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General set of traveling-wave solutions for amplitude equations in the phase field crystal model

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Abstract. Fronts dynamics of periodic crystalline state, which invades the homogeneous state (liquid phase), are analysed. These fronts are considered as traveling waves of atomic density amplitudes. The propagation of amplitudes is described by the hyperbolic equation of an extended Allen-Cahn type for which the complete set of analytical traveling-wave solutions are obtained by tanh-method. The set of solutions includes previously known traveling waves for the parabolic Allen-Cahn equation of both extended and standard form.

1. Introduction

The phase field crystal model (PFC-model) has been used to examine the dynamics of liquid-solid transformations, grain boundary migration and dislocation motion [1,2]. The PFC model is a continuum model that describes processes on atomic length scales and pattern on the nano- and micro-length scales [3]. This model is characterized by a free energy which is represented by a functional of a conserved atomic density field that is periodic in the solid phase and uniform in a liquid state.

One of the simplest ways to analyze the PFC-model is to use the amplitude equations [4,5,6] which represent smooth profiles over picks of the density field. Taking into account slow and fast degrees of freedom for the crystal-liquid interface propagation, the amplitude equation of the PFC-model is described by the following partial differential equation (PDE) [7]:

$$\frac{\partial u}{\partial t} + \tau \frac{\partial^2 u}{\partial t^2} = \nabla^2 u - \mathrm{K}_0 u + b u^2 - u^3. \tag{1}$$

The following notations are introduced in Eq. (1): $u(\vec{r}, t)$ is the amplitude of atomic density (non-conserved order parameter), $\vec{r}$ is the radius-vector, t is the time, the parameter b can be written as

$$b = \frac{2a}{\sqrt{15v|\Delta B_0|}}, \tag{2}$$

in which the driving force ΔB_0 describes

$$\Delta B_0 = \begin{cases} \Delta B_0 > 0, \ the\ transition\ from\ a\ metastable\ state\ with\ K_0 = +1, \\ \Delta B_0 < 0, \ the\ transition\ from\ an\ unstable\ state\ with\ K_0 = -1, \end{cases} \tag{3}$$

a and v are the coefficients in the free energy density which has the form of Landau-de Gennes potential:

$$f(u) = \frac{K_0 \Delta B_0}{2} u^2 - \frac{2a}{3} u^3 + \frac{15v}{4} u^4. \tag{4}$$

In the equilibrium, the two states (liquid and solid) have the equal energy with the parameter $b = 8a^2 / 135\, v$ and the crystalline front has zero velocity. Finally, it should be noted that Eq. (1) can be considered as an extended Cahn-Allen equation which transforms to its standard form at $b = 0$ and $\tau = 0$ [8] that was suggested for the anti-phase boundary motion and then used in a wide spectrum of mathematical and physical applications [9], for instance, in the description of free-boundary problems by phase-field method [10]. In its complete form, Eq. (1) has been applied in the field of fast phase transitions [11,12], whose validity has been verified by comparison with experimental data [13], in molecular dynamics simulations [14] and by coarse graining derivations of the phase field equations [15]. For the parabolic type of the extended Allen-Cahn equation, i.e., for $\tau = 0$, traveling wave has already been obtained by Wazwaz [16].

Generally, PDE can be analyzed using an important class of traveling wave solutions which, in their particular form, include tanh-functions [16]. Particular solutions of Eq. (1) have also been found in the form of tanh-function [7]. However, so far, by the moment there exists no general set of exact traveling waves for the hyperbolic equation of Allen-Cahn type (1). Therefore, the main purpose of the present work is to find a complete set of traveling waves as the set of exact analytical solutions of Eq. (1). This complete set will be found using the tanh-method [16,17,18], which nowadays represents one of the simplest and the most convenient ways in searching for solutions of traveling waves. As a final result, the complete set of solutions will be checked on the existence of tanh-functions in the obtained traveling waves.

2. The tanh-method and traveling-wave solutions

One of the important solutions for the analysis of phase transformations is related to traveling waves [7,9,16-19]. To treat the non-linear PDEs, the traveling waves are obtained by the first integral method [19,20,21,22] (which can be considered as one of particular cases of the direct method [23], generalizing the use of equivalent methods in finding the exact solutions of PDE, which were reduced to ODE [24]), and also using G'/G-expansion method [25], the rank analytical technique [26,27], and the phase-plane analysis [28,29].

In the present work, we use the tanh-method as a useful tool for the computation of the exact travelling waves by introducing a power series in tanh-function (function of hyperbolic tangent). The efficiency of the tanh-method has been illustrated in Refs. [16,17,18] by applying it for a variety of selected equations, such as nonlinear equations of the Fischer's type and generalized Korteveg-de-Vries-equation (KdV-equation). Moreover, its modification, the tanh-coth-method [18,30], is used to derive the solitons and kink solutions for some of the well-known nonlinear parabolic partial differential equations (the Newell-Whitehead-, Fitz-Hugh-Nagumo-, and Burgers-Fisher-equation). The tanh-coth-method extends a set of the possible solutions and provides abundant solitons and kink solutions in addition to the existing ones. As a result, the power of the tanh-method is confirmed as the most direct and effective algebraic methods [30,31] for finding the exact solutions of nonlinear differential equations.

Let's consider spatially one-dimensional equation (1) for the atomic density amplitude $u(x,t)$, which is evolving in time t along spatial coordinate x. Following Wazwaz [18], we introduce a new independent variable

$$\xi = \frac{x-ct}{\delta}, \tag{5}$$

which describes propagation of the amplitude with the velocity c and transforms the amplitude $u(x,t) \rightarrow U(\xi)$. This transformation re-writes the derivatives as follows:

$$\frac{\partial}{\partial t} = -\frac{c}{\delta}\frac{d}{d\xi}, \ \frac{\partial^2}{\partial t^2} = \frac{\partial}{\partial t}\left(-\frac{c}{\delta}\frac{d}{d\xi}\right) = \frac{c^2}{\delta^2}\frac{d^2}{d\xi^2}, \tag{6}$$

$$\frac{\partial}{\partial x} = \frac{1}{\delta}\frac{d}{d\xi}, \ \frac{\partial^2}{\partial x^2} = \frac{1}{\delta^2}\frac{d^2}{d\xi^2}, \ \frac{\partial^3}{\partial x^3} = \frac{1}{\delta^3}\frac{d^3}{d\xi^3}. \tag{7}$$

Using (6) and (7), spatially one-dimensional equation (1) in the new variable looks like:

$$\frac{c}{\delta}\frac{dU(\xi)}{d\xi} - \tau\frac{c^2}{\delta^2}\frac{d^2U(\xi)}{d\xi^2} + \frac{1}{\delta^2}\frac{d^2U(\xi)}{d\xi^2} - U^3(\xi) - K_o U(\xi) + bU^2(\xi) = 0. \tag{8}$$

To solve (8), we shall apply now the tanh-method [16], introducing the finite expansion:

$$U(\xi) = S(Y) = \sum_{k=0}^{M} a_k Y^k + \sum_{k=1}^{M} b_k Y^{-k}, \tag{9}$$

$$M \in \mathbb{Z}, Y = \tanh(\xi). \tag{10}$$

Using new variable (5), the solution (10) and derivatives,

$$\frac{d}{d\xi} = (1-Y^2)\frac{d}{dY},$$

$$\frac{d^2}{d\xi^2} = (1-Y^2)\left(-2Y\frac{d}{dY} + (1-Y^2)\frac{d^2}{dY^2}\right),$$

one may find that Eq. (8) takes the following form

$$\frac{c}{\delta}(1-Y^2)\frac{dS}{dY} + \frac{1}{\delta^2}(1-\tau c^2)\left[(1-Y^2)(-2Y\frac{dS}{dY} + (1-Y^2)\frac{d^2S}{dY^2})\right] - S^3 - K_o S + bS^2 = 0. \tag{11}$$

The parameter M from Eq. (8) can be determined using the analysis of Wazwaz [16]. Indeed, balancing the linear terms of the highest order with the highest order nonlinear terms in Eq. (11) one can get $3M = 4 + M - 2$, therefore, $M = 1$, so the expansion (9) becomes

$$S(Y) = a_0 + a_1 Y, \tag{12}$$

with the following derivatives

$$S'(Y) = \sum_{k=0}^{M}\left(a_k Y^k\right)' = a_1, S''(Y) = 0. \tag{13}$$

Now, opening the braces in Eq. (11), using Eqs. (12) and (13), we collect the coefficients of powers of Y^n in the resulting equations as follows

$$\left(\frac{2}{\delta^2}(1-\tau c^2)a_1 - {a_1}^3\right)Y^3 - \left(\frac{c}{\delta}\,a_1 + 3a_0{a_1}^2\right)Y^2 + \left(\frac{2}{\delta^2}(1-\tau c^2)a_1 - 3{a_0}^2a_1 - K_o a_1 + 2ba_0a_1\right)Y$$

$$+\left(a_1\frac{c}{\delta} - {a_0}^3 - a_0K_o + b{a_0}^2\right)Y^0 = 0. \quad (14)$$

Equation (14) has a solution if the braces ahead of Y^k are placed to zero. Thus, the following system of equations for the parameters a_k, k=0..*M*, c and δ is obtained:

$$Y^3: \frac{2}{\delta^2}(1-\tau c^2)a_1 - {a_1}^3 = 0, \quad (15)$$

$$Y^2: -\frac{c}{\delta}a_1 - 3a_0{a_1}^2 + b{a_1}^2 = 0, \quad (16)$$

$$Y^1: -\frac{2}{\delta^2}(1-\tau c^2)a_1 - 3{a_0}^2a_1 - K_o a_1 + 2a_0a_1b = 0, \quad (17)$$

$$Y^0: a_1\frac{c}{\delta} - {a_0}^3 - a_0K_o + b{a_0}^2 = 0. \quad (18)$$

The system of equations (15)-(18) has a trivial solution a_1=0 and $a_0 = b/2\,(1 \pm \sqrt{1-4K_0/b^2})$ with the arbitrary values of c and δ. In this case, the amplitude has constant profile $u(x,t) = a_0$. This homogeneous solution has no interest for us because we are looking for amplitude's profiles of atomic density, which are moving through metastable/unstable homogeneous state (liquid phase). In the case $a_1 \neq 0$, equations (15)-(18) look like:

$${a_1}^2 = \frac{2}{\delta^2}(1-\tau c^2), \quad (19)$$

$$a_1 = \frac{\frac{c}{\delta}}{b-3a_0}, \quad (20)$$

$$3{a_0}^2 - 2a_0b + \frac{2}{\delta^2}(1-\tau c^2) + K_o = 0, \quad (21)$$

$${a_0}^3 - b{a_0}^2 + a_0K_o - a_1\frac{c}{\delta} = 0. \quad (22)$$

Determination of the parameters a_0, a_1, c and δ from Eqs. (19)-(22) leads us to the amplitude profiles of the form:

$$u(x,t) = a_0 + a_1\tanh\left[\frac{x-ct}{\delta}\right]. \quad (23)$$

Concrete values for a_0, a_1, c and δ represent different types of solutions, that is shown in the next two sections.

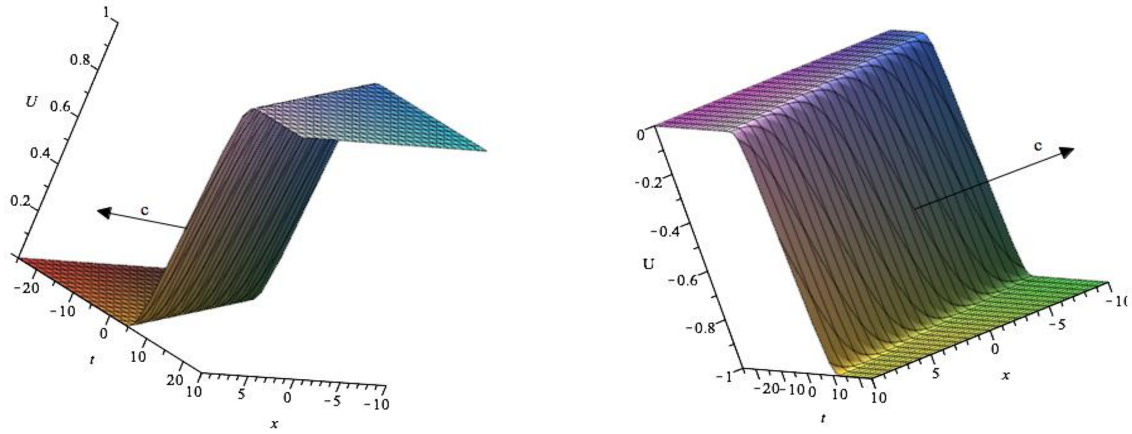

Figure 1. Smooth and continuous $\varphi -$ profiles calculated with the usage of *Solutions 3* and *4* from Table 1. Calculation were developed for fixed $\tau = 0.5$ and for the values of a_0, a_1 and δ given by $K_0 = 1$ and under the condition of $b^2 \geq 4K_0$ as from Eq. (2). (a) $\varphi -$ profile moves in direction of the x –axis with the constant negative velocity *c*. (b) $\varphi -$ profile moves in direction of the x –axis with the constant positive velocity *c*.

3. Set of solutions

A complete set of solutions consists of 12 decisions for the parameters K_0 and b, which are defined by Eqs. (2) and (3). This number of decisions follows from the degrees of Eqs. (19)-(22), where each (19) and (21) assume the existence of two roots (4 roots in total), multiplied by 3 decisions from the cubic equation (22). These 12 decisions can be divided into three sets, every one of which contains 4 similar by notation type of solution. All the coefficients from Eq. (23) are obtained for the following far field boundary conditions, $\xi \to \pm\infty: u \equiv const$, namely, for $u = 0$ or $u = \pm 1$.

3.1. Solutions 1-4

The first set of solutions can be recognized by the signs of the parameters a_1, c. As a result, solutions 1-4 are presented in Table 1.

Table 1. First set of solutions: solutions 1-4.

Values	Solutions 1 and 2	Solutions 3 and 4
a_0	$\frac{1}{2}b$	$\frac{1}{2}b$
a_1	$\pm\frac{1}{2}\sqrt{b^2 - 4K_0}$	$\frac{1}{2}\sqrt{b^2 - 4K_0}$
δ	$\frac{4}{\sqrt{2b^2 - 8K_0 + b^4\tau - 4b^2\tau K_0}}$	$-\frac{4}{\sqrt{2b^2 - 8K_0 + b^4\tau - 4b^2\tau K_0}}$
c	$\frac{b\sqrt{b^2 - 4K_0}}{\sqrt{2b^2 - 8K_0 + b^4\tau - 4b^2\tau K_0}}$	$\pm\frac{b\sqrt{b^2 - 4K_0}}{\sqrt{2b^2 - 8K_0 + b^4\tau - 4b^2\tau K_0}}$

With $b = 0$ and $K_0 = -1$, table 1 shows that $a_0 = 0$, $a_1 = \pm 1$, $\delta = \pm\sqrt{2}$ and $c = 0$. In this particular case, Eq. (23) predicts stationary profiles:

$$u(x,t) = \pm \tanh\left(\mp \frac{x}{\sqrt{2}}\right). \quad (24)$$

This profile is consistent with the steady solution of hyperbolic Allen-Cahn equation ($\tau \neq 0$) and parabolic Allen-Cahn equation ($\tau = 0$), which are obtained from (1) for the above accepted parameters $b = 0$ and $K_o = -1$.

3.2. Solutions 5-8

The second group of solution consist of solutions 5-8. It has the similar structure. In order to simplify the representation, we shall introduce the following notations for this set of solutions:

$$A_{5-8} = \left[-\left(10b^2 + 6b\sqrt{b^2 - 4K_0} + 162\tau {K_0}^2 - 36K_0 - 72b^2\tau K_0 + 8b^4\tau\right) \cdot \left(8b^2K_0 - b^4 - 6bK_0\sqrt{b^2 - 4K_0} + b^3\sqrt{b^2 - 4K_0} - 18{K_0}^2\right)\right]^{1/2}, \quad (25)$$

$$B_{5-8} = 5b^2 + 3b\sqrt{b^2 - 4K_0} + 81\tau {K_0}^2 - 18K_0 - 36b^2\tau K_0 + 4b^4\tau, \quad (26)$$

$$G_{5-8} = \sqrt{2b^2 + 2b\sqrt{b^2 - 4K_0} - 4K_0}. \quad (27)$$

Now using the parameters (25) - (27), we rewrite Solutions 5-8 in new designations:

$$a_0 = \frac{1}{4}b + \frac{1}{4}\sqrt{b^2 - 4K_0}, \quad a_1 = \frac{1}{4}G_{5-8}, \quad \delta = \frac{2A_{5-8}}{B_{5-8}K_0}, \quad c = -\frac{1}{4}\left(-\frac{1}{2}b + \frac{3}{2}\sqrt{b^2 - 4K_0}\right)G_{5-8}\frac{A_{5-8}}{B_{5-8}K_0}, \quad (28)$$

$$a_0 = \frac{1}{4}b + \frac{1}{4}\sqrt{b^2 - 4K_0}, \quad a_1 = \frac{1}{4}G_{5-8}, \quad \delta = -\frac{2A_{5-8}}{B_{5-8}K_0}, \quad c = \frac{1}{4}\left(-\frac{1}{2}b + \frac{3}{2}\sqrt{b^2 - 4K_0}\right)G_{5-8}\frac{A_{5-8}}{B_{5-8}K_0}, \quad (29)$$

$$a_0 = \frac{1}{4}b + \frac{1}{4}\sqrt{b^2 - 4K_0}, \quad a_1 = -\frac{1}{4}G_{5-8}, \quad \delta = \frac{2A_{5-8}}{B_{5-8}K_0}, \quad c = \frac{1}{4}\left(-\frac{1}{2}b + \frac{3}{2}\sqrt{b^2 - 4K_0}\right)G_{5-8}\frac{A_{5-8}}{B_{5-8}K_0}, \quad (30)$$

$$a_0 = \frac{1}{4}b + \frac{1}{4}\sqrt{b^2 - 4K_0}, \quad a_1 = -\frac{1}{4}G_{5-8}, \quad \delta = -\frac{2A_{5-8}}{B_{5-8}K_0}, \quad c = -\frac{1}{4}\left(-\frac{1}{2}b + \frac{3}{2}\sqrt{b^2 - 4K_0}\right)G_{5-8}\frac{A_{5-8}}{B_{5-8}K_0}. \quad (31)$$

3.3. Solutions 9-12

The third group consists of Solutions 9-12. It has the similar structure to the first group once again and is also similar
to the previous group of Solutions 5-8. Introducing the parameters,

$$A_{9-12} = \left[-\left(-10b^2 + 6b\sqrt{b^2-4K_0} - 162\tau K_0{}^2 + 36K_0 + 72b^2\tau K_0 - 8b^4\tau\right)\cdot\left(-8b^2K_0 + b^4 - 6bK_0\sqrt{b^2-4K_0} + b^3\sqrt{b^2-4K_0} + 18K_0{}^2\right)\right]^{1/2}, \tag{32}$$

$$B_{9-12} = -5b^2 + 3b\sqrt{b^2-4K_0} - 81\tau K_0{}^2 + 18K_0 + 36b^2\tau K_0 - 4b^4\tau, \tag{33}$$

$$G_{9-12} = \sqrt{2b^2 - 2b\sqrt{b^2-4K_0} - 4K_0}, \tag{34}$$

we, finally, rewrite parameters for a_0, a_1, c and δ for Solution 9-12 in the following form

$$a_0 = \frac{1}{4}b - \frac{1}{4}\sqrt{b^2-4K_0}, \qquad a_1 = \frac{1}{4}G_{9-12}, \qquad \delta = -\frac{2A_{9-12}}{BK_0}, \qquad c = \frac{1}{4}\left(-\frac{1}{2}b - \frac{3}{2}\sqrt{b^2-4K_0}\right)G_{9-12}\frac{A_{9-12}}{BK_0}, \tag{35}$$

$$a_0 = \frac{1}{4}b - \frac{1}{4}\sqrt{b^2-4K_0}, \qquad a_1 = \frac{1}{4}G_{9-12}, \qquad \delta = \frac{2A_{9-12}}{BK_0}, \qquad c = -\frac{1}{4}\left(-\frac{1}{2}b - \frac{3}{2}\sqrt{b^2-4K_0}\right)G_{9-12}\frac{A_{9-12}}{BK_0}, \tag{36}$$

$$a_0 = \frac{1}{4}b - \frac{1}{4}\sqrt{b^2-4K_0}, \qquad a_1 = -\frac{1}{4}G_{9-12}, \qquad \delta = -\frac{2A_{9-12}}{BK_0}, \qquad c = -\frac{1}{4}\left(-\frac{1}{2}b - \frac{3}{2}\sqrt{b^2-4K_0}\right)G_{9-12}\frac{A_{9-12}}{BK_0}, \tag{37}$$

$$a_0 = \frac{1}{4}b - \frac{1}{4}\sqrt{b^2-4K_0}, \qquad a_1 = -\frac{1}{4}G_{9-12}, \qquad \delta = \frac{2A_{9-12}}{BK_0}, \qquad c = \frac{1}{4}\left(-\frac{1}{2}b - \frac{3}{2}\sqrt{b^2-4K_0}\right)G_{9-12}\frac{A_{9-12}}{BK_0}. \tag{38}$$

4. Particular solutions

For the amplitude's equation (8) the whole set of 12 solutions of the form of Eq. (23) is presented by the coefficients summarized in Table 1, Eqs. (28) -(31) and Eqs. (35) -(38). Now, we compare special and particular cases of these solutions with corresponding results, which were obtained earlier.

Using the first integral method [19], traveling wave solutions have been obtained for the hyperbolic Allen-Cahn equation [20]. This equation is consistent with Eq. (1), if $b = 0$ and $K_0 = -1$. Indeed, if we substitute these values for b and K_0 into solutions (28)-(31), then solutions of the form (23) corresponds to those ones obtained in [20]. The graphical representation for this particular case is shown in Fig. 1, which gives a view for the atomic density profile, that invades the homogeneous phase with positive and negative values of c. Another pair of solutions could be obtained for $a_0 = a_1 = \pm 0.5$. Thus, in general, we have obtained 4 bounded solutions, which correspond to 4 bounded solutions of Ref. [20]. It should be noticed, that in [20] another 4 unbounded solutions were obtained. These solutions were extracted by us in [20] from the general set of solutions due to its physical and mathematical insolvency, namely, due to the absence of the physical sence and the violation of the mathematical problem statement. In the current work we do not obtain the unbounded solutions since tanh-method build (9)-(10) on the bounded set *a priori*. Therefore, solution (23) is always bounded.

With the zero relaxation time, namely $\tau = 0$, hyperbolic equation (1) transforms into parabolic partial differential type whose traveling wave solution has been previously found by Wazwaz [18]. Indeed, as it follows from our solutions (35)-(38), if we use $\tau = 0$ and take into account (32)-(34), solutions of [18] are covered for the extended Allen-Cahn equation.

In general, we have obtained traveling wave solutions represented by hyperbolic tanh-functions (23) that confirms the correctness of the particular solutions for the dynamical problem of fast diffuse interfaces [32-33].

5. Conclusions

We considered the atomic density amplitudes which represented by an extended hyperbolic Allen-Cahn equation (1). Using the tanh-method [16-18,30,31], we obtained traveling wave solutions for Eq. (1) as kink-profiles (step-profiles), which invade metastable or unstable homogeneous states (liquid phase). The kink-profiles are described by tanh-functions (23), which in its order confirms the correctness of the particular solutions [32,33], which were chosen for equations from the fields of rapid solidification and fast transformations. We have shown, that the presently obtained solutions indeed include as particular case the previously known sets of traveling waves, which have been found for (*i*) the extended parabolic Allen-Cahn equation [16] and (*ii*) the hyperbolic Allen-Cahn equation with a standard free energy density describing only the transitions from the unstable state [20].

6. References

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