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PROPAGATION OF SINGULARITIES AND RELATED PROBLEMS OF SOLIDIFICATION

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Abstract. We discuss some methods for computing the dynamics and interaction of singularities in nonlinear media. We also consider a physical problem (of solidification in a binary alloy), which has some discontinuous limit solutions.

1. Problems of propagation and interaction of singularities

One of the most interesting application of the theory of generalized functions is the problem of propagation and interaction of singularities. Nonsmooth solutions of nonlinear equations are very important from the physical viewpoint, since they describe such actual phenomena as shock waves, typhoons, hurricanes, tsunami waves, and so on. There are at least three different approaches to these problems.

The first approach is to consider the quasilinear hyperbolic equation (or the system of equations)

$$\frac{\partial u}{\partial t} + \frac{\partial}{\partial x} f(u) = 0, \qquad u\Big|_{t=0} = u^0(x), \tag{1}$$

with nonsmooth initial data. It is assumed that there exists a solution such that the nonlinearity in (1) is defined in some sense. A similar problem for linear equations was considered by Courant, Ludwig, Maslov, and Babich [1–4]. At present, it is well known that in the linear case the singularities propagate along the characteristics. In the nonlinear case, we do not have such a general description, since the trajectories of singularities depend on the solution (and on the type of the singularities). For example, for the shock wave problem ($u^0(x) = u^0_-(x)$ for $x < \psi_0$ and $u^0(x) = u^0_+(x)$ for $x > \psi_0$, where $\psi_0 = \text{const}$ and $[u^0]\big|_{x=\psi_0} = u^0_+(\psi_0 + 0) - u^0_-(\psi_0 - 0) < 0$), the solution of the Hopf equation ($f(u) = u^2/2$) has the form

$$\begin{aligned} u(x,t) &= u_-(x,t) \qquad \text{for} \quad x < \psi(t), \\ u(x,t) &= u_+(x,t) \qquad \text{for} \quad x > \psi(t), \end{aligned} \tag{2}$$

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and the trajectory $x = \psi(t)$ of the jump satisfies the Hugoniot condition

$$\dot{\psi} = \frac{1}{2}[u^2]\big|_{x=\psi} / [u]\big|_{x=\psi}. \tag{3}$$

So, the problem is to find the trajectory of the singularity for sufficiently general equations. At present, there exist some methods for calculating the dynamics of singularities. The most suitable method was developed by Maslov [5,6]. The main idea of this method is to represent the solution (from a suitable subalgebra) in the form of an asymptotic expansion with respect to smoothness. For example, for the solution (2) in a neighborhood of the trajectory $x = \psi(t)$, we have

$$u(x,t) = u_-^0(t) + (x-\psi)u_-^1(t) + \cdots + \theta(x-\psi)v^0(t) + (x-\psi)_+ v^1(t) + \cdots, \tag{4}$$

where $u_-^i = (i!)^{-1}\partial^i u(x,t)/\partial x^i\big|_{x=\psi}$, $\theta(\tau)$ is the Heaviside function, $\tau_+ = \tau$ for $\tau > 0$, $\tau_+ = 0$ for $\tau < 0$, and $v^i = (i!)^{-1}\partial^i\big(u_+(x,t) - u_-(x,t)\big)/\partial x^i\big|_{x=\psi}$. Substituting (4) into equation (1), we obtain a chain of necessary conditions for the existence of a solution of the form (4). These so-called Hugoniot-type conditions ((3) is the first of them) allow us to calculate the dynamics of the singularity. This scheme has been successfully used for solving the shock wave problem (the gas dynamics system) [5,7] and the typhoon problem (the shallow water system) [8], however this scheme is not general. So, to consider an arbitrary singularity (for example, the so-called $\varepsilon\delta$-singularity: $u^0(x)$ is smooth for $x \neq \psi_0$ and $u\big|_{t=0} = u^0(\psi_0) + A_0$ at the point $x = \psi_0$), we have to take the second approach. Namely, we need to consider equation (1) completed by a regularized initial value:

$$\frac{\partial}{\partial t}u_\varepsilon + \frac{\partial}{\partial x}f(u_\varepsilon) = 0, \qquad u_\varepsilon\Big|_{t=0} = u^0(x,\varepsilon), \tag{5}$$

where $u^0(x,\varepsilon)$ tends to $u^0(x)$ as $\varepsilon \to 0$ in some sense.

This approach is related to the construction of algebras of generalized functions developed by Ivanov, Colombeau, Egorov, Marti, Pilipovič, and others [9–14]. If $u_\varepsilon(x,t)$ is an element of the algebra, one can calculate $f(u_\varepsilon)$, substitute u_ε and $f(u_\varepsilon)$ into equation (5), pass to the limit as $\varepsilon \to 0$, and thus, obtain a chain of necessary conditions similar to (4). This scheme was developed by Biagioni, Oberguggenberger, Danilov and Shelkovich, and others [14–17]. In particular, in [15], both the trajectory of a $\varepsilon\delta$-singularity and the interaction of such singularities were calculated for general quasilinear hyperbolic equations of the first order. However, if we use this scheme, we have to take into account the following considerations.

Let u^0 be a shock wave and let u_ε^0 be a regularization of u^0. Then, after some necessary calculations, we obtain the same Hugoniot condition (3) independently of the choice of the regularization u_ε^0 [19]. At the same time, let u^0 be an $\varepsilon\delta$-singularity and let $\varphi(x/\varepsilon)/\varepsilon$ be a family of δ-type functions, where $\int_{-\infty}^{\infty}\varphi(\tau)\,d\tau = 1$. Then the regularization of the initial value has the form

$$u_\varepsilon\Big|_{t=0} = \overline{u}^0(x) + A_0\varphi\big((x-\psi_0)/\varepsilon\big), \tag{6}$$

where $\overline{u}^0 = w\text{–}\lim_{\varepsilon\to 0} u_\varepsilon^0(x,\varepsilon)$. The asymptotic solution of (1), (6) has the following self-similar form

$$u = \overline{u}_0(x,t) + A(t)\varphi\big((x-\psi(t))/\varepsilon\big) + O(\varepsilon),$$

where $\overline{u}_0$ is the smooth solution of the Hopf equation with the initial value $\overline{u}^0$. After some necessary calculations, we readily obtain the first Hugoniot-type condition

$$\dot{\psi} = \overline{u}_0(\psi,t) + \frac{1}{2}A(t)\int_{-\infty}^{\infty}\varphi^2(\tau)\,d\tau. \tag{7}$$

It is easy to see that the trajectory of the $\varepsilon\delta$-singularity depends on the choice of $u^0(x,\varepsilon)$. In other words, the result depends on the choice of the algebra, and we arrive at the question: what algebra do we have to choose?

To answer this question, let us recall that the quasilinear hyperbolic equations give only the simplest model, whereas more realistic models of actual phenomena include some additional terms. Assuming that these terms are small in some sense, we obtain the equation

$$\frac{\partial}{\partial t}u_\varepsilon + \frac{\partial}{\partial x}f(u_\varepsilon) = L_\varepsilon\Big(\varepsilon\frac{\partial}{\partial x}\Big)u, \qquad u_\varepsilon\Big|_{t=0} = u^0(x,\varepsilon), \tag{8}$$

where the term on the right-hand side corresponds to the phenomenon considered. For example, for phenomena in media with small viscosity, $L_\varepsilon(\varepsilon\partial/\partial x) = \varepsilon\partial^2/\partial x^2$ and (8) is the Burgers equation. If we consider waves on a surface, then

$$L_\varepsilon(\varepsilon\partial/\partial x) = \varepsilon^2\partial^3/\partial x^3 \tag{9}$$

and (8) is the KdV equation with small dispersion. Finally, if we consider interior waves in a liquid, then

$$L_\varepsilon(\varepsilon\partial/\partial x) = F^{-1}_{\xi\to x}a(\varepsilon\xi)F_{x\to\xi} \tag{10}$$

(F is the Fourier transform, $a(\zeta) = \zeta\coth\zeta - 1$), and (8) is the so-called Whitham equation [18].

So, we can understand problem (8) in two ways: on the one hand, (8) is a more or less realistic model for the actual phenomenon. On the other hand, (8) is a regularization for problem (1). Problem (8) provides the third approach to the consideration of propagation of singularities: we look for a smooth solution of the regularized problem and then pass to the limit as $\varepsilon\to 0$. This approach was developed by Hopf, Oleinik, Kruzhkov, Lax, Maslov and Omel'yanov, and others [19–21].

At the same time, from the viewpoint of the problem of singularity propagation, we do not need an arbitrary solution of (8), but we have to construct a solution whose property of being self-similar is preserved in time: $\lim_{\varepsilon\to 0} u_\varepsilon(x,t)$ has the same singularity as $u^0(x)$. This means that we need to have some special initial value. In general, we do not know beforehand how to choose such an initial value. Thus, we arrive at a nonstandard problem of obtaining a solution of equation (8) such that it satisfies some prescribed limiting properties. The value of this solution at the initial instant of time gives the initial value both for (8) and for (5). In general, it is impossible to find the explicit solution of such problem, however, it is possible to construct an asymptotic solution. A suitable method has been developed by Maslov and Omel'yanov [20]. In particular, constructing the asymptotic solution, we obtain

$$u = \overline{u}_0(x,t) + A(t)\cosh^{-2}(\mu\tau) + O(\varepsilon), \quad \tau = (x-\psi)/\varepsilon, \quad \mu = \sqrt{A/12}, \tag{11}$$

$$\dot{\psi} = \overline{u}_0(\psi,t) + A(t)/3, \qquad A(t) + 2\overline{u}_0(\psi,t) = \text{const}, \tag{12}$$

for the solitons of the KdV equation [20] and

$$u = \overline{u}_0(x,t) + A(t)\{\cosh^2(\mu\tau) + \sigma(t)\sinh^2(\mu\tau)\}^{-1} + O(\varepsilon), \tag{13}$$

$$\dot{\psi} = \overline{u}_0(\psi,t) + 1 - \delta\coth\delta, \qquad \ln(\delta/\sin\delta) - \delta\coth\delta + \overline{u}_0(\psi,t) = 0, \tag{14}$$
$$\sigma = \tan(\delta/2), \qquad A = 2\delta\sigma, \qquad \mu = \delta/2,$$

for the solitons of the Whitham equation [22]. The justification of the asymptotic solutions [21,22] allows us to pass to the limit as $\varepsilon \to 0$ and to describe the propagation of $\varepsilon\delta$-singularities for the Hopf equation (1). One can easily see that, for the same limit equation (1), different ways of regularization ((9) and (10)) give different forms of the regularization of the solution and of the initial data ((11) and (13)), as well as different trajectories of propagation of this singularity ((12) and (14)).

The method [20] for constructing an asymptotic solution with localized "fast" variation allows us to calculate the propagation of singularities. However, the problem of interaction is more complicated. In fact, only the first steps in this direction have been taken [20] (see also [23] about similar problems). At the same time, by using algebraic constructions, it is relatively simple (for the approach (5)) to calculate the interaction of singularities [15].

So, returning to the question about the regularization of the initial data in (5) and considering the application of the algebraic construction, one can suggest the following method. By choosing the physical meaning of the constructed solution, we determine the way of regularization of the equation. Then, constructing a self-similar asymptotic solution, we find the method of regularization of the initial data and the trajectories of propagation of the corresponding singularities. Finally, using an appropriate algebraic construction, we can calculate the interaction of the singularities.

2. Problems of solidification

Now let us consider a preliminary model of form other than (8)

$$\frac{\partial}{\partial t}(\theta + \varphi) = \Delta\theta, \qquad x \in \Omega, \quad t > 0, \tag{15}$$
$$\frac{\partial \varphi}{\partial t} + \Delta(\varepsilon^2\Delta\varphi + \varphi - \varphi^3 + \varepsilon\kappa\theta) = 0.$$

This model describes the problem of first-kind phase transitions in a binary alloy [24]. Here $\Omega \subset R^n$, $n \leq 3$, is a bounded domain with smooth boundary, θ is the normalized temperature, the so-called function of order φ characterizes the concentration in the binary alloy, the values $\varphi = +1$ and $\varphi = -1$ correspond to the pure phases, whereas the value $\varphi = 0$ corresponds to the uniform mixture, $\kappa > 0$ is a constant, and ε is a small parameter. Equations (15) are completed by natural initial and boundary conditions. The main purpose is to describe the evolution of the alloy from small perturbations of the state of a uniform mixture to the final state of separate phases.

Using the Whitham method, one can construct an asymptotic almost periodic solution of system (15)

$$\varphi = \Phi_0(S(x,t)/\varepsilon, x, t) + O(\varepsilon), \qquad \theta = \theta_0(x,t) + O(\varepsilon) \tag{16}$$

that describes the evolution of the system from the state $\overline{\varphi} = 0$, $|\varphi| \ll 1$ to the state $\overline{\varphi} = O(1)$, $|\varphi| = O(1)$. Here θ_0 is the smooth solution of the heat equation

$$\frac{\partial \theta_0}{\partial t} = \Delta\theta_0 + \overline{\frac{\partial}{\partial t}\Phi_0},$$

the bar denotes the weak limit as $\varepsilon \to 0$,

$$\Phi_0(\tau, x, t) = \frac{\gamma - \sigma\rho\,\mathrm{sn}^2(\mu\tau \mid m)}{1 - \sigma\mathrm{sn}^2(\mu\tau \mid m)}, \qquad \mu = \frac{\sqrt{(\beta-\rho)(\alpha-\gamma)}}{2\sqrt{2}|\nabla S|}, \tag{17}$$

$$m = (\beta-\gamma)(\alpha-\rho)/(\beta-\rho)(\alpha-\gamma),$$

and $\rho < \gamma < \beta < \alpha$ are the roots (depending on the parameters $c = c(x,t)$ and $E = E(x,t)$) of the equation $-z^4 + 2z^2 - 4cz = 4E$. The phase S of oscillations and the additional functions c and E satisfy the model equations

$$\frac{\partial S}{\partial t} = f_1 \operatorname{div}(f_2 \nabla S), \qquad \frac{\partial c}{\partial t} + f_3 \frac{\partial E}{\partial t} = f_4 \Delta c, \qquad |\nabla S| = f_5, \tag{18}$$

where the coefficients f_j depend on c and E. An analysis of formulas (17), (18) shows that this process is unstable and the oscillation amplitude $A = \beta - \gamma$ and the energy E increase very fast. At the critical instant of time t_1^* such that $\alpha - \beta \to 0$ as $t \to t^*$, the oscillation solution (16) transforms (at the corresponding point x) into the soliton type solution [25]

$$\varphi = \varphi_0(x,t) + \chi(\mu\tau) + O(\varepsilon), \qquad \theta = \theta_0(x,t) + O(\varepsilon). \tag{19}$$

Here $\tau = (t - \psi(x))/\varepsilon$,

$$\chi(\eta, x) = -8Q^2\{\exp(\eta) + 8b\exp(-\eta) + 8\check{\varphi}_0\}^{-1}, \qquad \mu = Q/|\nabla\psi|,$$

$$\check{\varphi}_0 = \varphi_0(x, \psi(x)), \qquad Q = \sqrt{3\check{\varphi}_0^2 - 1}, \qquad b = 1 - \check{\varphi}_0^2,$$

and θ_0 and $\varphi_0 \in (1/\sqrt{3}, 1)$ are solutions of the equations

$$\frac{\partial \varphi_0}{\partial t} = \Delta(\varphi_0^3 - \varphi_0), \qquad \frac{\partial \theta_0}{\partial t} = \Delta\theta_0 - \frac{\partial \varphi_0}{\partial t}, \tag{20}$$

completed by natural initial and boundary conditions.

The function ψ describes the front $\Gamma_t = \{x, \psi(x) = t\}$ of the solitary wave χ and satisfies the geometric problem

$$V_\nu = \frac{1}{3}\mathcal{K}(1+G) + G\frac{\partial}{\partial \nu}\ln \check{\varphi}_0, \qquad \psi\Big|_{\Gamma_0} = 0, \tag{21}$$

where $V_\nu = 1/|\nabla\psi|$ is the normal velocity of Γ_t, $\mathcal{K} = \operatorname{div}\nu$ is the mean curvature of Γ_t, $\nu = \nabla\psi/|\nabla\psi|$, $\partial/\partial\nu = \langle \nu, \nabla\rangle$, $G = IQ^2/2(Q-I)$, and $I = \sqrt{2}\check{\varphi}_0 \ln\{(\sqrt{2}\check{\varphi}_0 + Q)/\sqrt{b}\}$.

The self-similar asymptotic solution (19) was constructed (by the method developed in [26]) and justified in [25]. It is also proved that problems (20) and (21) are well posed and solution (19) is stable, that is, this solution exists during the time T independent of ε. However, the mean value $|\overline{\varphi}| = |\varphi_0|$ also increases and the second process of bifurcation starts at a critical time t_2^* such that $|\varphi_0| \to 1$ as $t \to t_2^*$. During this time interval, the soliton-type solution (19) transforms into the tanh-type solution [27]

$$\varphi = \tanh(\mu\tau) + O(\varepsilon), \qquad \theta = \theta_0(x) + O(\varepsilon), \tag{22}$$

where θ_0 is a function harmonic in Ω, $\mu = 1/\sqrt{2}|\nabla\psi|$, $\tau = (t-\psi(x))/\varepsilon$, and the function ψ describes the free boundary $\Gamma_t = \{x, \psi(x) = t\}$ between the domains $\Omega_t^\pm$ occupied by "pure" phases (that is $\overline{\varphi} = \pm 1$ in $\Omega_t^\pm$). The function $\psi(x)$ and auxiliary functions $\Phi_1^\pm$ are the solution of the Mullins–Sekerka problem

$$\Delta\Phi_1^\pm = 0, \qquad x \in \Omega_t^\pm, \qquad t > 0, \tag{23}$$
$$[\Phi_1^\pm]\Big|_{\Gamma_t} = 0, \qquad \Big[\frac{\partial \Phi_1^\pm}{\partial\nu}\Big]\Big|_{\Gamma_t} = V_\nu, \qquad \mathcal{K} = \tfrac{3}{\sqrt{2}}\Phi_1^\pm\Big|_{\Gamma_t}, \qquad \psi\Big|_{\Gamma_0} = 0.$$

The asymptotic solution (22) is also stable and justified [27]. So, asymptotic solutions (16), (19), and (22) describe three different stages of solidification in a binary alloy. An analysis of formulas (17)–(19) provides a formal description of the bifurcations from one state to another. However, the problem of explicit description of these bifurcations is open at present.

At the same time, from the limit viewpoint as $\varepsilon \to 0$, the constructed solutions are singular: solution (22) corresponds to a shock wave, (19) corresponds to the $\varepsilon\delta$-type of singularities, and (17) can be treated in terms of an oscillating wave front. In turn, the model problems (18), and (20), (21), and (23) are Hugoniot-type conditions for these singularities. One can conjecture that such singular solutions can be derived by algebraic methods for the limiting equations corresponding to (15). It also looks reasonable that these methods may be fruitful for the description of interactions and bifurcations.

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