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Analytical Approximation for Cahn-Hillard Phase-Field Model for Spinodal Decomposition of a Binary System

Ali Tozar[1], **Orkun Taşbozan**[2], **Ali Kurt**[3]

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Abstract — Phase transformations which lead to dramatical property change are very important for engineering materials. Phase-field methods are one of the most successful and practical methods for modelling phase transformations in materials. The Cahn-Hillard phase-field model is among the most promising phase-field models. The most successful aspect of the model is that it can predict spinodal decomposition (which is essential to determining the microstructure of an alloy) in a binary system. It is used in both materials science and many other fields, such as polymer science, astrophysics, and computer science. In this study, the Cahn-Hillard phase-field model is evaluated by an analytical approach using the $(1/G')$-expansion method. The solutions obtained are tested for certain thermodynamic conditions, and their accuracy of predicting the spidonal decomposition of a binary system is confirmed.

Keywords — *Cahn-Hillard phase field model, spidonal decomposition,* $(1/G')$*-expansion method*

Mathematics Subject Classification (2020) — 35R11, 34A08

1. Introduction

Foreseeing phase transformations is very important for tailoring the properties of engineering materials. For instance, occurrence of domains may determine magnetic properties of a metallic material [1]. On the other hand, mechanical properties of a material can be altered by a phase transformation [2]. Because of having a significant impact on the physical and chemical properties of the material, phase transformations, which are changes in the microstructure at equilibrium or non- equilibrium states, are the primary and most important concern of a materials engineering scientist. There are certain difficulties that this issue brings along with its importance. A method developed to model phase transformations to predict the properties of the material needs to take into account many thermal, electromagnetic, elastic and chemical effects. Hence, the issue is getting very difficult mathematically.

Phase-field methods are one of the most successful and practical methods for modeling phase transformations in materials. A phase field model can be described as spatiotemporal treating of the microstructure of a material as a scalar field (concentration, strain temperature, etc.). Phase field models have attracted much attention in recent years due to their versatility [3–5]. In these models, the free energy equation based on the thermodynamic state of the system is given in terms of phase fields. Nonlinear partial differential equations play an important role in the phase-field model due to dynamical governing of one or more order parameters as well as heat or mass transfer. These

[1]tozarali@gmail.com; [2]otasbozan@mku.edu.tr; [3]pau.dr.alikurt@gmail.com(Corresponding Author)
[1]Department of Physics, Hatay Mustafa Kemal University, Hatay, Turkey
[2]Department of Mathematics, Hatay Mustafa Kemal University, Hatay, Turkey
[3]Department of Mathematics, Pamukkale University, Denizli, Turkey

dynamical interactions of the parameters are based on the tendency of free energy to reach to its possible minimum value.

Cahn-Hillard phase field model is the one of the most promising phase field models [6,7]. The most successful aspect of the model is that it can predict spinodal decomposition (which is very essential for determining the microstructure of an alloy) in a binary system [8]. Due to the success of the model in this regard, it is being used both in materials science [9, 10] and in many fields such as polymer science [11], astrophysics [12], computer science [13] and astrophysics [12]. The simple structure of the model is mainly due to the fact that it is based on the diffusion laws in the Ginzburg-Landau theorem [14, 15]. Total energy of a binary alloy is illustrated by the sum of two parts which are the bulk part depending on local energy difference and the interfacial part depending on concentration gradient. In summary, the total energy expression can be written as follows:

$$E = \int_{\Omega} f(\varphi) d\Omega + \int_{\Omega} \frac{\epsilon^2}{2} |\nabla \varphi|^2 d\Omega \tag{1}$$

where the first term is bulk and second term is interfacial energy ($\epsilon > 0$ represents the interfacial parameter). In order to evaluate the thermodynamic conditions, on the $f(\varphi)$ which is the free energy function is considered as follows according to Flory-Huggins model [16];

$$f(\varphi) = \frac{1}{2}((1+\varphi)\ln(1+\varphi) + (1-\varphi)\ln(1-\varphi) - \theta\varphi^2)$$

where $\theta = T/T_{critical}$ and φ is the phase field.

In the literature, different numerical techniques such as radial basis functions differential quadrature [17], finite element [18] and reduced differential transform [19] methods have been employed for the solution of Cahn-Hillard equation. Unfortunately, numerical methods give approximate results. Analytical methods can give precise predictions to phase separation processes. Thus, Cahn-Hillard phase field model is evaluated by an analytical approach using the $(1/G')$-expansion method in this study. The obtained analytical solutions are firstly appeared in the literature.

2. Governing Equation

Authors considered the general form of the Cahn-Hillard [20];

$$\varphi_t + \varphi_{xxxx} = (A(\varphi))_{xx} + l\varphi_x . l > 0 \tag{2}$$

In this equation $A(\varphi(x,t))$ denotes an inherent chemical potential arising from driven forces (such as thermodynamic) that has the form of $A(\varphi(x,t)) = \varphi^3(x,t) - \varphi(x,t)$ and $\varphi(x,t)$ states phase field of a binary system that the components are having separated and $l\varphi_x$ indicates the diffusion induced kinetics of the mixture(such as a binary alloy).

3. $(1/G')$-Expansion Method

Many authors used The $(1/G')$-expansion method as a tool to get the exact solutions of various differential equations [21–23]. These studies represent that considered method is a powerful and effective while obtaining the analytical solutions of partial differential equations (PDEs). Suppose that nonlinear PDE for $\varphi(x,t)$ is given in the form

$$H\left(\varphi, \frac{\partial\varphi}{\partial t}, \frac{\partial\varphi}{\partial x}, \frac{\partial^2\varphi}{\partial t^2}, \frac{\partial^2\varphi}{\partial x^2}, \ldots\right) = 0 \tag{3}$$

that the unknown function $\varphi(x,t)$ is the function of two independent the variables x, t and also H is the polynomial of the function $\varphi(x,t)$ and its higher order partial derivatives.

Regarding the wave variable as

$$\varphi(x,t) = \varphi(\xi), \xi = kx + ct \tag{4}$$

where k and c can be described as free constants. By using Equation (4) and Equation (3) changes into an nonlinear ordinary differential equation (ODE) with respect to $\varphi = \varphi(\xi)$

$$F\left(\varphi, \varphi', \varphi'', \varphi''', \ldots\right) = 0 \tag{5}$$

where prime indicates Newtonian concept derivative due to ξ. According to considered method the traveling wave solutions of Equation (5) can be expressed as a polynomial of $(1/G')$ as follows

$$\varphi(\xi) = \sum_{i=0}^{n} a_i \left(\frac{1}{G'}\right)^i, \quad a_n \neq 0 \tag{6}$$

where $G = G(\xi)$ satisfies the following differential equation

$$G'' + \lambda G' + \mu = 0 \tag{7}$$

and $a_i (i = 0, \ldots, n), \lambda, \mu$ are random constants to be examined later. To represent the solution of Equation (7) with $G = G(\xi)$, the Equation (6) will include the following equation

$$\frac{1}{G'(\xi)} = \frac{1}{-\frac{\mu}{\lambda} + A\tanh(\lambda\xi) - A\sinh(\lambda\xi)} \tag{8}$$

where A is integral constant.

Step 1. By using the homogeneous balance principle between the highest nonlinear terms and the highest order derivatives of $\varphi(\xi)$ in Equation (5), the positive integer n in Equation (6) can be determined.

Step 2. Subrogating (6) with Equation (7) into Equation (5) and collecting together all the same powered terms of $(1/G')$ together, the left hand side of Equation (5) is turns into a polynomial with respect to $(1/G')$. After equating each coefficient of this polynomial to zero, we handle an algebraic equation system with respect to $a_i (i = 0, \ldots, n), \lambda, \mu, c, k$.

Step 3. In this step symbolic computer software is used to solve the algebraic equations system with respect to arbitrary constants $a_i (i = 0, \ldots, n), \lambda, \mu, c, k$, then subrogating the results with the solutions of Equation (7) into Equation (6) led to traveling wave solutions of Equation (5).

4. The Analytical Solution of Cahn-Hillard Equation

The transformation

$$\varphi(x,t) = \varphi(\xi), \xi = kx + ct \tag{9}$$

converts Equation (2) into nonlinear differential equation as

$$(c-l)\varphi + \varphi''' - \left(\varphi^3 - \varphi\right)' = 0 \tag{10}$$

Now, considering the homogeneous balance principle between φ''' and $\varphi^2\varphi'$ appearing in Equation (10), we get $n = 1$. Consequently, we can write the equation:

$$\varphi(\xi) = a_1 \left(\frac{1}{G'(\xi)}\right) + a_0, \quad a_1 \neq 0 \tag{11}$$

and therefore

$$\varphi'(\xi) = a_1\mu \left(\frac{1}{G'(\xi)}\right)^2 + a_1\lambda \left(\frac{1}{G'(\xi)}\right) \tag{12}$$

$$\varphi'''(\xi) = 6a_1\mu^3 \left(\frac{1}{G'(\xi)}\right)^4 + 12a_1\mu^2\lambda \left(\frac{1}{G'(\xi)}\right)^3 + 7a_1\lambda^2\mu \left(\frac{1}{G'(\xi)}\right)^2 + a_1\lambda^3 \left(\frac{1}{G'(\xi)}\right) \tag{13}$$

By substituting Equations (11)-(13) into Equation (10) and bringing all terms with the same power of $(1/G')$ together, the left-hand side of Equation (10) is changes into another polynomial in $(1/G')$.

Equating each coefficient of this polynomial to zero, yields a set of simultaneous algebraic equations for a_0, a_1, k, c, λ and μ follows:

$$\begin{aligned}
\left(\frac{1}{G'(\xi)}\right)^0 &: \quad ca_0 - lka_0 = 0 \\
\left(\frac{1}{G'(\xi)}\right)^1 &: \quad ca_1 - lka_1 - 3k^2a_1a_0^2\lambda + k^2a_1\lambda + k^4a_1\lambda^3 = 0 \\
\left(\frac{1}{G'(\xi)}\right)^2 &: \quad -3k^2a_1a_0^2\mu + 7k^4a_1\lambda^2\mu + k^2a_1\mu - 6k^2a_1^2a_0\lambda = 0 \\
\left(\frac{1}{G'(\xi)}\right)^3 &: \quad -3k^2a_1^3\lambda + 12k^4a_1\mu^2\lambda - 6k^2a_1^2a_0\mu = 0 \\
\left(\frac{1}{G'(\xi)}\right)^4 &: \quad 6k^4a_1\mu^3 - 3k^2a_1^3\mu = 0
\end{aligned}$$

Solving the algebraic equations above, yields

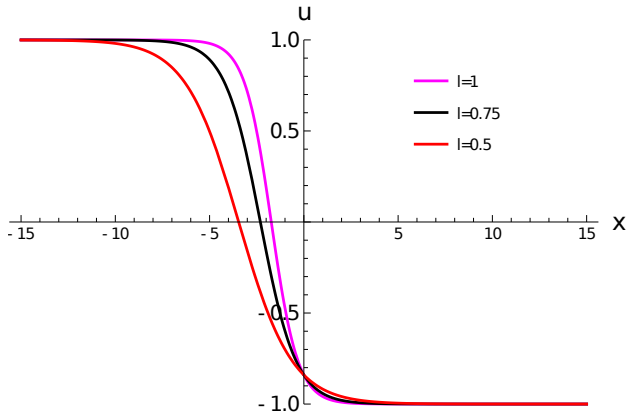
$$c = \pm\frac{l\sqrt{2}}{\lambda}, \quad k = \pm\frac{\sqrt{2}}{\lambda}, \quad a_0 = \pm 1, \quad a_1 = \pm\frac{2\mu}{\lambda} \tag{14}$$

and λ, μ are arbitrary constants. By using (14), expression (11) and (8), we have of travelling wave solutions of Equation (2) as follows:

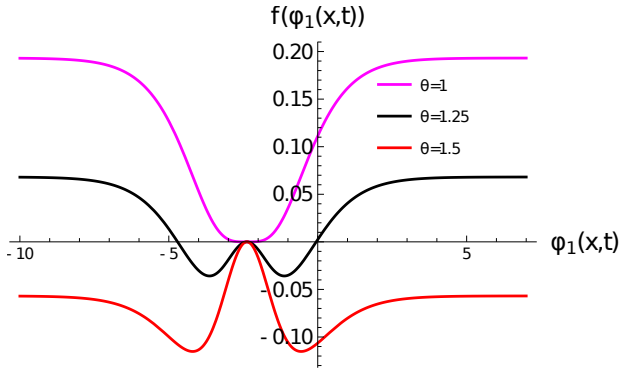
$$\varphi_{1,2}(x,t) = \pm 1 \pm \frac{2\mu}{-\mu + A\lambda\cosh\left(\sqrt{2}lt + \sqrt{2}x\right) \mp A\lambda\sinh\left(\sqrt{2}lt + \sqrt{2}x\right)} \tag{15}$$

5. Graphical Representation of $\varphi_1(x,t)$ for Some Thermodynamic Conditions

Interfacial parameter ϵ thickening with the decrease in the l parameter can be seen in Figure 1(a). It can be said that in a binary system interfacial region where the metastable phase exist narrows with the increasing l values. As it is expected from the model that the double-well structure for the θ values bigger than one can be seen in the Figure 1(b). The peak between the troughs of the wells corresponds to the metastable phase in the interfacial region. This issue can be more clearly in Figure 2(a-c) which show the energy density distribution for the corresponding θ values of $1, 1.25$, and 1.5.

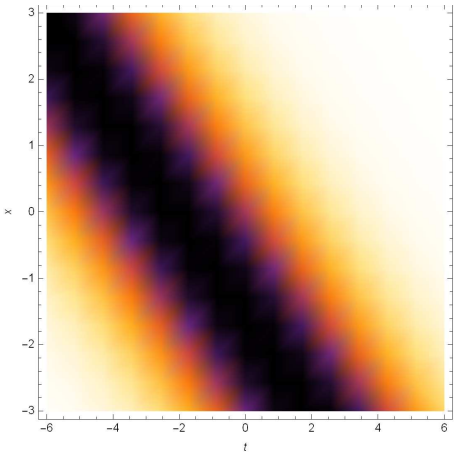


(a) $t = 0.1$

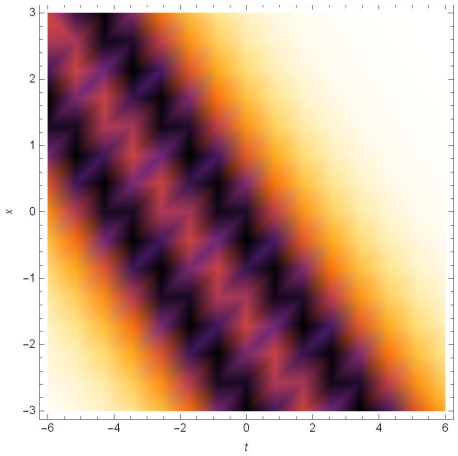


(b) $l = 0.75, x = 0.1, t = 1$

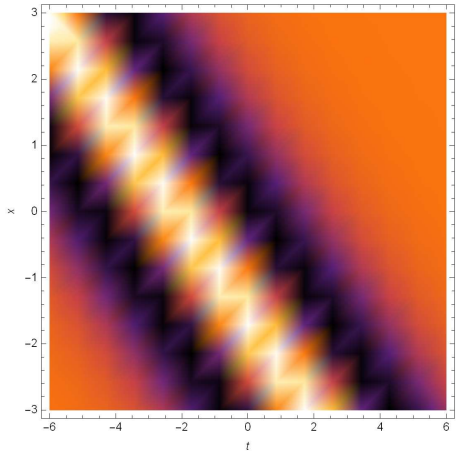
Fig. 1. Phase field (a), free energy (b) for the solution $\varphi_1(x,t)$ for $\mu = -0.1, \lambda = 0.1, A = 0.1$.



(a) $l = 0.75, \theta = 1$



(b) $l = 0.75, \theta = 1.25$



(c) $l = 0.75, \theta = 1.5$

Fig. 2. Spatiotemporal energy distribution (a-c) for the solution $\varphi_1(x,t)$ for $\mu = -0.1, \lambda = 0.1, A = 0.1$.

6. Conclusion

The exact solutions of Cahn-Hillard model have been achieved by the $(1/G')$-expansion method. An energy equation based on Flory-Huggins model was employed for evaluation of the solutions in certain thermodynamic conditions. As it is expected from the model double-well structure of the energy density distribution which corresponds to spinodal decomposition and occurrence of a metastable phase was seen. The results obtained in this study were shown to be accurate in predicting spinodal decomposition phenomenon. Also, some 2D graphical representations and contour plots of the obtained solutions are given for different values of l and θ. These results may be used by material engineers for tailoring the materials properties.

Author Contributions

All the authors contributed equally to this work. They all read and approved the last version of the manuscript.

Conflicts of Interest

The authors declare no conflict of interest.

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