ファセット結晶形状の不安定性と非強圧的ハミルトン・ヤコビ方程式

三竹 大寿 (MITAKE Hiroyoshi)
(福岡大学 応用数学科)

Joint work with

儀我 美一 (東京大学), Q. Liu (U. Pittsburgh)

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§0 Introduction (Physical Background)

Morphological stability (形状安定性) in crystal growth: Burton, Cabrera, Frank '51 (Micro Level), Chernov '74, E, Yip '01 (Macro Level).

$$V = \sigma(x) m(p),$$
$$m(p) = \frac{p}{p_s} \tanh(\frac{p_s}{p}),$$
$$p_s = \frac{d}{2x_s} \approx \ \varepsilon.$$

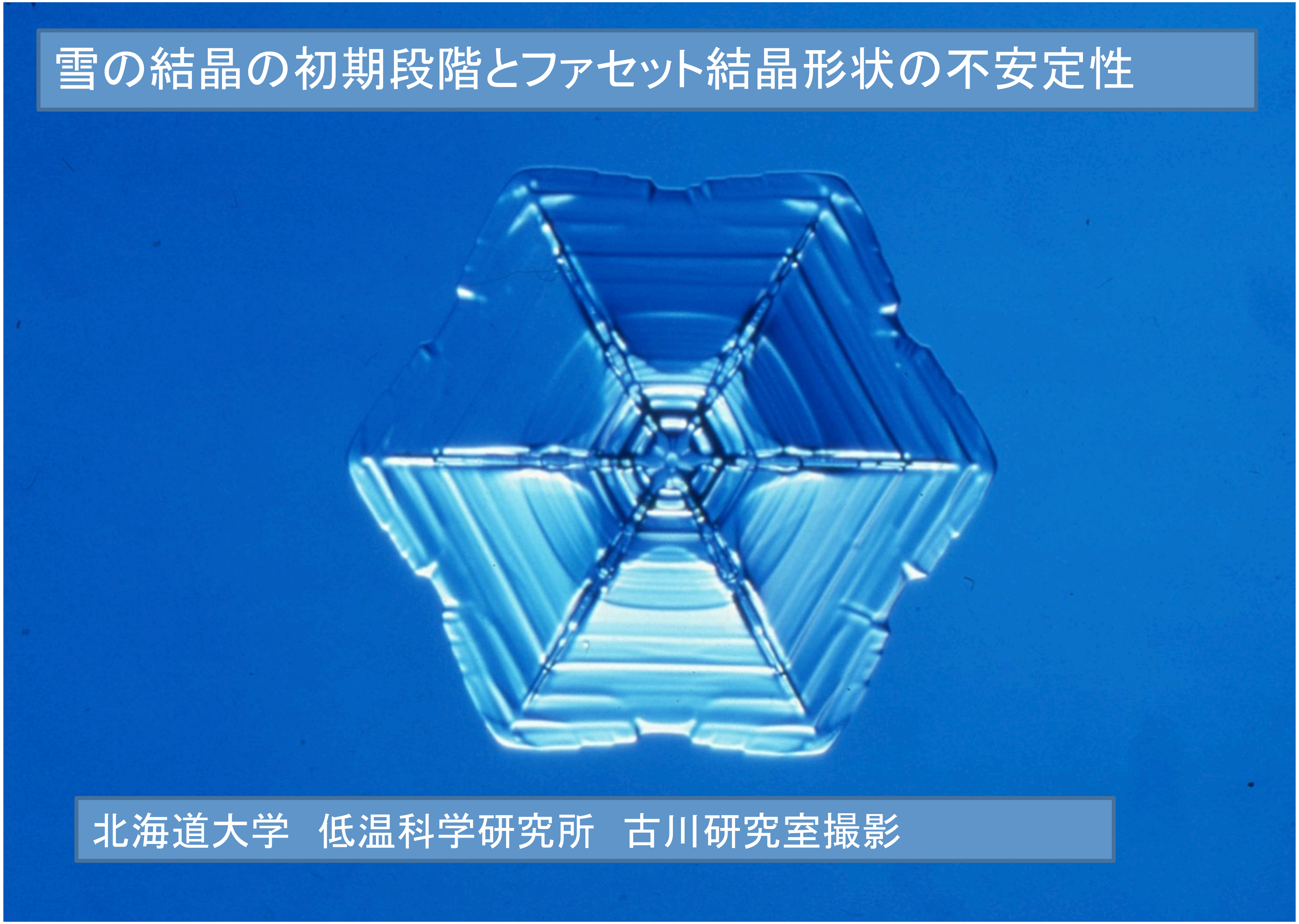
V: growth speed in the direction normal to a crystal surface Γ_t.

m: anisotropy of the kinetic energy.

σ: supersaturation (過飽和度).

d: step height, x_s: surface diffusion distance of a molecule.

p: local slope of the crystal surface.


雪の結晶の初期段階とファセット結晶形状の不安定性
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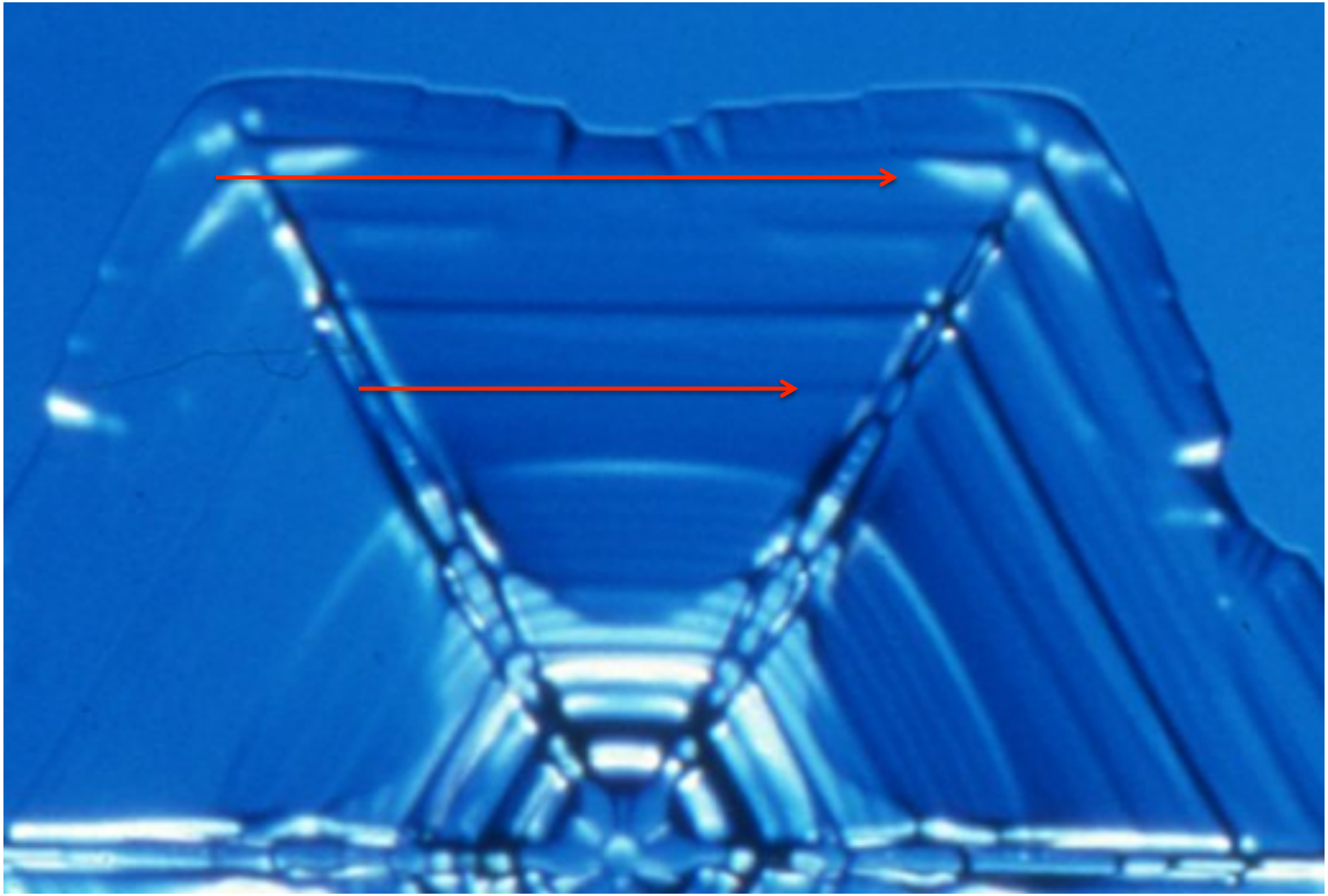


We consider

$$V = \sigma(x)m(|p|/\varepsilon) - f(x) \quad \text{on } \Gamma_t. \tag{1}$$

Graph Representation. Introduce the function z^ε which satisfies

$$\Gamma_t = \{(x, z^\varepsilon(x,t)) \mid x \in \mathbb{R}^N\}.$$

Then we have

$$p = Dz^\varepsilon(x) \text{ and } V = \frac{z_t^\varepsilon}{\sqrt{1+|Dz^\varepsilon|^2}}.$$

Thus, the above surface evolution equation can be written by

$$z_t^\varepsilon - \sigma(x)m(\frac{|Dz^\varepsilon|}{\varepsilon})\sqrt{1+|Dz^\varepsilon|^2} = f(x)\sqrt{1+|Dz^\varepsilon|^2} \tag{2}$$

References:

1. **儀我,「動く曲面を追いかけて」, 日本評論社**

2. **儀我,「曲面の発展方程式における等高面の方法」,「非等方的曲率による界面運動方程式」, 石井,「非線形偏微分方程式の粘性解について」　（雑誌　数学）**

3. Giga, 「Surface Evolution Equations」, Springer.

Yokoyama-Giga-Rybka '08

Investigate the behavior of u^ε in the ε-time scale, i.e.,

$$\tilde{u}^\varepsilon(x,\tau) = -z^\varepsilon(x,\varepsilon\tau)/\varepsilon \text{ (microscopic height)}$$

and a new independent variable $\tau = t/\varepsilon$ (microscopic time). Then $\tilde{u}^\varepsilon$ satisfies

$$\tilde{u}^\varepsilon_\tau + \sigma(x)m(|D\tilde{u}^\varepsilon|)\sqrt{1+\varepsilon|D\tilde{u}^\varepsilon|^2} = f(x)\sqrt{1+\varepsilon|D\tilde{u}^\varepsilon|^2}$$

Thus, (at least formally) $\tilde{u}^\varepsilon$ converges to a solution of

$$\tilde{u}_\tau + \sigma(x)m(|D\tilde{u}|) = f(x) \text{ in } \mathbb{R}^N \times (0,\infty).$$

A typical example is

$$\sigma(x) := \overline{\sigma}(1-|x|^2)_+,$$
$$m(r) := r\tanh(1/r) \ (r \gg 1) \text{ and},$$
f : nucleation (核生成) density.

§1 Main Result

We consider HJ equations of the form

$$u_t + \sigma(x)m(|Du|) = f(x). \tag{3}$$

(A1) $m : [0, \infty) \to [0, 1)$ is strictly increasing, Lipschitz continuous with $m(0) =: m_0 \in [0, 1)$ and $m(r) \to 1$ as $r \to \infty$.

(A2) $f : \mathbb{R}^n \to \mathbb{R}$ is continuous and satisfies

$$\mathcal{A} := \{x \in \mathbb{R}^n : f(x) = \min f, \sigma(x) = \overline{\sigma}\} \neq \emptyset, (\text{Revisit})$$

where $\overline{\sigma} := \max \sigma$.

(A3) u_0 is Lipschitz continuous in $\mathbb{R}^n$.

(A4) Set $c := \overline{\sigma} m_0 - \min f$. $\Omega_e := \{\sigma(\cdot) - f(\cdot) > c\}$ is bounded and $\sigma \in C^1(\mathbb{R}^N)$ satisfies $D\sigma(x) \neq 0$ on $\partial\Omega_e$.

Remark. Ω_e is called a *maximal stable region*.

Theorem 1 (Giga-Liu-M., JDE 2012, Trans. AMS to appear). *Assume that* (A1)–(A4). *Let* u *be a solution of* (3) *with* $u(\cdot,0) = u_0 \in W^{1,\infty}(\mathbb{R}^N)$. *Then,*

$$u(\cdot,t) + ct \to \phi_\infty \text{ loc. uniformly on } \Omega_e,$$

$$u(\cdot,t) + ct \to +\infty \text{ loc. uniformly on } \mathbb{R}^n \setminus \overline{\Omega}_e$$

as $t \to +\infty$, *where* ϕ_∞ *is a solution of*

$$(\mathrm{S}) \quad \begin{cases} |Dv| = m^{-1}\left(\dfrac{f(x)+c}{\sigma(x)}\right) =: h(x) & \text{in } \Omega_e, \\ \dfrac{\partial v}{\partial n} = +\infty & \text{on } \partial\Omega_e, \\ \sup\limits_{\Omega_e} |v(x)| < +\infty. & \end{cases}$$

Interpretation:

Theorem 1 now gives a clear view of z^ε on the effective domain Ω_e. We have

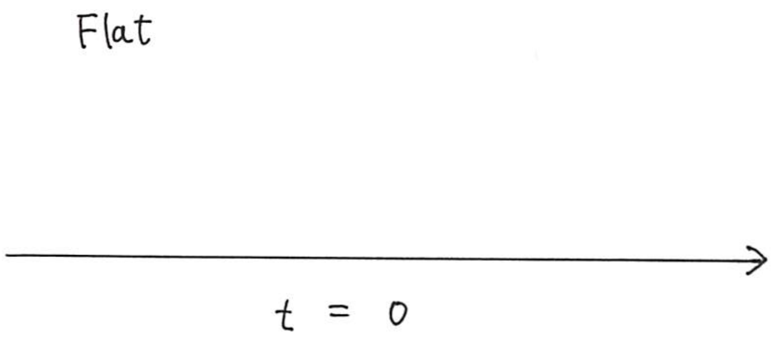
$$\begin{aligned} z^\varepsilon(x,t) &= -\varepsilon\tilde{u}^\varepsilon(x,\frac{t}{\varepsilon}) \\ &= -\varepsilon\tilde{u}(x,\frac{t}{\varepsilon}) + o(\varepsilon) \\ &= -\varepsilon(\phi_\infty(x) - \frac{ct}{\varepsilon} + m(\frac{\varepsilon}{t})) + o(\varepsilon) \\ &= -\varepsilon\phi_\infty(x) + ct + o(\varepsilon). \end{aligned}$$

Therefore, roughly speaking, the growing facet moving according to (1) is flat up to order ε with speed c on the effective domain Ω_e.

Remember $c = \overline{\sigma}m_0 - \min f$.

Crystal Growth

$$\Gamma_t = \{ (x, z^{\varepsilon}(x,t)) \mid x \in \mathbb{R}^N \}$$



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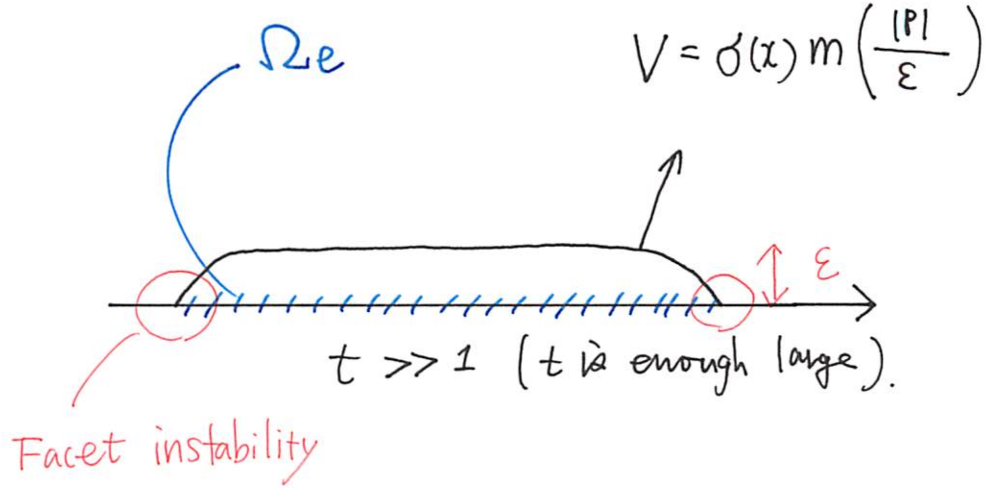

Result.

$$z^{\varepsilon}(x,t) = -\varepsilon \tilde{u}\left(x, \frac{t}{\varepsilon}\right) + O(\varepsilon)$$

$$\simeq -\varepsilon \phi_{\infty}(x) + ct + o(\varepsilon).$$

Interpretation.

1. Asymptotically, the facet is flat up to order ε with speed c on Ω_e.

2. Outside of Ω_e, growth speed is much slower.

Asymptotic Profile on the Effective Domain Ω_e.

We define the functions $\phi_-, \phi_\infty \in C(\overline{\Omega}_e)$ by

$$\phi_-(x) := \inf_{t\geq 0}(u(x,t) + ct),$$

$$\phi_\infty(x) := \min\{d(x,y) + \phi_-(y) \mid y \in \mathcal{A}\},$$

$$d(x,y) := \inf\{\int_0^t h(\gamma(s))\, ds \mid t > 0, \gamma(t) = x, \gamma(0) = y, |\dot{\gamma}(s)| \leq 1\}.$$

Theorem 2 (Asymptotic Profile). *We have*

$$\phi_\infty(x) = \lim_{t\to\infty}(u(x,t) + ct) \quad \textit{for all } x \in \Omega_e.$$

Example. Let $n = 1$, $u_0 = f \equiv 0$, $\sigma(x) = \overline{\sigma}(1 - x^2)_+$.
Then we have $c = \overline{\sigma} m_0$, $\Omega_e = (-\sqrt{1 - m_0}, \sqrt{1 - m_0})$, $\mathcal{A} = \{0\}$.
Moreover, $\phi_\infty(x) = \min_{y\in\mathcal{A}}\{d(x,y) + \phi_-(y)\} = d(x,0)$. Thus we obtain

$$\phi_\infty(x) = \int_0^x m^{-1}(\frac{m_0}{(1 - s^2)_+})\, ds \text{ for all } x \in \overline{\Omega}_e.$$

Discussion 1 (Morphological Stability).

In the theory of crystal growth, it is known that as long as the non-uniformity in supersaturation on the facet is not too large, the faceted crystal can grow in a stable manner.

Question. How much of non-uniformity implies a stable morphology?

Answer.

$$\frac{f(x)+c}{\sigma(x)} < 1 \ \forall x \in \mathbb{R}^n \iff$$
$$f(x) - \min f + \overline{\sigma} m_0 < \sigma(x) \le \overline{\sigma} \ \forall x \in \mathbb{R}^n.$$

In this case, we can expect we have the large-time asymptotic

$$u(x,t) + ct \to v(x) \quad \text{uniformly for } x \in \mathbb{R}^N$$

as $t \to \infty$

Discussion 2 (Step Source).

Revisit Assumption (A2):

$$\mathcal{A} := \{x \in \mathbb{R}^n : f(x) = \min f, \sigma(x) = \overline{\sigma}\} \neq \emptyset.$$

First Case: $f \equiv 0$.

The set $\mathcal{A}$ is considered as a step source in the theory of crystal growth.

Mathematically, we can see that $u + ct$ is non-increasing as $t \to \infty$.

The function f gives a nucleation density of crystal. Our assumption (A2) says that there is a step source in the place where no nucleation occurs.

Question. If this is not the case?

Reconsider $c := \max_x(\sigma(x)m_0 - f(x))$, $\mathcal{A} := \{x \mid \sigma(x)m_0 - f(x) = c\}$.

We don't know the uniform continuity of u on $\mathcal{A}$ yet.

Discussion 3 (Mean Curvature effect).

Effect of tension. Consider

$$V_\varepsilon = \big(\sigma(x) - \mathrm{div}\,(n(x))\big)m(\frac{|p|}{\varepsilon}) - f(x) \quad \text{on } \Gamma_t.$$

If we use the microscopic time and height, i.e.,

$$\tilde{u}^\varepsilon(x,\tau) = -z^\varepsilon(x,\varepsilon\tau)/\varepsilon$$

then we cannot see the difference, since

$$\tilde{u}^\varepsilon_t + ... - m(|D\tilde{u}^\varepsilon|)\mathrm{div}\Big(\frac{\varepsilon D\tilde{u}^\varepsilon}{\sqrt{\varepsilon|D\tilde{u}|^2+1}}\Big)\sqrt{\varepsilon|D\tilde{u}|^2+1} = 0.$$

Thank you for
your kind attention!