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Mullinsによる結晶の蒸発・凝固モデルに現れる一般化された曲率流方程式
(Generalized curvature flow equations appearing in evaporation-condensation model by Mullins)

東京大学 大学院数理科学研究科 博士課程２年

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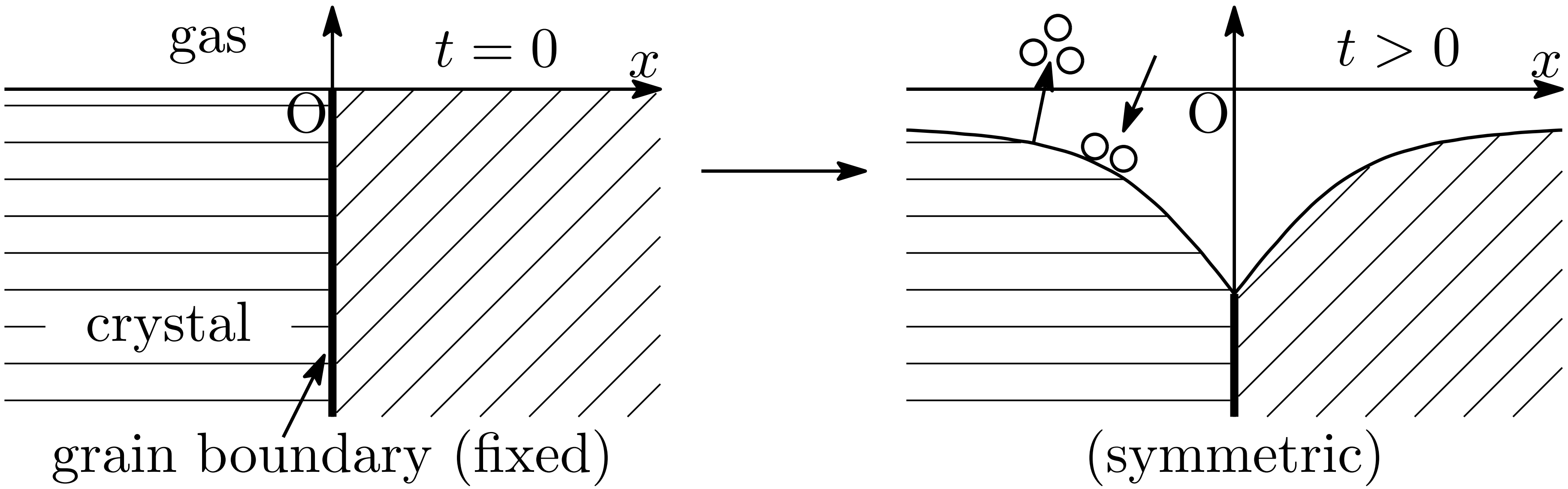
1 Introduction

Evaporation-condensation model

[Mullins '57] **William W. Mullins** (1927–2001), Materials Scientist.



Surface diffusion model is also proposed in [Mullins '57].
(∵ 4th order eq.)

∗ Mg & high air pressure ⇝ evaporation-condensation.
Au & low air pressure ⇝ surface diffusion.

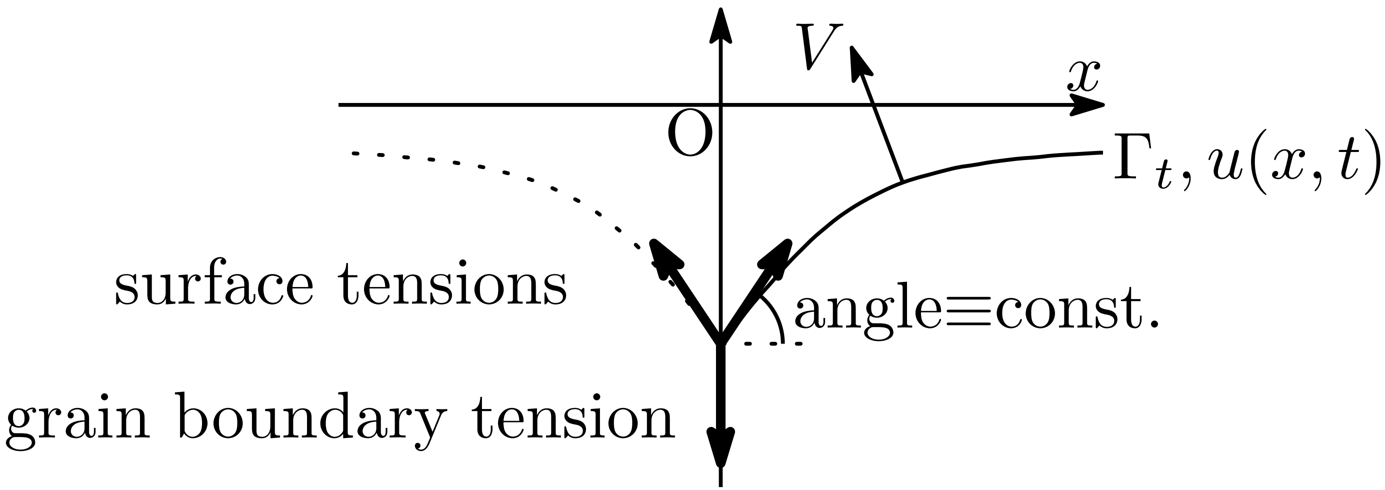
Equation and its derivation

$\Gamma_t = \{(x, u(x,t)) \mid x \geqq 0, t \geqq 0\}$: surface (curve).
V: upward normal velocity. k: upward curvature.

Generalized curvature flow equation: $V = 1 - e^{-k} \quad$ on Γ_t, i.e.,

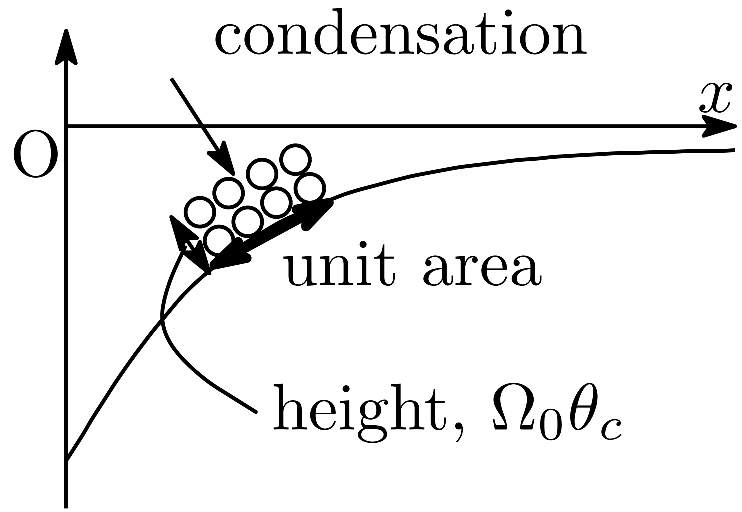
$$\boxed{\frac{u_t}{\sqrt{1+u_x^2}} = 1 - e^{-k}} \qquad \text{with } k = \frac{u_{xx}}{\sqrt{1+u_x^2}^{\,3}}.$$

Boundary condition: By equilibrium of tensions $\boxed{u_x(0,t) \equiv \beta} > 0$.



Derivation.

- Upward normal velocity V.



$$V = (\text{condensation}) - (\text{evaporation})$$
$$= \Omega_0(\theta_c - \theta_e)$$
$$= \Omega_0 \cdot C_1(p_0 - p). \quad (C_1 > 0) \qquad (*1)$$

$*$ Here Ω_0: molecular volume,

θ_c (θ_e): number of impinging (emitted) atoms per unit time and unit area,

p_0 (p): vapor pressure in the atmosphere (in equilibrium with the surface).

- **Gibbs-Thompson formula**: $\boxed{\log \dfrac{p}{p_0} = -C_2 k}$ $(C_2 > 0)$. $(*2)$

(k: upward curvature)

$$(*1)\ \&\ (*2) \implies V = \Omega_0 C_1 p_0 \left(1 - e^{-C_2 k}\right).$$

Generalization.

[Srolovitz '89] strain energy. [Ogasawara '03] temperature gradient.

Approximations by Mullins

$u(x,0) \equiv 0,\ u_x(0,t) \equiv \beta \ll 1.$

$$\frac{u_t}{\sqrt{1+u_x^2}} = 1 - e^{-k} \quad \overset{1-e^{-k}\approx k}{\dashrightarrow} \quad v_t = \frac{v_{xx}}{1+v_x^2} \quad \overset{v_x\approx 0}{\dashrightarrow} \quad w_t = w_{xx}$$

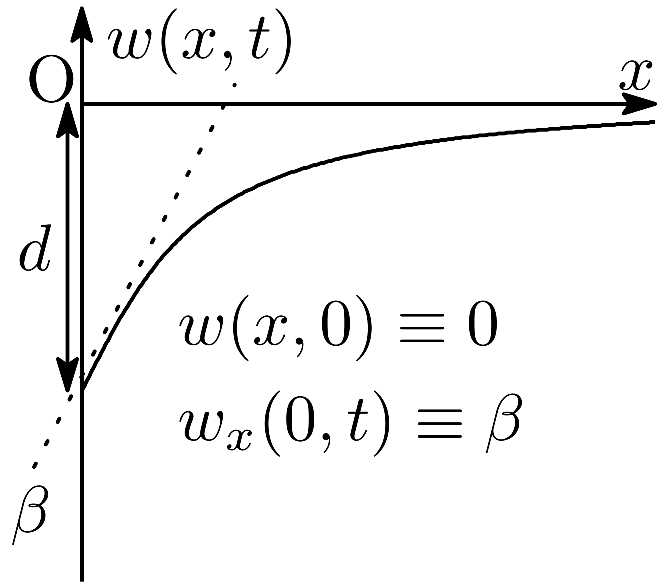
generalized curvature flow eq.   curvature flow eq. for graph   heat eq.

Solving the heat equation, Mullins concludes the groove profile is

$$w(x,t) = -2\beta\sqrt{t}\cdot \mathrm{ierfc}\left(\frac{x}{2\sqrt{t}}\right).$$

In particular, the depth at the origin is

$$d := -w(0,t) = 2\beta\sqrt{\frac{t}{\pi}} \approx 1.13\beta\sqrt{t}.$$



$*$ Here $\mathrm{ierfc}(x)$ is the **integral error function**:

$$\mathrm{ierfc}(x) = \int_x^\infty \mathrm{erfc}(z)dz, \quad \mathrm{erfc}(x) = \frac{2}{\sqrt{\pi}}\int_x^\infty e^{-z^2}dz.$$

Our aims

- **Justification of Mullins's two approximations.**

$$\boxed{\frac{u_t}{\sqrt{1+u_x^2}} = 1 - e^{-k}} \overset{1-e^{-k}\approx k}{\dashrightarrow} \boxed{v_t = \frac{v_{xx}}{1+v_x^2}} \overset{v_x\approx 0}{\dashrightarrow} \boxed{w_t = w_{xx}}$$

Point. v & w are self-similar (if initial data is 0), i.e.,

$$v(x,t) = \sqrt{t}V\left(\frac{x}{\sqrt{t}}\right), \quad w(x,t) = \sqrt{t}W\left(\frac{x}{\sqrt{t}}\right).$$

1. $u \approx v$? ⋆[Ans.] u is asymptotically self-similar, i.e.,

$$\frac{1}{\sqrt{t}}u(\sqrt{t}x,t) \overset{t\to\infty}{\longrightarrow} V(x).$$

2. $-V(0) \approx -W(0)$ (: depth of the groove) if $\beta \ll 1$? ⋆[Ans.] $o(\beta)$.

- **Degenerate cases.** ⋆[Ans.] V has a corner.

2 Neumann boundary problems

Let $F : \mathbf{R}^n \times \mathbf{S}^n \to \mathbf{R}$ be continuous & degenerate elliptic.

$$\text{(NP)} \quad \begin{cases} u_t(x,t) = F(\nabla_x u(x,t), \nabla_x^2 u(x,t)) & \text{in } \{x_1 > 0\} \times (0,\infty), \\ u(x,0) = u_0(x) \in BUC & \text{on } \{x_1 \geqq 0\}, \\ u_{x_1}(x,t) = \beta > 0 & \text{on } \{x_1 = 0\} \times (0,\infty). \end{cases}$$

Theorem. (NP)=(NP;F, u_0) admits a unique viscosity solution.

∗ The boundary condition is interpreted as the viscosity sense.

∗ BUC =bounded & uniformly continuous.

cf. (Neumann problems and viscosity sol.)

- [Lions '85] pioneer.
- [Barles '99], [Ishii-Sato '04] general singular 2nd order eq.

} bounded domain

- [Sato '96] half space, capillary boundary condition: $u_{x_1} - k|\nabla u| = 0$.

3 Asymptotic behavior

Structure of equations. $F, G : \mathbf{R}^n \times \mathbf{S}^n \to \mathbf{R}$.

- F: homogeneous (hom.) $\overset{\text{def.}}{\Longleftrightarrow}$ $F(p, \lambda X) = \lambda F(p, X)$, $\forall \lambda > 0$.
- G: asymptotically homogeneous (a-hom.)

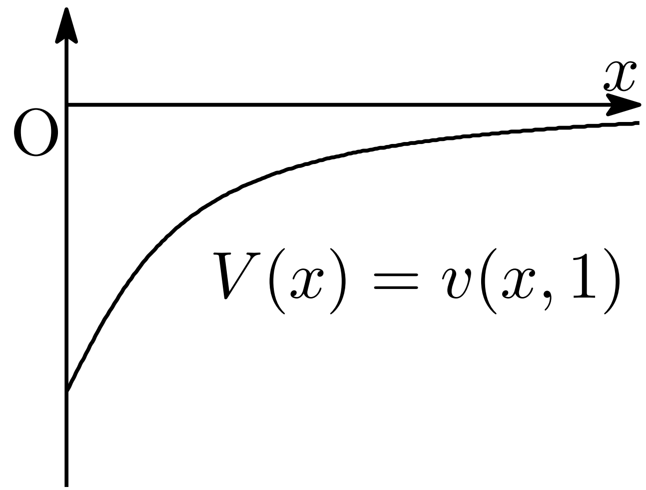
$\overset{\text{def.}}{\Longleftrightarrow}$ $\exists F$: hom., $\lambda G(p, X/\lambda) \overset{\lambda\to\infty}{\longrightarrow} F(p, X)$ loc. unif. in $\mathbf{R}^n \times \mathbf{S}^n$.

⋆ Mullins's 1st approx. $(G \approx F)$

$*$ $G(p, X) = \sqrt{1 + p^2}(1 - e^{-k})$ is a-hom. with the limit $F(p, X) = \dfrac{X}{1 + p^2}$.

Self-similar solution.

- v: self-similar $\overset{\text{def.}}{\Longleftrightarrow}$ $\exists V$, $v(x, t) = \sqrt{t} V\left(\dfrac{x}{\sqrt{t}}\right)$.



V is called a profile function.

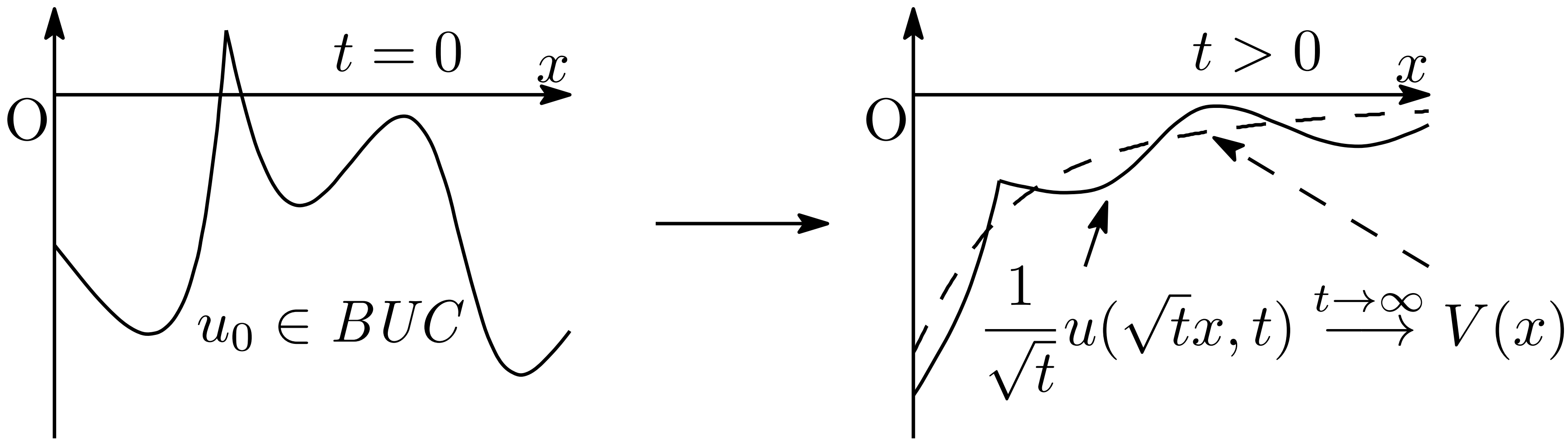
Fact.

If F is hom., the unique sol. of (NP; $F, u_0 \equiv 0$) is self-similar.

Theorem (Asymptotic convergence).
Assume G is a-hom. with the limit F. Let u solve (NP; G, u_0), v solve (NP; $F, u_0 \equiv 0$) and V be the profile function of v. Then

$$\frac{1}{\sqrt{t}} u(\sqrt{t}x, t) \overset{t\to\infty}{\longrightarrow} V(x) \quad \text{locally uniformly on } \{x_1 \geqq 0\}.$$

Remark. The limit is common to all initial data!!



Proof. (u solves (NP; G,u_0), v solves (NP; F,0).)

1. **Rescale function**: $u_{(\lambda)}(x,t) := \dfrac{1}{\lambda}u(\lambda x, \lambda^2 t)$ $(\lambda > 0)$.

It suffices to show "$u_{(\lambda)} \overset{\lambda\to\infty}{\longrightarrow} v$ loc. unif. on $\{x_1 \geqq 0\} \times [0,\infty)$".

$\star$ $u_{(\lambda)}$ is a solution of (NP; $\underbrace{\lambda G(p, X/\lambda)}_{\to F}$, $u_0(\lambda x)/\lambda$).

2. **Relaxed limits**: $\overline{u} := \limsup^*_{\lambda\to\infty} u_{(\lambda)}$ & $\underline{u} := \liminf_{*\lambda\to\infty} u_{(\lambda)}$.

$\star$ Construct suitable barriers $U^\pm(x,t)$ so that $U^\pm = O(\sqrt{t})$ as $t \to \infty$.

$\Longrightarrow U^\pm$: unif. bounded w.r.t. rescaling.

$-\infty < \overline{u}$(subsol.) $\overset{\mathrm{CP}}{\equiv}$ $\underline{u}$(supersol.) $< \infty$, i.e., loc. unif. convergence!! $\square$

Remark. If G is hom. (i.e. $G \equiv F$), then

$$\frac{1}{\sqrt{t}}u(\sqrt{t}x, t) \overset{t\to\infty}{\longrightarrow} V(x) \quad \text{~~locally~~ uniformly on } \{x_1 \geqq 0\}.$$

Contraction property: $\boxed{\|u_{(\lambda)} - v\|_{L^\infty} \leqq \|u_0(\lambda x)/\lambda - 0\|_{L^\infty}} \overset{\lambda\to\infty}{\longrightarrow} 0.$

"(difference of sol.) $\leqq$ (difference of data)"

4 Profile functions

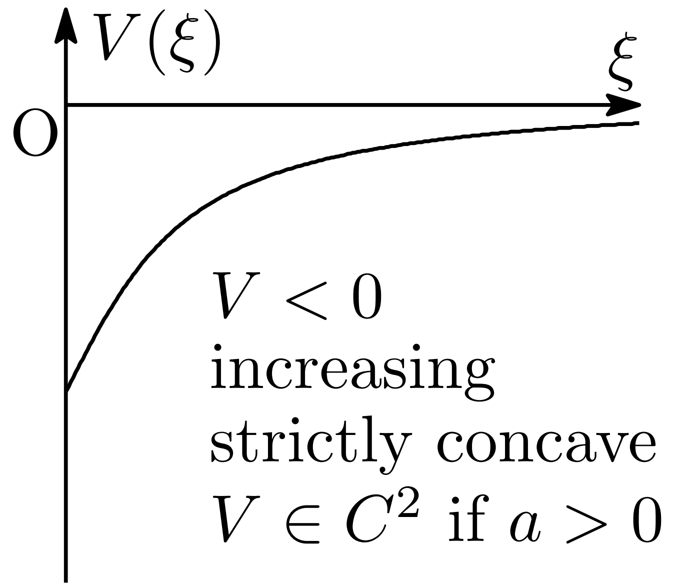
Let $n = 1$. The profile function V ($V(x) = v(x, 1)$) satisfies

$$\text{(ODE)} \begin{cases} V(\xi) - \xi V'(\xi) = a(V'(\xi))V''(\xi) \quad \text{in } (0, \infty), \\ V'(0) = \beta > 0, \\ \lim_{\xi \to \infty} V(\xi) = 0, \end{cases}$$

$$v_t = \frac{v_{xx}}{1 + v_x^2}$$

where $a(p) = -2F(p, -1)$. In Mullins's case $\boxed{a(p) = \dfrac{2}{1 + p^2}}$.

Conversely, solving (ODE) gives the self-similar sol.
(Recall $v(x, t) = \sqrt{t} V\left(x / \sqrt{t}\right)$.)



Assumptions (on given a.)
$a \in C(\mathbf{R})$, $a \geqq 0$ & $a(0) > 0$.

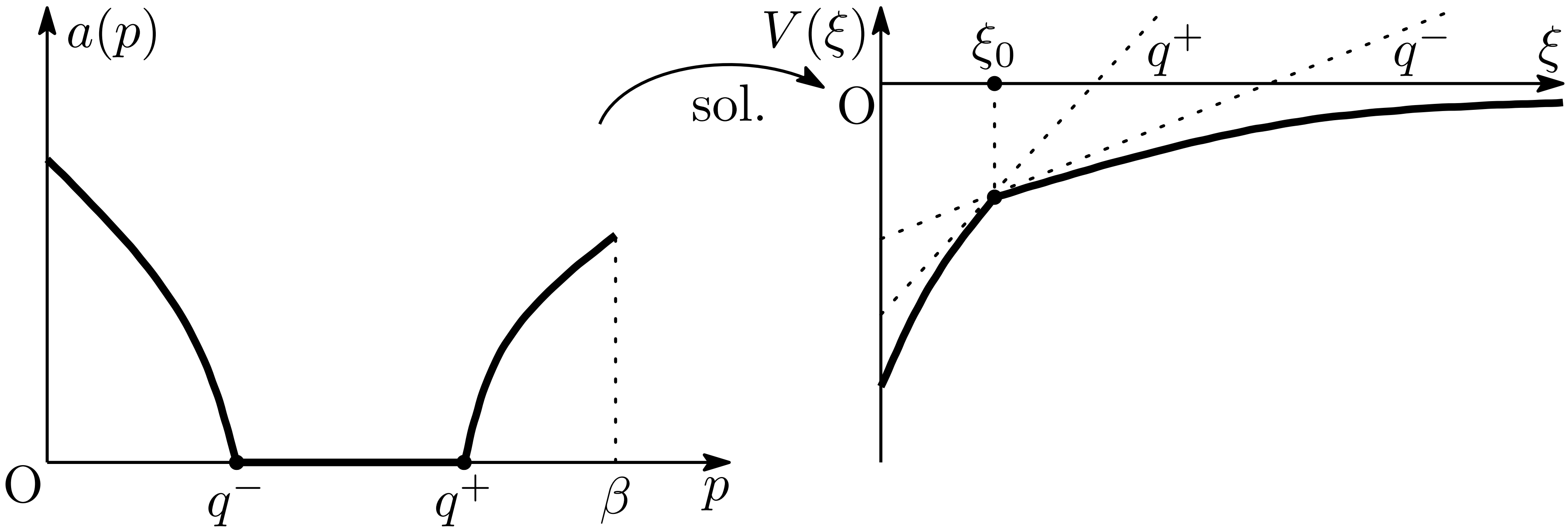
Fact. (ODE) has a unique viscosity sol., and the sol. V satisfies $\rightarrow$

(ODE) $V(\xi) - \xi V'(\xi) = \underline{\underline{a(V'(\xi))}} V''(\xi)$.

Theorem (Corner of profile functions).
Assume $a(p) = 0$ $(p \in [q^-, q^+] \subset (0, \beta))$, $a(p) > 0$ (otherwise).
Let V be the unique vis. sol. of (ODE). Then $\exists! \xi_0 \in (0, \infty)$ s.t.

$$q^+ = \lim_{\xi \uparrow \xi_0} \frac{V(\xi) - V(\xi_0)}{\xi - \xi_0}, \quad q^- = \lim_{\xi \downarrow \xi_0} \frac{V(\xi) - V(\xi_0)}{\xi - \xi_0}.$$

(left derivative) (right derivative)



5 Depth of the groove

Let $d(\beta) := -V(0)$, where V solves (ODE): non-linear eq.
(= depth at time $t = 1$ at the origin.)

Let $L(\beta) := -W(0)$, where W solves ("$= \underline{\underline{a(V'(\xi))}}V''(\xi)$" (ODE))

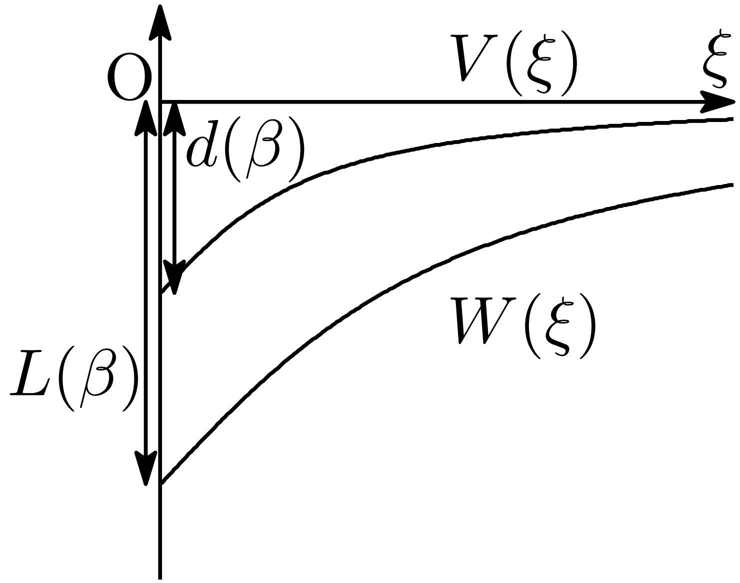
⋆ Mullins's 2nd approx.

$$\text{(L-ODE)} \quad \begin{cases} W(\xi) - \xi W'(\xi) = \underline{\underline{a(0)}}W''(\xi) \quad \text{in } (0, \infty), \\ W'(0) = \beta > 0, \\ \lim_{\xi \to \infty} W(\xi) = 0. \end{cases}$$

: linear eq.

W is the profile function of the heat eq.

$$\Longrightarrow \boxed{L(\beta) = \beta\sqrt{\frac{2a(0)}{\pi}}}$$



Want to

- study $d(\beta)$ as a function of β.
- compare $d(\beta)$ and $L(\beta)$ when $\beta \ll 1$.

Theorem (Depth of the groove).
Assume $a(p) \leqq a(0)$ $(\forall p \geqq 0)$.
Define $d(\beta)$ and $L(\beta)$ as before.

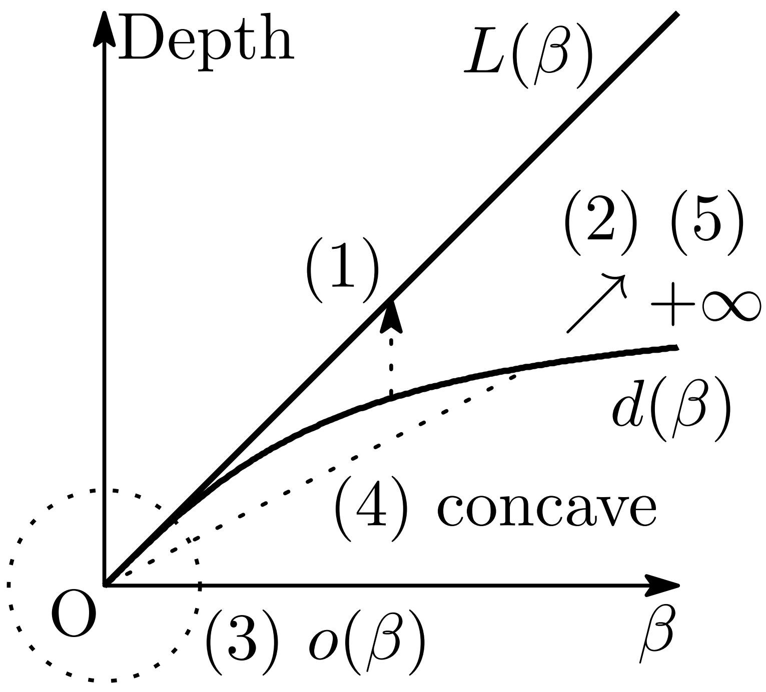
(1) $0 < d(\beta) \leqq L(\beta)$.

(2) d is nondecreasing in $(0, \infty)$.

(3) $$\frac{L(\beta) - d(\beta)}{\beta} \leqq {}^{\exists}C \left(a(0) - \min_{[0,\beta]} a \right).$$

(4) $\lambda d(\beta) \leqq d(\lambda\beta)$ $(\forall \lambda \in [0,1])$ if a is nonincreasing.

(5) $\lim_{\beta\to\infty} d(\beta) = +\infty$ if $a(p) \geqq \dfrac{c}{1+p^2}$ $(\forall p \gg 1)$.



Proof. **Comparison principle**.
Find a suitable subsol. V_1 and supersol. V_2 of (ODE). $\Longrightarrow V_1 \leqq V_2$. $\square$

Remark. In Mullins's case $L(\beta) - d(\beta) = O(\beta^{1+2})$ as $\beta \to 0$ by (3).