Growth rate of crystal surface by several screw dislocations and grouping of dislocation centers by the effective growth rate

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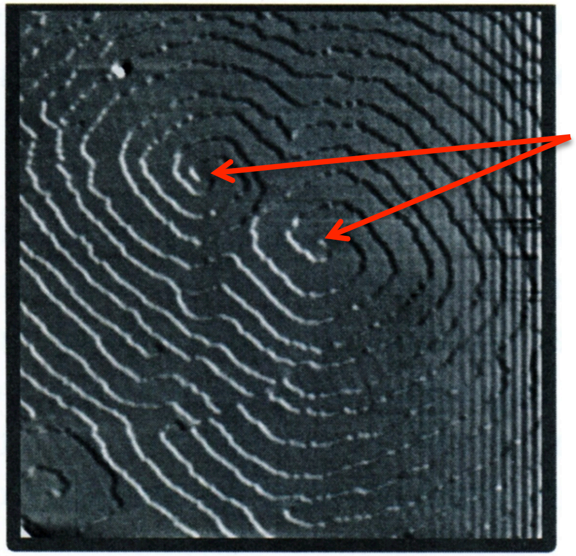
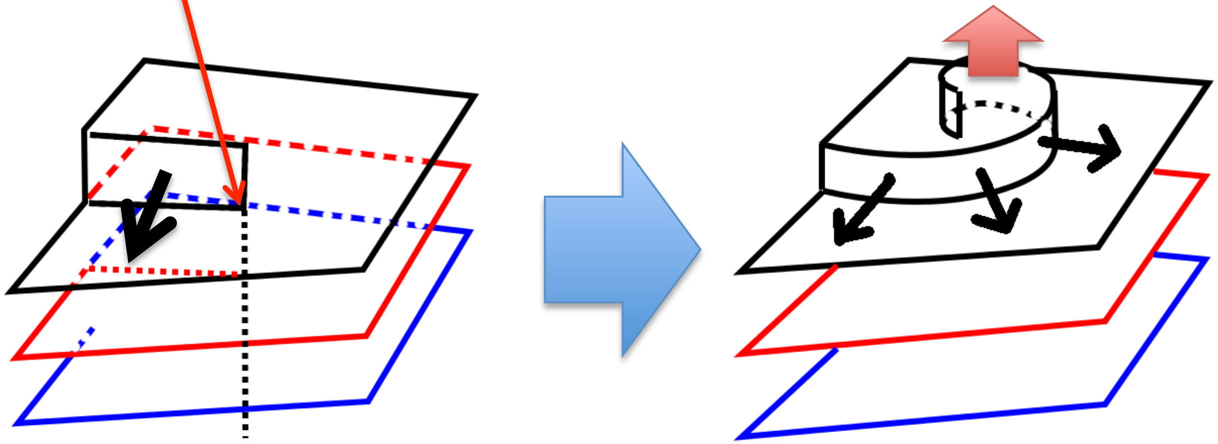
Spiral crystal growth



A. McPherson, *Crystallization of biological macromolecules,* 1999, Cold Spring Harbor Laboratory Press

Burton-Cabrera-Frank (1951, BCF paper)

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



[Gibbs-Thomson effect] Steps evolve with

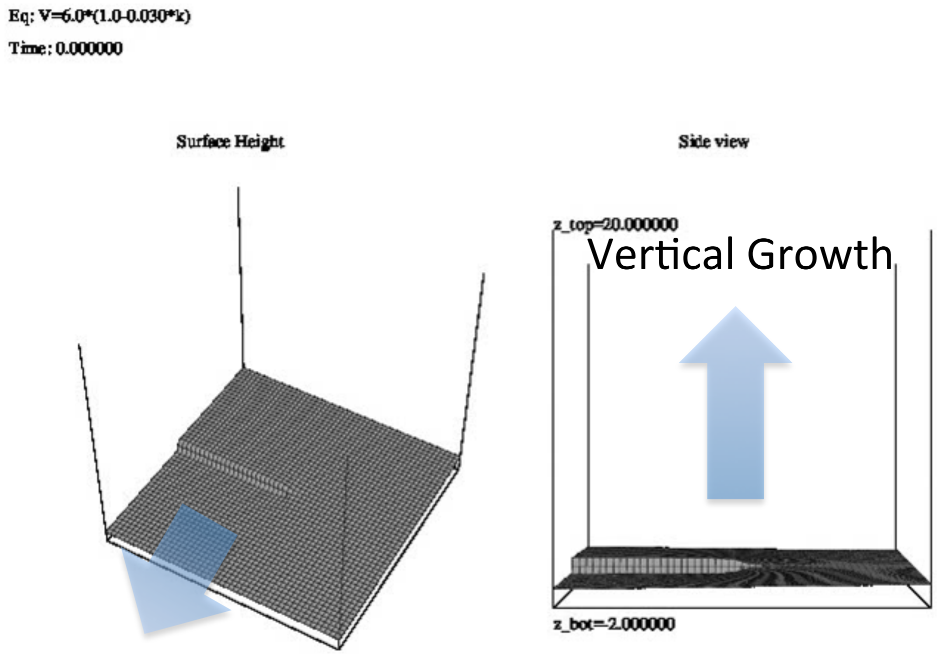
$$V = v_\infty(1 - \rho_c \kappa)$$ (steps = spiral curve $\Gamma_t \subset \mathbb{R}^2$)

V : Normal velocity, κ : curvature

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

Vertical Growth Rate

In this talk we are interested in the growth rate of the crystal surface by MANY (>=3) spiral steps.



(Horizontal Growth)

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

For single rotational spirals:

$$R^{(0)} = h_0 \times \frac{\omega}{2\pi} = \frac{h_0 \omega_1 v_\infty}{2\pi \rho_c}.$$

$\omega = \dfrac{\omega_1 v_\infty}{\rho_c}$:angular velocity

ω_1 :numerical constant

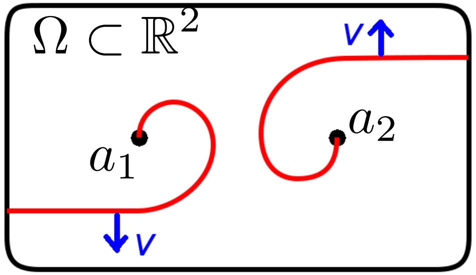
h_0 :height of the step

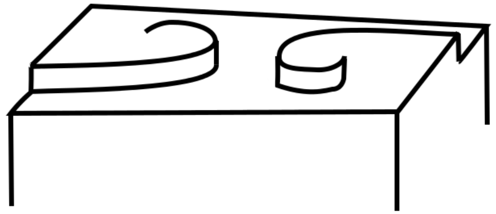
Estimate of ω_1

- Burton-Cabrera-Frank('51): $\omega_1 = 1/2.$
- Cabrera-Levine('56): $\omega_1 = 2\pi/19 \approx 0.330694.$
- Ohara-Reid('73): $\omega_1 = 0.330958061.$

Review: A co-rotating pair

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





Predictions by Burton et al. ('51) R: the effective growth rate

- If $d := |a_1 - a_2| \to 0$, then $R \to 2R^{(0)}$.
- If $d \geq d_c = 2\pi\rho_c$, then $R \approx R^{(0)}$.
- For $0 < d < d_c$, no estimate is given. But, by applying the formula for N-co-rotating spirals on a line,

$$R = \frac{2}{1 + d/(2\pi\rho_c)} R^{(0)}.$$

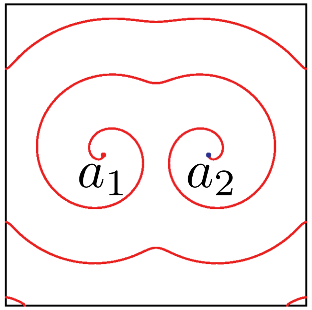
O-Tsai-Giga(arXiv:1612.08924(2016)) give an improved estimate:

$$R^{(2)}(d) = \begin{cases} \dfrac{2}{1 + d\omega_1/(\pi\rho_c)} R^{(0)} & \text{if } d < \tilde{d}_c = \dfrac{\pi\rho_c}{\omega_1}, \\ R^{(0)} & \text{otherwise.} \end{cases}$$

$$\omega_1 = 0.330958061.$$

Review: a pair with opposite rotation

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



opposite rotations

Predictions by Burton et al.

- If $d := |a_1 - a_2| < 2\rho_c$, then no growth occurs. (Inactive pair)
- If $d \approx 3\rho_c$, then $R \approx 1.1 \times R^{(0)}$.
- If $d \to \infty$, then $R \searrow R^{(0)}$ (exponential decay).

The above is verified by Miura-Kobayashi ('15), O-Tsai-Giga (arXiv).
A stationary solution for an inactive pair exists. (O, 2014(in Japanese))

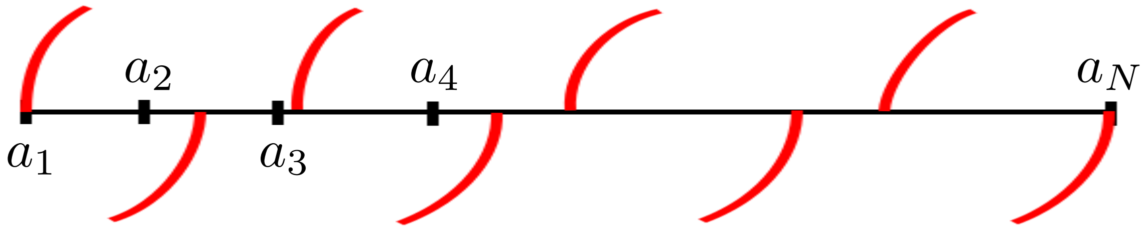
Summary for a pair

- Co-rotating pair when $d := |a_1 - a_2| < \tilde{d}_c := \dfrac{\pi \rho_c}{\omega_1} (\approx 3\pi\rho_c)$.
  - Independent two centers when $d \geq \tilde{d}_c$.
- A pair with opposite rotations is inactive when $d < 2\rho_c (< \tilde{d}_c)$.

Co-rotating group on a line

Consider the situation such that N co-rotating centers are on a line whose length is L, i.e.,

- $a_1, a_2, \ldots, a_N$ are ordered on a line with $|a_1 - a_N| = L$,
- $|a_{i+1} - a_i| < \tilde{d}_c = \pi\rho_c/\omega_1$ for every $j = 1, 2, \ldots, N$.



Burton et al.('51): $R^{(N)}(L) = \dfrac{N}{1 + L\omega_1/(\pi\rho_c)} R^{(0)}.$
$(\text{with } \omega_1 = 1/2)$

Miura-Kobayashi('15) verified the above formula with equally arranged centers by phase-field model. $(\text{with } \omega_1 = 2\pi/19)$

Question:
Is the growth rate independent of the distribution of centers?

General group

Consider N-screw dislocations $\mathcal{A} = \{a_1, a_2, \ldots, a_N\}$ with

$$a_j = (\alpha_j, \beta_j; m_j).$$

$$((\alpha_j, \beta_j) \in \Omega : \text{Location of } a_j,\ \ m_j : \text{strength(Burgers vector)})$$

Predictions by BCF: Classify the centers as follows:

1. Inactive: $\{a_j;\ \ j \in \mathcal{I}\}$ which are connected by lines which are shorter than $2\rho_c$, and $\sum_{j\in\mathcal{I}} m_j = 0$.
   →No growth occurs.
2. Group: $\{a_j;\ \ j \in \mathcal{I}\}$ which are connected by lines which are shorter than $\tilde{d}_c$, and $\sum_{j\in\mathcal{I}} m_j = n$ (possibly 0).
   →The effective growth rate is:

$$R = |n|R^{(0)} \text{ if } n \neq 0,\ \ R \approx R^{(0)} \text{ if } n = 0.$$

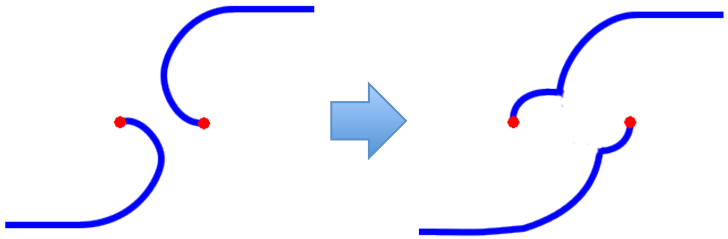
Question:

Does the centers a_i and a_j with opposite rotation also make a group when $|a_i - a_j| < \tilde{d}_c$?

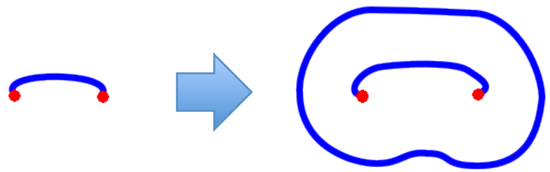
Does that cancel the effective growth rate?

Difficulties on the formulation

- Difficulty by several screw dislocations
  … Merging (with topological change)



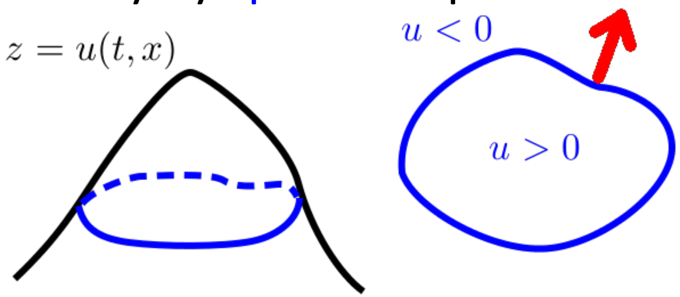
co-rotating



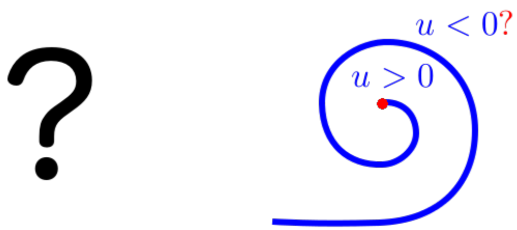
opposite rotational pair

Implicit representation (level set, phase field) of spirals are necessary.

- Difficulty by spirals … spiral is NOT closed curve



Usual level set method

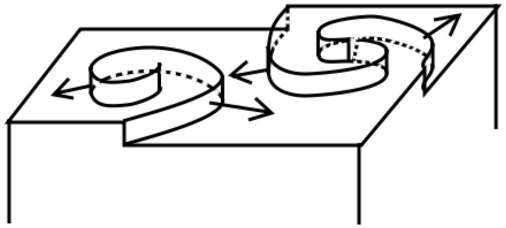


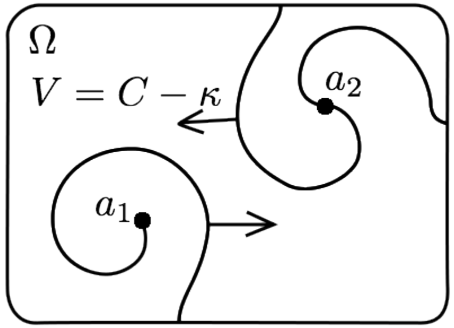
level set for spiral?

- Known formulations
  - Parametric curve: Burton-Cabrera-Frank('51)
  - Phase field method: Karma-Plapp('98), Miura-Kobayashi('15)
  - Level set method: Smereka('00), O-Tsai-Giga('15)

Level set formulation for spirals

Notations:





- Domain: $\Omega \subset \mathbb{R}^2$ is bdd. dmn.
  (Surface is on Ω.)
- Centers: $a_1, a_2, \ldots, a_N \in \Omega$
  - Region the spirals are located:

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

$$\left(B_\rho(a) = \{ x \in \mathbb{R}^2;\ |x - a| < \rho \} \right)$$

(For the technical reason we remove a disk surrounding a_j from the surface.)

- Sheet structure function (due to '90th Kobayashi)

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

- Level set formulation:

$$\Gamma_t = \{ x \in \overline{W};\ u(t,x) - \theta(x) = 2\pi n \ (n : \text{integer}) \}, \ \mathbf{n} = -\frac{\nabla(u - \theta)}{|\nabla(u - \theta)|}.$$

Role of the sheet structure function

$$\Gamma_t = \{x \in \overline{W};\ u(t,x) - \theta(x) = 2\pi n\ (n: \text{integer})\},\ \mathbf{n} = -\frac{\nabla(u-\theta)}{|\nabla(u-\theta)|}.$$

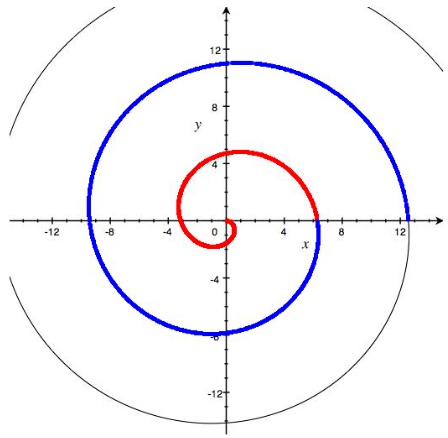
- Key observation: Rotating Archimedean spiral is given as

$\{x \in \overline{W};\ t - |x| - \arg x \equiv 0 \mod 2\pi\mathbb{Z}\}$, or

(counter-clockwise)

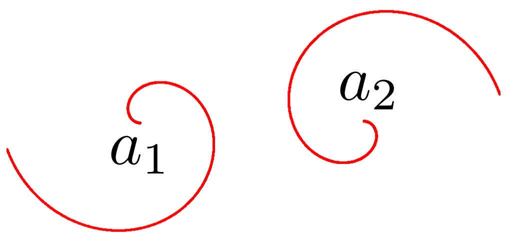
$\{x \in \overline{W};\ t - |x| + \arg x \equiv 0 \mod 2\pi\mathbb{Z}\}$.

(clockwise)

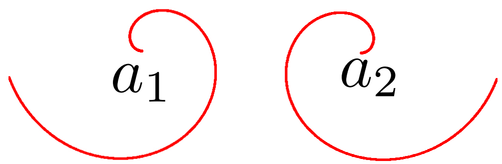


Remark: θ should be a multi-valued function.

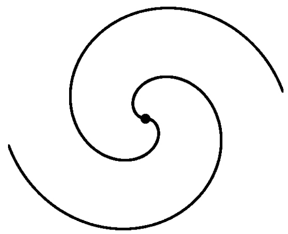
- The coefficient m_j configurates the number $(= |m_j|)$ and rotational orientation $(= \mathrm{sgn}(m_j))$ of spirals associated with a_j.



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



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



$\theta = 2\arg x$

Level set equation

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

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

Level set equation for $V = C - \kappa$ and right-angle condition:

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

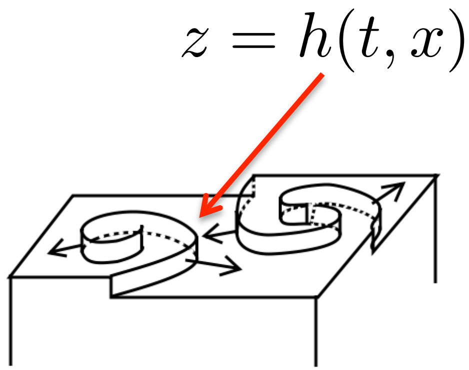
(cf. Y. Giga, *Surface evolution equation: a level set approach*, Birkhäuser, 2006)

Summary of mathematical results

- ('03 O) There exists a unique solution globally-in-time for every continuous initial data (u(0,x)) (in viscosity sense).
- ('08 Goto-Nakagawa-O) Level set is unique for every initial data describing the same initial curve. (It is unnecessary to take the distance function for level set method.)

Surface height

The surface height function $h(t,x)$ should satisfy



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

$$\Leftrightarrow \begin{cases} \Delta h = 0 \quad \text{in } W \setminus \Gamma_t, \\ h(t,x) \text{ has } h_0 > 0 \text{ jump discontinuity} \\ \text{only on } \Gamma_t \text{ in the direction of } -\mathbf{n}. \end{cases}$$

(h_0 is the diameter of the atom.)

(cf. Smereka('00), Hirth and Lothe, *Theory of dislocations*, Krieger)

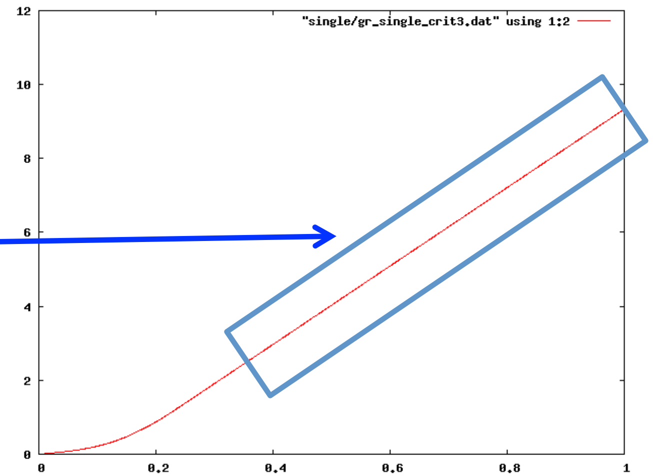
$$\Rightarrow h(t,x) = \frac{h_0}{2\pi}\theta_{\Gamma_t}$$

$$(\theta_{\Gamma_t}: \text{branch of } \theta \text{ whose discontinuity is only on } \Gamma_t)$$

Once we obtain the height function, the mean growth height is calculated as

$$H(t) = \frac{1}{|W|}\int_W (h(t,x) - h(0,x))dx.$$

Then the slope $R_\triangle$ of the linear approximation of $H(t)(\approx R_\triangle t + C_0)$ expresses the growth rate of the surface.

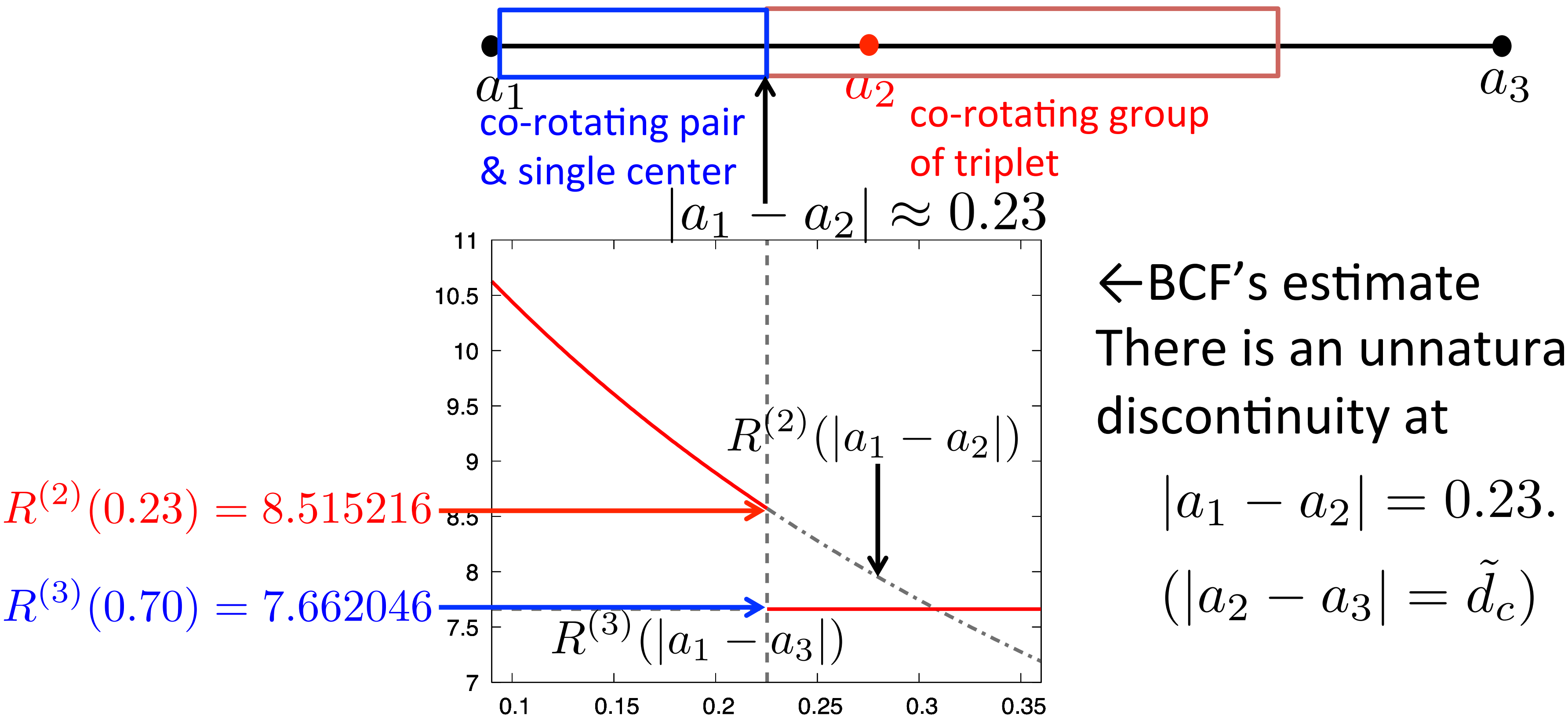


Influence of the distribution

For the evolution equation $V = 6(1 - 0.05\kappa)$ $(\rho_c = 0.05)$, consider a co-rotating triplet

$$a_1 = (-0.35, 0),\ a_2 = (-\beta, 0),\ a_3 = (0.35, 0)\ (0 < \beta < 0.35).$$

Claim: $\tilde{d}_c = 0.05 \times \pi / 0.330958061 \approx 0.474650. \Rightarrow \tilde{d}_c < |a_1 - a_3| < 2\tilde{d}_c.$



←BCF's estimate

There is an unnatural discontinuity at

$$|a_1 - a_2| = 0.23.$$

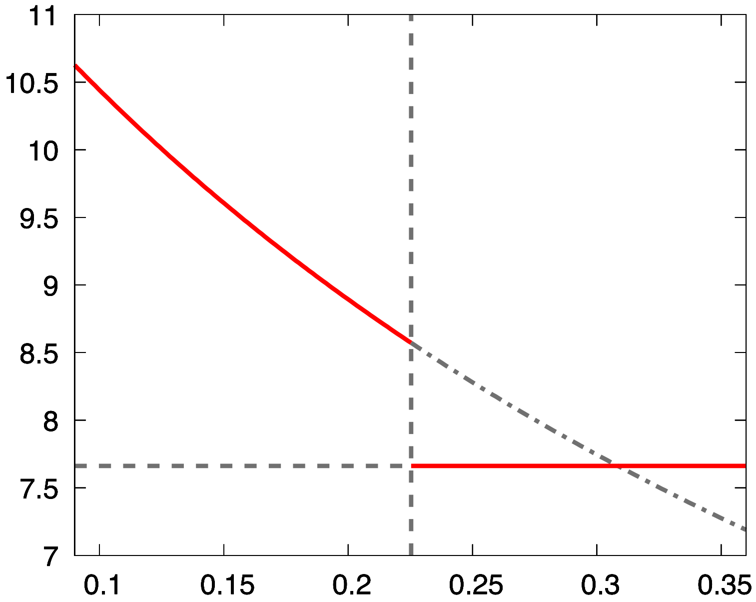
$$(|a_2 - a_3| = \tilde{d}_c)$$

Numerical results: co-rotating triplets

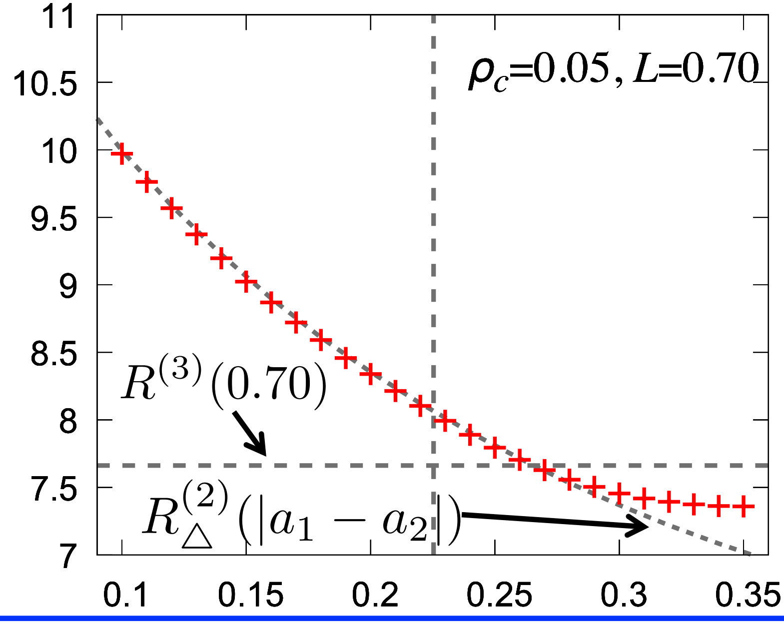
Evolution equation: $V = 6(1 - 0.05\kappa)$ $(\rho_c = 0.05)$,

$$\tilde{d}_c = 0.05 \times \pi/0.330958061 \approx 0.474650. \Rightarrow \tilde{d}_c < |a_1 - a_3| < 2\tilde{d}_c.$$

BCF's estimate



Numerical results



Summary:

- The effective growth rate is almost agree with $R^{(2)}_{\triangle}(|a_1 - a_2|)$ while
  $R^{(2)}_{\triangle}(|a_1 - a_2|) > R^{(3)}(|a_1 - a_3|)$.
- If $R^{(2)}_{\triangle}(|a_1 - a_2|) < R^{(3)}(|a_1 - a_3|)$, then the growth rate satisfies
  $R^{(2)}_{\triangle}(|a_1 - a_2|) < R_{\triangle} < R^{(3)}(|a_1 - a_3|)$.

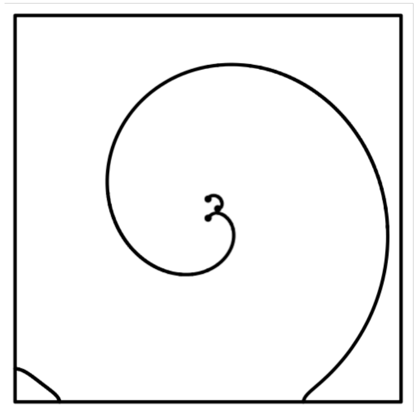
The effective growth rate depends on the distribution of screw dislocations.

Cancellation of the growth rate

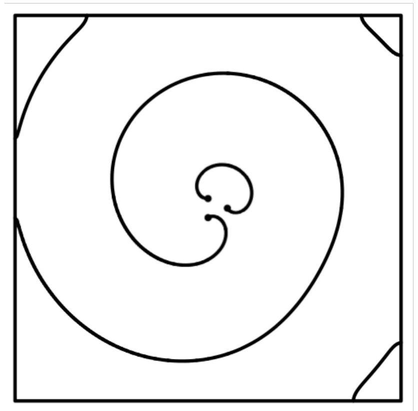
For the evolution equation $V = 6(1 - 0.05\kappa)$, consider a triplet

$$a_1 = (0, -0.05; 1),\ a_2 = (0, 0.05; 1),\ a_3 = (\beta, 0; -1).\ (0 \le \beta \le 0.5)$$

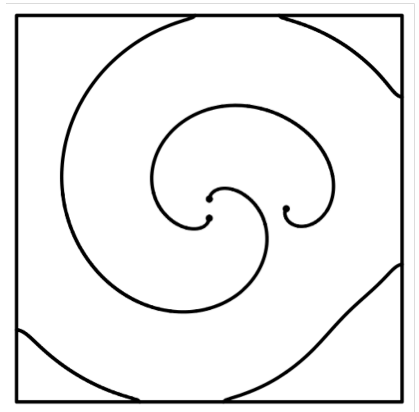
Approach the center with opposite rotation to a co-rotating pair.



$\beta = 0.05$

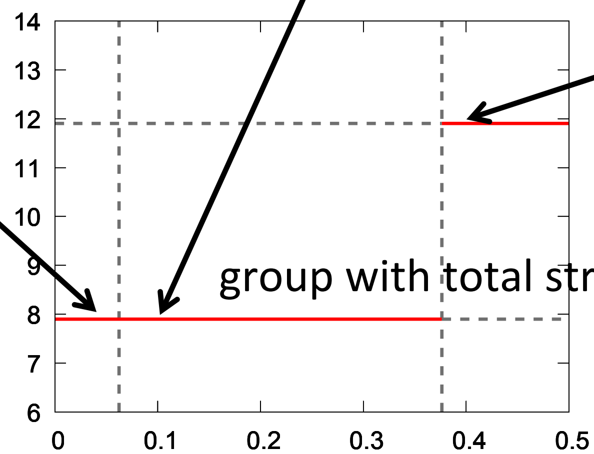


$\beta = 0.10$



$\beta = 0.40$

BCF's estimate:

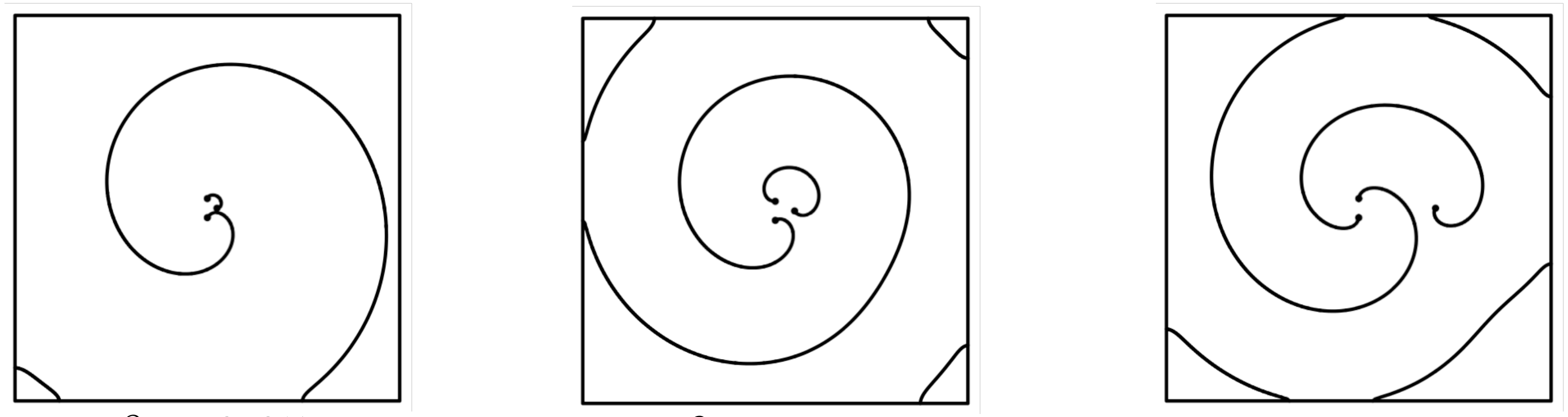


inactive pair + single

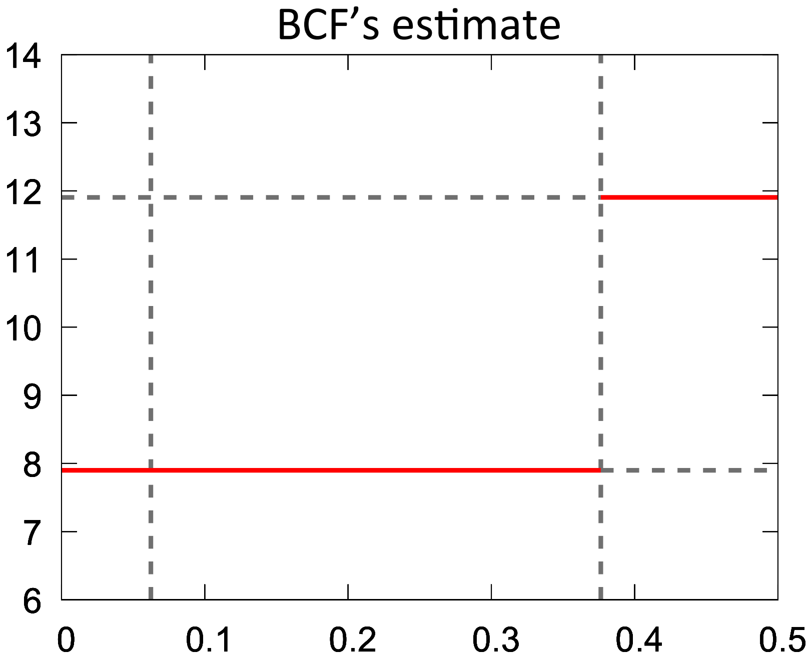
group with total strength=1

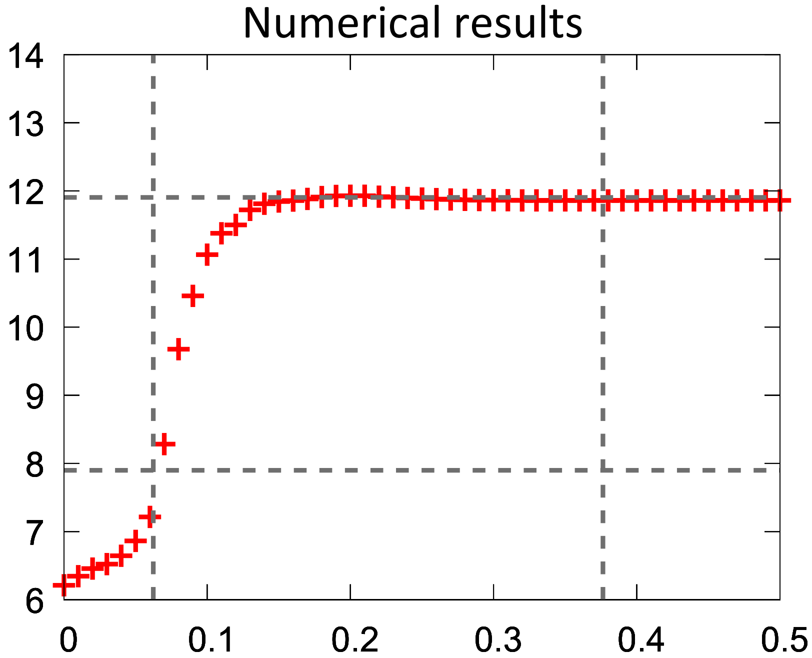
co-rotating pair + single
total strength=2

Numerical results: cancellation



$\beta = 0.05$ $\beta = 0.10$ $\beta = 0.40$



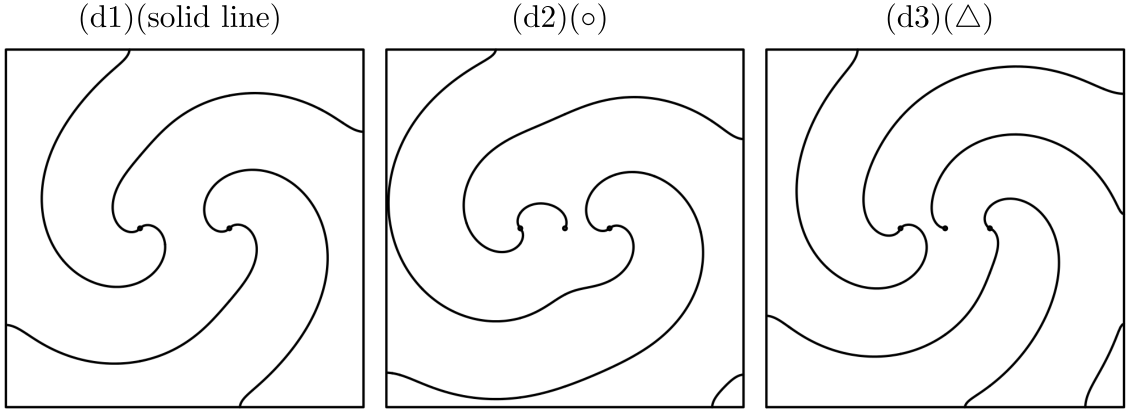


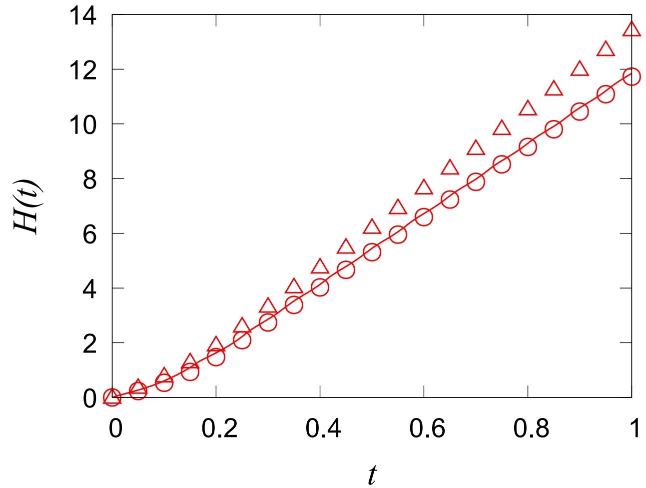
Cancellation of the growth rate occurs when $|a_i - a_j| < 2\rho_c$.

Connection of centers

To verify the connection of centers, we consider the following 3 situations.

Evolution equation: $V = 6(1 - 0.05\kappa), \qquad (\tilde{d}_c \approx 0.474650)$





- (d1): Independent two centers with strength=2

  $a_1 = (-0.25, 0; 2), \; a_2 = (0.25, 0; 2)$

- (d2): A center with opposite rotation between the pair (d1)

  $a_1 = (-0.25, 0; 2), \; a_2 = (0.25, 0; 2), \; a_3 = (0, 0; -1) \; (\text{Total strength} = 3)$

- (d3): Co-rotating triplet with total strength=5:

  $a_1 = (-0.25, 0; 2), \; a_2 = (0.25, 0; 2), \; a_3 = (0, 0; 1) \; (\text{Total strength} = 5)$

BCF's estimate:

$$(\text{d1}) \; 2R^{(0)} \approx 12.641667, \; (\text{d2}) \; R^{(3)}(0.5) \approx 9.234359, \; (\text{d3}) \; R^{(5)}(0.5) \approx 15.390599.$$

Numerical results: A center with opposite rotation does not make connections.

$$(\text{d1}) \; R_{\triangle} \approx 12.846801, \; (\text{d2}) \; R_{\triangle} \approx 12.841811, \; (\text{d3}) \; R_{\triangle} \approx 14.445982.$$

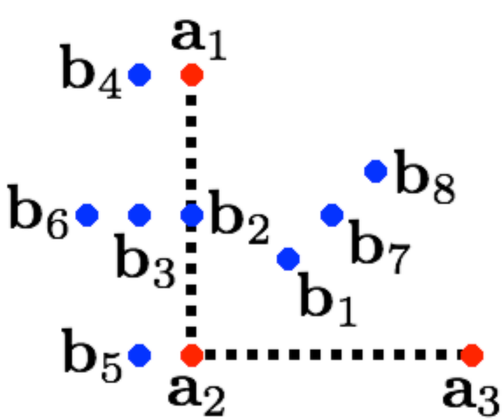
Reduction of the growth rate

There is a case the effective growth rate of co-rotating group is reduced by a center with opposite rotation around the convex hull of the group.

Evolution equation: $V = 6(1 - 0.05\kappa)$,
Co-rotating group (total strength=6):

$$a_1 = (-0.21, 0.21; 2),\ a_2 = (-0.21, -0.21; 2),\ a_3 = (0.21, 0.21; 2).$$

(Co-rotating connection between a_1-a_2, a_2-a_3, but no connection between a_1-a_3)
Opposite rotating center: $b = (\alpha, \beta; -1)$ as follows.

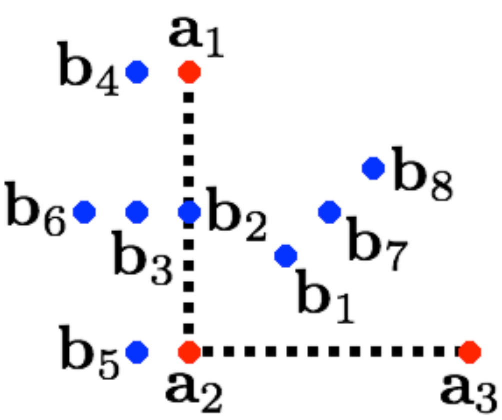


$\{a_1, a_2, a_3\}$ with
b_1: the mass center of a_1, a_2, a_3
b_2: on the convex hull & the c-line
b_3: out but close to the convex hull
b_4: cancel the strength of a_1
b_5: cancel the strength of a_2
b_6: far away from the convex hull
b_7: in the convex hull, not on the c-line
b_8: far away from the convex hull

c-line=connection line(dotted)

Claim: every b_j reduces the strength of a group $\{a_1, a_2, a_3\}$ to 5.

Numerical results: Reduction of rates



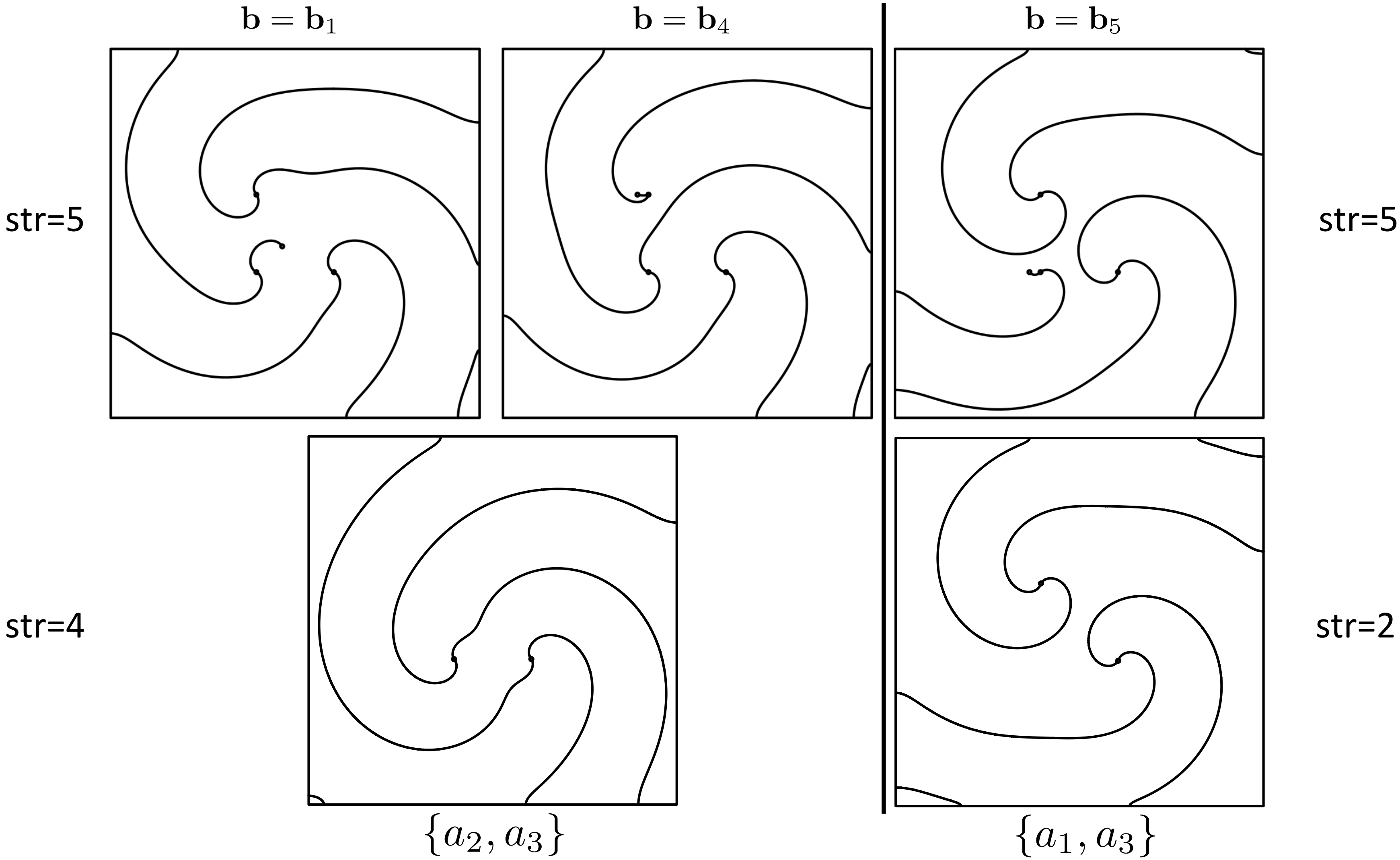
$\{a_1, a_2, a_3\}$ with	$R_\triangle$
b_1: the mass center of a_1, a_2, a_3	13.268728
b_2: on the convex hull & the c-line	13.383400
b_3: out but close to the convex hull	13.580583
b_4: cancel the strength of a_1	13.283504
b_5: cancel the strength of a_2	12.811923
b_6: far away from the convex hull	13.833242
b_7: in the convex hull, not on the c-line	13.553001
b_8: far away from the convex hull	13.808827
Just co-rotating centers	$R_\triangle$
$\{a_1, a_3\}$: independent two centers	12.724605
$\{a_2, a_3\}$: co-rotating pair	13.283220
$\{a_1, a_2, a_3\}$: co-rotating group	14.195001

- The all cases of $\{a_1, a_2, a_3\}$ with b_j reduces the effective growth rate. But, the all rates are higher than $(5/6) \times R_\triangle(\{a_1, a_2, a_3\}) = 11.8291675.$
  → Reduction of the growth rate is not caused by the reduction of strength.
- Important consistency:

$$R_\triangle(\{a_1, a_2, a_3, b_j\})(j = 1, 2, 4) = R_\triangle(\{a_2, a_3\}) \approx R^{(4)}(0.42) \approx 13.413502.$$

$$R_\triangle(\{a_1, a_2, a_3, b_5\}) = R_\triangle(\{a_1, a_3\}) \approx 2R^{(0)} \approx 12.641667.$$

Profiles



- Strength is refrected to the numbers of spirals
- The growth rate of a group should be the maximum of rates of the subgroups.

Summary on Grouping

1. Each pair of a_i, a_j with strength m_i, m_j should be regarded as a single center with the strength m_i+m_j if $|a_i - a_j| < 2\rho_c$. If m_i+m_j=0, then the pair should be discarded from the surface.
2. After the reduction described in 1., groups of co-rotating spirals are identified by connecting the co-rotating centers with lines whose length is shorter than $\tilde{d}_c = \pi\rho_c/\omega_1$.
3. If there is a group $\mathcal{A} = \{a_1, \ldots, a_N\}$ with the strength $n \geq 1$, and a center b with negative strength $-m$ with $m \geq 1$ nearby $\mathcal{A}$, then they seem to be a single center with $|n - m|$ spiral steps. If $|n - m| = 0$, then closed loops stem out from the group.
4. If the center b is in a covex hull of $\mathcal{A}$ in 3. and $n>m$, then the effective growth rate by $\mathcal{A}$ and b should be reduced from that of $\mathcal{A}$ in a more elaborate fashion.
   - Consider a subgroup of $\mathcal{A}$. We call the subgroup is b-pure when b is out of the convex hull of this subgroup.
   - Then, the effective growth rate of $\mathcal{A}$ is the maximum of the rates of b-pure subgroups and $(n - m)R^{(0)}$.

Concluding remarks

1. Conclusions
    1. Not only the Burgers vectors and density(number) but also the distribution of screw dislocations has an influence to the effective growth rate of the crystal surface.
        - The center with opposite rotation between co-rotating centers does not make a connection of a group.
        - Strength (total norm of Burgers vector) of the group has influence to the number of spirals, but does not affect to the growth rate.
    2. A new procedure estimating the growth rate of the surface is proposed.
2. Further works
    1. Rigorous mathematical analysis
    2. Extention to the crystalline motion (polygonal steps)

Thank you for your attention.

Appendix: Mathematical results

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* $u(0,x) \leq v(0,x)$ *for* $x \in \overline{W}$, *then* $u(t,x) \leq v(t,x)$ *for* $(t,x) \in (0,T) \times \overline{W}$.

(⇒Uniqueness of solution to (LV))

(Remark: USC(D) (resp. LSC(D)) ⇔ Upper (resp. Lower) Semi Continuous on D)

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* $u(0,\cdot) = u_0$.

Uniqueness of level sets ('08 Goto-Nakagawa-O)
The spiral Γ_t depends only on Γ_0, i.e., is independent of the choice of $u_0 \in C(\overline{W})$.

'15 O-Tsai-Giga: Numerical simulations and giving a practical way to construct an initial data.