On growth speed of a birth-spread model for two-dimensional nucleation on a crystal surface

Yoshikazu Giga (University of Tokyo)
Joint work with
Hiroyoshi Mitake (Hiroshima University)
Hung V. Tran (University of Wisconsin)

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Contents

1. Introduction
1.1 Models (for growth of a crystal surface)

Two-dimensional nucleation: A flat crystal surface grows by adatoms over the surface. How should one model this phenomenon to measure the growth rate?

There are several models. A typical one is "Birth and Spread Model" (cf. M. Ohara – R. C. Reid (1973))

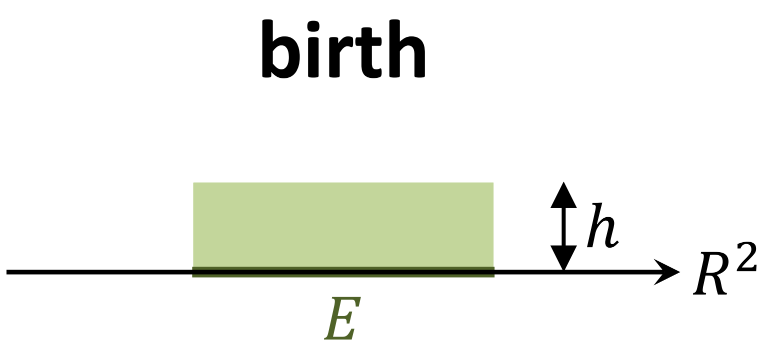
Birth and Spread Model

1. Birth

Adatoms touch to the crystal surface on a set E.

The set E is a set of nucleation centers.

The height is assumed to be $h > 0$.



Birth and Spread Model (continued)

2. Spread / propagation

Each layer (step) moves horizontally with horizontal normal speed:

$$V = v_\infty \left(\rho_c \kappa + 1 \right).$$

Here κ : the mean curvature (sum of principal curvature)

$v_\infty > 0$: step velocity

$\rho_c > 0$: critical radius

spread

Birth and Spread Model (continued)

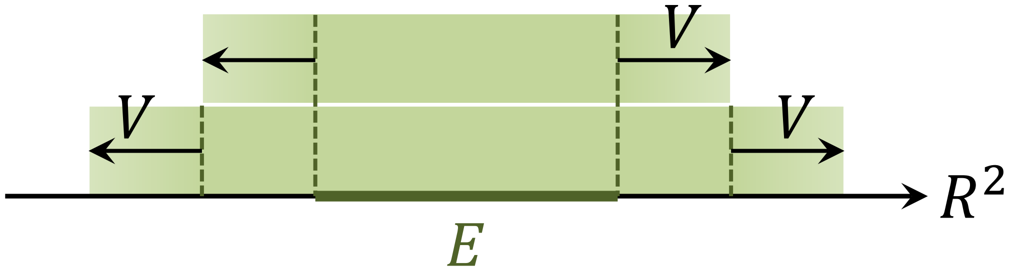
3. **Repeat the Step 1 (Forming the second layer)**
4. **Repeat the Step 2**

and repeat 3 and 4 successively.

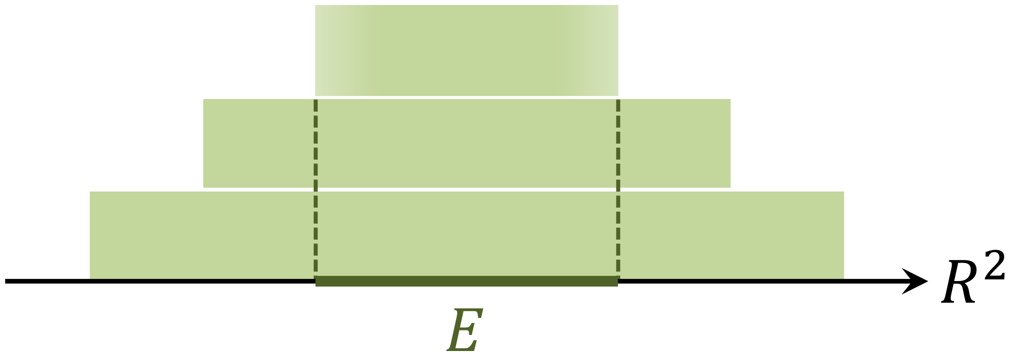
Step 3

Birth and Spread Model (continued)

Step 4



Step 5



Derivation of PDE model

Let $w = w(x,t)$ be the height function at the place $x \in R^2$ and the time $t > 0$.

1. Birth (with speed $c > 0$)

$$u(x,t) = c1_E t, \quad 1_E(x) = \begin{cases} 1, x \in E \\ 0, x \notin E \end{cases}$$

or $u_t = c\, 1_E$

2. Spread

$$u_t = v_\infty \left(\rho_c \operatorname{div}\left(\frac{Du}{|Du|} \right) + 1 \right) |Du|$$

Repeating these processes alternatively with the time grid τ and sending $\tau \to 0$ to get the equation

$$w_t - v_\infty \left(\rho_c \operatorname{div}\left(\frac{Dw}{|Dw|} \right) + 1 \right) |Dw| = c1_E$$

(Trotter-Kato product formula)

Problem

Consider

$$\begin{cases} w_t - v_\infty \left(\rho_c \operatorname{div}\left(\dfrac{Dw}{|Dw|} \right) + 1 \right) |Dw| = c 1_E \\ w\Big|_{t=0} = 0. \end{cases}$$

What is the large time behavior of w? For example, investigate the asymptotic speed (growth rate)

$$\lim_{t\to\infty} \frac{w(x,t)}{t} = ?$$

(The value may not be c.)

2. The case of no curvature and spherical symmetric case

2.1 The case $\rho_c = 0$

Equation becomes

$$\begin{cases} w_t - v_\infty |Dw| = c 1_E \quad (\, E : \text{bounded closed set}\,) \\ w\big|_{t=0} = 0 \end{cases}$$

The unique “envelope” solution is

$$w(x,t) = c(t - v_\infty \operatorname{dist}(x, E))_+$$

so that $w/t \to c$ as $t \to \infty$. The set E can be a point or a discrete set, so we need a notion of an envelope solution (Y. G. – N. Hamamuki (2013))

Asymptotic speed in the case $\rho_c = 0$

$$\begin{cases} w_t - v_\infty |Dw| = \sum_{i=1}^{m} c_i \, 1_{\{a_i\}}, \quad c_i > 0 \\ w\big|_{t=0} = 0 \end{cases}$$

The unique envelope solution is given

$$w(x,t) = \max_{1 \le i \le m} c_i (t - v_\infty |x - a_i|)_+$$

(cf. T. P. Schulze – R. Kohn (1999))

The problem is **coercive** so general growth rate can be obtained. (N. Hamamuki (2014))

Large-time asymptotics for non-coercive Hamiltonians (e.g. Y. G. – Q. Liu – H. Mitake (2012), (2014). E. Yokoyama – Y. G. – P. Rybka (2008))

2.2 Spherical symmetric case

From now on, we assume $\rho_c = 1, v_\infty = 1$.

Consider the level-set flow equation of the eikonal-curvature flow $V = \kappa + 1$ with source term f :

$$
\text{(P)} \quad \begin{cases} w_t - \left(\operatorname{div}\left(\dfrac{Dw}{|Dw|} \right) + 1 \right) |Dw| = f(x) & \text{in } R^n \times (0, \infty), \\ w\Big|_{t=0} = w_0 & \text{in } R^n. \end{cases}
$$

Assumptions on f and w_0

Here f is bounded and $f \geq 0$, $\operatorname{supp} f$ is compact, w_0 is continuous, $\operatorname{supp} w_0$ is compact.

Basic properties

- Even if f is discontinuous, there exists a global-in-time viscosity solution, which may not be unique (Y. G. – Mitake – Tran)
- Weak comparison principle holds.

Spherical symmetric case

A non-coercive equation :

$$w_t - \left(1 - \frac{n-1}{r}\right) w_r = c1_{B(0,R_0)}.$$

Assume that $E = B(0, R_0)$ a closed ball of radius R_0 centered at zero. Let w be the maximum solution of (P) with $f = c1_E, w_0 = 0$. The solution w can be obtained by an explicit calculation.

- $R_0 < n - 1 \Rightarrow$ the growth is completed in finite time
- $R_0 > n - 1 \Rightarrow$ the growth rate equals c
- $R_0 = n - 1 \Rightarrow w(x, t) = tc1_{B(0,R_0)}$

  It grows with speed c in $B(0, R_0)$ but never grows outside $B(0, R_0)$

Spherical symmetric case

Theorem 2.1. (i) If $R_0 < n-1$, then

$$w(x,t) = \min(ct, \varphi(r))$$

φ: stationary solution

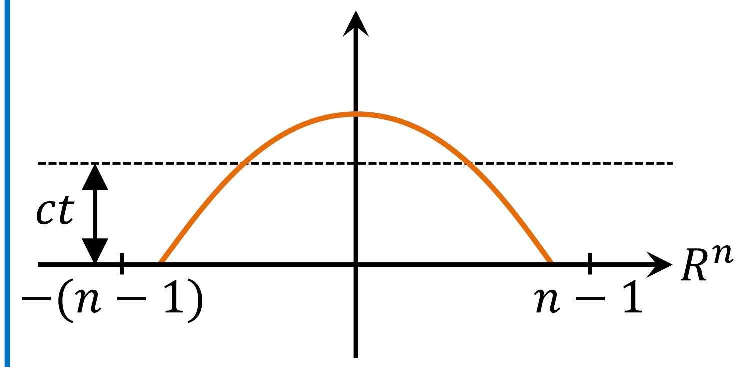
(ii) If $R_0 > n-1$, then

$$\lim_{t\to\infty} \frac{w(x,t)}{t} = c \quad \text{(locally uniformly)}$$

(There is an explicit formula for w)

(iii) If $R_0 = n-1$, $w(x,t) = t\, c 1_{B(0,R_0)}$

Here w is the maximal viscosity solution.



graph of φ

Note that even if $E = \partial B(0,R_0)$ with $R_0 > n-1$, we get $\frac{w(x,t)}{t} \to c$.

3. Existence of asymptotics speed for a Lipschitz source term (work in progress)

Consider

$$(\mathrm{P})\quad \begin{cases} w_t - \left(\operatorname{div}\left(\dfrac{Dw}{|Dw|}\right) + 1\right)|Dw| = f(x) & \text{in } R^n \times (0,\infty) \\ w\big|_{t=0} = w_0 & \text{in } R^n \end{cases}$$

f : bounded, $f \not\equiv 0$, $\operatorname{supp} f$: compact

w_0 : continuous, $\operatorname{supp} w_0$: compact

(There is a unique viscosity solution if f is Lipschitz.)

Theorem 3.1. Assume that f is Lipschitz. Let w be the viscosity solution of (P). Then $\lim_{t\to\infty} w(x,t)/t = a$ exists and the convergence is locally uniform.

What is the growth rate a?

Let $\phi(t)$ be the maximum value of w at time t, i.e.,

$$\phi(t) := \max_{x \in R^n} w(x,t)$$

Theorem 3.2 (Subadditivity of ϕ). $\phi(t+s) \le \phi(t) + \phi(s)$ $t, s > 0$

Proof. Set $v(x,t) := w(x,t+s) - \phi(s)$ so that $v(x,0) \le 0$. By the comparison principle, $v(x,t) \le w(x,t)$, which implies

$$w(x,t+s) \le w(x,t) + \phi(s)$$

for all $x \in R^n$. □

What is the growth rate a? (continued)

Lemma 3.3.

$$a = \lim_{t\to\infty} \frac{\phi(t)}{t} = \inf_{t>0} \frac{\phi(t)}{t}$$

Proof. Fekete's lemma on subadditivity says that $\phi(t)/t$ is nonincreasing. Thus $\lim_{t\to\infty} \phi(t)/t$ exists. $\square$

The growth rate in Theorem 3.1 must be $\inf \phi(t)/t$.

Idea of the proof of Theorem 3.1

Lemma 3.4 (Lipschitz bound). There exists $C > 0$ depending on f and w_0 such that

$$\|w_t\|_{L^\infty(R^n\times[0,\infty))} + \|Dw\|_{L^\infty(R^n\times[0,\infty))} \leq C$$

Proof of Theorem 3.1. For any fixed $R > 0$ we have, by Lemma 3.4,

$$|w(x,t) - \phi(t)| = \left|w(x,t) - \max_{y\in[-d,d]^n} w(y,t)\right| \leq \mathrm{L}(R+d)$$

where d is taken so that $\mathrm{supp}\, f, \mathrm{supp}\, w_0 \subset [-d,d]^n$. Thus

$$\lim_{t\to\infty} \sup_{|x|<R} \left|\frac{w(x,t) - \phi(t)}{t}\right| = 0,$$

which yields Theorem 3.1. □

Bernstein's argument to get a Lipschitz bound (formal proof of Lemma 3.4)

We recall that our equation can be written as

$$w_t - \sum_{i,j} a_{ij}(Dw)\, w_{x_i x_j} - |Dw| - f = 0$$

with $a_{ij}(p) = \delta_{ij} - p_i p_j/|p|^2$. We set $U = |Dw|^2/2$ and differentiate in x_k the above equation and multiply w_{x_k} to get

$$2U_t - \sum_{i,j,k,\ell} a_{ij}\left(U_{x_i x_j} - w_{x_i x_k} w_{x_j x_k}\right) - f_{x_k} w_{x_k} - \left\{\left(a_{ij}\right)_{p_\ell} w_{x_i x_j} + \frac{2 w_{x_\ell}}{|Dw|}\right\} U_{x_\ell} = 0$$

Formal proof continued 1

Take max point $(x_0, t_0) \in R^n \times (0, T]$ of U, i.e.,

$$U(x_0, t_0) = \max_{R^n \times [0,T]} U \, .$$

(We may assume that $t_0 > 0$.) At this point $U_t \le 0$, $DU = 0$, $D^2 U \le 0$. Thus

$$\sum_{i,j,k} a_{ij} \, w_{x_i x_h} w_{x_j x_k} - f_{x_k} w_{x_k} \le 0. \qquad (*)$$

Note that $0 \le A \le I$ for $A = (a_{ij})$.

A linear algebra inequality $(\operatorname{tr} AB)^2 \le \operatorname{tr} A \operatorname{tr} AB^2$ for $A \ge 0$ implies

$$\left(\sum a_{ij} \, w_{x_i x_j} \right)^2 \le n \sum a_{ij} \, w_{x_i x_k} w_{x_j x_k}.$$

Formal proof continued 2

Note that

$$\left(\sum a_{ij}\, w_{x_i x_j}\right)^2 = (w_t - |Dw| - f)^2 \geq \frac{1}{2}|Dw|^2 - {}^{\exists}M_0$$

provided that $|w_t| \leq M_1$ (since f is Lipschitz).

Thus (*) implies

$$\frac{1}{2n}|Dw|^2 - Df \cdot Dw \leq M_2 \quad \text{at} \quad (x_0, t_0).$$

This implies a bound for $|Dw|$ (or U). (The bound for $|w_t| \leq M_1$ is easier.) □

Actual proof needs approximation of the equation so that the equation is parabolic e.g. $|Dw|$ is approximated by $(|Dw|^2 + \varepsilon^2)^{1/2}$.

4. Estimate for asymptotic speed (Y. G. – H. Mitake – H. Tran, preprint)

Problem. If $f(x) = c1_E$, in what E

$$\limsup_{t\to\infty} \frac{w(x,t)}{t} < c \quad \text{and} \quad \liminf_{t\to\infty} \frac{w(x,t)}{t} > 0?$$

We have studied this problem when E is a ball. In this case

$$\frac{w(x,t)}{t} \to 0 \quad \text{or} \quad \frac{w(x,t)}{t} \to c.$$

Are there any intermediate situation?

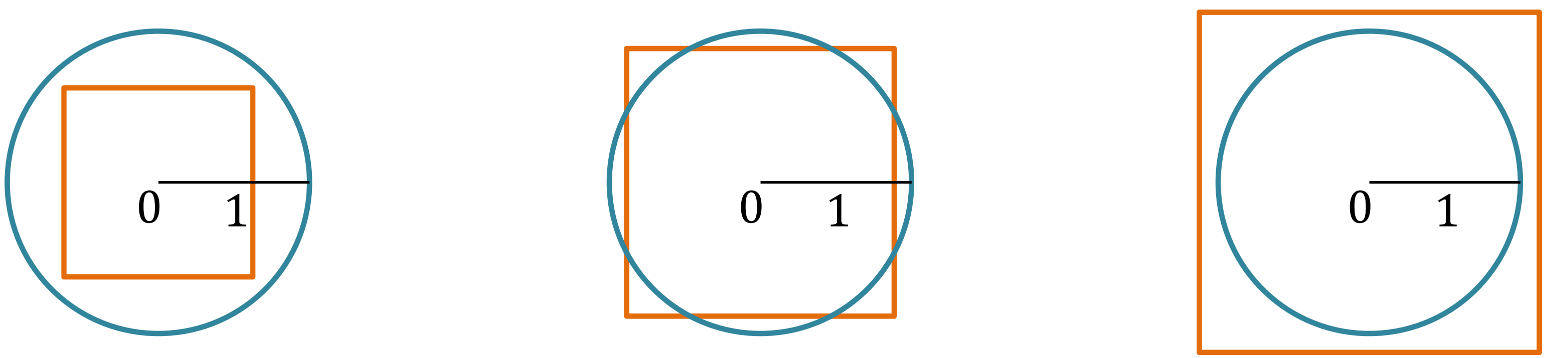
4.1 In the case of square

Assume that $E = \{(x_1, x_2) || x_i| \leq d, i = 1, z\}$. Let w be the maximal solution of

$$w_t - \left(\operatorname{div}\frac{Dw}{|Dw|} + 1\right)|Dw| = c1_E,$$

$$w\Big|_{t=0} = 0.$$

$d < 1/\sqrt{2}$ $\quad$ $1/\sqrt{2} < d < 1$ $\quad$ $d > 1$



Intermediate situation

Theorem 4.1 (Y. G. – H. Mitake – H. Tran, preprint). Assume that $1/\sqrt{2} < d < 1$. Then there exists α and β such that $0 < \alpha < \beta < c$ at

$$\alpha \leq \liminf_{t\to\infty} \frac{w(x,t)}{t} \leq \limsup_{t\to\infty} \frac{w(x,t)}{t} \leq \beta$$

locally uniformly for $x \in R^2$.

Growth speed seriously depends on the shape of E.

4.2 Motion of the top – flow with obstacle

We consider

$$w_t - \left(\operatorname{div}\frac{Dw}{|Dw|} + 1\right)|Dw| = c1_E, \quad w\Big|_{t=0} = 0$$

for a general compact set E in R^n.

By comparison, $w^*(x,t) \le ct$ in $R^n \times (0,\infty)$.

Notation:

$$A_{\max}(t) = \{x \in R^n | w^*(x,t) = ct\}.$$

Curvature flow with obstacle

Lemma 4.2. The set $A_{\max}(t)$ is a set theoretic solution of $V = \kappa + 1$ (i.e., $h(x,t) = 1_{A_{\max}(t)}(x)$ is a viscosity subsolution of

(L) $$h_t - \left(\operatorname{div}\frac{Dh}{|Dh|} + 1\right)|Dh| = 0.$$

Moreover, $A_{\max}(t) \subset E$.

Actually, h is a subsolution of the obstacle problem

$$\max\left\{h_t - \left(\operatorname{div}\frac{Dh}{|Dh|} + 1\right)|Dh|, h - 1_E\right\} = 0 \ \text{ in } \ R^n \times (0,\infty)$$

Curvature flow with an obstacle: G. Mercier……

Idea of proof

Note that

$$w_c(x,t) := w(x,t) - ct$$

is a viscosity subsolution of (L) and $w_c \leq 0$. Moreover, $A_{\max}(t) = \{x \in R^n | w_c^*(x,t) = 0\}$. Thus $A_{\max}$ is a set theoretic subsolution (cf. Y. G., Surface Evolution Equations, 2006).

Proof for $\boldsymbol{A_{max}} \subset \boldsymbol{E}$. If not, $^{\exists}x_0 \in A_{\max}(t_0) \cap E^c$ with some $t_0 > 0$. Then $\varphi(x,t) = ct$ is a test function of w^* from above. This is a contradiction

$$c = \varphi_t - \left(\mathrm{div}\frac{D\varphi}{|D\varphi|} + 1\right)|D\varphi|\Big|_{(x_0,t_0)} \leq c1_E(x_0) = 0. \quad \square$$

4.3 Upper estimate

Lemma 4.3. Assume that a flow $V = \kappa + 1$ with obstacle E starting from E vanishes at $t = t_0$. Then there exists $b \in (0, c)$ such that $\max_x w(x, t_0) \leq bt_0$.

Proof. Since $A_{\max}(t_0) = \phi$, we have

$$\max_x w(x, t_0) < ct_0.$$

We set

$$b = \max_x \frac{w(x, t_0)}{t_0}$$

to get the desired result. □

Global upper estimate

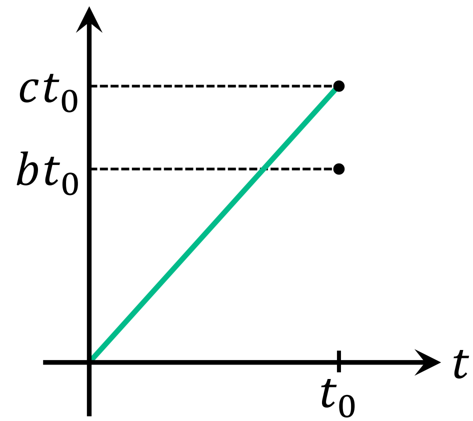
Theorem 4.4. Under the assumption of Lemma 4.3 with t_0. There exists $b \in (0, c)$ such that

$$w(x,t) \leq bt + (c-b)t_0, \quad (x,t) \in R^n \times (0,\infty).$$

In particular,

$$\limsup_{t\to\infty} \frac{w(x,t)}{t} \leq b.$$

Global upper estimate (continued)



Since

$$\max_x w(x, t_0) \leq bt_0,$$

by induction we have

$$w(x, mt_0 + t) \leq w(x, t) + mbt_0 \text{ on } R^n \times (0, \infty)$$

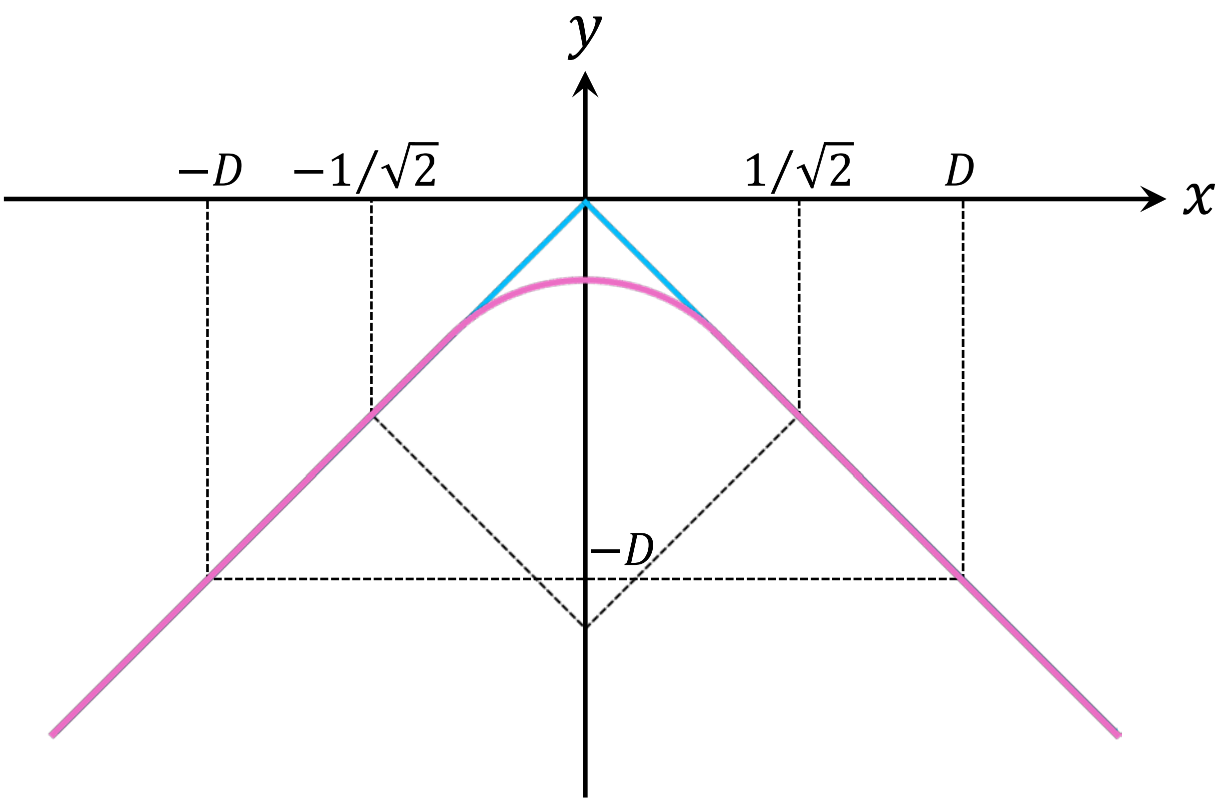
In particular, $w(x, mt_0) \leq mbt_0$. Thus for $t \in (mt_0, (m+1)t_0)$, $m \in \mathbf{N}$, we observe that

$$w(x, t) \leq w(x, mt_0) + c(t - mt_0) \leq bmt_0 + c(t - mt_0)$$
$$= bt + (c - b)(t - mt_0) \leq bt + (c - b)t_0$$

Estimate from below is similar. Theorem 4.1 now follows.

4.4 In the case of square of medium size

Lemma 4.5. If $D > 1$ with $d < 1$, $D = \sqrt{2}d$, then there exists $t_0 > 0$ such that $A_{\max}(t_0) = \phi$.



Obstacle problem

We shall construct a supersolution of the obstacle problem

$$\max\left\{y_t - \frac{y_{xx}}{1+y_x^2} - (1+y_x^2)^{1/2},\, y - g(x)\right\} = 0$$

$$\text{in } (-D, D) \times (0, \infty)$$

where $g(x) = -|x|$, $D = \sqrt{2}d$.

To simplify the work, we seek a self-similar solution of form

$$y(x,t) = \lambda(t) Y\left(\frac{x}{\lambda(t)}\right), \quad \lambda'(t) = \frac{1}{\lambda(t)} - 1.$$

Idea of the proof of Theorem 4.1

[$1/\sqrt{2} < d < 1$ yields an intermediate speed]

Lemma 4.5 together with Theorem 4.4 yields an upper bound for w.

We construct a supersolution for the obstacle problem outside E for $V = \kappa + 1$ which leads the estimate for w/t from below.

Open issues

- **Growth rate**. If $f = c1_E$, we do not know the existence of the growth rate $\lim_{t\to\infty} w/t$. (One has to be careful that in the case of $E = B(0, n-1)$ critical size the growth rate depends on the place.)
- **Dependence**. does the growth rate depend on f or E continuously?
- **The value of the growth rate**. Is it possible to characterize this quantity?

5. More examples (work in progress)

Consider for $1/2 < R_0 < 1, a > 0$

$$E = B\big((-a,0), R_0\big) \cup B\big((a,0), R_0\big)$$

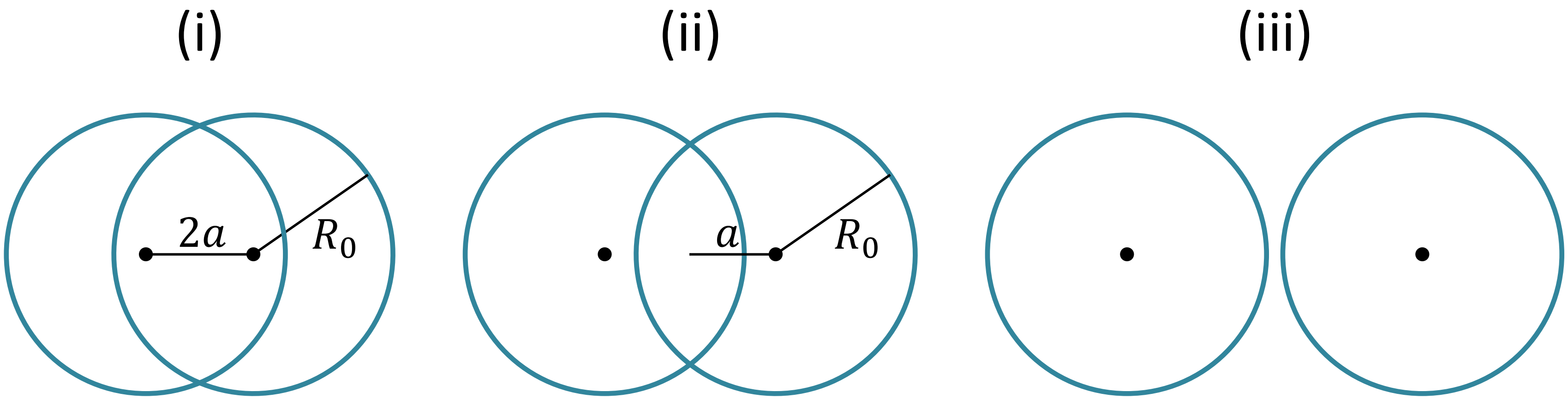
Corollary 5.1. (i) If $a > 0$ is small enough to satisfy $a + R_0 < 1$, then w is bounded in R^2.

(ii) If $a > 0$ a middle length, more precisely, $1 < a + R_0 < 2R_0$. Then there exists $0 < \alpha \leq \beta < c$ such that

$$\alpha \leq \liminf_{t\to\infty} \frac{w(x,t)}{t} \leq \limsup_{t\to\infty} \frac{w(x,t)}{t} \leq \beta.$$

(iii) If $a > 0$ is large enough so that $R_0 < a$, then w is bounded.

Figure of two disks



$$1 < a + R_0 < 2R_0$$

Other examples

Time dependent source term $c1_{E(t)}$

First example

$$E(t) = \begin{cases} B(a_1, R_1) & \text{for } \ 0 \le t \le t_1 \\ B(a_1, R_1) \cup B(a_2, R_2) & \text{for } \ t_1 \le t \le t_2 \\ B(a_1, R_1) \cup B(a_2, R_2) \cup B(a_3, R_3) & \text{for } \ t_2 \le t \le t_3 \end{cases}$$

Corollary 5.2. If there exists i such that $R_i > 1$, then

$$w(x,t)/t \to c \quad \text{as} \quad t \to \infty.$$

If $B(a_i, R_i) \cap B(a_j, R_j) = \emptyset$ for all i, j, $i \ne j$, then $w(x,t)$ is bounded if $R_i < 1$ for all i.

Open problem

If $B(a_iR_i) \cap B(a_jR_j) \neq \emptyset$ for some i, j with $i \neq j$ and $R_i < 1$ for all i, what is the growth rate?

Second example

The source term is

$$c1_{B(0,R(t))}$$

with a continuous function $t \mapsto R(t)$.

Asymptotic speed

Corollary 5.3. Assume that there exists

$$\lim_{T\to\infty} \frac{|\{t \in [0,T] | R(t) < 1\}|}{T} =: \alpha_-$$

$$\lim_{T\to\infty} \frac{|\{t \in [0,T] | R(t) = 1\}|}{T} =: \alpha$$

$$\lim_{T\to\infty} \frac{|\{t \in [0,T] | R(t) > 1\}|}{T} =: \alpha_+.$$

Then

$$\lim_{t\to\infty} \frac{w(x,t)}{t} = c(\alpha + \alpha_+) \text{ for } x \in B(0,1)$$

$$= c(1 - \alpha_-)$$

$$\lim_{t\to\infty} \frac{w(x,t)}{t} = c\alpha_+ \qquad \text{for } x \in R^2 \setminus B(0,1).$$

Summary

We have studied asymptotic speed for the level-set equation of the eikonal curvature flow equation with source term.

- Spherical symmetric case: asymptotic speed is computable.
- Lipschitz source term: existence of asymptotic speed
- Case of intermediate speed: application of eikonal curvature flow equation with obstacle.