH models

What about

- $\mathcal{F}[u_\lambda(x)]$ vs λ
- $\mathcal{F}[(1+\delta)u_\lambda(x)]$ vs δ

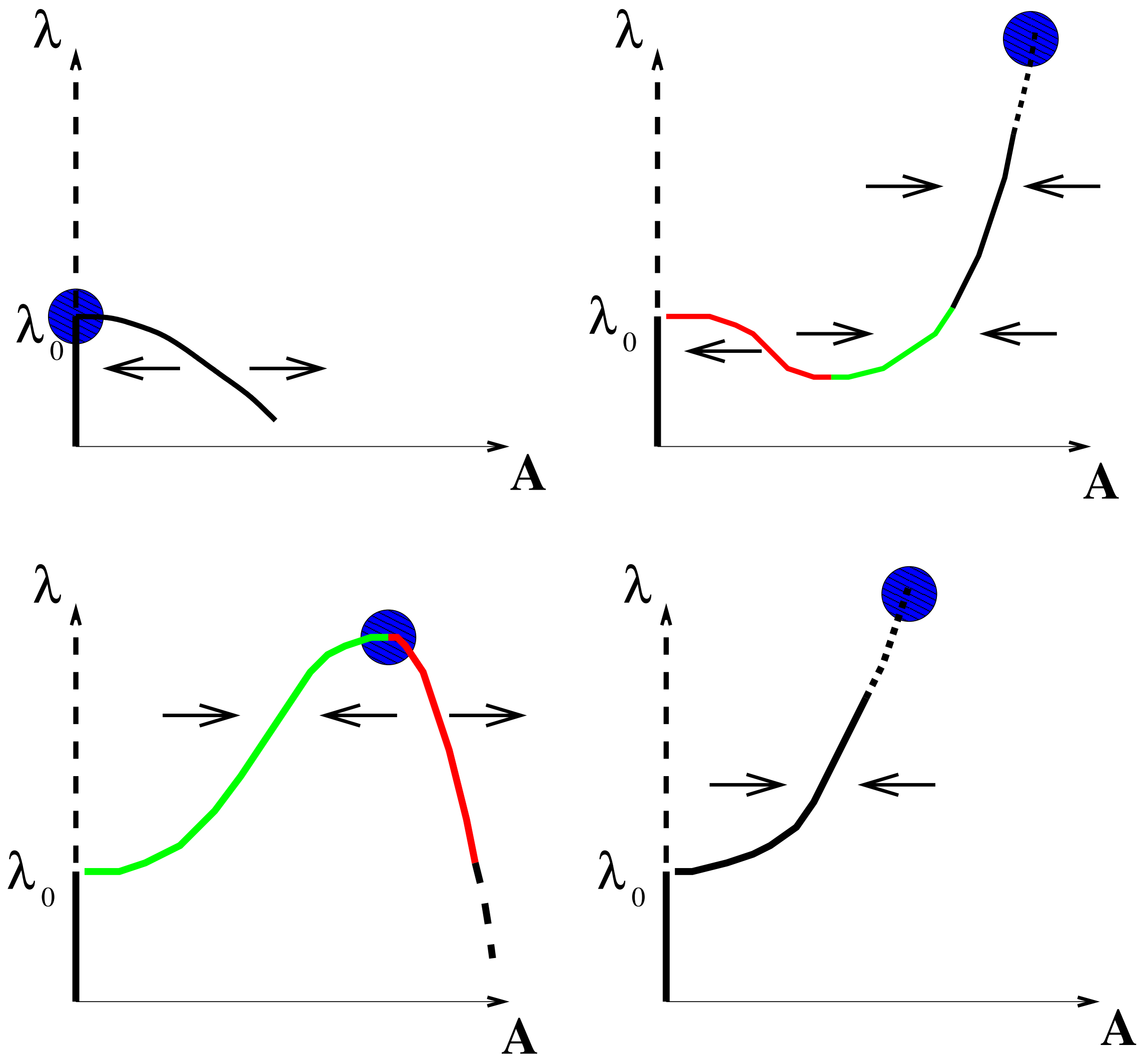


- $\mathcal{F}[u_\lambda(x)]$ vs λ

$$\begin{aligned}\mathcal{F}[u_\lambda(x)] &= \frac{J}{\lambda} - E \\ \frac{d\mathcal{F}}{d\lambda} &= -\frac{J}{\lambda^2} + \frac{1}{\lambda}\frac{dJ}{d\lambda} - \frac{dE}{d\lambda} = -\frac{J}{\lambda^2} < 0\end{aligned}$$

- $\mathcal{F}[(1+\delta)u_\lambda(x)]$ vs δ

$$\mathcal{F}[(1+\delta)u_\lambda(x)] - \mathcal{F}[u_\lambda(x)] = \frac{\delta^2}{2}\underbrace{\int dx\left[u_\lambda^2(x)F'(u_\lambda(x)) - u_\lambda(x)F(u_\lambda(x))\right]}_{\text{same sign as } d\lambda/dA}$$


λ
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A

Phase dynamics of the GL equations

$$\partial_x^2 u_0 - F(u_0) = 0 \quad V(u) = -\int du\, F(u)$$

$$u_0(x+\lambda) = u_0(x) \qquad \phi = qx \quad q = 2\pi/\lambda$$

Phase equation: perturbative treatment of weak distorsions of a regular pattern
$\epsilon \equiv$ smallness of the phase modulation

$$X = \epsilon x \quad T = \epsilon^2 t \quad \psi(X,T) = \epsilon\phi(x,t)$$

$$q(X,T) = \partial_x \phi = \partial_X \psi$$

$$\partial_x \to q\partial_\phi + \epsilon\partial_X \qquad \partial_t \to \epsilon^2 \partial_T \phi \partial_\phi + \epsilon^2 \partial_T$$

$$u = u_0 + \epsilon u_1 + \dots$$

Zero order: $\quad L[u_0] = q^2 \partial_{\phi\phi} - F(u_0) = 0$

First order: $\quad \tilde{L}[u_1] = f(u_0)$

$$\tilde{L} = q^2 \partial_{\phi\phi} - F'(u_0)$$

$$f(u_0) = \partial_T \psi \partial_\phi u_0 - [\partial_\phi u_0 + 2q\partial_{\phi q} u_0]\partial_{XX}\psi$$

$$\tilde{L}[\partial_\phi u_0] = 0 \implies (\partial_\phi u_0) \text{ and } f(u_0) \text{ are orthogonal}$$

$$\partial_T \psi = D\, \partial_{XX} \psi \ , \qquad D = \frac{\partial_q \langle q(\partial_\phi u_0)^2 \rangle}{\langle (\partial_\phi u_0)^2 \rangle} \equiv \frac{D_1}{D_2}$$

$$\langle \dots \rangle = (2\pi)^{-1} \textstyle\int_0^{2\pi} \dots d\phi$$

$$\langle q(\partial_\phi u_0)^2 \rangle = \frac{1}{2\pi} \int_0^{2\pi/q} d\tau (\partial_\tau u_0)^2 = \frac{J}{2\pi}$$

$$D_1 = \frac{1}{2\pi} \partial_q J = \frac{1}{2\pi} \left(\frac{\partial J}{\partial E} \right) \left(\frac{\partial q}{\partial E} \right)^{-1} = -\frac{\lambda^3}{4\pi^2} \left(\frac{\partial \lambda}{\partial E} \right)^{-1}$$

$$D = \ - \frac{\lambda^3}{4\pi^2 \langle (\partial_\phi u_0)^2 \rangle} \left(\frac{\partial \lambda}{\partial E} \right)^{-1}$$

Conclusion: The sign of D is always opposite to the sign of $\partial_E \lambda$

$\partial_E \lambda > 0 \implies D < 0$ coarsening

$\partial_E \lambda < 0 \implies D > 0$ phase stability

Phase dynamics of conserved equations

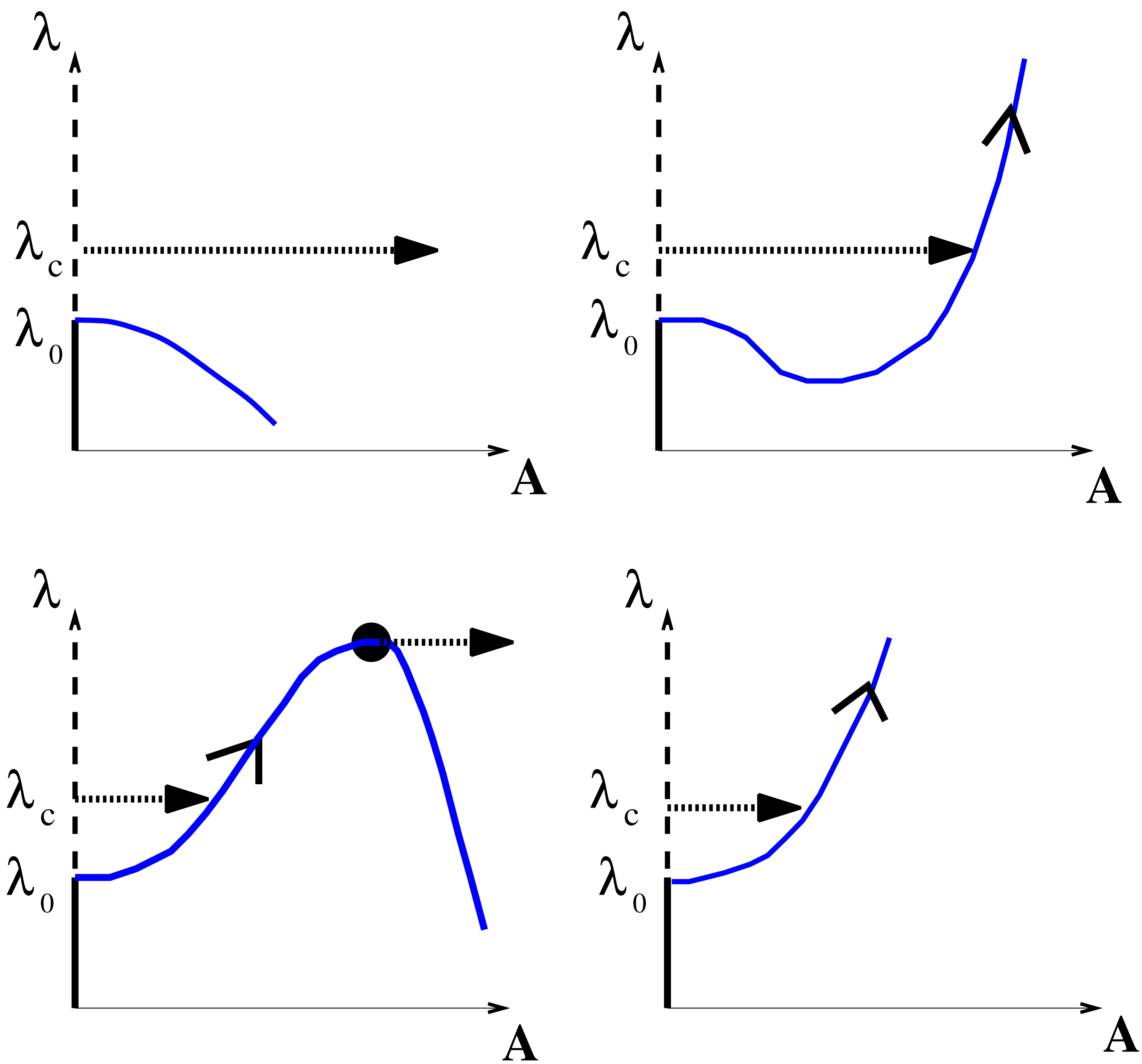
$$D = \frac{q^2 \partial_q \langle q(\partial_\phi u_0)^2 \rangle}{\langle u_0^2 \rangle} = -\frac{\lambda}{\langle u_0^2 \rangle} \left(\frac{\partial \lambda}{\partial E} \right)^{-1}$$

Conclusion: `Coarsening takes place`
<u>`if and only if`</u> $\partial_E \lambda > 0$

Steady states and dynamical behavior

Fixed wavelength
Diverging amplitude

Perpetual coarsening



Interrupted coarsening

Perpetual coarsening

[P. Politi and C. Misbah, arXiv:cond-mat/0307072 (2003)]

Time dependence of coarsening

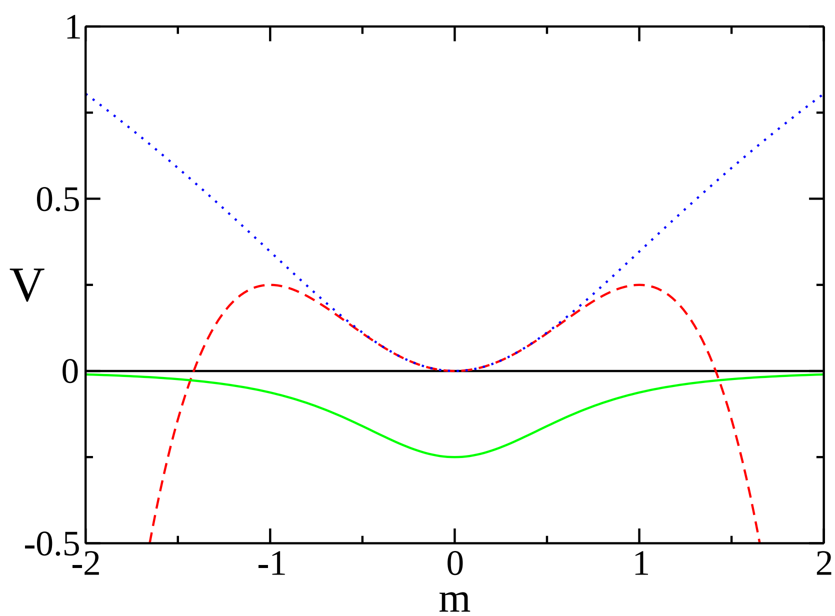
[In collaboration with Alessandro Torcini]

For perpetual coarsening, $\lambda(t) \approx$??

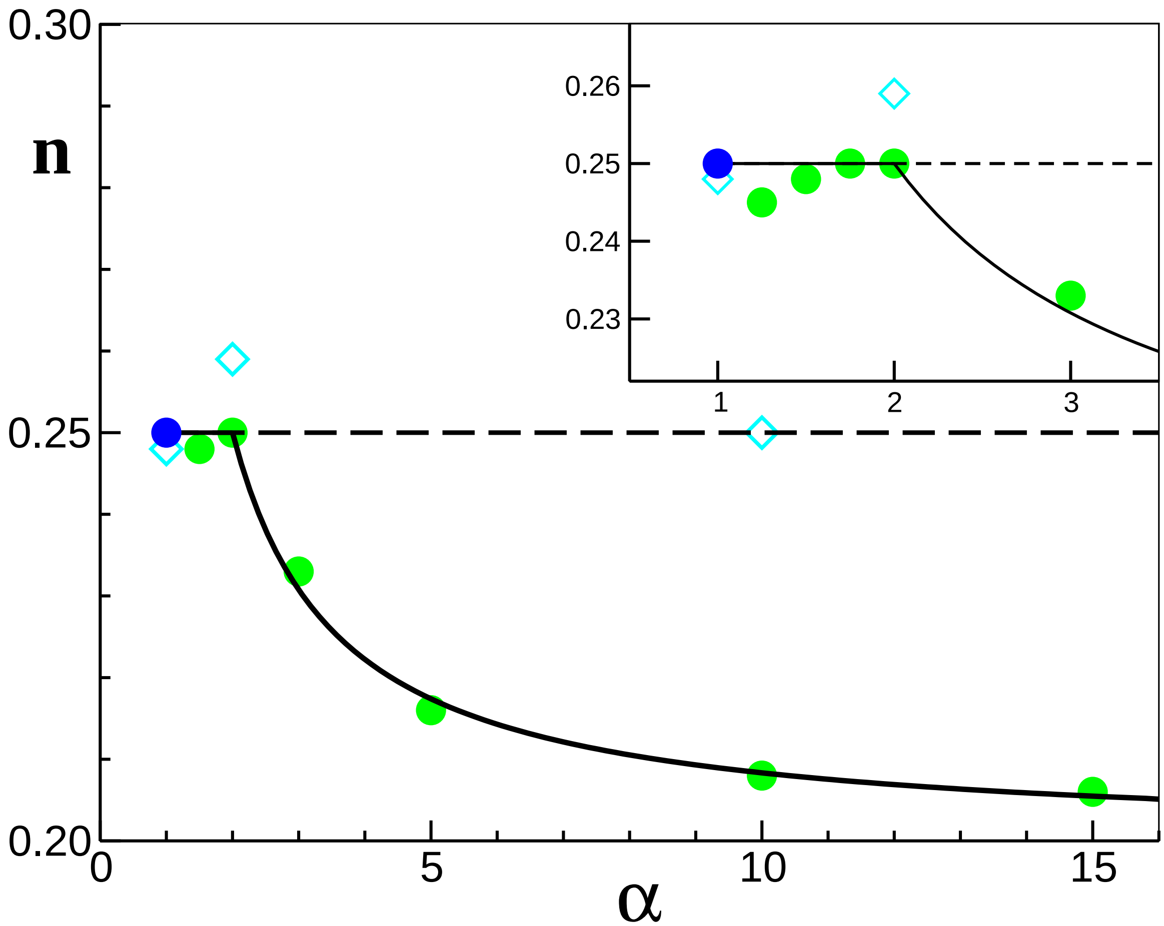
$$\partial_t z(x,t) = -\partial_x j(x,t) + \eta(x,t)$$

$$j(x,t) = \begin{cases} \partial_x^2 m + m(1-m^2) & \text{model 0} \\ \partial_x^2 m + \frac{m}{(1+m^2)^\alpha} & \text{model } \alpha \end{cases}$$

$$V(m) = \begin{cases} m^2/2 - m^4/4 & \text{model 0} \\ (1/2)\ln(1+m^2) & \text{model 1} \\ -(1+m^2)^{1-\alpha}/[2(\alpha-1)] & \text{model } \alpha > 1 \end{cases}$$



The coarsening exponent



[A. Torcini and P. Politi, Eur. Phys. J. B **25**, 519 (2002)]

Conclusions

- Steady state properties $\Longleftrightarrow$ Dynamical behavior
- Coarsening occurs if and only if $d\lambda/dA > 0$

Perspectives

- How general this relation is ?

$$\partial_t u = -\partial_x^2[\partial_x^2 u + u - u^3] + \nu u \partial_x u \qquad \omega = q^2 - q^4$$

$$\partial_t u = \epsilon u - (1 + \partial_x^2)^2 u - u^3 \qquad \omega = \epsilon - (1 - q^2)^2$$

- Is it possible to gain information on $L(t)$ from the phase diffusion equation ?