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Exact solutions for a nonstandard viscous Cahn—Hilliard system

Presented by Academician of the NAS of Ukraine N.F. Shulga

The one-dimensional version of a nonstandard viscous Cahn–Hilliard system (proposed by Colli et al.) for the order parameter and chemical potential with a generally asymmetric polynomial double-well potential is considered. For this system, an exact travelling wave solution, which describes the advancing front of a phase transformation in an infinite domain, is found.

Keywords: *Cahn—Hilliard equation, phase transition, travelling wave solution.*

Introduction. The Cahn—Hilliard equation [1, 2] is now the well-established phenomenological model in the theory of phase transitions. The basic underlying idea of this model is that, for an inhomogeneous system, e.g., a system undergoing a phase transition, the thermodynamic potential (e.g., free energy) should depend not only on the order parameter (here, the term "order parameter" denotes a field, whose values characterize the phase), but also on its gradient as well. The idea of such dependence was introduced by van der Waals [3] in his theory of capillarity. Due to this dependence, instead of the usual second order, the resulting diffusion equation for the order parameter becomes a fourth-order PDE.

The stationary form of this equation was introduced in [1]. In [2], a linearized version of the time-dependent equation was treated, and the corresponding instability ("spinodal decomposition") of the homogeneous state was identified. However, it was only much later on that the intense study of the fully nonlinear form of this equation was started [4]. The impressive amount of work has now been done on the nonlinear Cahn–Hilliard equation (see [5]), as well as on its numerous modifications. One of the most interesting modifications was introduced by Gurtin [6]. Following the general trend in the development of nonlinear continuous mechanics, he based his derivation "on the separation of the basic balance laws (such as those for mass and force), which are general and hold for large classes of materials, from the constitutive equations (such as those for elastic solids and viscous fluids), which delineate specific classes of material behavior", see [6, p. 179]. Additionally, he introduced a new balance law for microforces and used the second law of thermodynamics in the form of a dissipation inequality, see [6] for details. Then he obtained the standard Cahn—Hilliard equation and the viscous Cahn—Hilliard equation [7] as special cases of his model.

The next step was done by Podio-Guidugli [8]: keeping the balance of microforces as in [6], he replaced the dissipation inequality by the imbalance of entropy and the mass balance by the energy balance. In his derivation, the chemical potential plays the same role as the "coldness" (inverse absolute temperature) in the derivation of the heat equation. Based on the latter approach, Colli et al. [9] introduced and studied the following system of governing equations for two unknowns, the chemical potential μ and the order parameter ρ:

$$(\varepsilon+2\rho)\frac{\partial\mu}{\partial t}+\mu\frac{\partial\rho}{\partial t}-\Delta\mu=0\,, \tag{1}$$

$$\delta\frac{\partial\rho}{\partial t}-\Delta\rho+f'(\rho)=\mu\,. \tag{2}$$

Here, ε is a regularization constant introduced to preserve the parabolic structure of Eq. (1) (see [9]), δ is the characteristic time for the evolution of the order parameter, and $f(\rho)$ is some double-well potential. They proved the existence and uniqueness of a global-in-time smooth solution to the associated initial-boundary-value problem and studied the long-time behavior of the solution.

In the present communication, we consider the one-dimensional version of this system with a generally asymmetric polynomial double-well potential $f(\rho)$, i.e.

$$f'(\rho)=\rho^3-r\rho^2-q\rho+\eta\,. \tag{3}$$

For this system, we give the exact travelling wave solution, which describes the advancing phase transformation in an infinite domain.

Travelling wave solution. Looking for the travelling-wave solution $\mu(z),\rho(z)$, where $z=$ $=x-vt$, Eqs. (1) and (2) yield

$$v(\varepsilon+2\rho)\frac{d\mu}{dz}+v\mu\frac{d\rho}{dz}+\frac{d^2\mu}{dz^2}=0\,, \tag{4}$$

$$-v\delta\frac{d\rho}{dz}-\frac{d^2\rho}{dz^2}+\rho^3-r\rho^2-q\rho+\eta=\mu\,. \tag{5}$$

Now, we introduce our ansatz, by presuming that μ is the n-th power polynomial of ρ, $\mu=P_n(\rho)$. Comparing the powers of the nonlinearities, it is easily seen that it should be $n\leqslant 3$; postponing the discussion of other possibilities to the further communications, we consider the simplest case $n=1$:

$$\mu=\gamma\rho+\omega\,. \tag{6}$$

Let us first consider Eq. (4). The substitution of (6) into (4) for μ yields

$$v\left[3\gamma\rho+(\varepsilon\gamma+\omega)\right]\frac{d\rho}{dz}=-\gamma\frac{d^2\rho}{dz^2}\,. \tag{7}$$

Integrating Eq. (7) once, we get

$$-\frac{3}{2}v\left[\rho^2+\frac{2}{3\gamma}(\varepsilon\gamma+\omega)\rho+C_1\right]=\frac{d\rho}{dz}, \tag{8}$$

where C_1 is the integration constant. We are looking for the monotone “kink-” or “antikink-”like solution approaching the limiting values

$$\rho\big|_{z\to-\infty} = \rho_1, \quad \rho\big|_{z\to+\infty} = \rho_2 . \tag{9}$$

At this level of phenomenology, there is no reason to attach any particular value neither to ρ_1, nor to ρ_2. It is important only that the different values are assigned to different homogeneous phases. For definiteness, we presume $\rho_1 < \rho_2$, i.e. the kink solution. We will get such a solution for ρ, if Eq. (8) takes the form

$$\frac{d\rho}{dz} = -\kappa(\rho-\rho_1)(\rho-\rho_2); \quad \rho_1 \leqslant \rho \leqslant \rho_2 . \tag{10}$$

For Eq. (8) to take form of (10), the following constraints should be satisfied:

$$\kappa = \frac{3}{2}v , \tag{11}$$

$$\frac{2}{3\gamma}(\varepsilon\gamma+\omega) = -X . \tag{12}$$

Here, we have denoted $X = (\rho_1+\rho_2)$ for brevity. Because C_1 is an arbitrary constant, there are only two constraints, (11) and (12). The integration of Eq. (10) yields

$$\rho = \frac{\rho_1+\rho_2}{2} + \frac{\rho_2-\rho_1}{2}\tanh\left[\frac{\kappa}{2}(\rho_2-\rho_1)(z+c)\right], \tag{13}$$

where c is the integration constant. It is natural to take the position of the maximal value of the derivative $\frac{d\rho}{dz}$ (where $\frac{d^2\rho}{dz^2}=0$) as $z=0$; then $c=0$. The constant κ has the same sign as the velocity v [see (11)], so solution (13) is a kink for positive v, and an antikink for negative v. In other words, the state with a lower value of the order parameter is always advancing. The evident formal reason for this is that Eq. (4) is linear and homogeneous in μ.

Now, let us consider Eq. (5). Using (10), the second derivative $\frac{d^2\rho}{dz^2}$ is easily calculated:

$$\frac{d^2\rho}{dz^2} = \kappa^2\left[2\rho^3 - 3X\rho^2 + (2Y+X^2)\rho - XY\right], \tag{14}$$

where $Y = \rho_1\rho_2$. Substituting expressions (6), (10), and (14) for μ, $\frac{d\rho}{dz}$, and $\frac{d^2\rho}{dz^2}$, respectively, into Eq. (5) and equating the coefficients at all powers of ρ to zero yield four constraints

$$1-2\kappa^2 = 0 , \tag{15}$$

$$v\delta\kappa + 3\kappa^2 X - r = 0 , \tag{16}$$

$$-v\delta\kappa X - \kappa^2[2Y+X^2] - q = \gamma , \tag{17}$$

$$v\delta\kappa Y + \kappa^2 XY + \eta = \omega . \tag{18}$$

For definiteness, we will presume $\kappa > 0$ below, i.e., we consider the kink solution.

The substitution of expressions (11) and (15) for v and κ into (16) yields

$$X = \frac{2}{3}\left(r - \frac{\delta}{3}\right). \tag{19}$$

Substituting expressions (17) and (18) for γ and ω into constraint (12), we get

$$Y = \frac{1}{4(\delta - 3X - 3\varepsilon)}\left[9X^3 + 6(\delta + \varepsilon)X^2 + 2(9q + 2\delta\varepsilon)X + 12(q\varepsilon - \eta)\right]. \tag{20}$$

The detailed study of the parametric dependence of ρ_1, ρ_2, i.e. of X and Y, will be given elsewhere. Here, we present the short version only. In system (1—2), the terms proportional to ε and δ were introduced in [9] for the purpose of regularization of this system, with some a posteriori justification. Setting $\varepsilon = \delta = 0$ simplifies expressions (19) and (20) for X and Y substantially:

$$X = \frac{2}{3}r, \tag{21}$$

$$Y = -\left[\frac{1}{3}r^2 + \frac{3}{2}q - \frac{3\eta}{2r}\right]. \tag{22}$$

Correspondingly, the limiting values of the order parameter at $\mp\infty$ are

$$\rho_{1,2} = \frac{1}{3}r \mp \sqrt{\frac{4}{9}r^2 + \frac{3}{2}q - \frac{3\eta}{2r}}. \tag{23}$$

Using Eqs. (21) and (22), the coefficients γ and ω in ansatz (6) are easily calculated as

$$\gamma = \frac{1}{9}r^2 + \frac{1}{2}q - \frac{3\eta}{2r}; \quad \omega = -\gamma r. \tag{24}$$

So, finally, the solution for the chemical potential μ is

$$\mu = \left(\frac{1}{9}r^2 + \frac{1}{2}q - \frac{3\eta}{2r}\right)(\rho - r), \tag{25}$$

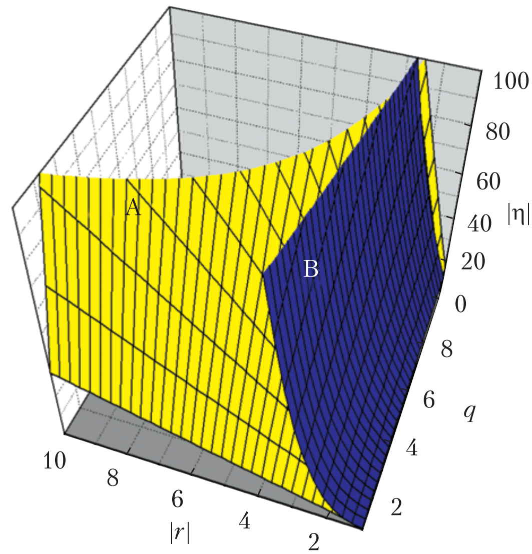
where the order parameter ρ is given by Eq. (13).

Discussion. It is reasonable to presume that the phase with the lower value of the chemical potential μ is advancing, so it should be $\gamma > 0$. This imposes the following condition on the coefficients of the polynomial potential:

$$\frac{1}{9}r^2 + \frac{1}{2}q > \frac{3\eta}{2r}. \tag{26}$$

Here, q is positive. So, if the last inequality is fulfilled, (23) always yields real ρ_1, ρ_2. If $\eta = 0$, then ρ_1, ρ_2 are real independently of the sign of r. So, formally, the solution exists. However, the case where $\eta = 0$ results in the negative values of the chemical potential μ. Indeed, the lowest value of the chemical potential, which corresponds to $\rho = \rho_1$, is

$$\mu_1 = \gamma\left(-\frac{2}{3}r - \sqrt{\frac{4}{9}r^2 + \frac{3}{2}q - \frac{3\eta}{2r}}\right). \tag{27}$$



Surfaces *A* and *B* correspond to the lower limit in the first inequality of (28) and to the upper limit in the second inequality, respectively

For μ_1 to be nonnegative, both r and η should be negative, and it should be additionally

$$\frac{3}{2}q < \frac{3}{2}\left|\frac{\eta}{r}\right| < \frac{1}{9}r^2 + \frac{1}{2}q\,. \tag{28}$$

Figure shows the surfaces A $|\eta| = q|r|$ and B

$$|\eta| = \frac{2}{27}|r|^3 + \frac{1}{3}q|r|,$$

corresponding to the lower limit in the first inequality of (28), and to the upper limit in the second inequality, respectively. For values of the coefficients corresponding to the points $q, |r|$, and $|\eta|$ in the space between these surfaces, the physically reasonable solutions exist.

So, the physically reasonable exact solution exists for an essentially asymmetric potential $f(\rho)$ only. This is somewhat reminiscent of the situation with the convective Cahn—Hilliard equation, where the exact travelling-wave solutions exist only for the asymmetric potential [10].

In the sequence of works, Colli et al. [11—15] introduced and studied the following generalization of system (1—2):

$$(1 + 2g(\rho))\frac{\partial \mu}{\partial t} + \mu g'(\rho)\frac{\partial \rho}{\partial t} - \operatorname{div}(k(\mu,\rho)\nabla\mu) = 0\,, \tag{29}$$

$$\delta\frac{\partial \rho}{\partial t} - \Delta\rho + f'(\rho) = \mu g'(\rho)\,. \tag{30}$$

If $g(\rho)$ and $\kappa(\mu,\rho)$ are polynomials in ρ of the powers m and l, respectively, and if $\kappa(\mu,\rho)$ is a polynomial in μ of the power s, for several sets of m, l, and s, the above method is applicable finding the exact travelling wave solutions of system (29)—(30) as well. These solutions will be systematically studied in the following publications.

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ТОЧНЕ РОЗВ’ЯЗАННЯ СИСТЕМИ
НЕСТАНДАРТНИХ В’ЯЗКИХ РІВНЯНЬ КАНА—ХІЛЛІАРДА

Розглянуто одновимірний варіант нестандартної системи рівнянь Кана—Хілліарда (запропонованої Colli et al.) для параметра порядку і хімічного потенціалу з асиметричним поліномним двоямним потенціалом. Для цієї системи знайдено точне розв’язання вигляду рухомої хвилі, що описує рух фронту фазового перетворення в нескінченній області.

Ключові слова: *рівняння Кана—Хілліарда, фазові перетворення, розв’язання виду рухомої хвилі.*

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ТОЧНОЕ РЕШЕНИЕ СИСТЕМЫ НЕСТАНДАРТНЫХ
ВЯЗКИХ УРАВНЕНИЙ КАНА—ХИЛЛИАРДА

Рассмотрен одномерный вариант нестандартной системы уравнений Кана—Хиллиарда (предложенной Colli et al.) для параметра порядка и химического потенциала с асимметричным полиномиальным двуямным потенциалом. Для этой системы найдено точное решение вида бегущей волны, которое описывает движение фронта фазового превращения в бесконечной области.

Ключевые слова: *уравнение Кана—Хиллиарда, фазовые превращения, решение вида бегущей волны.*