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Merging and interacting wave fronts for reaction – diffusion equations

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IN THIS PAPER the merging and interacting kink-type solution for general reaction diffusion equations are considered. Both the analytical and numerical investigations are presented. In particular, the existence of the complicated merging, elliptic and hyperbolic fronts in two dimensions is shown.

1. Introduction

IN THIS PAPER the Cauchy problem for the reaction-diffusion equations is considered:

$$\frac{\partial u}{\partial t} = \Delta u + h^2(x) f(u), \qquad x \in R^n, \quad t \geqslant 0, \tag{1.1}$$

$$u(x,0) = u_0(x), \tag{1.2}$$

where $f(u)$ and h^2 are smooth functions.

These equations play an important role in a number of applications such as the theory of combustion, phase transitions, polymer science, chemical kinetics and many others.

Here we shall study some special kind of solutions for problem (1.1) – (1.2) describing the motion, the interaction and merging of well localized wave fronts (interfaces). These fronts are involved in many mechanical, physical and biological phenomena.

The asymptotical theory of the interface propagation was developed in numerous papers, for example, [9, 10, 11, 6]. The first rigorous proof of existence of such fronts was given by [10] in the pioneering work on the scalar systems of Ginzburg-Landau type. Another approach for more general scalar equations, based on the comparison principle, was suggested in [1]. By this principle, Z. PERADZYŃSKI and B. KAŹMIERCZAK [12] have considered monotone parabolic systems of very general form. These results describe the localized fronts of a small curvature and do not pretend to describe completely the front interaction and the front merging.

At the present time, the theory of the front interaction in one-dimensional case is extensively developed (see, for example, [2, 7, 9]). However, all analytical results hold only when the travelling fronts (kinks) are separated by large distances (weak interaction). The first goal of this paper is to present an effective semi-analytic, semi-numerical method that allows to analyze the process of interaction and merging of two kinks completely, up to the final stage.

The theory of interaction of localized fronts in 2D is much less developed as compared to 1D. In fact, there exist only a few results in this field. The first of them was obtained by Z. PERADZYŃSKI [13] and concerned the 2D merging kink solutions. Physically, such solution describes a moving interface (with a constant velocity) between two phases. This interface has a form close to two lines intersecting at an angle $\alpha \neq \pi$. At the intersection point such an interface can have a large curvature, what makes the investigation especially difficult. In particular, the well known methods ([10, 11, 9]) cannot be applied. Let us also notice that the existence of some special odd 2D solutions was shown in [4]; however, it is well known that these solutions are unstable [14].

The second aim of the paper is to construct new *exact* analytic 2D solutions describing the complex effects of the interaction and merging of the kinks. This holds for some special coefficients h (for example, quadratic). These solutions can describe a compression of curved kinks of elliptic form; an interaction of two kinks with fronts of hyperbolic type; and at last, merging of two kinks with asymptotically planar fronts.

The paper is organized as follows. In Section 1 we describe the case of interaction of two one-dimensional kinks. In Section 2, we give the analytic approach that allows us to describe a class of exact 2D solutions.

2. Approximate solution of the kink – antikink collision problem for real Ginzburg-Landau model. Merging kinks in one dimension.

In this section we consider the kink - antikink collision problem for the real Ginzburg-Landau model. Mathematically, this problem can be written as the Cauchy problem

(2.1) $$u_t = u_{xx} + u - u^3, \qquad x \in R, \qquad t > 0,$$

(2.2) $$u_0 = 1 + \mathrm{tgh}(p_0(x - q_0)) - \mathrm{tgh}(p_0(x + q_0)),$$

where $|q_0| >> 1$, $p_0 = 1/\sqrt{2}$ are constants. This problem enables the following equivalent variational formulation

$$\frac{\delta D}{\delta u_t} = -\frac{\delta F}{\delta u}, \tag{2.3}$$

where D and F are functionals of dissipation and free energy:

$$D[u_t] = \frac{1}{2}\int\limits_{-\infty}^{\infty} u_t^2 dx, \tag{2.4}$$

$$F[u] = \int\limits_{-\infty}^{\infty} \left(\frac{u_x^2}{2} + \frac{(u^2-1)^2}{4}\right) dx. \tag{2.5}$$

Such a formulation is rather important both for the mathematical description of solutions and the physical understanding of underlying phenomena. The aim of this section is to construct an approximate solution of Eq. (2.1) with initial data (2.2).

Firstly let us describe some physical effects appearing in (2.1) – (2.2). Suppose the Eq. (2.1) describes a state of bistable (two-phase) medium. The stable phases of this matter correspond to stationary solutions of Eq. (2.2) $u = u^+ = 1$ and $u = u^- = -1$. From this viewpoint, initial data (2.2) describe the case when a large interval of space $d \simeq 2q_0$ is filled by phase $u = u^-$ and surrounded on both sides by semi-infinite regions by the phase u^+, these phases being separated by the boundary layers (fronts). Although the initial data (2.2) almost exactly satisfy Eq. (2.1), Eq. (2.2) is an unstable solution. In fact, as time passes, the fronts approaching each other, and the distance between them reduces progressively, and when $t \to \infty$, the solution approach $u = u^+$ exponentially in time and uniformly in space. Physically, this process describes an absorption of phase u^- by phase u^+. When the distance between fronts is sufficiently large, one can describe its motion asymptotically. Then the principal part of the asymptotic solution is given by

$$u_0 = 1 + \mathrm{tgh}(p_0(x-q)) - \mathrm{tgh}(p_0(x+q)), \tag{2.6}$$

where $p_0 = 1/\sqrt{2}$ is a constant, $q = q(t)$ is the following function:

$$q(t) = \frac{1}{2\sqrt{2}} \ln\left(\exp(2\sqrt{2}q_0) - 48t\right). \tag{2.7}$$

This well – known result (see, for example, [2, 9, 7]) holds only when q_0 is sufficiently large. When the fronts approach each other at the distances comparable to 1, solution (2.6), (2.7) fails. In fact, the interaction of the fronts at these distances changes the character and analytical description of such interaction becomes more complicated.

In order to describe the entire process of fronts motion for the system (2.1) - (2.2) from weak interaction to collision, we apply the generalized Whitham principle [9, 18].

According to this principle, variational Eq. (2.3) can be approximated as follows:

$$\frac{\partial \bar{D}(\mathbf{s}, \dot{\mathbf{s}})}{\partial \dot{s}_i} = -\frac{\partial \bar{F}(\mathbf{s})}{\partial s_i}, \tag{2.8}$$

where $\bar{D}$, $\bar{F}$ are the functionals D and F "Whitham averaged" on the approximation $U(x, \mathbf{s}(t))$. In other words,

$$\bar{D}(\mathbf{s}, \dot{\mathbf{s}}) = \frac{1}{2} \int_{-\infty}^{\infty} U_t^2 dx, \tag{2.9}$$

$$\bar{F}(\mathbf{s}) = \int_{-\infty}^{\infty} \left(\frac{U_x^2}{2} + \frac{(U^2 - 1)^2}{4} \right) dx, \tag{2.10}$$

where $\mathbf{s} = \mathbf{s}(t)$ is an unknown time - dependent vector function, which should be obtained from the system (1.8).

The approximation $U(x, \mathbf{s})$ depends explicitly on the space coordinate and implicitly, via $\mathbf{s}$, on time that allows us to make an approximate reduction from infinite - dimensional system (1.3) to finite-dimensional one (1.8).

Practically an approximation $U(x, \mathbf{s})$ will be as good as our prediction a real space shape of solution $u(x, t)$. The generalized Whitham principle helps us only to find the best approximation of exact solution $u(x, t)$ among the functions $U(x, \mathbf{s})$ where $\mathbf{s} = \mathbf{s}(t)$ is any time-dependent function. Let us note here that choice of the shape function U, number of components in $\mathbf{s}$ and dependence of $U(x, \mathbf{s})$ on $\mathbf{s}$ is a quite complicated problem. This is similar, in a sense, to the choice of a proper basis for the Galerkin approximation. In fact there exist no general rules to define these quantities and such a selection is more an art than a science.

Here we are going to describe a function U which is, according to the numerical grid solution of Eq. (2.1), a very good approximation of the true solution.

This approximation is as follows:

$$U(x, q, p) = 1 + \operatorname{tgh}(p(x - q)) - \operatorname{tgh}(p(x + q)), \qquad \mathbf{s}(t) = (q(t), p(t)). \tag{2.11}$$

The choice of this function (2.11) is mainly inspired by initial conditions and the physical nature of the problem. Both the unknown functions have a clear physical interpretation: q, as it was mentioned above, is the front coordinate and p is the slope of the front. This means that, in this approximation, the fronts can move and that all front distortions are reduced to the change of their slope. Direct numerical computation by the grid method shows that such a presumption is very close to the real front behaviour. According to the numerical results, the front generally moves according to our predictions but with a small distortion at the same time. Such a distortion level may reach about three percent of the solution and is strongly localized at the center of symmetry (Fig. 1).

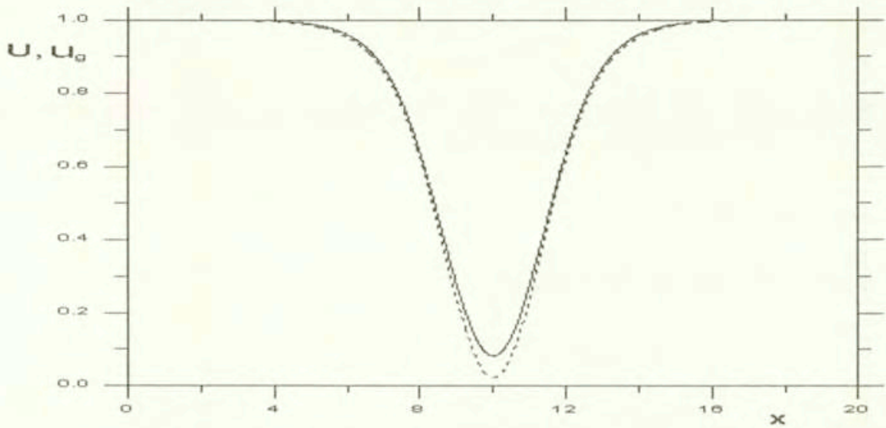

FIG. 1. Comparison of the grid solution u_g (dashed line) and approximate solution U, given by the formula (2.11) (solid line) at the moment corresponding to the final stage of the kink — antikink collision.

Let us describe now how the parameters q and p behave during the collision. At the initial stage of the front motion while the kink distance q is large (practically for $|q| > 3$), the motion goes as it is predicted by asymptotic formulas (1.7): the slope of the fronts remains constant and the coordinate q slowly decreases. When the fronts approaching each other are close enough, the slope starts to be involved in dynamics. Motion becomes faster and faster and the slope decreases making them wider. At the final stage, both parameters $p, q \to 0$ and the stable state $u = u^+$ appears.

The agreement between true and approximate solutions may be called quite good. Apparently the approximation preserves the main features of the front collision, nonetheless it would be helpful to find an algorithm to improve the accuracy of the approximation. In fact, such a refinement must give a more detailed description of the front distortion. Our numerical experiment shows that such an improved approximation can be given in the following form:

$$u_{ia} = \sum_{k=1}^{N} z_k(t)[\cosh^{-2}(p(t)(x - c_k q(t))) + \cosh^{-2}(p(t)(x + c_k q(t)))], \tag{2.12}$$

where c_k are some *a priori* given numbers and z_k are some time-dependent functions which can be defined by the Galerkin method from linearized at U Eq. (2.1). For example, if we take $N = 3$ and $\mathbf{c} = (c_1, c_2, c_3) = (0, 1, 2)$, the accuracy of solution will increase from three percent to 0.05 percent.

We should notice that a similar approximation has been used in [3] to understand qualitative behaviour of the kinks connected states for ϕ^4 model which is $u_{tt} - u_{xx} = u - u^3$. In this work such a approximation is called "parametric collective coordinate" (PCC). However, the agreement between numerical simulations and the result of PCC approach is only of a qualitative character.

3. Exact analytic solutions describing the interaction and merging of kinks in some inhomogeneous 2D-media

2.1. General approach

Consider the following equation:

$$u_t = \Delta u + h^2(x,y)f(u). \tag{3.1}$$

Suppose there exists a kink-type function satisfying the equation

$$-cU' = U'' + f(U). \tag{3.2}$$

The kink-type function is here a function $u(x)$ that is monotone and approaching exponentially its limits $u^{\pm}$, $u^+ \neq u^-$ as $x \to \pm\infty$. Under natural conditions of bistability (for example, see [5, 16, 17, 15] among others and references given therein), such a solution U exists and is globally stable.

Let us seek a solution of (3.1) in the following form:

$$u = U(\theta), \quad \theta = \phi(x,y) - vt. \tag{3.3}$$

Substitution of (3.3) to (3.1) leads to

$$-vU' = \Delta\phi U' + (\nabla\phi)^2 U'' + h^2(x,y)f(U). \tag{3.4}$$

Using condition (3.2) and equating coefficients at U' and U'' to zero, we obtain the following equations for ϕ

$$\Delta\phi + v - ch^2(x,y) = 0, \tag{3.5}$$

$$(\nabla\phi)^2 = h^2(x,y). \tag{3.6}$$

Certainly, the system (3.5) – (3.6) can not be solved for a general function h^2 because one function ϕ should satisfy two equations. Nevertheless, at least for some functions h^2 it is possible to construct phase ϕ which satisfies both Eqs. (3.5) and (3.6). It allows us to find a new class of exact solution describing the interesting physical effects.

2.2. Examples of curved fronts and merging kink solutions

In this section we consider two examples of Eq. (3.1) with different functions h^2 which lead to curved fronts and merging kink solutions.

Our first example concerns two simple terms h^2 which are quadratic functions of x and y. In this example, we intend to show that, even in such simple cases, one can observe a number of new non-trivial physical effects. In particular, we show that such a term generates solutions of (3.1) with moving curved fronts. These fronts are plane second-order curves.

The function h^2 is a sufficiently nonlocal function. In the second example we consider a case where h^2 is localized along some line. This means that asymptotically, at an exponential rate, h^2 tends to a constant as $x \to \infty$. This localization leads to merging front formation.

The first example deals with two types of Eq. (3.1) with polynomial h^2 functions. The first one (case A) leads to a kink-type solution with elliptic and hyperbolic fronts, the second type (case B) to a parabolic one.

Case A. Elliptic and hyperbolic fronts

As the first step let us consider Eq. (3.1) with

$$h^2 = (ax)^2 + (by)^2. \tag{3.7}$$

We suppose also that velocity of the initiated kink solution $c = 0$ (see Eq. (3.2)). It is easy to check that phase ϕ nucleated by such a term h^2 can be expressed in a way similar to h^2 as a quadratic function

$$\phi = \phi_0 + \alpha x^2 + \beta y^2, \tag{3.8}$$

where

$$\alpha = \pm\frac{a}{2}, \qquad \beta = \pm\frac{b}{2}, \qquad v = -2(\alpha + \beta). \tag{3.9}$$

Here we need to distinguish two different cases: $\mathrm{sign}(\alpha) = \mathrm{sign}(\beta)$, $\mathrm{sign}(\alpha) = -\mathrm{sign}(\beta)$.

The first case is especially simple and corresponds to the compressive elliptic front solution (see Fig. 2). Such a solution has a simple physical interpretation in the framework of the phase transition theory. Assume that Eq. (3.1) describes a two-phase nonlinear medium. In this sense, solution $u = u^+$ corresponds to one

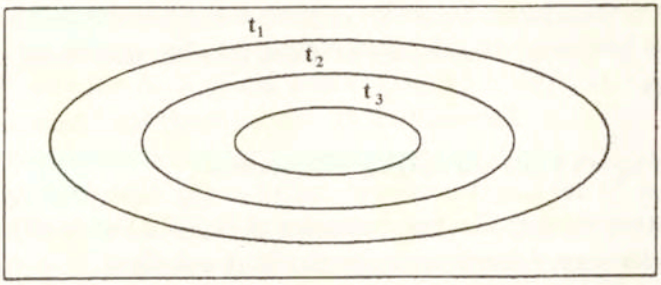

FIG. 2. Elliptic front behaviour.

phase, $u = u^-$ to another. At the initial moment, we have two regions consisting of different phases u^+ and u^-.

These regions are separated by a thin boundary layer (the phase front) which has an elliptic shape. In other words, the elliptic area consisting of one of the phases (say u^-) is surrounded by an infinite area with the u^+ phase. As time passes, the phase front is compressing which means that phase u^+ captures the region filled by phase u^- and as $t \to \infty$, the phase u^- vanishes and phase u^+ fills all the space. Such an effect is well known in the asymptotic theory of interface propagation [9].

The second case describes moving hyperbolic fronts and is slightly more complicated. Such fronts depending on a, b can behave in two different manners. Let us describe this motion by an example. Suppose that $a, b > 0$ and $\alpha > 0$, $\beta < 0$. Assume also ϕ_0 to be a large negative number. In this case the front positions are determined by:

$$\frac{a}{2}x^2 - \frac{b}{2}y^2 = -\phi_0 + (b-a)t.$$

At the initial stage the fronts are hyperbolic, symmetrical about the y - axis. The time evolution of this front is completely determined by the sign of difference $d = b - a$. When d is positive, the fronts are moving away from each other and the distance between them is increasing (see Fig. 3b). More complicated behaviour occurs when d is negative. In this case, the fronts are approaching each other and at a certain moment of time $t^* = d - \phi_0$, they degenerate into two crossing lines. After $t = t^*$, these fronts take a hyperbolic shape again but now symmetrical about the x-axis (Fig. 3a). The motion of these fronts is inverse compared to the initial stage and the fronts are moving away from each other (see Fig. 3).

Case B. Parabolic fronts.

Let us consider another polynomial function

$$h^2 = h_0^2 + (ax)^2. \tag{3.10}$$

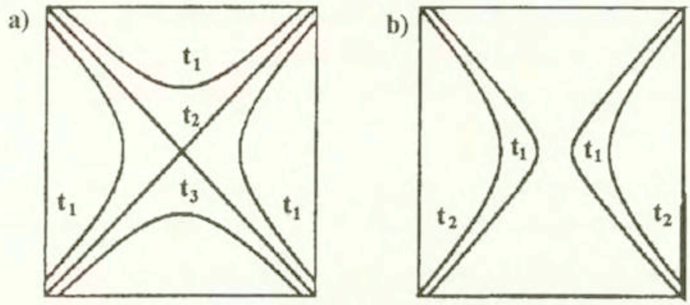

FIG. 3. Hyperbolic fronts behaviour.

Similarly to the previous case, we suppose the velocity c of initial solution (3.2) to be zero.

Substitution of (3.10) into conditions (3.5), (3.6) leads to the following expression for the phase ϕ:

$$\phi = \phi_0 + \alpha x^2 + \beta y, \tag{3.11}$$

where

$$\alpha = \pm\frac{a}{2}, \quad \beta = \pm h_0^2, \quad v = \pm a.$$

From expression (3.11) we see that the front has a parabolic shape moving towards large positive y values, see Fig 4.

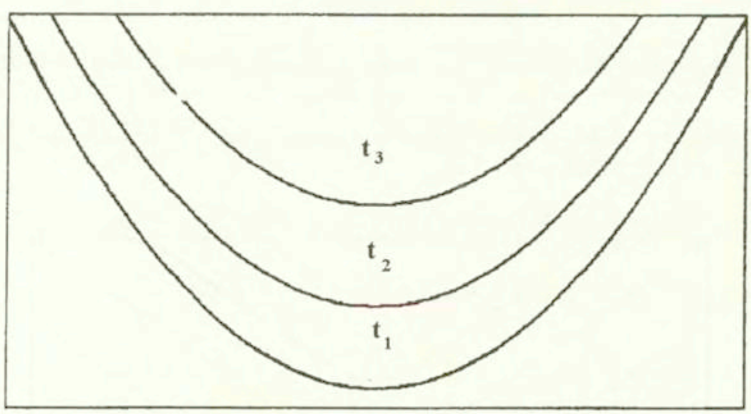

FIG. 4. Parabolic front behaviour.

In order to understand the physical nature of these phenomena, we again need to return to the phase transition theory. Consider a two-phase matter whose behaviour is governed by Eq. (3.1) with h^2 given by (3.10). At the initial time, both phases are present and divided by a parabolic interface (say, u^+ inside the interface and u^- outside it). In this interpretation, the front motion means that the phase u^+ located inside the parabolic area is driven out by the phase u_-.

Case C: Localized h and merging solutions

In the previous example function h^2 was strongly nonlocal. In the following example we consider a localized function h^2. This function can be defined as follows:

$$h^2 = A^2 + \left(\frac{a}{c}\right)^2 \operatorname{tgh}^2(ax), \tag{3.12}$$

where A and a are some constants and $c \neq 0$ is the initial velocity.

Let us notice that such an Eq. (3.1) can describe an almost homogenous medium, with linear inclusion (inhomogeneity) given by $\left(\frac{a}{c}\right)^2 \operatorname{tgh}^2(ax)$ where a is the width of inhomogeneity, $\left(\frac{a}{c}\right)^2$ is the amplitude.

Substitution of (3.12) into Eqs. (3.5) and (3.6) sets the following expression to the phase

$$\phi = \phi_0 + \alpha \ln(\cosh(ax)) + \beta y, \tag{3.13}$$

where

$$\alpha = -\frac{1}{c}, \qquad \beta = \pm A, \qquad v = \frac{(cA)^2 + a^2}{c}. \tag{3.14}$$

From Eq. (3.13) it is clear that the front is close to merging lines $y = \pm\frac{a}{cA}x + st$, as x, y tend to infinity (see Fig. 5). The angle γ of merging is equal to $\operatorname{arctg}(a/c)$. If the defect vanishes ($a = 0$), then the front becomes linear ($\gamma = \pi$) and moves in y-direction. If $a \to \infty$ (the defect of large amplitude), the angle γ tends to 0 and the front moves in y- direction along the defect and resembles a very narrow cone, almost a needle.

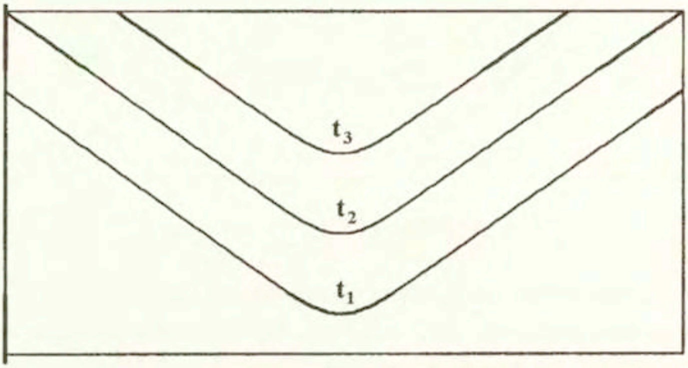

FIG. 5. The merging front behaviour.

The front moves as a whole with the speed v which also depends on the amplitude of the defect. The localization of the front grows as a increases.

One can give the following simple interpretation of these results. To move along the defect, the merging kink should have the appropriate velocity and the angle of merging. For higher and sharper defects, narrow and quick kinks move along the defect.

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