Article

NONCLASSICAL SYMMETRY SOLUTIONS FOR 4TH ORDER PHASE FIELD REACTION-DIFFUSION

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Abstract: Using a nonclassical symmetry of nonlinear reaction-diffusion equations, some exact multi-dimensional time-dependent solutions are constructed for a fourth-order Allen-Cahn-Hilliard equation. This models a phase field that gives a phenomenological description of a two-phase system near the critical temperature. Solutions are given for the changing phase of a cylindrical or spherical inclusion, allowing for a ’mushy zone’ with mixed state that is controlled by imposing a pure state at the boundary. The diffusion coefficients for transport of one phase through the mixture, depend on the phase field value, since the physical structure of the mixture depends on the relative proportions of the two phases. A source term promotes stability of both of the pure phases but this tendency may be controlled or even reversed through the boundary conditions.

Keywords: Fourth-order diffusion; Allen-Cahn equation; Cahn-Hilliard equation; phase field, nonlinear reaction-diffusion.

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1. Introduction

Material transport problems with phase change are conveniently modelled by Stefan free boundary conditions, in which there is assumed to be a moving sharp interface between phases. In practice, the interface of solidification may consist of a ‘mushy’ zone, within which there is dendritic infiltration of the liquid by the solid. Similarly, crystal dislocations may migrate between one solid crystal phase and another through a region of crystal overlap that may be extensive at the micro-scale (e.g. [1]). Extended transition zones with two-phase mixtures may occur in environments wherein the temperature varies little from its critical value. For multi-phase dynamical modelling, the next level of realism beyond

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sharp interfaces is phase-field theory, in which a continuously varying scalar field $\theta(\mathbf{x},t)$ interpolates Phase 1 ($\theta = 1$) and Phase 0 ($\theta = 0$). θ is a monotonic function of the concentration of Phase 1. It may be regarded as a surrogate for the relative concentration of one phase. Following the seminal works by Allen and Cahn [2], and by Cahn and Hilliard [3], phase-field theories have been studied for several decades [4–7].

The core of usual simplified versions of Allen-Cahn (or of Ginzburg-Landau [8]), is an equation for direct relaxation to the minima of a double-well potential. The resulting partial differential equation (PDE) is a standard reaction-diffusion equation of Fitzhugh-Nagumo type,

$$\theta_t = \beta \nabla^2 \theta + s\theta(1-\theta)\,(\theta - 0.5)\,, \tag{1}$$

where $\beta > 0$ and s are constants. Here, the two stable steady states are the pure phases $\theta = 0$ and $\theta = 1$. Without loss of generality, $s > 0$; otherwise we could interchange the labels of the two phases. The cubic source term drives the dynamics towards bi-stable fixed points, with the zones of attraction separated by the unstable fixed-point at $\theta = 0.5$. The diffusion term allows for forward transport of existing Phase 1 material through the mixture, opposite to the direction of its own concentration gradient. Equivalently, Phase 0 diffuses in the opposite direction, counter to the direction of its own complementary concentration gradient. Note also that the cubic source term has also appeared in the context of population genetics, as a correct modification to Fisher's equation for gene frequencies when the genes are not Mendelian but are neither fully dominant nor fully recessive [9–11]

The usual simplified Cahn-Hilliard equation is

$$\theta_t = a\nabla^4\theta + b\nabla^2\theta. \tag{2}$$

The operator ∇^2 is the Laplacian and ∇^4 is the square of the Laplacian. The negative Laplacian term (with b<0) is destabilising, and generates time-reversed diffusion. It has positive spectrum, with amplification of perturbations at high spatial frequency. However when the spatial frequency is high enough, the instability is restrained by an opposing negative squared Laplacian term (with a<0) which has negative spectrum, and at high spatial frequencies, the overall spectral values are negative rather than positive.

Although these diffusion equations do not minimise any action functional, they do result ultimately from an energy functional. In the Cahn-Hilliard approach, the phase flux is the negative gradient of a chemical potential multiplied by a conductivity function (e.g. [3,4,6,12,13]). The chemical potential Φ is the variational derivative $\Phi = \delta\mathcal{E}/\delta\theta$, where $\mathcal{E}$ is the energy functional. Further, it is reasonable to include within $\mathcal{E}$, a component of strain energy $B(\theta)|\nabla\theta|^2$ that depends locally on the phase field value as well as on its squared gradient. Karali and Katsoulakis [13] showed that in some cases, a combined Allen-Cahn-Hilliard equation could indeed be derived from an energy principle, allowing for both a gradient flow and a reaction term that allows for relaxation towards equilibrium:

$$\theta_t = \nabla \cdot \left[-M(\theta)\nabla\nabla^2\theta + D(\theta)\nabla\theta \right] - W'(\theta). \tag{3}$$

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Comparatively few exact solutions are known for time-dependent multi-dimensional fourth-order nonlinear reaction-diffusion equations. Galaktionov and Svirshchevskii (Example 6.72 of [14]) constructed some solutions for the thin-film equation with absorption term $-W'(\theta) = -\sqrt{(}\theta)$, allowing for θ simply to be quadratic in Cartesian coordinates x^i. These solutions, along with a number of others, were derived by Cherniha and Myroniuk [15] in a comprehensive Lie symmetry classification. In the current article, some more realistic explicit solutions, with meaningful boundary conditions, will be constructed after a reduction by a strictly nonclassical symmetry. The solutions have nontrivial spatial structure but they approach the pure phase $\theta = 0$, exponentially in time.

In Section 2, we show that a nonclassical symmetry allows one to separate variables to linear equations in each of space and time, when the nonlinear reaction and diffusivity obey a single relationship. This allows us, in Section 3, to construct solutions that approach the phase $\theta = 0$ asymptotically in time when the Allen-Cahn source term is exactly the cubic function that was given in ([2]).

In Section 4, we show how these fourth-order reaction-diffusion equations relate to an energy principle for a flux potential variable that is the analogue of the matric flux potential that is well-known from nonlinear porous media studies [16,17].

In Section 5, we conclude with a discussion of the solutions, and some open problems.

2. Nonclassical symmetry reduction

2.1. Role of a fourth-order Kirchhoff-Helmholtz equation

Classical point symmetries were originally conceived by Lie [18,19] as the analytical group of invariance transformations of a differential equation, from which one can achieve a reduction of order, or more generally, a reduction in the number of variables of a system. Lie already realised [18] that point symmetries could be extended to contact symmetries. Contact transformations arise naturally in Hamiltonian dynamics wherein phase space includes generalised position coordinate variables and conjugate momentum variables, the latter being expressible in terms of first-order velocity variables (e.g. [20]). They were considered by Noether [21] as possible contact symmetries for the purpose of finding conservation laws and first integrals of dynamical systems. For some special PDEs, higher-order extended symmetries, or "Lie-Bäcklund" symmetries were found [22–25]. Later, the theory of potential symmetries was developed (Chap. 7 of [26]), to open new possibilities to reduce partial differential equations that had a conservation law. In the aforementioned developments, the focus of attention was on the group of transformations under which any solution of the target equation transforms to another solution. This concept allowed one to view the symmetry as a geometric transformation on a hypersurface defined by algebraic constraints within a jet space, co-ordinatised by the system variables and their derivatives up to some order at least as high as the order of the target PDE. However, for the purposes of reducing the number of variables and producing special symmetric solutions, the

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requirement of leaving the whole solution manifold invariant, could be weakened, so that only a subset of solutions were invariant. For example, the sub-manifold could be defined by imposing a compatible differential constraint. General ideas on partial symmetries and conditional symmetries were espoused by Ovsiannikov [27] and Fushchych [28]. In general, it is difficult to find those differential constraints that are compatible. However, if a symmetric solution can be constructed, then by definition, the target equation must be compatible with the invariant surface condition that is simply an expression of that invariance. This led Bluman and Cole [29] to the definition of a *nonclassical symmetry* as a one-parameter transformation, an analytic function of a single real parameter ϵ, connected to the identity transformation at $\epsilon = 0$, that leaves invariant the system consisting of a target PDE together with the invariant surface condition. The first example to be considered [29] was the linear heat equation supplemented by the invariant surface condition:

$$\begin{aligned} u_t &= u_{xx}, \\ \eta(x,t,u) &= \xi_1(x,t,u)u_t + \xi_2(x,t,u)u_x. \end{aligned}$$

Subscripts will denote partial derivatives with respect to the subscripted variables. A full set of determining equations was constructed for the coefficients (ξ_1, ξ_2, η) of the infinitesimal symmetry generator

$$\Gamma = \xi_0\frac{\partial}{\partial t} + \xi_1\frac{\partial}{\partial x} + \eta\frac{\partial}{\partial u}\ .$$

Unlike the determining relations of the classical symmetries that are linear PDEs, the nonclassical determining relations for (ξ_1, ξ_2, η) are nonlinear. The nonclassical determining relations for the linear heat equation were not solved for three decades [30]. The very first class of nonlinear PDEs that was fully classified by solving the nonclassical determining relations, was the class of semi-linear $(1 + 1)$-dimensional reaction diffusion equations with linear diffusion term and general nonlinear reaction term [31,32]. This demonstrated possibility, along with the Clarkson-Kruskal direct method of variable reduction [33], opened up the nonclassical method for practical applications. A more extensive account is given in the recent book by Cherniha and Davydovych [34]. Higher-order conditional symmetries appeared in the theory of generalised conditional symmetries (GCS) [35]. Solutions that are invariant under GCS may be obtained from compatibility with a higher-order differential constraint [36].

Pertinent to the current study, a general nonclassical symmetry classification of fully nonlinear reaction-diffusion equations in (2+1) -dimensions was completed in [37]. The class of target PDEs was

$$\begin{aligned} \theta_t(\mathbf{x},t) &= \nabla\cdot(D(\theta)\nabla\theta) + R(\theta) \\ &= -\nabla\cdot\mathbf{J} + R\,; \qquad J = -D(\theta)\nabla\theta. \end{aligned} \tag{4}$$

It is convenient to change the dependent variable to the Kirchhoff (ref 1896) variable

$$u = \int_{\theta_0}^{\theta} D(\bar\theta)d\bar\theta, \tag{5}$$

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so that the class of PDE (4) is expressed as

$$\frac{1}{D(u)}u_t = \nabla^2 u + R(u). \tag{6}$$

Not only does this reduce the number of terms in the PDE but it also simplifies the flux to $J = -\nabla u$. Since $\theta = 0$ is a stable stationary state, θ_0 is henceforth chosen to be 0.
Without loss of generality, nonclassical symmetries have $\xi_0 = 1$ or $\xi_0 = 0$. Hence, in [37], the system to be analysed was (6), combined with

$$u_t + \xi_1(t, \mathbf{x}, u)u_{x_1} + \xi_2(t, \mathbf{x}, u)u_{x_2} = \eta(t, \mathbf{x}, u). \tag{7}$$

Among the compatible nonclassical symmetry generators, there was the unexpected simple combination

$$\xi_0 = 1\,; \quad \xi_1 = \xi_2 = 0\,; \quad \eta = Au\ (A \in \mathbb{R}), \tag{8}$$

$$u'(\theta) = D(\theta) = \frac{Au}{R(\theta) - \kappa u}. \tag{9}$$

Note that if $D(\theta)$ is specified, then (9) gives $R(\theta)$ explicitly. However, if $R(\theta)$ is specified, then (9) must be treated as a differential equation, to solve for $u(\theta)$, after which $D(\theta) = u'(\theta)$. The symmetry reduction gives

$$u = e^{At}\Phi(\mathbf{x}), \quad \text{where} \quad \nabla^2\Phi + \kappa\Phi = 0. \tag{10}$$

Provided the nonlinear diffusivity function and the nonlinear reaction function are related as in (9), the nonlinear reaction-diffusion equation is amenable to separation of variables to two linear equations, allowing an arbitrary solution of the Helmholtz equation (10). This led to the only known exact time-dependent solution of Arrhenius combustion with diffusion [38], by a symmetry reduction that applies in $n \geq 1$ spatial dimensions.

At this point, it is important to note that provided (9) holds, the same nonclassical symmetry applies when the Laplacian operator in the PDE (6) is replaced by any linear operator, that is, Lu can be any time-independent linear combination of u and its spatial derivatives,

$$\frac{1}{D(u)}u_t = Lu + R(u). \tag{11}$$

In a recent article (ref PB et al 2017), this was applied directly to a soil-water-crop system, by choosing L to be the Kirchhoff operator $Lu = \nabla^2 u - u_{x_3}$.
Now we choose $Lu = a\nabla^4 u + b\nabla^2 u$ with $a, b \in \mathbb{R}$, so that u and θ satisfy

$$\frac{1}{D(u)}u_t = a\nabla^2\nabla\cdot\nabla u + b\nabla\cdot\nabla u + R(u), \tag{12}$$

$$\theta_t = a\nabla^2(\nabla\cdot[D(\theta)\nabla\theta]) + b\nabla\cdot[D(\theta)\nabla\theta] + R(\theta). \tag{13}$$

A direct substitution of

$$u = e^{At}\Phi(\mathbf{x})\,; \quad a\nabla^2\nabla\cdot\nabla\Phi + b\nabla\cdot\nabla\Phi + \kappa\Phi = 0, \tag{14}$$

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into (12) leads to the single requirement (9). Eq. (14) could be regarded as a *fourth-order Helmholtz equation*.

The constrained system consisting of (6) with $R(\theta)$ and $D(\theta)$ satisfying (9), supplemented by the simple invariant surface condition $u_t = Au$, has an infinite dimensional point symmetry group

$$\bar{t} = t + \epsilon\,; \quad \bar{u} = e^{A\epsilon}[u + e^{At}\Phi(\mathbf{x}, t)], \tag{15}$$

where $\Phi(\mathbf{x}, t)$ is an arbitrary solution of the linear equation (14). However this type of symmetry does not appear in the classical symmetry group of the original unconstrained PDE (6) that is not integrable. In the sense that we can construct an infinite dimensional sub-manifold of the solution manifold that is also a linear space, the unconstrained PDE is semi-integrable. The linear space of constructed solutions originates from a linear PDE in two independent variables, compared to the original three independent variables.

2.2. *Amenable diffusivity and reaction functions*

The amenable diffusivity function for the second-order multi-dimensional nonlinear reaction-diffusion equation with cubic reaction term, was already investigated in [39], in the context of population genetics. However, in that application the steady state $\theta = 0$ (meaning no advantageous genes present) is unstable, whereas in the current application, $\theta = 0$ is a stable pure phase.
First consider the canonical cubic reaction term that appears in (1),

$$R = s\theta(\theta - 0.5)(1 - \theta). \tag{16}$$

We assume that the phase that is approached exponentially is $\theta = 0$, requiring $A = -|A| < 0$. In phase pattern formation, there is some interest in the case that the fourth-order diffusion is dissipative ($aD < 0$) whereas the second-order diffusion is backwards in time ($bD < 0$), giving a negative contribution to entropy production [40]. We will focus on this case below, and assume that these sign properties are determined by the parameters a and b taking negative values after assigning $D > 0$.

At this point it is convenient to introduce dimensionless variables. We assume $D(\theta)$ has the usual dimensions of diffusivity, $[D] = L^2T^{-1}$. From (13), b is dimensionless, $[\sqrt{b/a}] = L^{-1}$ and $[s] = T^{-1}$. This inverse length is around the critical wave number, above which the fourth-order diffusion overcomes the second-order backward diffusion, resulting in attenuation and stability. A natural choice of length and time scales is $\ell_s = \sqrt{a/b}$ and $t_s = 1/s$. Define dimensionless coordinates $(x^*, y^*, z^*) = (x, y, z)/\ell_s$ and $t^* = t/t_s$, with dimensionless Laplacian $\Delta^* = \ell_s^2\Delta$. In that system of units, s is scaled to 1, whereas the time scale for the particular solution to decrease exponentially is written as $1/|A^*|$ with $A^* = At_s$. Defining

$$D^* = \frac{D\,b^2}{|a|s}\,, \quad u^* = \frac{u\,b^2}{|a|s}\,, \quad \Phi^* = \frac{\Phi\,b^2}{|a|s}\,, \quad R* = \frac{R}{s}\,, \tag{17}$$

equation (13) reduces to

$$\theta_{t*} = -\nabla^{*2}(\nabla^* \cdot [D*(\theta)\nabla^*\theta]) - \nabla \cdot [D^*(\theta)\nabla^*\theta] + R^*(\theta). \tag{18}$$

With $A^* = A/s$ and $\kappa^* = \kappa|a|/b^2$, equation (9) can also be written in using dimensionless variables, without a, b, or s occurring explicitly, as can other equations of interest above. From here on, non-dimensional coordinates will be assumed, and asterisks will be dropped.

Before solving Eq. (9) for $D(\theta)$, the values $D(0)$, $D(0.5)$ and $D(1)$ can be deduced immediately. First assume that $D(0) \neq 0$, so that $D(0) > 0$ as above. Since at $\theta = 1$, $R = 0$, (9) immediately implies $D(1) = |A|/\kappa$. By the same argument, $D(0.5) = |A|/\kappa$. From here on, we need to assume $\kappa > 0$. Since $R(0) = 0$ and $u(\theta) = 0 + D(0)\theta + O(\theta^2)$, (9) implies

$$D(0) = \frac{AD(0)\theta}{R'(0)\theta - \kappa D(0)\theta} + O(\theta)$$
$$\implies D(0) = \frac{-A - \frac{1}{2}}{\kappa}.$$

In summary,

$$D(0.5) = D(1) = \frac{|A|}{\kappa}, \quad D(0) = \frac{-A - \frac{1}{2}}{\kappa} = D(0.5) - \frac{1}{2\kappa}. \tag{19}$$

From here on, we require $|A| > 1/2$. Naturally, the rate of exponential decay (with time scale $1/|A|$), will be related to the strength of the sink term (with time scale 1/s). (19) shows that the diffusivity must be increasing from $\theta = 0$ to some value $\theta_m \in (0.5, 1)$ where D reaches a maximum. It is physically reasonable to expect that the mobility of one phase through a mixture will change, resulting in a change of diffusivity, as the composition of the mixture changes. For example, take $|A| = 5/2$. This results in $D(0)$ being $4|A|/(5\kappa)$, which is 20% lower than $D(0.5)$.

The required solution of the differential equation (9), is the fixed point of the map

$$D_{j+1}(\theta) = \frac{A\int_0^\theta D_j(\bar{\theta})d\bar{\theta}}{R(\theta) - \kappa\int_0^\theta D_j(\bar{\theta})d\bar{\theta}} \,. \tag{20}$$

It is convenient to choose $D_0(\theta) = D(0) = -(A + \frac{1}{2})/\kappa$ (constant). Then

$$D_1(\theta) = \frac{-A\theta(A + \frac{1}{2})/\kappa}{R(\theta) + (A + \frac{1}{2})\theta} = \frac{-A(A + \frac{1}{2})/\kappa}{(\theta - \frac{1}{2})(1 - \theta) + A + \frac{1}{2}}\,, \tag{21}$$

$$= \frac{A(A + \frac{1}{2})}{\kappa\left(\theta - \frac{3}{4} + \sqrt{A + \frac{9}{16}}\right)\left(\theta - \frac{3}{4} - \sqrt{A + \frac{9}{16}}\right)}\,. \tag{22}$$

This already has the correct values at the three locations given in (19), however we now require $|A| > 9/16$ to avoid singularities in the region $\theta \in (0.5, 1)$. From $D_1(\theta)$ we can calculate the corresponding

$$u_1(\theta) = \int_0^\theta D_1(\bar{\theta})d\bar{\theta} = \frac{-A\left(-A - \frac{1}{2}\right)}{\kappa\sqrt{-A - \frac{9}{16}}}\left[\arctan\left(\frac{\frac{3}{4}}{\sqrt{-A - \frac{9}{16}}}\right) + \arctan\left(\frac{\theta - \frac{3}{4}}{\sqrt{-A - \frac{9}{16}}}\right)\right], \tag{23}$$

so that the next iterate $D_2(\theta)$ can also be calculated explicitly from (20).

As demonstrated in [39], these iterates may converge rapidly to the exact solution. In this example, although the analytic expressions for $D_1(\theta)$ and $D_2(\theta)$ are quite different, numerically they may be practically indistinguishable, as illustrated in Figure 1 for $A = -5/2$, $\kappa = 1$.

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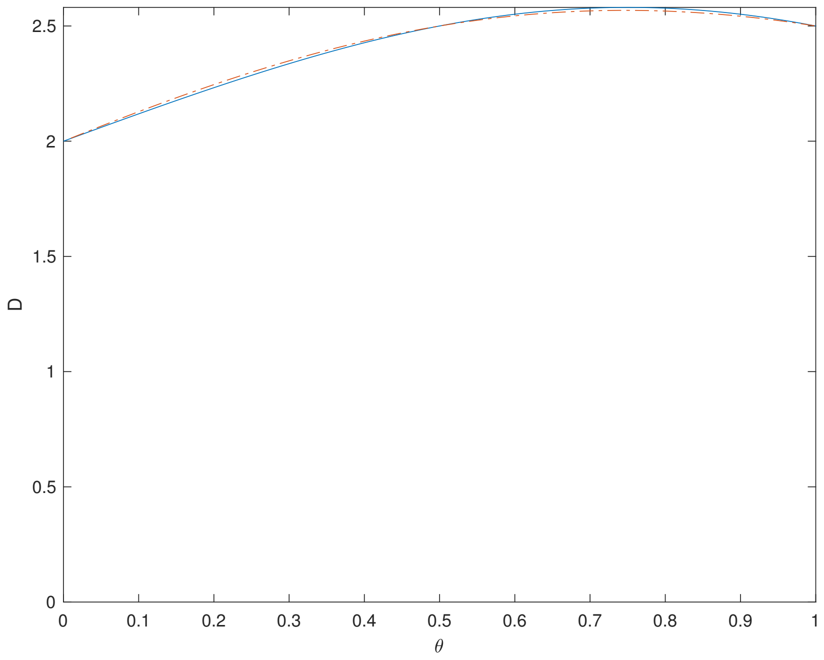

Figure 1. Iterated approximations to diffusivity function: D_1 (solid), D_2 (dash dot) with $\kappa = 1$, $A = -5/2$.

Given the cubic reaction term (16), $D_1(\theta)$ is already a good approximation for the diffusivity function that leads to our exact solution for the phase field. Conversely, we may choose the diffusivity function to be $D_1(\theta)$ and then exactly construct a reaction function $R_1(\theta)$ that has the same generic properties as the canonical cubic function, but which exactly leads to the analytic solution for the phase field. From (9),

$$R_1(\theta) = \frac{-A(\theta - 1/2)(1-\theta)}{\sqrt{-A - \frac{9}{16}}} \left[\arctan\left(\frac{\frac{3}{4}}{\sqrt{-A - \frac{9}{16}}} \right) + \arctan\left(\frac{\theta - \frac{3}{4}}{\sqrt{-A - \frac{9}{16}}} \right) \right]. \qquad (24)$$

Figure 2 plots the cubic $R(\theta)$ along with $R_1(\theta)$ for $A = -5/2$.

3. Interior solutions for slabs, cylinders and spheres.

In order to gain some understanding of the nature of the solutions, we consider interior solutions for slabs, cylinders and spheres in dimensions $n = 1, 2$ and 3 respectively. The four independent solutions will be trigonometric and hyperbolic functions (n=1), Bessel and modified Bessel (n=2) and spherical Bessel and modified spherical Bessel functions (n=3). The solutions decrease uniformly in t towards $\theta = 0$ even if the initial condition has $\theta > 0.5$ in some significant sub-domain, the region wherein the source term tends to stabilise the phase $\theta = 1$. Therefore this global approach to Phase 0 should be controlled by the boundary conditions which may include, for example, ideal contact with the exterior pure phase at $\theta = 0$, or a Robin boundary condition for extraction of Phase 1.

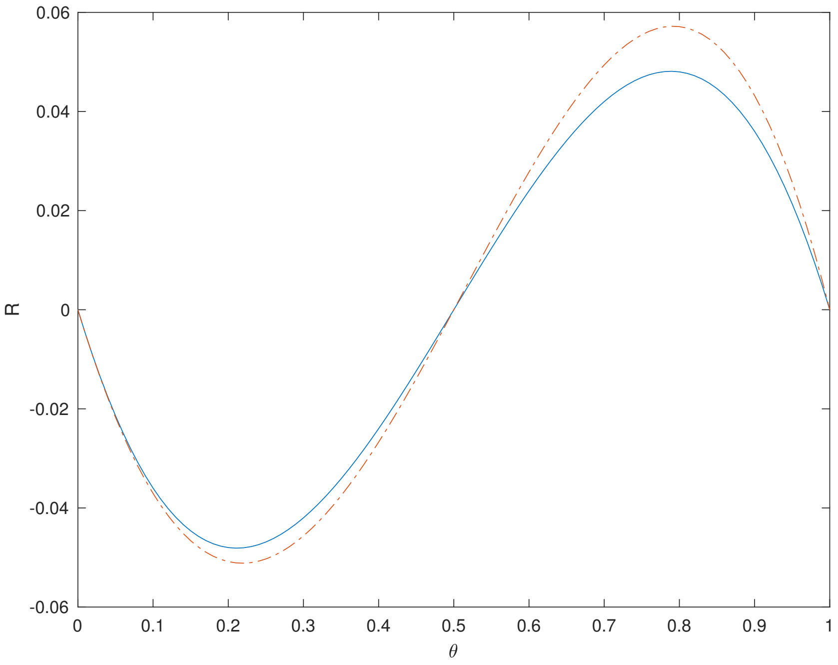

Figure 2. Cubic reaction term R (solid); Exact matching partner R_1 (dash dot) for D_1 with $A = -5/2$.

125 *The Case:* $a, b < 0$.

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In general coordinate systems with our adopted dimensionless variables, the simplified form of Equation (14) factorizes as

$$(-\Delta^2 - \Delta + \kappa)\Phi = 0 \quad \Rightarrow \quad (\Delta - \gamma^2)(\Delta + \omega^2)\Phi = 0, \tag{25}$$

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$$\omega = \left(\frac{1 + \sqrt{1 + 4\kappa}}{2}\right)^{1/2}, \qquad \gamma = \left(\frac{-1 + \sqrt{1 + 4\kappa}}{2}\right)^{1/2}. \tag{26}$$

For radial flow within the ball $\sqrt{\sum_{i=1}^{n} x_i^2} = r \in (0, r_0)$, the Laplacian operator within (25) is $r^{1-n}\frac{d}{dr}[r^{n-1}\frac{d}{dr}]$. The two operator factors commute so (25) reduces simply to a system of two alternative second-order Helmholtz equations.The general solution $\Phi(r)$ of (25) in one, two and three dimensions, with four free parameters $c_i \in \mathbb{R}$, is

$$\begin{aligned} \Phi &= c_1 \cos(\omega r) + c_2 \sin(\omega r) + c_3 \cosh(\gamma r) + c_4 \sinh(\gamma r) && \text{(n=1)}, \\ \Phi &= c_1\, J_0(\omega r) + c_2\, Y_0(\omega r) + c_3\, I_0(\gamma r) + c_4\, K_0(\gamma r) && \text{(n=2)}, \\ \Phi &= c_1\, j_0(\omega r) + c_2\, y_0(\omega r) + c_3\, i_0(\gamma r) + c_4\, k_0(\gamma r) && \text{(n=3)}. \end{aligned} \tag{27}$$

Here, the spherical Bessel functions are defined simply as $j_0(r) = \sin(r)/r$, $y_0(r) = \cos(r)/r$, $i_0(r) = \sinh(r)/r$ and $k_0(r) = \cosh(r)/r$.

For radial flows, the flux density of Phase 1 is

$$\mathbf{J} = J(r)\, \mathbf{e}_r = \left[-a\frac{\partial^3 u}{\partial r^3} - a(n-1)\frac{1}{r}\frac{\partial^2 u}{\partial r^2} + ([n-1]a\frac{1}{r^2} - b)\frac{\partial u}{\partial r}\right] \mathbf{e}_r \,.$$

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For all values of n we impose zero flux at $r = 0$. For $n = 3$, considering the asymptotic behaviour of $J(r)$ as $r \to 0$ shows that $J(0) = 0$ imposes two conditions on c_2 and c_4

$$\begin{aligned} 0 &= \gamma^3 c_2 - \omega^3 c_4, \\ 0 &= \gamma c_3 + \omega c_4. \end{aligned} \tag{28}$$

These admit no non-trivial solutions, so $c_2 = c_4 = 0$. For $n = 3$ alternatively imposing either $\Phi'(0) = 0$ or $\Phi'''(0) = 0$ also gives two conditions on c_2 and c_4 similar to those above, which also imply $c_2 = c_4 = 0$.

For $n = 2$ imposing $J(0) = 0$ only implies a single condition

$$0 = \frac{2\gamma^2}{\pi} c_2 + \omega^2 c_4. \tag{29}$$

However, $\Phi(0)$ is unbounded and hence unphysical in this context, unless

$$0 = \frac{2}{\pi} c_2 - c_4, \tag{30}$$

which also ensures that $\Phi'(0) = 0$. Again the above two equations only admit the trivial solution $c_2 = c_4 = 0$.

For $n = 1$, $J(0) = 0$ only implies the condition

$$0 = \gamma c_2 - \omega c_4. \tag{31}$$

As $\Phi(0)$ is finite, the $n = 1$ case does admit physical solutions where $J(0) = 0$ and $\Phi'(0) \neq 0$. We can eliminate this extra degree of freedom by imposing $\Phi'(0) = 0$, to match the admissible solutions discussed above for $n = 2$ and $n = 3$. This gives an extra condition on c_2 and c_4

$$0 = \omega c_2 + \gamma c_4, \tag{32}$$

so that again only $c_2 = c_4 = 0$ is possible.

The boundary $r = r_0$ is in contact with pure Phase 0. Imposing $\Phi(r_0) = 0$, implies

$$\begin{aligned} c_3 &= -c_1 \cos(\omega r_0)/\cosh(\gamma r_0) && \text{(n=1)}, \\ c_3 &= -c_1 J_0(\omega r_0)/I_0(\gamma r_0) && \text{(n=2)}, \\ c_3 &= -c_1 j_0(\omega r_0)/i_0(\gamma r_0) && \text{(n=3)}. \end{aligned}$$

We have found in examples that the zero-flux boundary condition at $r = r_0$ will result in an inadmissible solution that is not positive semi-definite. However there is a solution that connects smoothly with an external slab of Phase 0, beginning at the boundary $r = r_0$. Assuming $\Phi'(r_0) = 0$, we deduce

$$\begin{aligned} \omega \tan(\omega r_0) &= -\gamma \tanh(\gamma r_0) && \text{(n=1)}, \\ \omega \frac{J_1(\omega r_0)}{J_0(\omega r_0)} &= -\gamma \frac{I_1(\gamma r_0)}{I_0(\gamma r_0)} && \text{(n=2)}, \\ \omega \cot(\omega r_0) &= \gamma \coth(\gamma r_0) && \text{(n=3)}. \end{aligned} \tag{33}$$

This has a sequence of solutions for r_0. With $\kappa = 1$, the first of these are $r_0 \approx 2.0616, 2.7012$ and 3.2653 for $n = 1, 2$ and 3 respectively, showing significant increase with dimensionality. Higher values

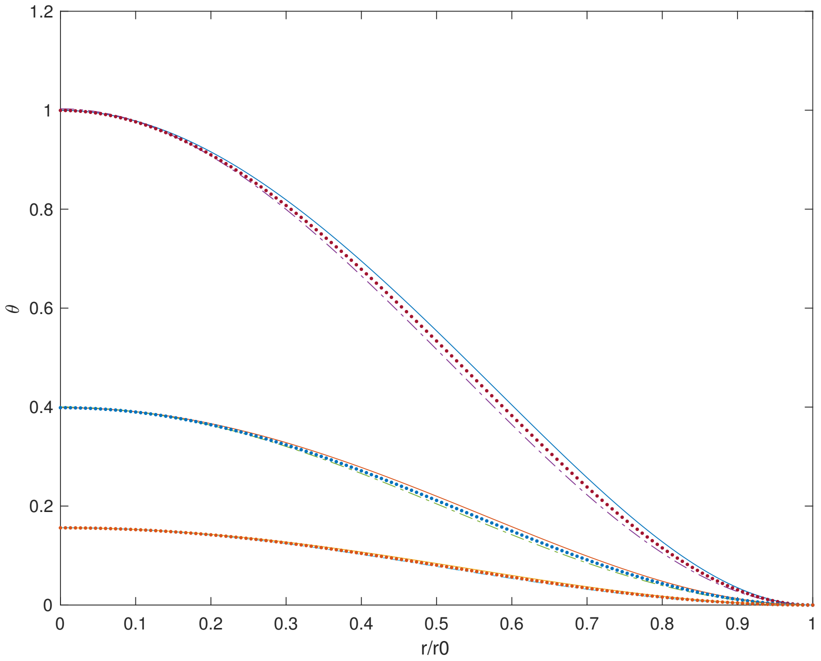

Figure 3. Exact spherical radial (dash-dot), cylindrical radial (dot) and 1D slab (solid) solutions $\theta(r,t)$, at output times $-At = 0,1,2$. Diffusivity and reaction terms are D_1 and R_1 depicted in Figures (1) and (2).

in the sequence of solutions for r_0 are found to produce unphysical solutions exhibiting negative values of u. With diffusivity $D_1(\theta)$ and reaction term $R_1(\theta)$ shown in Figures 1 and 2 respectively, θ is given explicitly in terms of u as

$$\theta = \frac{3}{4} + \sqrt{-A - \frac{9}{16}} \tan\left[\frac{\kappa u\sqrt{-A-\frac{9}{16}}}{A(A+\frac{1}{2})} - \arctan\left(\frac{\frac{3}{4}}{\sqrt{-A-\frac{9}{16}}}\right)\right]. \tag{34}$$

Although solutions for $u(x,t)$ at different times are geometrically similar, this is not true for $\theta(x,t)$ which is related to u by a nonlinear transformation. The solution for $\theta(x,t)$ is depicted in Figure 3 for $A = -5/2$, $\kappa = 1$. The solutions in dimensions $n = 1,2,3$ are close after the three different domain radii r_0 are rescaled to the same value.

Unphysical solutions were found for large values of r_0 above. If one attempts to find the largest possible value of r_0 that produces a physically valid (non-negative) solution for a given κ, it soon becomes clear that for the class of solutions considered above, this corresponds to the first non-zero solution r_0, of the above conditions $\Phi'(r_0) = 0$ shown in (33). This is a consequence of our solutions being a linear combination of one oscillatory, and one monotonically increasing function that take finite values at $r = 0$. As such, Figure 3 shows scaled examples of solutions with the maximum possible value of r_0. Selecting smaller values of r_0 produces solutions with a non-zero negative slope at $r = r_0$. Figure 4 shows variation of the maximum possible r_0 value as κ varies. In all cases $\max r_0 \to 0$ as $\kappa \to \infty$. The

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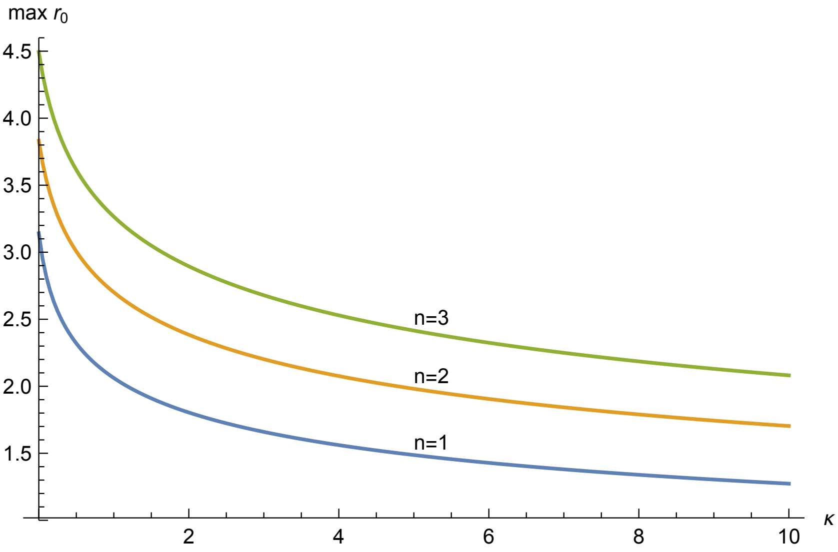

Figure 4. Largest possible values of r_0 for various values of κ.

case $\kappa = 0$ does not produce valid solutions via our methods above, however the largest possible values of r_0 are obtained as $\kappa \to 0$ and equations (33) approach the following simple conditions respectively

$$\begin{aligned} 0 &= \sin(r_0) &\Rightarrow\quad r_0 &= \pi &\text{(n=1)},\\ 0 &= J_1(r_0) &\Rightarrow\quad r_0 &\simeq 3.8317 &\text{(n=2)},\\ r_0 &= \tan(r_0) &\Rightarrow\quad r_0 &\simeq 4.4934 &\text{(n=3)}. \end{aligned} \tag{35}$$

4. Energy Formulation

Let us consider the original Eq. (13),

$$\theta_t = a\nabla^2(\nabla\cdot[D(\theta)\nabla\theta]) + b\nabla\cdot[D(\theta)\nabla\theta] + R(\theta), \quad \theta : \Omega\times(0,T)\to\mathbb{R}. \tag{36}$$

In this section we assume Ω is an open, bounded subset of $\mathbb{R}^n$ with smooth boundary ($\partial\Omega \in C^\infty$). Conforming to Section 3, $a < 0$ so that the fourth-order diffusion term, which dominates at high wave numbers, has negative spectrum, generating a diffusion process that propagates forward in time. With no loss of generality, we set $a = -1$. Eq. (36) is a fourth-order quasi-linear equation in divergence form. Although the fourth order term $L_4(\theta) := -\nabla^2\nabla\cdot(D(\theta)\nabla\theta)$ can be written as $L_4 = -\nabla^2(L_2)$, that is, the cascade of two symmetric second order operators with $L_2(\theta) = \nabla\cdot(D(\theta)\nabla\theta)$, it turns out that L_4 is not symmetric and therefore there is no associated energy functional of which $L_4(\theta)$ is the first variation. We introduce the flux potential variable $u : \Omega\times(0,T)\to\mathbb{R}$ defined as $u(x,t) = \mathcal{D}(\theta(x,t))$ where $\mathcal{D}(\theta) := \int_{\theta_o}^{\theta} D(s)ds$, ($\mathcal{D}(\theta_o) = 0$). We also assume $D(\theta)$ is smooth and strictly positive, implying that $\mathcal{D}$ is 1-1 and globally invertible. By substituting $\theta = \mathcal{D}^{-1}(u)$ into Eq. (36) we obtain

$$\frac{u_t}{\tilde{D}(u)} = -\nabla^4 u + b\nabla^2 u + \tilde{R}(u). \tag{37}$$

Here we have defined $\tilde{D}(u) := D(\mathcal{D}^{-1}(u))$ and $\tilde{R}(u) := R(\mathcal{D}^{-1}(u))$. With some abuse of notation -and to keep the notation consistent with the previous sections- in what follows we drop tildas. We remark

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the approach leading to writing Eq. (37) is essentially the substitution method largely employed in the theory of porous medium equations [41]. In soil physics, the variable u is well known as the matric flux potential [16,17]. It is relevant to the physics of the flow since $-\nabla u$ is the soil-water flux driven by the intrinsic capillary action of the soil matrix, without gravity.

By exploiting the linear structure of the right hand side of (37) the investigation of existence results of the solution becomes more transparent. Let us consider the static problem when $u(x,t) \equiv u(x)$ obtained by setting $u_t \equiv 0$ in Eq. (37). Although in this paper we are mainly concerned with time-dependent problems, the static regime is of interest as the solutions of it represent ground-state configurations for the physical system. Eliminating time-dependence in (37) yields

$$-\nabla^4 u + b\nabla^2 u + R(u) = 0. \tag{38}$$

Eq. (38) is obtained as the linear combination of symmetric operators and it does have a variational structure. Indeed, it coincides with the first variation of the functional

$$I(u) := \int_\Omega \Big(\frac{1}{2}|\nabla^2 u|^2 + \frac{b}{2}|\nabla u|^2 - \mathcal{R}(u)\Big)dx \tag{39}$$

where $\mathcal{R}(u) = \int_{u_o}^{u} R(s)ds$. The derivation of (38) from (39) has been performed formally. Under the regularity assumptions on Ω and if $\mathcal{R}$ verifies suitable growth conditions (here unspecified), the derivation of the Euler-Lagrange equations (38) is exact in $H^2_0(\Omega)$, the subspace of H^2-Sobolev functions $u : \Omega \to \mathbb{R}$ with higher-order energy norm $\max(\|u\|_{L^2(\Omega)}, \|\nabla u\|_{L^2(\Omega,\mathbb{R}^n)}, \|\nabla\nabla u\|_{L^2(\Omega,\mathbb{R}^{n\times n})}) \leq C < +\infty$ (where $L^2(\Omega,\cdot)$ denotes the Lebesgue space of square-integrable functions) with zero boundary conditions for u and $\frac{\partial u}{\partial \nu}$, where ν is the outward normal to $\partial\Omega$. Non-homogenous boundary conditions are incorporated by introducing $H^2_\varphi(\Omega)$, the set contaning all the H^2-functions u such that $u - \varphi \in H^2_0(\Omega)$, with $\varphi \in H^2(\Omega)$ representing the boundary datum. By exploiting the variational structure of the problem, one may look for solutions to (38) as the critical points of (39) and vice-versa. The nature of the critical points of I is determined by the sign of b as well as the shape of $\mathcal{R}$. As an example, when $b \geq 0$ and $-\mathcal{R} = cu^2$ with $c \geq 0$, the Lax-Milgram Lemma ensures that there exists a unique solution of Eq. (38), denoted with $\overline{u}$, and that $\overline{u}$ is the unique minimizer of $I(u)$ in $H^2_\varphi(\Omega)$. Furthermore, when $\varphi \in C^\infty(\overline{\Omega})$, by elliptic bootstrapping we recover that $\overline{u}$ is the classical (indeed in $C^\infty(\overline{\Omega})$) solution to Eq. (38). From the knowledge of the solution $\overline{u}$ to Eq. (38), one is able to recover information on a function $\theta(x,t)$ which solves the original Eq. (36) in the static regime (i.e., $\theta_t \equiv 0$) by simply plugging $\theta = \mathcal{D}^{-1}(u)$ into Eq. (36). In more physically relevant situations $\mathcal{R}$ represents a competing energy contribution usually in the form of a non-negative multi-well function in the variable u. When $-\mathcal{R}$ is a non-convex non-negative polynomial it may still be possible to ensure existence (although not the uniqueness) of the solution $\overline{u}$ to the minimum problem for $I(u)$ possibly in a subset of $H^2_\varphi(\Omega)$ and characterize $\overline{u}$ as a solution to Eq. (38). Instead, when $b < 0$ and $-\mathcal{R} = -cu^2$ with $c > 0$ we have genuine competition in the summands of the energy I and in turn I may fail to be positive-definite. Under these circumstances solutions to Eq. (38) correspond to various critical points of I including saddles or more intricate situations. In those cases, existence theorems should be investigated by methods possibly based on min-max principles.

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An alternative approach (e.g. [12,13]) is to express the phase flux density as being proportional to the negative gradient of a chemical potential energy density that is itself the variational derivative of a total internal energy functional. This comes about because the drift velocity of the mobile particles of Phase 1 quickly reaches a terminal velocity that enables the driving gradient of chemical potential energy to be balanced by a mechanical resistance force that is proportional to velocity and in the opposite direction. The new element that we need here to justify the non-standard Equation (6), is that the variational derivative is taken with respect to the flux potential u, rather than the phase variable θ. Then we choose

$$E = \int_\Omega -\frac{1}{2}a\nabla u \cdot \nabla u + \frac{1}{2}bu^2 \, dV, \tag{40}$$

$$\Phi = \frac{\delta}{\delta u}E = a\nabla^2 u + bu, \tag{41}$$

$$\mathbf{J} = -\nabla\Phi = -a\nabla\nabla^2 u - b\nabla u, \tag{42}$$

$$\frac{d\theta}{dt} + \nabla \cdot \mathbf{J} = R(\theta). \tag{43}$$

In this set-up, $R(\theta)$ must be regarded as an externally driven Phase 1 production term that assists relaxation towards the stable fixed points.

5. Conclusion

A nonclassical symmetry reduction has led to some exact positive solutions for multi-dimensional nonlinear reaction-diffusion equations with both fourth-order diffusion and second-order backward diffusion. In all likelihood, these are the only known exact solutions for equations of the Allen-Cahn-Hilliard type that have meaningful boundary conditions. The presented solutions have zero flux and zero gradient at one central boundary point, plus a prescribed value, representing a pure phase, as well as zero gradient at the other boundary. The initial condition has the phase field taking the value $\theta = 1$ at $r = 0$. Even though Phase 1 is stabilised by the reaction term, the boundary conditions force the solution to have the system uniformly approaching Phase 0. An interior cylindrical or spherical inclusion with a mixed phase could not withstand the inward advance of Phase 0 from the outer boundary.

These idealised solutions do not have structured phase domain patterns that have been seen in numerical solutions of the Cahn-Hilliard equation. However, since the exact solution involves a general solution of the fourth-order linear Helmholtz equation for the flux potential, it is possible that more complex patterns could be incorporated in the future.

We remark the approach based on the Helmholtz substitution adds additional structure to the model in terms of a variational principle as the by-product of symmetry and linearity. Although the thorough investigation of the relation between the non-linear model in the unknown variable θ and the transformed model in u is not the scope of the present contribution, in Section 4 some insight is provided for some special situations. The construction used here, became possible because of a nonclassical symmetry that applies when the nonlinear diffusivity and the nonlinear reaction term together obey a single relationship. Then an additional constraint

$$\theta_t/D(\theta) = A\int_{\theta_0}^{\theta} D(s)ds,$$

added to the governing PDE, results in an integrable system. Reduction of variables then results in the linear fourth-order Helmholtz equation. In that sense, the original multidimensional nonlinear scalar PDE is partially integrable because one additional constraint leads to a linear PDE in one fewer independent variables. It is an open question as to whether nonclassical symmetry classification can unearth other semi-integrable PDEs -possibly defined by different fourth-order non-linear operators- in this way, and more generally, how to select compatible constraints.

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Conflicts of Interest

The authors declare no conflict of interest.

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