Growth rate of a surface by a co-rotating pair of spiral steps evolving by an eikonal-curvature equation

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Mathematical aspects on boundary layer
in reaction-diffusion phenomena,
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Joint work with
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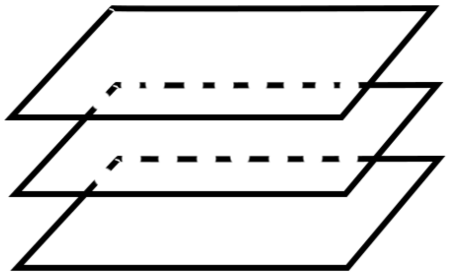
and Y. Giga(Univ. Tokyo)

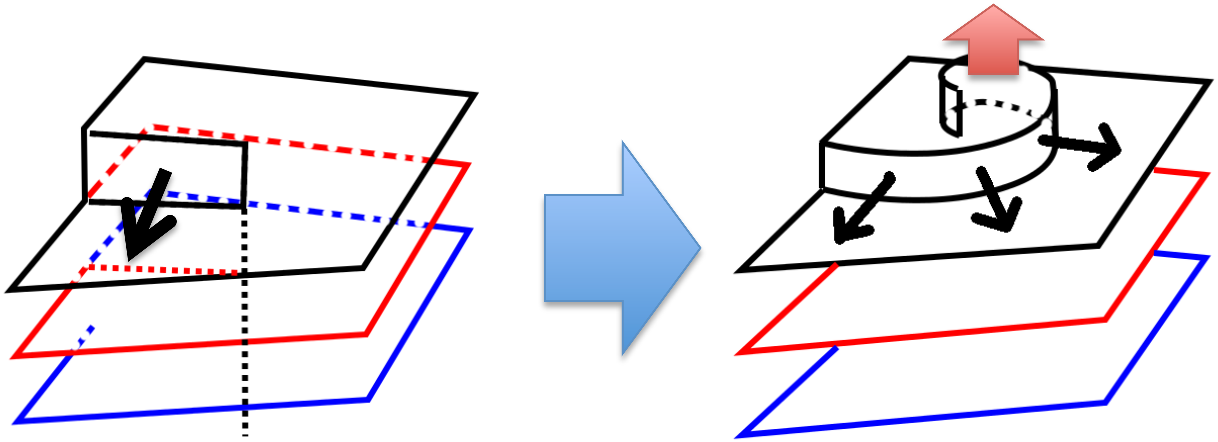
Spiral crystal growth

Burton-Cabrera-Frank (1951, BCF paper)

Layer structure of a complete (without dislocations) crystal



Screw dislocations provide helical surface structure and spiral steps on the crystal surface.



- Holizontal evolution: Steps evolve with

$$V = v_\infty(1 - \rho_c \kappa) \qquad \text{(steps = spiral curve } \Gamma_t \subset \mathbb{R}^2 \text{)}$$

V : Normal velocity, κ : curvature

(v_∞ : velocity of straight steps, ρ_c : critical radius (constants))

- Vertical evolution: the step climbs the helical surface.

Growth rate of the surface = angle velocity × step height

Evolution of "crystal surface"

Question: How fast the "surface" evolve?

Single spiral case (1 screw dislocation, 1 spiral step)

Approximation by a rotating spiral:

$$\Gamma_t = \{r(\cos(\theta(r) + \omega t), \sin(\theta(r) + \omega t));\ \ r > 0\}$$

$\Rightarrow$ Growth rate: $R_S = \dfrac{\omega}{2\pi} \times h_0$ ($h_0 > 0$: step height)

Known results

- BCF(1951): Approximation by Archimedean spiral

$$\Rightarrow r = 2\rho_c \theta, \quad \omega = \frac{v_\infty}{2\rho_c} \qquad \left(\omega = \omega_1 \frac{v_\infty}{\rho_c}, \quad \omega_1 = \frac{1}{2}\right)$$

- BCF(1951): Better approximation $\omega_1 = \dfrac{\sqrt{3}}{2(1+\sqrt{3})} \approx 0.315.$

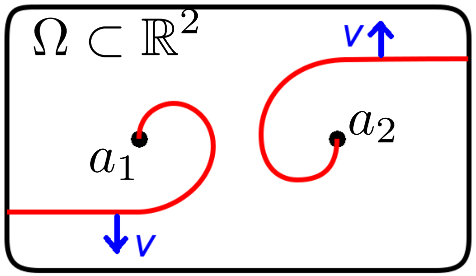
- Ohara-Reid(1973): Shooting method with ODE model:

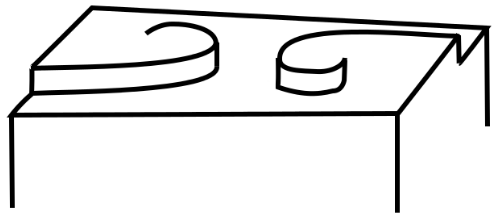
$$\Rightarrow \omega_1 = 0.330958061$$

Surface evolution by a co-rotating pair

THE GOAL of this talk is to know the growth rate of the surface by a co-rotating pair.

Evolution equation
$$V = v_\infty(1-\rho_c\kappa)$$





$\Omega \subset \mathbb{R}^2$: Crystal surface(view from above)

$a_1, a_2 \in \Omega$: a pair of centers with co-rotating spirals

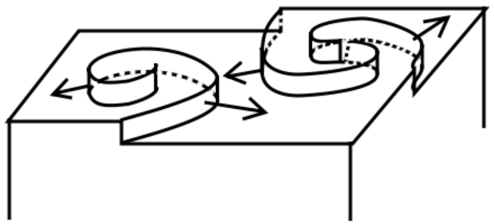
$\Rightarrow R_p = R_p(d)$: Growth rate(activity) depends on the distance $d := |a_1 - a_2|$ of a pair.

Speculations by BCF:

- [far apart] $d > 2\pi\rho_c \Rightarrow R_p(d) \approx R_S$
- [limiting case] $d \to 0 \Rightarrow R_p(d) \to 2R_S$
- [close, but...] $d \le 2\pi\rho_c \Rightarrow$ No estimates.

Goal: Verify these speculations, and give an estimates of $R_p(d)$.

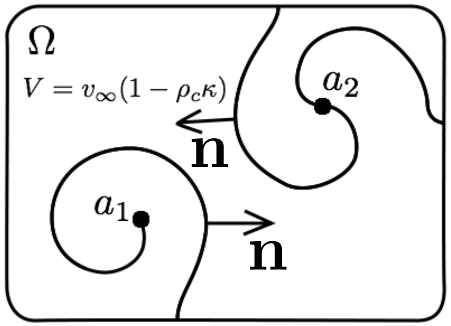
Level set method for spiral steps



(O(2003), O-Tsai-Giga(preprint))

Domain: $\Omega \subset \mathbb{R}^2$ bounded with smooth $\partial\Omega$.

Centers: $a_1, \ldots, a_N \in \Omega \ (N \geq 1)$,

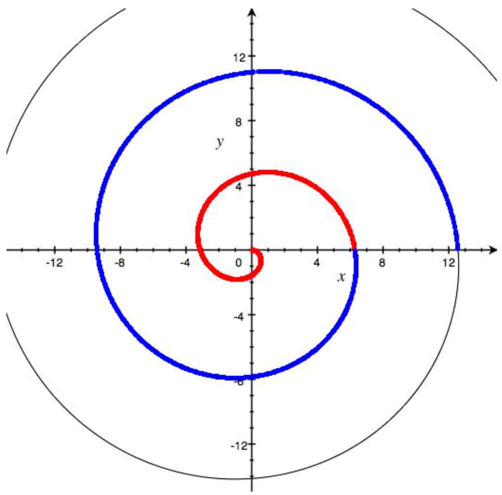


$$W = \Omega \setminus \left[\bigcup_{j=1}^{N} \overline{B_{\rho_j}(a_j)} \right]$$

$$\rho_j > 0 \ (j = 1, \ldots, N)$$

$$\Gamma_t = \{x \in \overline{W};\ u(t,x) - \theta(x) \equiv 0 \mod 2\pi\mathbb{Z}\},\ \mathbf{n} = -\frac{\nabla(u-\theta)}{|\nabla(u-\theta)|}$$

$$\theta(x) = \sum_{j=1}^{N} m_j \arg(x - a_j) \quad (m_j \in \mathbb{Z} \setminus \{0\})$$

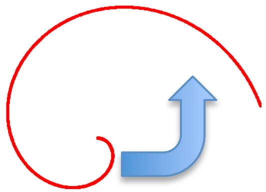


ex. Archimedean spiral :

$$\Gamma_t = \{x \in \mathbb{R}^2;\ -|x| - \arg x \equiv 0 \mod 2\pi\mathbb{Z}\}$$

Description of spirals

Archimedean spiral:

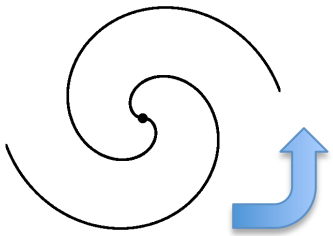


$$(\text{Polar coordinate}):\ \theta = -r + \omega t$$

$$(\text{Level set}):\ \Gamma_t = \{x;\ \boxed{\omega t - |x|} - \arg x \equiv 0\}$$

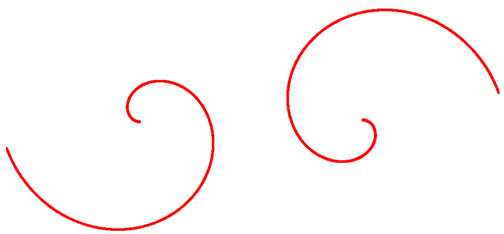
$u(t,x)$

2 Archimedean spirals:



$$(\text{Polar coordinate}):\ \theta = -r + \omega t, \theta = -r + \omega t + \pi$$

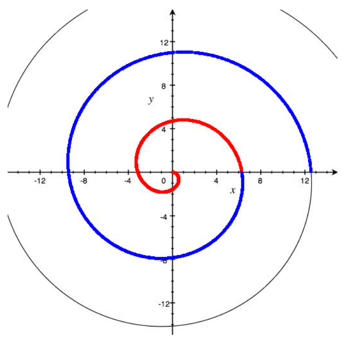
$$(\text{Level set}):\ \Gamma_t = \{x;\ \boxed{2(\omega t - |x|)} - 2\arg x \equiv 0 \mod 2\pi\mathbb{Z}\}$$



$$(\text{Level set}):$$

$$\Gamma_t = \{x;\ u(t,x) - \theta(x) \equiv 0 \mod 2\pi\mathbb{Z}\}$$

$$\theta(x) = \arg(x - a_1) + \arg(x - a_2)$$



Claim: θ should be a multiple-valued function.

Level set equation

$$\Gamma_t = \{x \in \overline{W};\ u(t,x) - \theta(x) \equiv 0 \mod 2\pi\mathbb{Z}\},\ \ \mathbf{n} = -\frac{\nabla(u-\theta)}{|\nabla(u-\theta)|}$$

It is roughly regard as the usual level set of $u-\theta$.

$$\Rightarrow V = \frac{u_t}{|\nabla(u-\theta)|}, \quad \kappa = \mathrm{div}\frac{\nabla(u-\theta)}{|\nabla(u-\theta)|}.$$

Level set equation: $V = v_\infty(1-\rho_c\kappa)$ and right-angle condition

$$\Rightarrow \begin{cases} u_t - v_\infty|\nabla(u-\theta)|\left\{\rho_c \mathrm{div}\dfrac{\nabla(u-\theta)}{|\nabla(u-\theta)|} + 1\right\} = 0 & \text{in } (0,T)\times W, \\ \langle \vec{\nu}, \nabla(u-\theta)\rangle = 0 & \text{on } (0,T)\times \partial W. \end{cases}$$

(cf. Y. Giga, *Surface evolution equation: a level set approach*, Birkhäuser, 2006)

Remark

- This equation works well because $\nabla\theta$ or $\nabla^2\theta$ are single-valued.
- The solution is in viscosity solution sense since the above is degenerate parabolic equation.

(cf. Chen-Giga-Goto(1991), Evans-Spruck(1991), Crandall-Ishii-Lions(1992).)

Mathematical analysis

$$\text{(LV)}\begin{cases} u_t - v_\infty|\nabla(u-\theta)|\left\{\rho_c \mathrm{div}\dfrac{\nabla(u-\theta)}{|\nabla(u-\theta)|}+1\right\}=0 & \text{in } (0,T)\times W,\\ \langle\vec{\nu},\nabla(u-\theta)\rangle = 0 & \text{on } (0,T)\times\partial W.\end{cases}$$

Comparison.('03 O) *Assume that ∂W is C^2. Let $u \in USC([0,T)\times\overline{W})$ and $v \in LSC([0,T)\times\overline{W})$ be a viscosity sub- and super-solutions of (LV). Then, if $u(0,x)\le v(0,x)$ for $x\in\overline{W}$, then $u(t,x)\le v(t,x)$ for $(t,x)\in(0,T)\times\overline{W}$.*

Existence and uniqueness('03 O) *For $u_0\in C(\overline{W})$ there exists a viscosity solution $u\in C([0,\infty)\times\overline{W})$ globally-in-time satisfying $u(0,\cdot)=u_0$.*

Global solution exists uniquely with respect to the continuous initial data.

Problem:
- Continuous initial data is NOT unique w.r.t. an initial curve.
- Construction of a continuous initial data is NOT trivial.

Uniqueness of level sets

Comparison of interior.('08 Goto-Nakagawa-O)
Assume that ∂W is C^2. Let $u \in USC([0,T) \times \overline{W})$ and $v \in LSC([0,T) \times \overline{W})$ be a viscosity sub- and super-solutions of (LV). Then, if

$$\{(x,\xi) \in \mathfrak{X};\ \tilde{u}(0,x,\xi) > 0\} \subset \{(x,\xi) \in \mathfrak{X};\ \tilde{v}(0,x,\xi) > 0\},$$

then $\{(x,\xi) \in \mathfrak{X};\ \tilde{u}(t,x,\xi) > 0\} \subset \{(x,\xi) \in \mathfrak{X};\ \tilde{v}(t,x,\xi) > 0\}$

for $t \in (0,T)$. *Also, if*

$$\{(x,\xi) \in \mathfrak{X};\ \tilde{u}(0,x,\xi) < 0\} \supset \{(x,\xi) \in \mathfrak{X};\ \tilde{v}(0,x,\xi) < 0\},$$

then $\{(x,\xi) \in \mathfrak{X};\ \tilde{u}(t,x,\xi) < 0\} \supset \{(x,\xi) \in \mathfrak{X};\ \tilde{v}(t,x,\xi) < 0\}$

for $t \in (0,T)$.

$$\mathfrak{X} = \{(x,\xi) \in \overline{W} \times \mathbb{R}^N;\ \xi_j \text{`} = \text{'} \arg(x - a_j)\ (j = 1,\ldots,N, \xi = (\xi_1,\ldots,\xi_N))\}$$

=helical (crystal) lattice of atoms

$$u(t,x,\xi) = u(t,x) - \sum_{j=1}^{N} m_j \xi_j \approx u(t,x) - \theta(x)$$

→ The level set is unique with respect to an initial curve.

Surface height

Assumption: There is no horizontal and enough small vertical displacement of atom by screw dislocation.

The surface height function $h(t,x)$ satisfies

$$\Delta h = -h_0 \mathrm{div} \delta_{\Gamma_t} \mathbf{n} \quad \text{in } W.$$

$$\Leftrightarrow \begin{cases} \Delta h = 0 \quad \text{a.e. in } W, \\ h_0 > 0 \text{ jump discontinuity only on } \Gamma_t \\ \qquad \text{in the direction of } -\mathbf{n}. \end{cases}$$

If $\Gamma_t = \{x \in \overline{W};\ u(t,x) - \theta(x) \equiv 0 \mod 2\pi\mathbb{Z}\}$,

$$h(t,x) = \frac{h_0}{2\pi} \theta_{\Gamma_t}(x),$$

$$\theta_{\Gamma_t}(x) = \Theta(x) + 2\pi k(t,x) + \pi \vartheta(u(t,x) - [\Theta(x) + 2\pi k(t,x)])$$

($\theta_{\Gamma_t}(x)$ is a branch of θ whose discontinuity is only on Γ_t)

ϑ : Heavyside function, $\Theta(x)$: a branch of θ (fix),

$k(t,x)$: a branch number of the location of the step, i.e.,

$$k(t,x) \in \mathbb{Z} \text{ s.t. } -\pi \le u(t,x) - (\Theta(x) + 2\pi k(t,x)) < \pi.$$

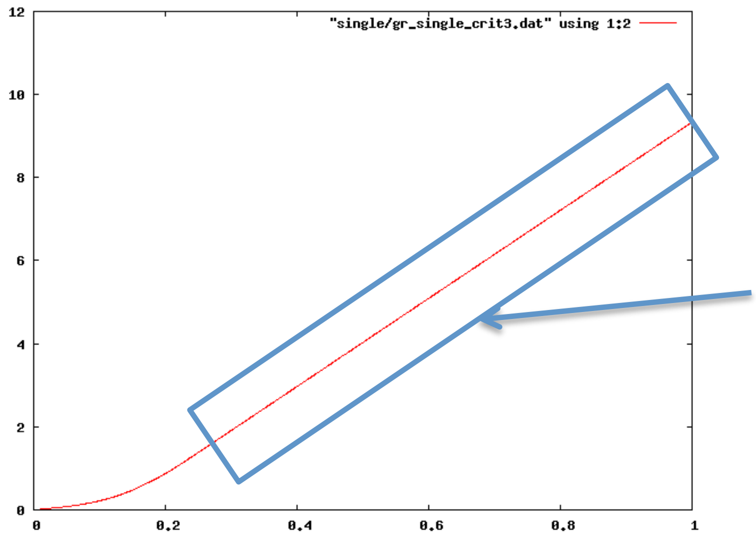
Growth rate

Mean growth height: $H(t;t_0) = \frac{1}{|W|}\int_W [h(t,x) - h(t_0,x)]\mathrm{d}x$

$$\Rightarrow \text{Growth rate} \approx H'(t;t_0).$$

From numerical data we derive two kinds of the growth rate.

(1)[Quantity]
Linear approximation



Sample: surface evolution by a single spiral step

Evolution equation: $V = 6(1 - 0.03\kappa)$

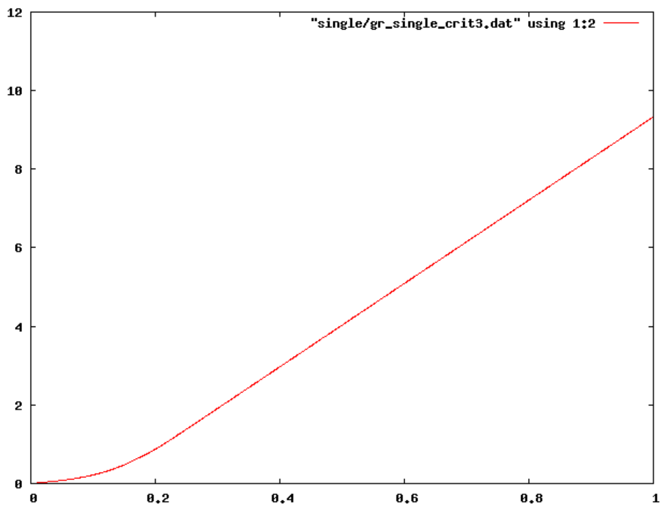
$$\Rightarrow R_S = 10.534722$$

Approximation: $H(t;0) \approx R_\ell t + b$ with data in [0.3,1].

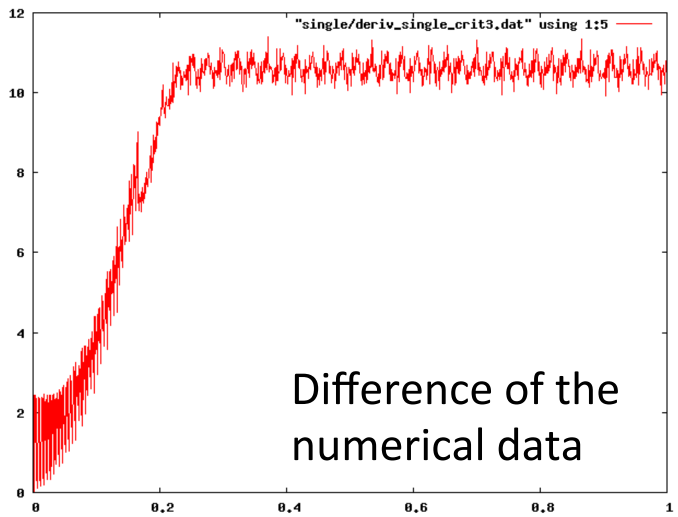
$$\Rightarrow R_\ell = 10.606435$$

Graph of the growth rate

Surface evolution by a single spiral step with $V = 6(1 - 0.03\kappa)$.



Difference

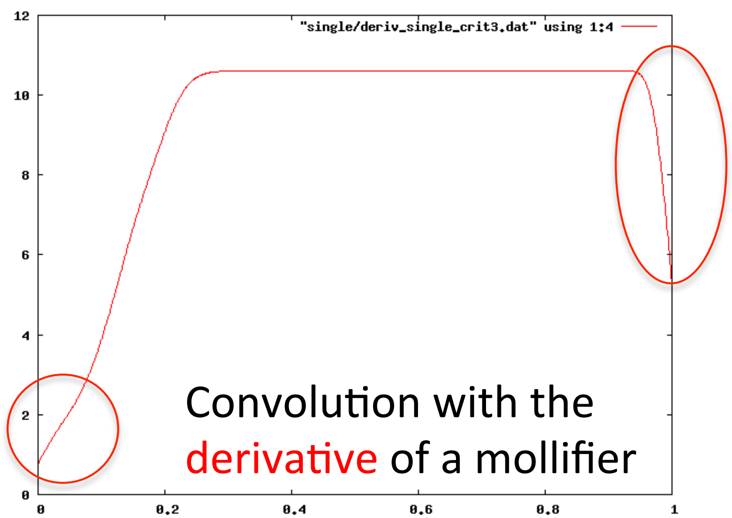


Calculate $R_w(t) = (H * \psi'_\mu)$ with

$$\psi_\mu(t) = \begin{cases} C_\mu \cos^4(t/\mu) & (|t/\mu| < \pi/2, \\ 0 & (\text{otherwise}). \end{cases}$$

$$(C_\mu \text{ is the constant s.t. } \int \psi_\mu = 1.)$$

$$\Rightarrow R_w \approx H'$$



Remark: R_w around initial and terminal time should be avoided.

Technical remarks on discretization

For numerical simulations we discretize the level set equation with an usual explicit finite difference scheme.

Technical remarks

- Equation: $V = 6(1-\rho_c\kappa)\ (v_\infty = 6,\ \rho_c > 0(\text{parameter}))$
- Regularization of the curvature term:

$$k_{i,j} := \left[\operatorname{div}\frac{\nabla(u-\theta)}{|\nabla(u-\theta)|}\right]_{i,j} \approx \left[\operatorname{div}\frac{\nabla(u-\theta)}{\sqrt{\varepsilon^2+|\nabla(u-\theta)|^2}}\right]_{i,j}$$

- Lattice points

$$\Omega \approx [-1,1]^2 \approx D_s = \{(i\Delta x, j\Delta x);\ -100s \le i,j \le 100s\},$$

$$\Delta x = 1/(100s),\ s = 1,2,4.$$

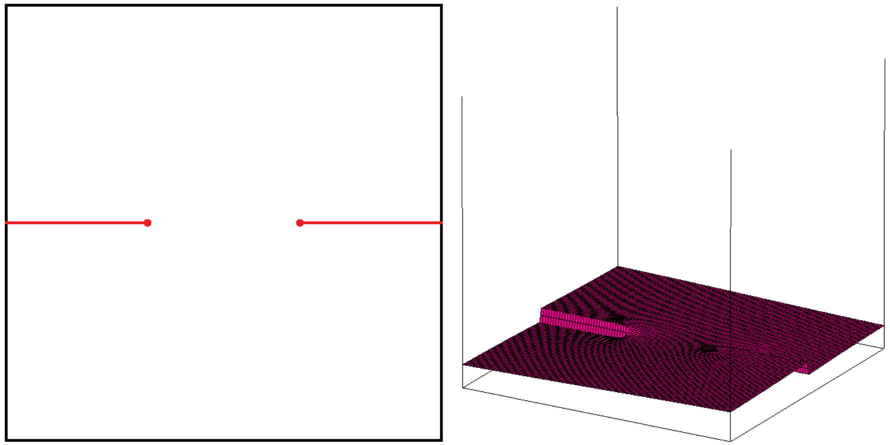
- Centers are located only on D_s, and only centers are removed.
  - Single case: $a_1 = (0,0)$, $(\rho_j = \Delta x)$
  - Co-rotating pair:

$$a_1 = (-k\Delta x, 0),\ a_2 = (k\Delta x, 0),\ 2 \le k \le 50s.$$

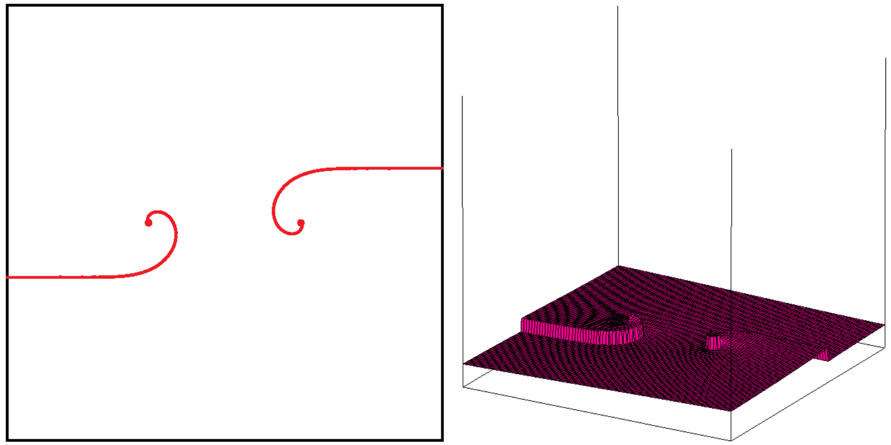
- Step heights: $h_0 = 1$. (Growth rate = Rotating number)

Co-rotating pair

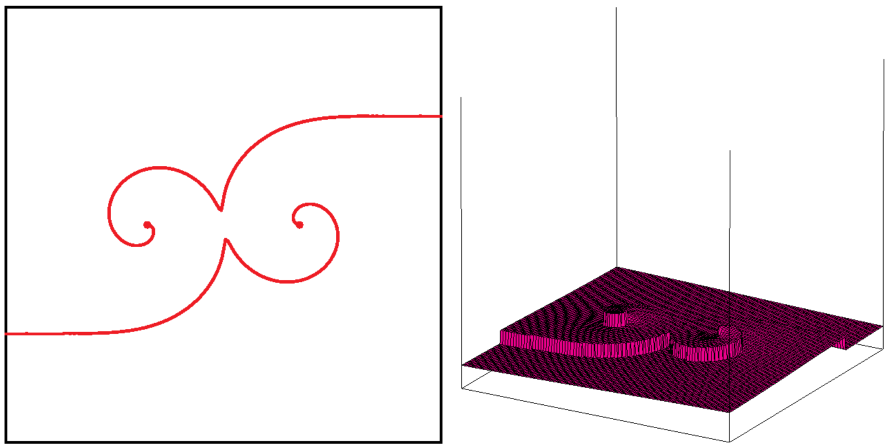
Evolution eq. $V = 5(1 - 0.02\kappa)$ $(v_\infty = 5, \rho_c = 0.02)$.



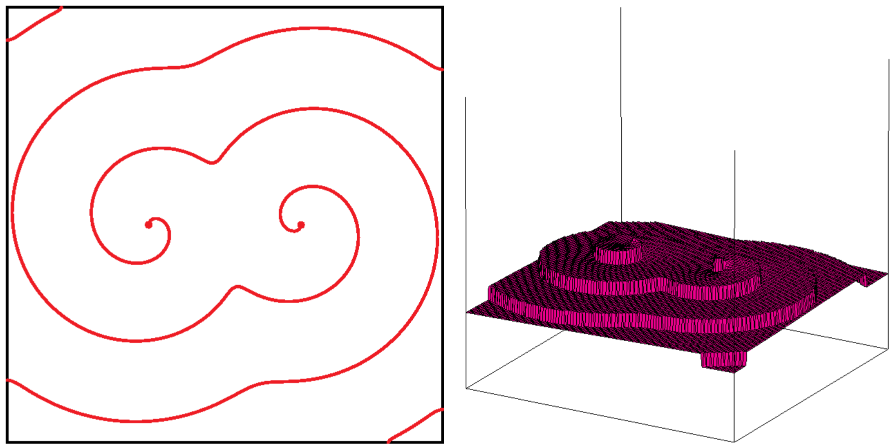
t=0



t=0.05



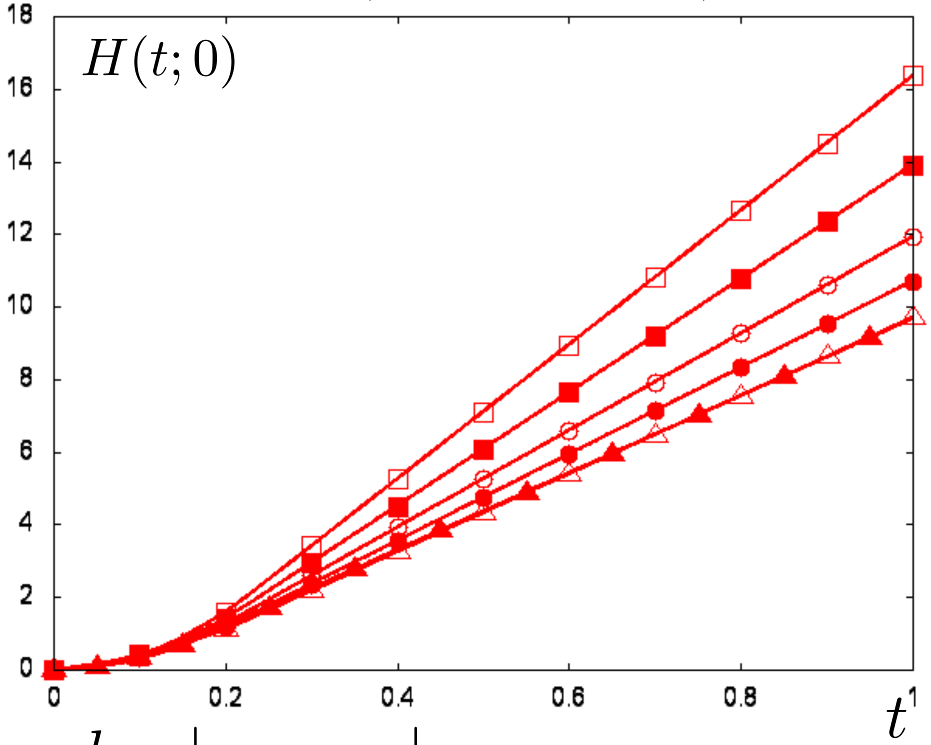
t=0.1

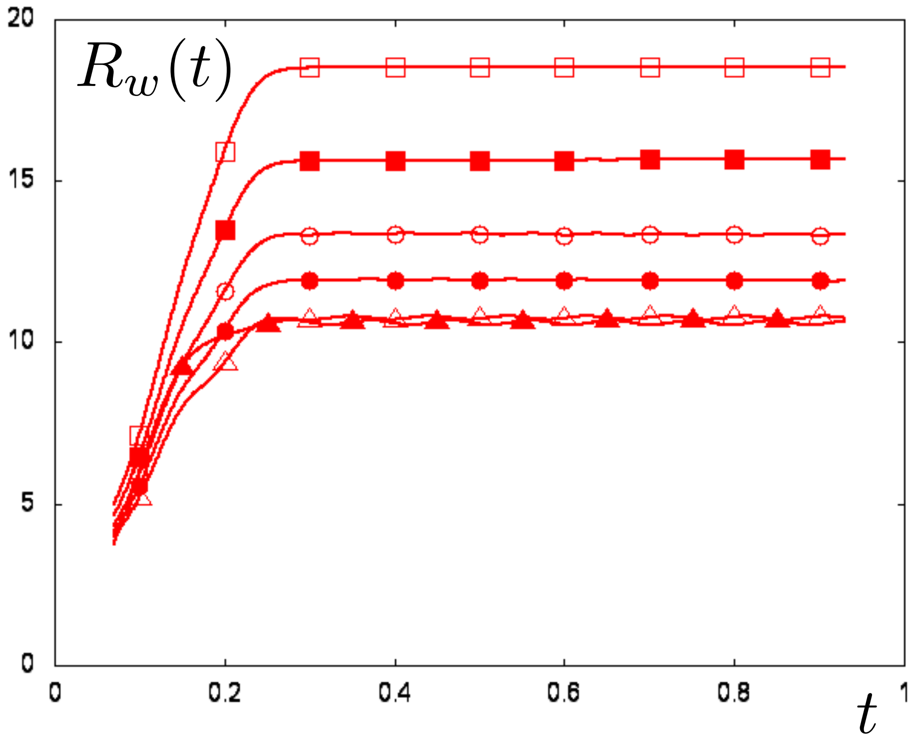


t=0.5

Surface evolution by a co-rotating pair

$\rho_c = 0.03 \quad (2\pi\rho_c \approx 0.1884)$

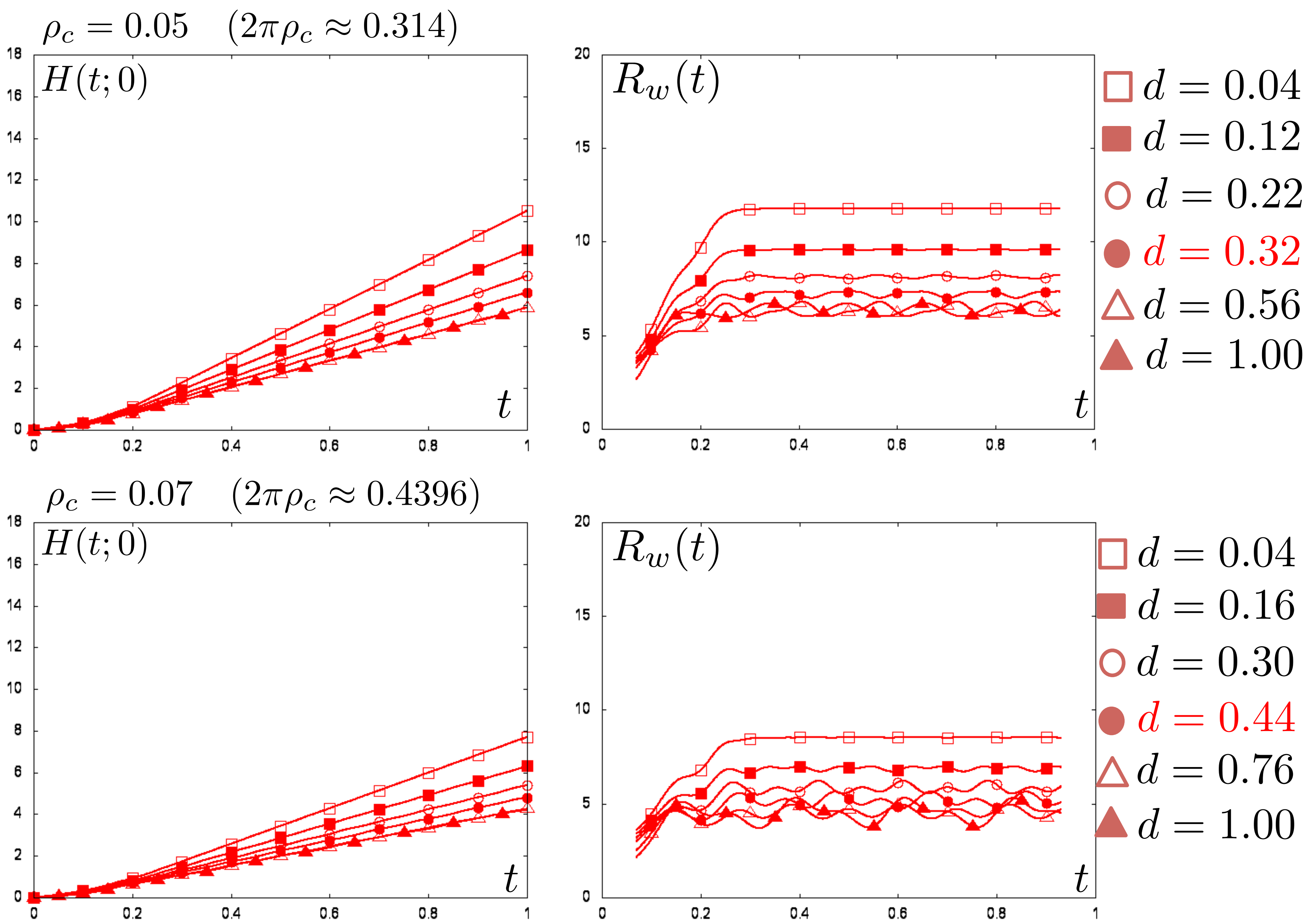




$d = |a_1 - a_2|$

- □ $d = 0.04$
- ■ $d = 0.08$
- ○ $d = 0.14$
- ● $d = 0.20 \approx 2\pi\rho_c$
- △ $d = 0.30$
- ▲ $d = 1.00$

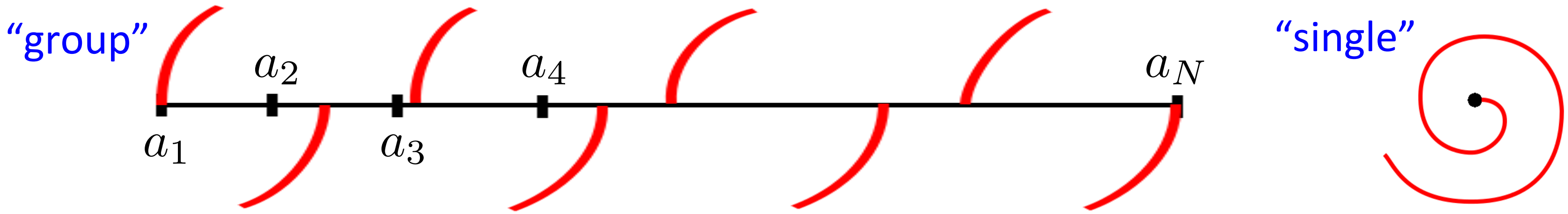
The evolution is faster than the single one when $d>2\pi\rho_c$ but $d \fallingdotseq 2\pi\rho_c$.



$\rho_c = 0.05 \quad (2\pi\rho_c \approx 0.314)$
$H(t;0)$
$R_w(t)$
t
$d = 0.04$
$d = 0.12$
$d = 0.22$
$d = 0.32$
$d = 0.56$
$d = 1.00$
$\rho_c = 0.07 \quad (2\pi\rho_c \approx 0.4396)$
$H(t;0)$
$R_w(t)$
t
$d = 0.04$
$d = 0.16$
$d = 0.30$
$d = 0.44$
$d = 0.76$
$d = 1.00$

Activity formula by a group

Assume that a group N –single screw dislocations are on line with length L.



Then, the activities of a group and a single are as follows:

Activity of a group $R_L = \frac{N h_0}{T_L}$

Activity of a single $R_S = \frac{\omega}{2\pi} h_0 = \frac{\omega_1 v_\infty h_0}{2\pi \rho_c}$

T_L is a duration a single spiral go around the line with length L.

$\omega = \omega_1 v_\infty / \rho_c$ is the angle velocity of a single spiral.

$T_L = T_1 + T_2$:

- T_1 : time for half turn at the terminal of L.
- T_2 : both way on L.(Claim: the velocity is v_∞.)

$$T_1 = \frac{2\pi}{\omega} = \frac{2\pi\rho_c}{\omega_1 v_\infty}, \quad T_2 = \frac{2L}{v_\infty}$$

$$T_L = \frac{2\pi\rho_c}{\omega_1 v_\infty} + \frac{2L}{v_\infty} = \frac{2\pi\rho_c}{\omega_1 v_\infty}(1 + L\omega_1/(\pi\rho_c))$$

$$\Rightarrow \; R_L = \frac{N}{1 + L\omega_1/(\pi\rho_c)} \cdot \frac{\omega_1 v_\infty h_0}{2\pi\rho_c} = \frac{N}{1 + L\omega_1/(\pi\rho_c)} R_S$$

$N = 2, L = d$
⇒Activity by a co-rotating pair

Relative errors

Activity formula by a co-rotating pair

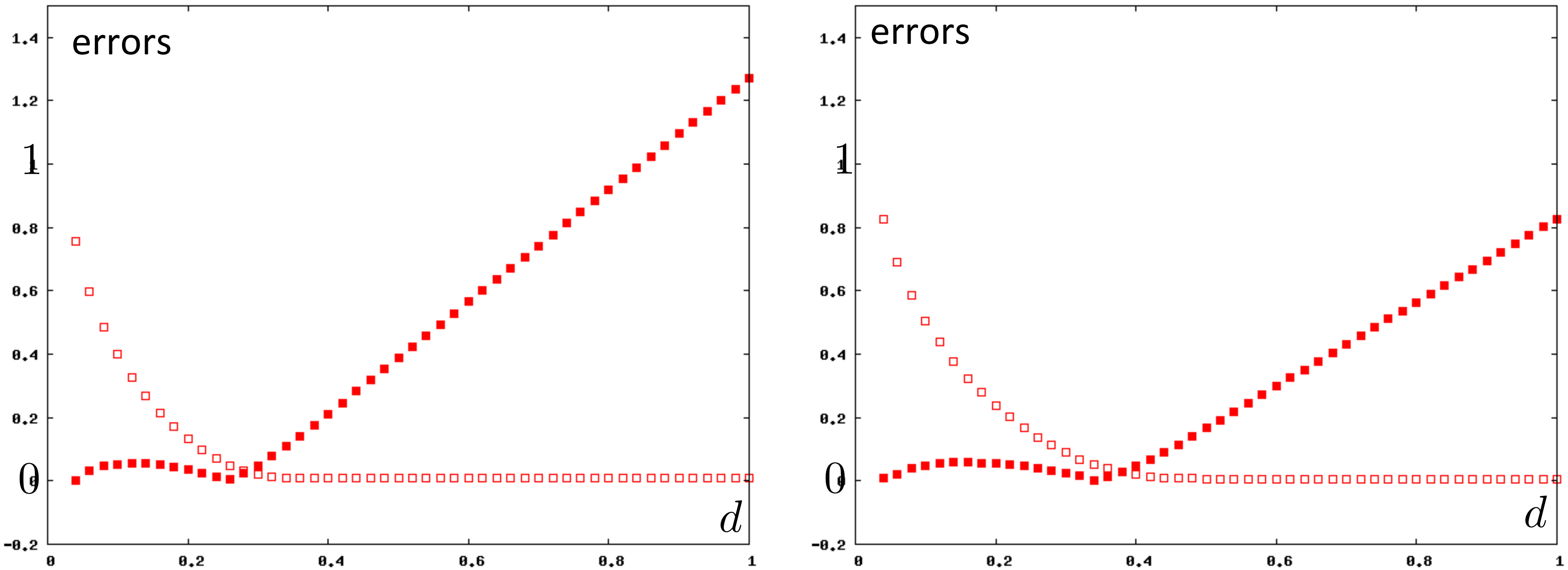
$$R_p(d) = \frac{2}{1 + d\,\omega_1/(\pi\rho_c)} R_S \quad (d < \frac{\pi\rho_c}{\omega_1})$$

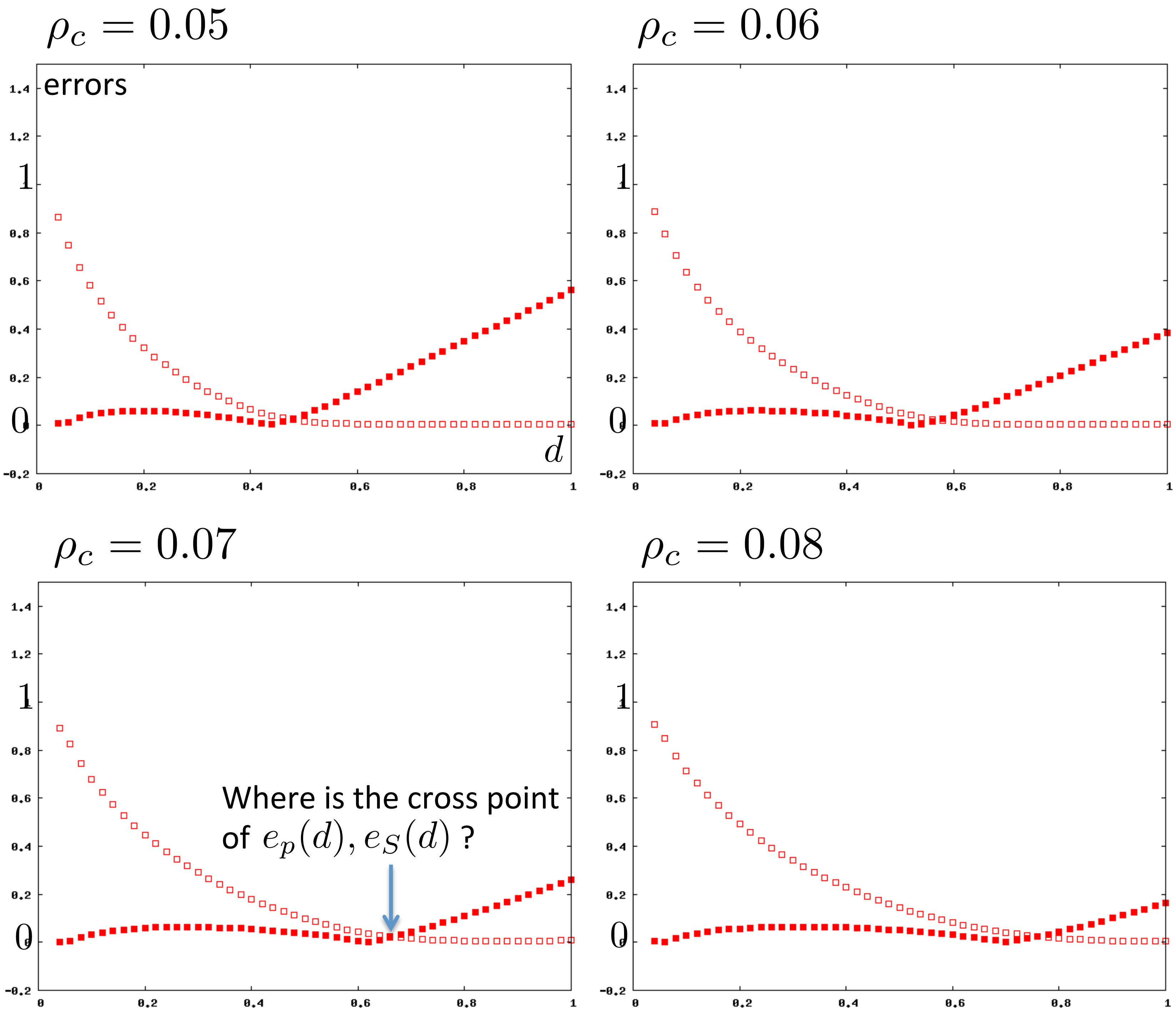
$$\omega_1 = 0.330958061$$

Relative errors between $R_\ell(t \in [0.3, 1])$ and $R_p(d)$ or R_S .

■ $e_p(d) = \frac{|R_\ell(d) - R_p(d)|}{R_p(d)}$, □ $e_S(d) = \frac{|R_\ell(d) - R_S|}{R_S}$

$\rho_c = 0.03$ $\rho_c = 0.04$





ρc = 0.05
ρc = 0.06
ρc = 0.07
ρc = 0.08
errors
d
1.4
1.2
1
0.8
0.6
0.4
0.2
0
-0.2
0
0.2
0.4
0.6
0.8
1
Where is the cross point
of $e_p(d), e_S(d)$?

Critical disntance of a co-rotating pair

Critical distance of a co-rotating pair

$$d_c = \frac{\pi \rho_c}{\omega_1}, \quad \omega_1 = 0.330958061$$

$$\Leftrightarrow R_p(d_c) = R_S$$

Numerical critical distance $\tilde{d}_c$ is such that

$$\begin{cases} e_p(d) < e_S(d) & \text{if } d < \tilde{d}_c, \\ e_p(d) > e_S(d) & \text{if } d > \tilde{d}_c \end{cases}$$

$$(\text{Roughly, } e_p(\tilde{d}_c) = e_S(\tilde{d}_c))$$

ρ_c	$2\pi\rho_c$	$\pi\rho_c/\omega_1$	$\tilde{d}_c$
0.030	0.188496	0.284773	0.284813
0.040	0.251327	0.379697	0.379700
0.050	0.314159	0.474621	0.474650
0.060	0.376991	0.569545	0.569574
0.070	0.439823	0.664469	0.664486
0.080	0.502655	0.759394	0.759396

←Numerical critical distance is almost agree with ours.

Limiting case

Consider $N = 1, a_1 = 0 \in \Omega$, and $W = \{x \in \mathbb{R}^2;\ \rho < |x| < R\}$.

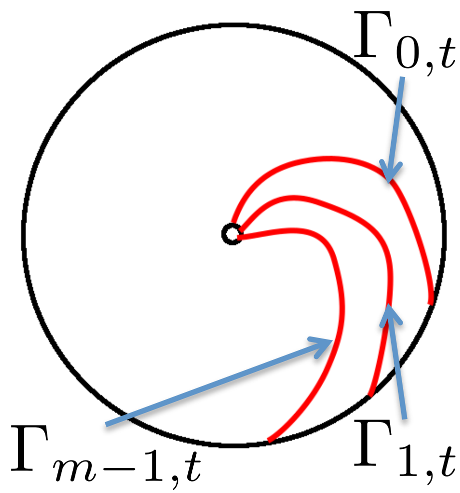
Level set equation:

$$(\mathrm{LV})_m \quad \begin{cases} u_t - v_\infty |\nabla(u - m\theta_0)| \left\{ 1 + \rho_c \mathrm{div} \dfrac{\nabla(u - m\theta_0)}{|\nabla(u - m\theta_0)|} \right\} = 0 \quad \text{in } (0,T) \times W, \\ \langle \nabla(u - m\theta_0), \vec{\nu} \rangle = 0 \quad \text{on } (0,T) \times \partial W. \end{cases}$$

$$(\theta_0(x) = \arg x)$$

Spirals:

$$\begin{aligned} \Gamma_t &= \{x \in \overline{W};\ u(t,x) - m\theta_0(x) \equiv 0 \mod 2\pi\mathbb{Z}\} \\ &= \bigcup_{j=0}^{m-1} \{x \in \overline{W};\ u(t,x) - m\theta_0(x) \equiv 2\pi j \mod 2\pi m\mathbb{Z}\} \\ &\left(=: \bigcup_{j=0}^{m-1} \Gamma_{j,t} \right). \end{aligned}$$



Claim. $\Gamma_{i,t} \cap \Gamma_{j,t} = \emptyset$ for $t > 0$ if $i \neq j$ provided that $u(0,\cdot) \in C(\overline{W})$.

Growth rate by N-spirals with a single center

Theorem.

Let H and H_j respectively be the mean growth height by m-spiral steps Γ_t, and only a single spiral step $\Gamma_{j,t}$. Then, $H(t) = \sum_{j=0}^{m} H_j(t)$.

In particular $H(t) = mH_0(t)$ if there exist $\alpha_j > 0$ for $j = 1, 2, \ldots, m-1$ such that $R_{\alpha_j}\Gamma_{0,0} = \Gamma_{j,0}$, where R_α is the rotation matrix with angle $\alpha \in \mathbb{R}$.

Claim: H and H_j is uniquely determined w.r.t. choice of solution u.

Key point: $\Gamma_{j,t} = \{x \in \overline{W};\ v_j(t,x) - \theta_0(x) \equiv 0 \mod 2\pi\mathbb{Z}\}$

$$\text{with } v_j(t,x) = \frac{u(t,x) - 2\pi j}{m}$$

$$\Longrightarrow v_j \text{ is a solution to } (\mathrm{LV})_1.$$

Claim. This result means that there is no interaction between spirals.
(This is different from the behavior by Allen-Cahn type equation by Kobayashi
(Ogiwara-Nakamura('02).)

Summary

- Rough estimate of the growth rate by a co-rotating pair.

$$\tilde{R}_p(d) = \begin{cases} \dfrac{2}{1 + d\,\omega_1/(\pi\rho_c)} R_S & (d < d_c = \pi\rho_c/\omega_1), \\ R_S & (d \geq d_c) \end{cases}$$

$$\omega_1 = 0.330958061 \text{(Ohara-Reid's constant)}$$

  - The relative error between the above and the numerical results are less than 7% for $\rho_c \in [0.03, 0.08]$.
- Introduce a new definition and quantity of the critical distance of a co-rotating pair.
  - Definition: $d = d_c$ s.t $R_p(d_c) := \dfrac{2}{1 + d_c\,\omega_1/(\pi\rho_c)} R_S = R_S$
  - Quantity: $d_c = \pi\rho_c/\omega_1 > 2\pi\rho_c.$
- Further problem
  - Mathematical analysis on the growth rate and the critical distance(finding exact limit and give a proof.)