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A VARIATIONAL APPROACH TO VERY SINGULAR GRADIENT FLOW EQUATIONS

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Abstract. We formulate singular gradient flow equations by the notion of subdifferential. Characterization of the subdifferential operator in the Sobolev space with negative power H^{-1} enables us to calculate the initial speed of a solution solving the subdifferential formulation of the fourth order singular parabolic equation which models a crystalline surface driven by surface diffusion.

Key words. subdifferential, fourth order equation, surface diffusion, singular parabolic equation

AMS subject classifications. 35G25,35K90,35R70

1. Introduction. Some mathematical models describing the motion of a crystalline surface have a strong singularity, therefore they do not have a clear notion of solution solving the equations. In this work we will study how to formulate such singular parabolic PDEs mathematically and observe the behaviour of the corresponding solutions. The models we are concerned with are written as follows.

$$u_t = \operatorname{div}\left(\frac{\nabla u}{|\nabla u|}\right) \text{ in } \Omega \times (0, +\infty), \tag{1.1}$$

$$u_t = \operatorname{div}\left(\frac{\nabla u}{|\nabla u|} + |\nabla u|^{\gamma-1}\frac{\nabla u}{|\nabla u|}\right) \text{ in } \Omega \times (0, +\infty), \tag{1.2}$$

$$u_t = -\Delta \operatorname{div}\left(\frac{\nabla u}{|\nabla u|} + |\nabla u|^{\gamma-1}\frac{\nabla u}{|\nabla u|}\right) \text{ in } \Omega \times (0, +\infty), \tag{1.3}$$

for the exponent $\gamma > 1$ and the domain $\Omega \subset \mathbb{R}^n$. The function $u : \Omega \times [0, +\infty) \to \mathbb{R}$ stands for the surface height on the domain Ω at time t.
H. Spohn [12] proposed the second order parabolic equation (1.2) as a model of the crystalline surface driven by evaporation of the surface atom and the fourth order equation (1.3) to describe the crystalline surface's motion caused by surface diffusion, respectively. Moreover, H. Spohn formulated these equations as free boundary value problems with evolving facets (flat portions on the surface).
On the other hand, M.-H. Giga, Y. Giga and R. Kobayashi [8] formulated (1.1) by the notion of subdifferential, which is an extended notion of differential, and constructed the global in time solution analytically. Their method is applicable to analyse these singular gradient flow equations and explained as follows. Since the right hand side of these equations are the gradients of convex energy functional with respect to the metric of the suitable Hilbert space, they can be written as the subdifferential of the energy. Then in the case that the dimension $n = 1$ by choosing the smallest element in

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the subdifferential, we can practically obtain the vertical speed of the solution whose unique existence is assured by the general existence framework from the nonlinear semigroup theory (see, eg, [3], [4], [11]).
Though the behaviour of the solution solving the equation (1.1) was studied in detail in [8] by the subdifferential formulation and the equation (1.2) was investigated in [12] by the free boundary formulation, the motion of the surface described by (1.3) is not known clearly. The free boundary formulation of (1.3) in [12] was done on the assumption that the facets on the initial surface would evolve spontaneously. We would like to see whether the facet on the initial profile will grow or not when we apply the method proposed in [8] to the fourth order singular equation (1.3).

2. The motion of the evaporation model. Let us review the approach by M.-H. Giga, Y. Giga and R. Kobayashi [8] to analyze the singular equation (1.1). Since the right hand side of the equation (1.2) is L^2-gradient of the energy functional

$$F(u) = \int_\Omega |\nabla u| dx,$$

we can introduce the notion of subdifferential to handle the singularity mathematically. The model (1.1) can be rewritten as an evolution equation whose right hand side is the subdifferential of the energy F in $L^2(\Omega)$. The general theory ([3]) says that the speed of the solution of the subdifferential formulation is expressed by the smallest element in the value of the subdifferential operator at each time. Therefore the procedure to construct the global in time solution is explained as follows.

(Step1) The subdifferential formulation of the singular gradient of the energy.

(Step2) Characterization of the subdifferential of the convex energy functional in the functional space where the functional is defined.

(Step3) Calculation of the smallest element in the subdifferential at each time.

If the speed obtained in (Step3) is a constant on the facetting parts and zero in the other parts, the facet will grow spontaneously. Therefore we can construct the solution by

(Step4) The free boundary problem with the growing facets written as the system of ODE, which practically enables us to calculate the global in time solution.

The characterization of subdifferential for a class of convex energies in L^2 space was established by H. Attouch and A. Damlamian in [2]. Their theory is applicable to the energy functional F defined in $L^2(\Omega)$ by modifying the energy density to be coercive and we can achieve (Step2). The next (Step3) actually shows the constant vertical speed on the facets for (1.1), which allows us to proceed to (Step4), and we can successfully obtain the global solution. The spontaneous growth of the facets of the solution was observed in [8], while H. Spohn arrived the same conclusion for the solution solving a free boundary value formulation of (1.2) in [12].

Remark 1. *The application of the theory of subdifferential operator to the second order singular crystalline curvature flow equation was initiated by T. Fukui and Y. Giga [7] in 1993 for one dimensional case. The motion of the surface solving their subdifferential formulation was numerically studied by C. M. Elliott, A. R. Gardiner and R. Schätzle in [5]. They observed the evolution of facets on the surface as well as the problem* (1.1) *shows.*

3. The application to the surface diffusion model. Let us study the fourth order problem (1.3) by this approach. In the fourth order problem, the right hand side term in (1.3) can be formally interpreted as the gradient of the energy functional

F_γ defined by

$$F_\gamma(u) = \int_\Omega \left(|\nabla u| + \frac{1}{\gamma} |\nabla u|^\gamma \right) dx$$

with respect to the metric of $H^{-1}(\Omega)$. The Hilbert space $H^{-1}(\Omega)$ is defined by

$$H^{-1}(\Omega) = \left\{ -\Delta u \mid u \in H_0^1(\Omega) \right\}$$

with the inner product $\langle u, v \rangle_{H^{-1}(\Omega)} := \langle (-\Delta)^{-1} u, v \rangle$, where $\langle \ , \ \rangle$ is the inner product of the duality between $H_0^1(\Omega)$ and $H^{-1}(\Omega)$. Indeed, the formal calculation shows

$$\frac{\delta F_\gamma(u)}{\delta u} \|_{H^{-1}(\Omega)} = \Delta \operatorname{div} \left(\frac{\nabla u}{|\nabla u|} + |\nabla u|^{\gamma - 1} \frac{\nabla u}{|\nabla u|} \right).$$

Now we define the energy functional F_γ in $H^{-1}(\Omega)$ imposing zero Dirichlet boundary condition to fix the problem.

$$F_\gamma(u) := \begin{cases} \displaystyle\int_\Omega |\nabla u| + \frac{1}{\gamma} |\nabla u|^\gamma dx & u \in W_0^{1,1}(\Omega), \ \nabla u \in L^\gamma(\Omega, \mathbb{R}^n), \\ +\infty & \text{otherwise.} \end{cases}$$
$$: H^{-1}(\Omega) \to \mathbb{R} \cup \{+\infty\}.$$

The subdifferential of F_γ at u is a set given by

$$\partial F_\gamma(u) = \left\{ v \in H^{-1}(\Omega) \mid \langle \phi, v \rangle_{H^{-1}(\Omega)} + F_\gamma(u) \le F_\gamma(u + \phi), \forall \phi \in H^{-1}(\Omega) \right\}.$$

The mathematical formulation of the surface diffusion model (1.3) is

$$\frac{du}{dt} \in -\partial F_\gamma(u), \tag{3.1}$$

which is an extended gradient flow equation in $H^{-1}(\Omega)$ requiring the surface to move in order to reduce the energy with respect to the metric of $H^{-1}(\Omega)$.
Since now F_γ satisfies the lower semicontinuity, the unique existence of a global solution for the initial value problem for (3.1) is an immediate consequence of the nonlinear semigroup theory ([3],[4], or [11]).
One remarkable property of (3.1) is the following stability theorem ([1],[13]). If we introduce the regularized energy functional

$$F_\gamma^m(u) := \begin{cases} \displaystyle\int_\Omega \left(|\nabla u|^2 + \frac{1}{m} \right)^{\frac{1}{2}} + \frac{1}{\gamma} \left(|\nabla u|^2 + \frac{1}{m} \right)^{\frac{\gamma}{2}} dx & u \in W_0^{1,1}(\Omega), \ \nabla u \in L^\gamma(\Omega, \mathbb{R}^n), \\ +\infty & \text{otherwise,} \end{cases}$$

and denote $u_m, u : \Omega \times [0, +\infty) \to \mathbb{R}$ as solutions of the initial value problems

$$\begin{cases} \dfrac{du_m(t)}{dt} \in -\partial F_\gamma^m(u_m(t)) \text{ a.e } t > 0, \\ u_m(0) = u_{0m}, \end{cases} \quad \begin{cases} \dfrac{du(t)}{dt} \in -\partial F_\gamma(u(t)) \text{ a.e } t > 0, \\ u(0) = u_0, \end{cases}$$

respectively, then we observe the next convergence.

PROPOSITION 3.1. *If the initial data u_{0m} converges to u_0 strongly in $H^{-1}(\Omega)$ as $m \to +\infty$, then for all $T > 0$,*

$$\lim_{m \to +\infty} \sup_{0 \le t \le T} \|u_m(t) - u(t)\|_{H^{-1}(\Omega)} = 0.$$

This proposition tells us that the solution of the subdifferential formulation (3.1) is a limit of some regularized smooth problems.

4. Characterization of the subdifferential in $H^{-1}(\Omega)$. To attain (Step2) for the surface diffusion model we need to determine the subdfferential $\partial F_\gamma(u)$ precisely. It is possible by extending the argument in [2] into the space $H^{-1}(\Omega)$ on the assumption that the space dimension $n \le 4$ to obtain the following characterization.

THEOREM 4.1. *If $n \le 4$, for any $u \in H^{-1}(\Omega)$ such that $\partial F_\gamma(u) \neq \emptyset$,*

$$\partial F_\gamma(u) = \Big\{ \Delta \operatorname{div} g \ \Big| \ g \in L^{\gamma/(\gamma-1)}(\Omega, \mathbb{R}^n), \ \operatorname{div} g \in H_0^1(\Omega),$$

$$g(x) \in \partial\sigma_\gamma(\nabla u(x)) \ \text{a.e.} x \in \Omega, \quad \text{and} \ \int_\Omega (u \cdot \operatorname{div} g + \langle g, \nabla u\rangle) dx = 0 \Big\},$$

where

$$\sigma_\gamma(p) = |p| + \frac{1}{\gamma}|p|^\gamma : \mathbb{R}^n \to \mathbb{R}.$$

If we restrict the dimension n to be one, we can erase the integral condition in the characterization.

COROLLARY 4.2. *When the space dimension $n = 1$, for any $u \in H^{-1}(\Omega)$ satisfying $\partial F_\gamma(u) \neq \emptyset$,*

$$\partial F_\gamma(u) = \{ g_{xxx} \mid g \in C^1(\bar{\Omega}), g_x \in H_0^1(\Omega), \ g(x) \in \partial\sigma_\gamma(u_x(x)) \ \text{a.e.} x \in \Omega\}.$$

REMARK 2. *More generally, we can calculate the subdifferential of convex functionals of the form*

$$E(u) := \begin{cases} \displaystyle\int_\Omega \tau(x, u(x), \nabla u(x)) dx & u \in W_0^{1,1}(\Omega), \\ +\infty & \text{otherwise}, \end{cases}$$
$$: H^{-1}(\Omega) \to \mathbb{R} \cup \{\infty\},$$

where the function $\tau : \Omega \times \mathbb{R} \times \mathbb{R}^n \to \mathbb{R}$ satisfies the integrability for the first variable, the convexity for the second and third variables, and the coercivity for the third variable, etc, on the same assumption that the space dimension $n \le 4$ ([10]).

5. Calculation of the initial speed. The consequence of (Step3) for the fourth order problem (1.3) will let us know whether it is possible to construct the solution as well as the second order's case and to see the behaviour of the surface in a next moment. What we are especially interested in is the speed in a facetting part on the initial profile, therefore, let us give an initial surface with one facet and calculate the initial speed in the case that $n = 1$, $\gamma = 2$, and the domain $\Omega = (0, l)$. The initial data u_0 is defined as

$$u_0(x) = \begin{cases} u_{01}(x) & (0 < x \le a), \\ h(>0) & (a \le x \le b), \\ u_{02}(x) & (b \le x < l), \end{cases}$$

where $u_{01} \in C^4([0, a])$ is a strictly monotone increasing function with $u_{01}(0) = 0$, $u_{01}(a) = h$, and $u_{01}^{(i)}(0) = u_{01}^{(i)}(a) = 0$ $(i = 1, 2, 3, 4)$. Similarly $u_{02} \in C^4([b, l])$

is a strictly monotone decreasing function with $u_{02}(b) = h,\ u_{02}(l) = 0$, and $u_{02}^{(i)}(b) = u_{02}^{(i)}(l) = 0$ $(i = 1, 2, 3, 4)$. Then we see

THEOREM 5.1. *In the situation stated above, the initial vertical speed of the solution of* (3.1) *for the initial data u_0 is given by*

$$\frac{d^+u_0}{dt} = -u_{0xxxx}\chi_{(0,a)\cup(b,l)} - \frac{24}{(b-a)^3}\chi_{(a,b)} + \frac{12}{(b-a)^2}\delta_a + \frac{12}{(b-a)^2}\delta_b, \tag{5.1}$$

where $\chi_{(0,a)\cup(b,l)}$ and $\chi_{(a,b)}$ are the characteristic functions of $(0,a)\cup(b,l)$ and (a,b), δ_a and δ_b stand for the Dirac distributions on a and b respectively, and d^+/dt is the right derivative in time.

REMARK 3. *More generally, it is possible to calculate the initial vertical speed for C^1-class initial profile. If we adopt an initial data $u_0 \in C^1(\overline{\Omega})$ such that $u_0|_{\partial\Omega} = 0$,*

$$u_0(x) = \begin{cases} u_{01}(x) & (0 < x \le a), \\ h(>0) & (a \le x \le b), \\ u_{02}(x) & (b \le x < l), \end{cases}$$

where u_{01} is strictly monotone increasing and u_{02} is strictly monotone decreasing. Then we see

$$\begin{aligned} \frac{d^+u_0}{dt} = &- u_{0xxxx}\chi_{(0,a)\cup(b,l)} - \frac{6}{(b-a)^2}\left(u_{02xx}(b) + u_{01xx}(a) + \frac{4}{b-a}\right)\chi_{(a,b)} \\ &+ \left(\frac{2}{b-a}u_{02xx}(b) + \frac{4}{b-a}u_{01xx}(a) + \frac{12}{(b-a)^2} + u_{01xxx}(a)\right)\delta_a \\ &+ \left(\frac{4}{b-a}u_{02xx}(b) + \frac{2}{b-a}u_{01xx}(a) + \frac{12}{(b-a)^2} - u_{02xxx}(b)\right)\delta_b. \end{aligned}$$

6. Conclusion. Our subdifferential formulation of (1.3) turned out to be difficult to be the system of ODE like the second order problem (1.1) since the initial vertical speed we obtained is not a constant on the facet and includes the delta functions depending on the profile and the facet growth is not visible.

Recently it was pointed out in [9] and [6] that it is natural to assume that the coefficients of the delta functions vanish for the global solution by taking the regularizing effect of parabolic equations into account. Assuming so and giving a symmetric initial data u_0, the problem becomes the following free boundary value problem in the domain $\Omega = (0, l/2)$.

$u_t = -u_{xxxx},\ (x,t) \in (0, \alpha(t)) \times [0, +\infty),$

boundary conditions:

$$\begin{cases} u(0,t) = u_{xx}(0,t) = u_x(\alpha(t),t) = 0, \\ u(\alpha(t),t) = -\displaystyle\int_0^t \frac{12}{(l-2\alpha(s))^2}\left(u_{xx}(\alpha(s),s) + \frac{2}{l-\alpha(s)}\right)ds + h, \\ \dfrac{6u_{xx}(\alpha(t),t)}{l-2\alpha(t)} + \dfrac{12}{(l-2\alpha(t))^2} + u_{xxx}(\alpha(t),t) = 0, \quad t \in [0, +\infty), \end{cases}$$

initial conditions:

$$\begin{cases} u(x,0) = u_0(x),\ x \in (0, l/2), \\ \alpha(0) = a, \end{cases}$$

where $\alpha(t)$ denotes the free boundary between the facet and the other region. Thus, we can conclude that our subdifferential formulation can be reformed in a free boundary value problem on the assumption that the facet grows.

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