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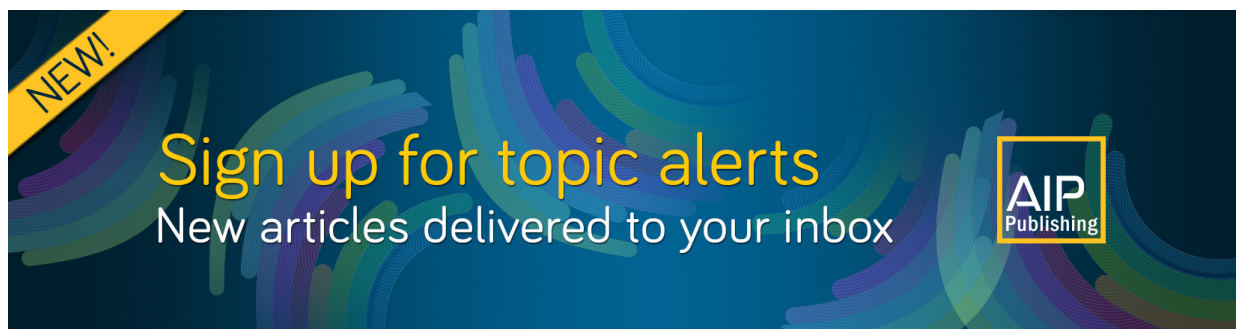
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ABSTRACT

The well-known cubic Allen–Cahn (AC) equation is a simple gradient dynamics (or variational) model for a nonconserved order parameter field. After revising main literature results for the occurrence of different types of moving fronts, we employ path continuation to determine their bifurcation diagram in dependence of the external field strength or chemical potential. We then employ the same methodology to systematically analyze fronts for more involved AC-type models. In particular, we consider a cubic–quintic variational AC model and two different nonvariational generalizations. We determine and compare the bifurcation diagrams of front solutions in the four considered models.

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The problem of front propagation has a very long history with essential contributions coming from different fields. One of the simplest variational model possessing front solutions is a so-called cubic Allen–Cahn (AC) equation for a nonconserved order parameter field. In this paper, we systematically analyze possible phase transitions in the AC equation employing analytical results given in the literature and compare them to results obtained with numerical path continuation techniques. Furthermore, we apply the same methodology to fronts occurring in more involved AC-type models, including a cubic–quintic variational AC model and two different nonvariational generalizations, where the AC equation is emended by a nonequilibrium chemical potential or is coupled to a polarization field.

I. INTRODUCTION

Many spatially extended systems can exist in different spatially homogeneous states that depend on various ambient parameters. In the absence of out-of-equilibrium driving forces, energy arguments hold, and the homogeneous states may be (globally) stable, metastable (nonlinearly unstable), or linearly unstable. In other words, they represent global minima, local minima, and maxima (or saddles), respectively, of an underlying energy functional. In general,

states of higher energy can be replaced through a moving front by states of lower energy. A simple well studied deterministic continuum model for such processes is the Allen–Cahn (AC) equation that reads in a nondimensional form in one spatial dimension [Ref. 1, their Eq. (11) with their Eqs. (3) and (4)] as

$$\frac{\partial \phi}{\partial t} = -\frac{\delta \mathcal{F}}{\delta \phi} \quad \text{with} \quad \mathcal{F} = \int \left[\frac{1}{2} |\partial_x \phi|^2 + f(\phi) - \mu \phi \right] dx. \quad (1)$$

It corresponds to a nonconserved gradient dynamics on an underlying energy functional $\mathcal{F}[\phi]$ that contains a square gradient term and a local energy $f(\phi)$. The equation arises in many different contexts and is, sometimes for specific, often quartic choices of $f(\phi)$, known as the Fisher–Kolmogorov,² Fife–Greenlee,³ Schlögl,⁴ or Zeldovich–Frank–Kamenetsky equation.⁵ It is studied as a model that describes dynamics in multistable systems close to phase transitions of a nonconserved order parameter field $\phi(x, t)$. By “nonconserved,” we refer to a dynamics like Eq. (1) that does not conserve the total “mass” $\int \phi(x, t) dx$ in the system. In its most common form, the AC equation features a double-well potential, i.e., a quartic $f(\phi)$. It may be symmetric with minima of equal energy at ϕ^- and $\phi^+ = -\phi^-$ or be tilted by a chemical potential or external field μ . Note that sometimes Eq. (1) with this specific $f(\phi)$ is referred to as the Allen–Cahn equation.⁶

For example, the behavior of the magnetization density in a ferromagnet can be described by a coarse-grained free energy density that is identical to such an energy functional. Moreover, the time evolution of this density can indeed be modeled by the AC equation.⁷ Although the global minimum for a symmetric double-well potential corresponds to homogeneous steady states of either ϕ^- or ϕ^+ , steady states consisting of arrangements of patches of ϕ^- and ϕ^+ do also exist. Here, we call the interfaces between the patches “fronts.” In the literature, the notions “kink” and “anti-kink” are also used. In a fully symmetric situation, the fronts are at rest. Otherwise, they move, e.g., driven by $\mu \neq 0$. For small driving, one can analytically determine the velocity of these fronts that connect two linearly stable states corresponding to local minima of $f(\phi)$, see, e.g., Refs. 8 and 9.

Via another type of moving front, a linearly stable state invades a linearly unstable state.¹⁰ Such fronts occur when systems are suddenly quenched into an initially homogeneous unstable state. Small local perturbations then grow and develop into patches of stable states that spread out over the whole domain. In general, the stable state may correspond to a pattern. This case can, for example, be found in the Taylor–Couette flow.¹¹ Fronts also appear in Rayleigh–Bénard systems when the heat flux is suddenly increased. Then, a convective vortex front propagates into the unstable conductive state.¹² Moreover, front propagation into unstable states is studied in crystal growth¹³ and in the context of chemical reactions.¹⁴ Note that the motion of fronts between homogeneous and spatially periodic states may be induced adding noise terms.¹⁵ Another distinction is between pulled and pushed fronts, where the velocity of the former is controlled by linear effects, while in the latter case, nonlinear effects dominate.^{8,9}

Here, we investigate the dependence of the motion of fronts on the strength of the external field or chemical potential $\mu \neq 0$. On the one hand, we consider the well-known case of a simple AC system with a double-well potential⁸ and use it to introduce our methodology that is based on numerical continuation.¹⁶ On the other hand, we consider AC models with more complicated local energy^{17,18} that allows for a larger number of front types and an active AC model that cannot be written as a gradient dynamics, i.e., in the variational form (1). We employ two ways to render the AC model nonvariationally. First, we add a nonvariational term analogously to Ref. 19, i.e., we incorporate a nonequilibrium chemical potential¹⁶ as also frequently done for mass-conserving Cahn–Hilliard-type dynamics.^{20–23} Such an amended AC equation may be employed to model, e.g., front propagation in a liquid crystal light valve.¹⁹ Second, we couple the AC equation for the order parameter to an evolution equation of a polarization field P in a similar spirit as in an active phase-field-crystal (PFC) model.^{24–26} For other models including an active Swift–Hohenberg equation, see Ref. 27; a tentative systematics in the case of single scalar fields is given in the introduction of Ref. 16. Taking the second option for an active AC model in one spatial dimension results in a system that is similar to the FitzHugh–Nagumo model,^{28,29} describing spike generation in squid axons. There, the evolution equation of the membrane potential corresponds to an AC equation with cubic nonlinearity. As the AC model with double-well local energy is arguably the simplest nonlinear gradient dynamics model for a parity symmetric spatially extended system with $\phi \rightarrow -\phi$ symmetry, its active generalizations are likely the simplest such active models.

Their detailed understanding will help us to extend our knowledge of the collective behavior of active systems consisting of a large number of active particles that are able to transform different types of energy into motion. Here, we focus on front motion; however, the range of phenomena in such systems is much richer. In general, the microscale constituents interact in such a way that on a macroscopic (collective) level directed collective motion and clustering phenomena may occur.³⁰ Different forms of interaction result in different phenomena, e.g., a purely repulsive interaction may give rise to motility-induced phase separation,²¹ whereas a combination of repulsive and attractive interaction allows for the formation of swarms, e.g., of fish or birds,³¹ bacteria colonies,³² or cell motion.^{33,34} The occurring collective structures may consist of disordered or well ordered arrangements that are referred to as active clusters and active crystals,³⁵ respectively. Our work is structured as follows: First, in Sec. II, we focus on the passive systems, i.e., AC systems that evolve toward equilibrium. In particular, Sec. II B introduces the cubic AC equation, briefly reviews linear and nonlinear marginal stability analyses and determines different front types and their velocities as a function of driving strength μ . In Sec. II C, we consider the cubic–quintic AC equation that has already attracted much interest, e.g., in Refs. 17, 18, and 36–38. In contrast to the literature, we focus on the transitions occurring in the behavior of fronts when the driving strength μ is changed. Second, Sec. III considers the two nonvariational amendments of the AC equation. Thereby, Sec. III A considers the first option, namely, the case of a nonequilibrium chemical potential. We discuss the analytical expression for the shift in front velocity close to the transition from the variational to the nonvariational case and compare this to our fully nonlinear numerical results. Section III B considers the second option, namely, the coupling of a cubic AC equation with the dynamics of a polarization field. It is shown that a condition for onset of motion can be determined analytically, similar to the case of the active PFC model in Ref. 25. Bifurcation diagrams are presented for both cases of active AC equations that summarize the behavior of all occurring front solutions when the driving strength is varied. Finally, in Sec. IV, we conclude and give an outlook to future works.

II. PASSIVE SYSTEMS

A. General form of Allen–Cahn-type models

We start our analysis with the well-known standard passive version of the AC equation that describes the time evolution of an one-dimensional nonconserved order parameter field $\phi = \phi(\tilde{x}, t)$. The general form is obtained by introducing the energy \mathcal{F} in Eq. (1) into the general gradient dynamics. It reads

$$\frac{\partial \phi}{\partial t} = \frac{\partial^2 \phi}{\partial \tilde{x}^2} - f'(\phi) + \mu, \quad (2)$$

where μ is the chemical potential, $f'(\phi)$ is the first derivative of the purely nonlinear local energy density f with respect to ϕ , and \tilde{x} is the coordinate in the laboratory frame. In order to find the velocity v of steadily traveling fronts propagating between two homogeneous steady states ϕ^s given by $-f'(\phi^s) + \mu = 0$, we transform system (2)

into a co-moving frame $x = \tilde{x} - vt$ and get

$$-v \frac{d\phi}{dx} = \frac{d^2\phi}{dx^2} - f(\phi) + \mu. \tag{3}$$

Multiplying Eq. (3) by $\frac{d\phi}{dx}$ and integrating (employing Neumann boundary conditions) yields the explicit expression for the velocity

$$v = \frac{f(\phi^{s1}) - f(\phi^{s2}) + \mu(\phi^{s2} - \phi^{s1})}{\int_{-\infty}^{\infty} \left(\frac{d\phi}{dx}\right)^2 dx}, \tag{4}$$

for a front propagating from ϕ^{s2} at $x \rightarrow -\infty$ into ϕ^{s1} at $x \rightarrow \infty$.

In the following, we consider two specific passive systems in Secs. II B and II C below, namely, AC equations with cubic and cubic–quintic nonlinearities, respectively. By employing μ as a main control parameter, we focus on the influence of a physically most relevant quantity that can be easily controlled externally. Note that this differs from most employed and well-known parametrizations.^{38–42}

B. The passive cubic Allen–Cahn equation

1. Model

In the case of the cubic Allen–Cahn equation, $f(\phi) = -\frac{1}{2}\phi^2 + \frac{1}{4}\phi^4$ and hence, in the co-moving frame, we obtain

$$-v \frac{d\phi}{dx} = \frac{d^2\phi}{dx^2} + \phi - \phi^3 + \mu. \tag{5}$$

As mentioned above, this equation is extensively studied in the literature. Here, we review some main approaches to introduce the methodology for our analysis of the more involved models, cf. e.g., Refs. 8 and 9. For the cubic nonlinearity, three homogeneous steady state solutions $\phi^0(\mu)$, $\phi^+(\mu)$, and $\phi^-(\mu)$ exist for $-\mu_c < \mu < \mu_c$ with $\mu_c = \frac{2}{3\sqrt{3}} \approx 0.385$. Here, ϕ^+ and ϕ^- are linearly stable states, while ϕ^0 is unstable. Equation (5) can be seen as a mechanical system, where ϕ corresponds to the position and x is time. In this framework, Eq. (5) describes a particle moving in a double-well potential $V(\phi) = -f(\phi) + \mu\phi$ with friction v . As for $\mu = 0$ the maxima of $V(\phi)$ are of equal height, we find that for any friction $v > 0$, the particle will always asymptotically approach “position” $\phi^0 = 0$, which corresponds to the unstable homogeneous state. However, in reality, one observes that such fronts, moving into the unstable state ϕ^0 , have a certain specific velocity,⁴¹ namely, $v = 2$. Hence, a dynamical selection of the front speed occurs (for details, see, e.g., Ref. 43), which we briefly discuss next.

2. Linear marginal stability analysis

The selection problem is tackled employing a linear marginal stability analysis: We consider the linearization of the fully time-dependent AC equation about the unstable homogeneous state ϕ^0 , i.e., we consider the leading edge of the front (cf. Ref. 43). Note that at the marginal stability point, i.e., the point where the resulting eigenvalues are zero, the group velocity of perturbations at the

leading edge of the front

$$v_g = \frac{d\omega^r(k)}{dk^r} \tag{6}$$

equals the velocity of the front

$$v_f = \frac{\omega^r(k)}{k^r}. \tag{7}$$

Here, k and ω are the wavenumber and frequency, respectively, and the superscript r denotes the real part. In this way, one obtains a linear marginal velocity

$$v_l := v_f = v_g = \pm 2\sqrt{-f'(\phi^0)}. \tag{8}$$

Thus, at the linear marginal stability, point perturbations can not grow above the moving front profile and any front with $v < v_l$ is unstable. Hence, Eq. (8) provides a criterion to determine the dynamically selected front velocity. In Ref. 43, it is shown that the linear marginal velocity is an attractive fixed point such that any front moving with $v > v_l$ eventually converges to one with $v = v_l$. This is referred to as a pulled front. Note that Ref. 44 investigates marginally stable fronts and transitions between different front types for several passive AC-type nonlinear diffusion equations as part of a study of heteroclinic orbits in various two-dimensional dynamical systems. Namely, they analyze the eigendirections in phase space of the homogeneous fixed points that correspond to front solutions and show that indeed the perpendicular direction, i.e., the direction corresponding to the marginal velocity is approached.

3. Numerical path continuation

Next, we determine fronts numerically and compare them to the analytical results. In particular, we employ path continuation techniques^{45,46} bundled in the MATLAB toolbox `pde2path`^{16,47} or in the continuation package `auto07p`^{48,49} to determine front profiles and velocities in dependence of the parameter μ that acts as the strength of a driving caused by an external field or chemical potential.⁵⁰

The resulting bifurcation diagram is shown in terms of the front velocity in Fig. 1(a). Interestingly, three branches exist corresponding to three different front types that are illustrated by the examples in panels (b)–(d). The overall symmetry of the bifurcation diagram reflects the symmetries $(x, v) \rightarrow (-x, -v)$ and $(\phi, \mu) \rightarrow (-\phi, -\mu)$ of Eq. (5). The three front types are a front between the two linearly stable homogeneous states ϕ^- and ϕ^+ indicated by the red dashed lines, and the two respective fronts corresponding to the two different linearly stable states invading the unstable state indicated by green dotted and blue solid lines. The velocity v of the front between stable states is determined as explained in Sec. II A. For the front that moves to the right at positive μ [red dashed line in the upper right quadrant of Fig. 1(a)], v first increases linearly than faster with increasing μ . The curve becomes vertical when μ reaches the critical value μ_c , where the lower maximum of the mechanical potential (ϕ^-) and the minimum (ϕ^0) annihilate [see Fig. 1(e)]. This implies that the bifurcation curve passes a saddle-node bifurcation and folds back. Then, it continues toward lower μ as the solid blue line representing fronts where the globally stable state (linearly stable and of lowest energy) invades the unstable state

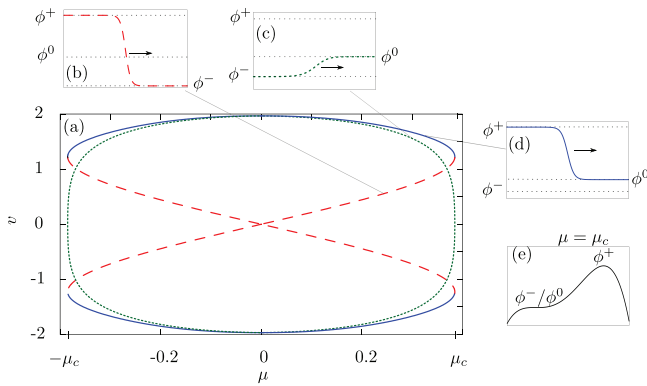


FIG. 1. The central panel (a) presents the bifurcation diagram of front states described by the cubic AC Eq. (5) in terms of the front velocity v as a function of the driving strength μ . The red dashed lines correspond to fronts between the two linearly stable homogeneous states ϕ^- and ϕ^+ with an example given in panel (b). The two respective fronts corresponding to the two different linearly stable states invading the unstable states are indicated by green dotted and blue solid lines with examples in panels (c) and (d), respectively. Panel (e) gives the equivalent mechanical potential $V(\phi)$ at the critical value $\mu = \mu_c$, where ϕ^- and ϕ^0 annihilate.

ϕ^0 . To understand its origin, in Sec. II B 4, we introduce the nonlinear marginal analysis. Decreasing μ further, when crossing $\mu = 0$, the fronts where the globally stable state ϕ^+ invades the unstable state ϕ^0 become fronts where the metastable state ϕ^- (linearly stable, but of higher energy than the globally stable state) invades ϕ^0 (green dotted lines).

Note, finally, that at the value of μ where the red dashed and green dotted line cross, fronts from ϕ^0 to ϕ^- and from ϕ^- to ϕ^+ have the same velocity.

This implies that in the vicinity of this point one may expect moving structures consisting of two fronts as depicted exemplarily in Fig. 2(a). To the left of this point, the ϕ^- to ϕ^+ front stays behind the ϕ^0 to ϕ^- front [cf. Fig. 3(a)], while to the right of this point the former catches up with the latter. Then, they merge as indicated in Fig. 3(b) and create the faster ϕ^0 to ϕ^+ front shown in Fig. 2(b).

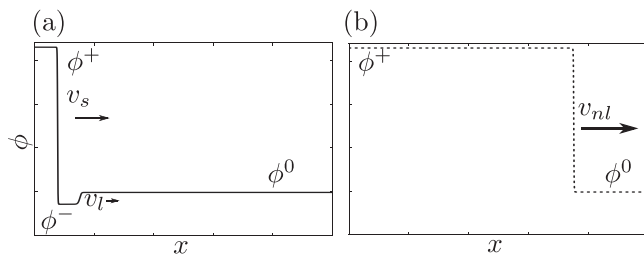


FIG. 2. Snapshots from a time simulation of Eq. (5) at $\mu = 0.377$ for a front initially composed of a front between the two stable states ϕ^+ and ϕ^- moving at v_s and the linear marginal front between ϕ^- and ϕ^0 moving at $v_l < v_s$ (a). At a later time, the two fronts merge into a single nonlinear marginal front between ϕ^+ and ϕ^0 moving at $v_{nl} > v_s$ (b).

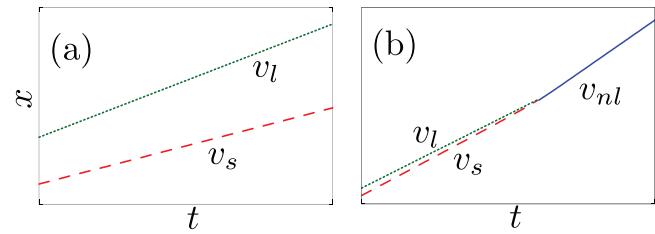


FIG. 3. The motion of the fronts illustrated in Fig. 2 is illustrated in space–time plots of the front position (a) at $\mu = 0.350$, where $v_l > v_s$, i.e., the fronts do not merge and (b) at $\mu = 0.375$, where $v_l < v_s$, i.e., the fronts eventually merge and move with v_{nl} .

4. Nonlinear marginal stability analysis

Using the mechanical analogy, we can also understand the second occurring front moving into the unstable state: a particle moving in this potential may start at either of the maxima corresponding to ϕ^+ or ϕ^- . In Refs. 36 and 43, it is shown that solving the fully nonlinear equation above a threshold μ one additionally finds a so-called invasion front, where ϕ^+ invades ϕ^0 , that is marginally stable and has a nonlinear velocity $v_{nl} > v_l$.

Therefore, we study (5) to find the front solution corresponding to the blue solid line in Fig. 1(a) following the ideas given in Refs. 8, 36, 39 and 43. We denote the two possible linearly stable states by ϕ^\pm . Because the front is monotonic, we can define

$$h(\phi) = \frac{d\phi}{dx} \tag{9}$$

as a function of ϕ . As the front connects two homogeneous states, we request

$$h(\phi^0) = h(\phi^\pm) = 0. \tag{10}$$

Deriving (9) with respect to x yields

$$\frac{d\phi}{dx} \frac{dh}{d\phi} = h(\phi) \frac{dh}{d\phi} = \frac{d^2\phi}{dx^2}. \tag{11}$$

Thus, inserting (9) and (11) into (5) we get

$$-vh(\phi) = h(\phi) \frac{dh}{d\phi} + \phi - \phi^3 + \mu. \tag{12}$$

Finally, with a power series ansatz up to second order for $h(\phi)$, we obtain

$$v_{nl}(\mu) = \frac{3}{\sqrt{2}} (\phi^0 + \phi^\pm), \tag{13}$$

for the nonlinear marginal velocity. Note that considering an ansatz of higher order, the comparison of coefficients always results in a second order polynomial. Therefore, the obtained expression is an exact solution to the cubic AC equation.

Figure 4(a) shows the linear marginal wave number k_l^r (solid green line, obtained in Sec. II B 2) and the here obtained nonlinear marginal wave numbers k_{nl+}^r and k_{nl-}^r (dashed blue and red line, respectively) as a function of μ , whereas Fig. 4(b) gives the corresponding velocities v_l , v_{nl+} , and v_{nl-} . Subscripts “+” and “−” refer to fronts where states ϕ^+ and ϕ^- invade state ϕ^0 , respectively.

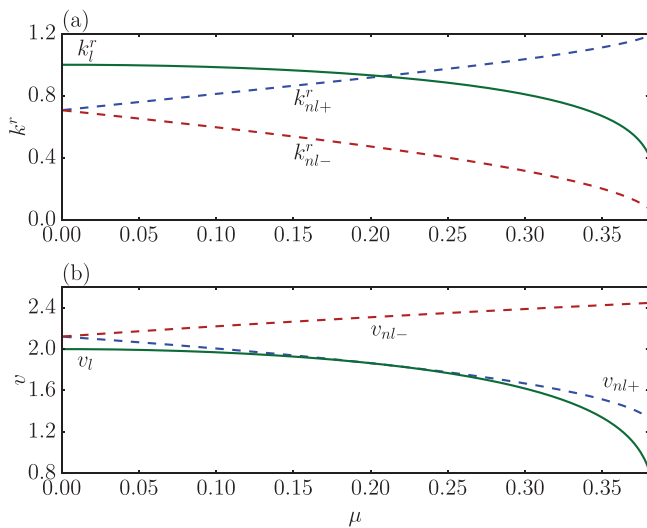


FIG. 4. Shown are the (a) real part of wave numbers $\text{Re}(k) = k^r$ and (b) velocities v of linear (subscript “l”) and nonlinear (subscript “nl”) marginal fronts as a function of driving strength μ . The nonlinear marginal results are given for fronts, where state ϕ^+ invades state ϕ^0 (subscript “+”) as well as for fronts where state ϕ^- invades state ϕ^0 (subscript “-”). The implication of the dependencies for the selection of front velocities is discussed in the main text.

The dynamical selection always implies that the steeper (larger wave number) and slower front is chosen. Considering the front connecting ϕ^- and ϕ^0 , we see that $k_l^r > k_{nl-}^r$ for all μ , i.e., at all μ where the front exists, the linear marginal velocity is selected [solid line in Fig. 4(b)], corresponding to the numerically obtained green dotted line in Fig. 1. In contrast, for the front connecting ϕ^+ and ϕ^0 , the condition $k_l^r > k_{nl+}^r$ only holds for $\mu < 0.2078$, while at larger μ one has $k_{nl+}^r > k_l^r$. This implies that for $\mu < 0.2078$, we find the linear marginal velocity [solid line in Fig. 4(b)], while for $\mu > 0.2078$, the nonlinear marginal velocity [dashed blue line in Fig. 4(b)] is selected. This perfectly agrees with the numerical results in Fig. 1 (solid blue line).

In summary, for $\mu < 0.2078$, the two fronts are degenerated as both move with the linear marginal velocity, while at larger μ , two distinct velocities are found, i.e., above $\mu = 0.2078$, the dotted green and the solid blue branch in Fig. 1(a) differ, while they exactly coincide below this value. Note that the $v(\mu)$ curves in Fig. 4 are tangential to each other where the two corresponding $k^r(\mu)$ curves cross. This implies that a clear transition in the corresponding numerically obtained curve can be best seen when inspecting the second derivative of v with respect to μ .

Note that all described front types are analytically studied in Ref. 8. We have seen that the numerical results obtained by path continuation well agree with the analytical results. The given brief review and comparison provides the starting point for our analysis of more complex models.

C. The passive cubic-quintic Allen-Cahn equation

Next, we analyze the cubic-quintic AC equation, i.e., Eq. (1) with $f(\phi) = \frac{1}{6}\phi^6 - \frac{a}{4}\phi^4 + \frac{b}{2}\phi^2$ similar to the one studied in Ref. 18

in the context of the creation of metastable phases in crystallization processes. It is also studied in Ref. 51 with the additional influence of stochastic noise. The equation for steadily moving fronts (3) is then

$$-v \frac{d\phi}{dx} = \frac{d^2\phi}{dx^2} - \phi^5 + a\phi^3 - b\phi + \mu. \quad (14)$$

It has stable homogeneous solutions $\phi_s^-, \phi_s^0, \phi_s^+$ and unstable homogeneous solutions ϕ_u^- and ϕ_u^+ , all depending on μ . As in Ref. 18, we use $a = 5/4$ and $b = 1/4$. The corresponding bifurcation diagram is depicted in Fig. 5(a) together with exemplary front profiles in panels (b)–(f). Panels (g) and (h) show the potential in the mechanical analogy at the critical values $\mu_{c1} \approx 0.044$ and $\mu_{c2} \approx 0.114$, where two homogeneous steady states annihilate. To understand the rich picture involving a number of different branches of front solutions, we first identify the two linear marginal velocities corresponding to fronts invading the two unstable states. We also characterize all nonlinear marginal velocities. Note that the overall symmetries of the bifurcation diagram correspond to the ones known from Fig. 1.

Because the nonlinear function in (14) is a quintic polynomial, the roots as a function of μ cannot be calculated analytically. Nevertheless, we can find them numerically, e.g., employing continuation. In consequence, we were able to study the linear marginal velocity by inserting the numerical results into the specific form of Eq. (8), i.e., into

$$v_{l+} = \pm 2\sqrt{-5\phi_u^{+4} + 3a\phi_u^{+2} - b}, \quad (15)$$

$$v_{l-} = \pm 2\sqrt{-5\phi_u^{-4} + 3a\phi_u^{-2} - b}, \quad (16)$$

where v_{l+} and v_{l-} are the linear marginal velocities for a front invading the unstable states ϕ_u^+ and ϕ_u^- , respectively. They are depicted in Fig. 6 as black dotted-dashed and dashed lines, respectively. The numerical results are indicated by the gray solid lines and, in particular, for the linear marginal velocities coincide well with the semi-analytical result.

In this way, we identify the gray dotted-dashed branches and the green solid branches for $|\mu| > \mu_{c1}$ in Fig. 5(a) as linear marginal, i.e., pulled fronts. We note that different parts of the structure of the bifurcation diagram for the simple cubic AC equation presented above in Fig. 1(a) can be recognized as substructures within the bifurcation diagram for the quintic case in Fig. 5(a). For instance, the red solid branches corresponding to fronts between the two stable states ϕ_s^+ and ϕ_s^- in Fig. 5(a) behave similarly to the red dashed branches in Fig. 1(a) over the entire μ -range. The blue dashed and green solid branches in Fig. 5(a) are similar to blue solid and green dotted branches in Fig. 5(a), however, only for $|\mu| > \mu_{c1}$.

Therefore, we expect the blue dashed branch in Fig. 5(a) to correspond to a nonlinear marginal front, as they can be identified as invasion fronts at the bifurcation point, where it merges with the red branch. Moreover, in the interval $-\mu_{c1} < \mu < \mu_{c1}$, we twice observe a structure similar to the one of the cubic AC equation, once for negative and once for positive velocities. Again, this can be explained referring to the mechanical analogy: In this μ -range, we can consider the potential as being composed of two cubic AC potentials. At the critical values $|\mu| = \mu_{c1}$, the metastable state merges with one of

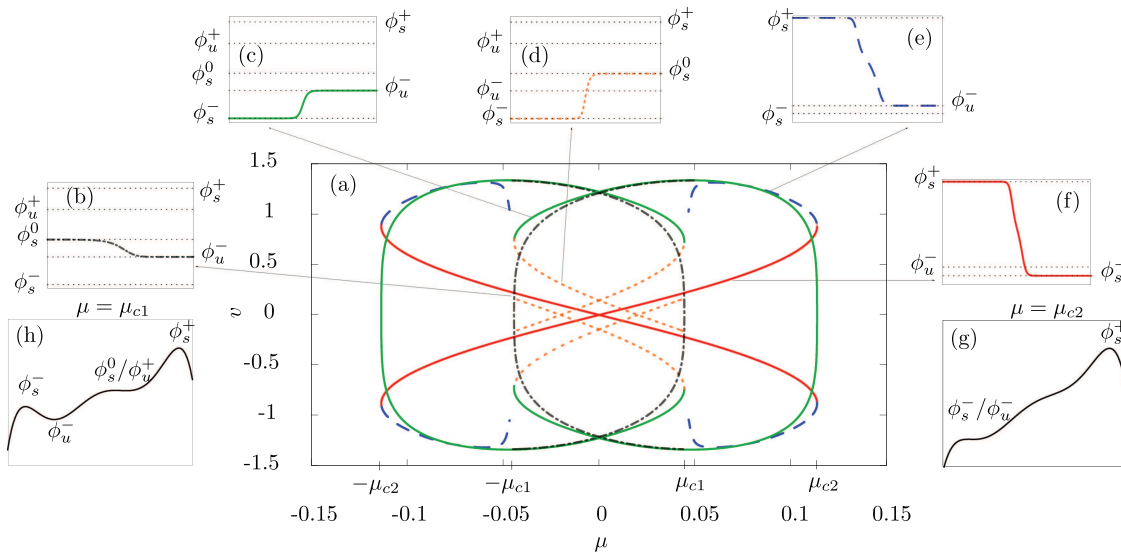


FIG. 5. The central panel (a) presents the bifurcation diagram of front states described by the cubic–quintic AC Eq. (14) in terms of the front velocity v as a function of the driving strength μ . The red solid lines correspond to fronts between the two linearly stable states ϕ_s^+ and ϕ_u^- with an example given in panel (f) for $\mu = 0.09$. At the saddle-node bifurcation at $\mu = \mu_{c2}$ the states ϕ_s^- and ϕ_u^- annihilate. The green solid lines corresponds to fronts between ϕ_s^- and ϕ_u^- [panel (c) for $\mu = -0.02$] or between ϕ_s^+ and ϕ_u^+ depending on the sign of μ . At the saddle-node bifurcation at $\mu = \mu_{c1}$ the states ϕ_s^0 and ϕ_u^+ annihilate (at $\mu = -\mu_{c1}$ the states ϕ_s^0 and ϕ_u^-). The orange dotted lines refer to front solutions between ϕ_s^+ and ϕ_s^0 or between ϕ_s^- and ϕ_s^0 [panel (d) for $\mu = -0.02$], again depending on the sign of μ . The blue dashed lines refer to front solutions between ϕ_s^+ and ϕ_u^- [panel (e) for $\mu = 0.09$]. Finally, the gray dotted-dashed lines represent front solutions between ϕ_s^0 and ϕ_u^+ or between ϕ_s^0 and ϕ_u^- [panel (b) for $\mu = -0.02$]. The thin horizontal black dotted lines in front profile panels represent the homogeneous steady states, i.e., the real roots of $f(\phi) - \mu$ in (14). Panels (g) and (h) gives the equivalent mechanical potential $-f(\phi) + \mu\phi$ at the critical values μ_{c1} and μ_{c2} , respectively.

the unstable states and, thus, for $|\mu| > \mu_{c1}$, there is only one “cubic” AC potential left.

We now return to the blue dashed front in Fig. 5(a), for a profile see Fig. 5(e). To understand why the front does not exist for $|\mu| < \mu_{c1}$, we study again the mechanical analogy at $\mu = \mu_{c1}$ illustrated in Fig. 5(h): consider a particle starting at ϕ_s^+ and just

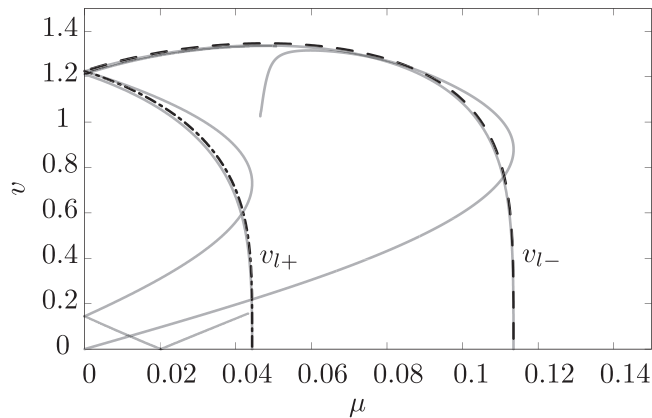


FIG. 6. The linear marginal velocity v_{l-} found in Eq. (14) corresponds to the black dashed line, whereas v_{l+} corresponds to the black dotted-dashed line. The results gained with `aut0-07p` are illustrated as the gray solid lines.

reaching ϕ_u^- without overshooting. Let the corresponding friction be v_1 . Considering now a particle that moves from ϕ_s^+ to ϕ_s^0 , the corresponding friction v_2 needs to satisfy $v_2 > v_1$. Moreover, a particle starting in ϕ_u^- requires more negative friction to move up to ϕ_s^+ than it does to move up to ϕ_s^0 . Hence, we claim $v_1 > v_3$, where v_3 is the friction to move from ϕ_s^0 to ϕ_u^- . That is, we require $v_3 < v_1 < v_2$, where v_3 corresponds to the velocity $v_3 \approx 1.33$ of a front on the gray dotted-dashed branch at μ_{c1} . However, v_2 is the velocity at the bifurcation point, where the orange dotted branch becomes the green solid branch with $v_2 \approx 0.73 < v_3$. Hence, v_1 , the velocity of the blue dashed solution does not satisfy the condition at $\mu = \mu_{c1}$ and, therefore, the branch cannot exist anymore. Note that this argument is similar to the one given in Ref. 18, and we can identify the blue dashed front solutions as being similar to those found there, however, as our equations slightly differs they are not identical. The question how exactly this branch ends is not easy to answer. Our calculations show that following the branch toward smaller μ , the slight shoulder visible in Fig. 5(e) develops into a long inclined plateau of increasing length. This indicates that even at $\mu > \mu_{c1}$, the front already “feels” the presence of the two additional homogeneous steady states that exist for $\mu \leq \mu_{c1}$. With other words, the spatial dynamics slows down close to these “ghost solutions” forming the sloped plateau. The slope gets smaller the longer the plateau becomes, i.e., the closer one approaches μ_{c1} from above. We are not able to follow the blue dashed branch further than shown in Fig. 5(a) as the plateau becomes too long for the largest of our numerical domain sizes. Our hypothesis is that the curve becomes

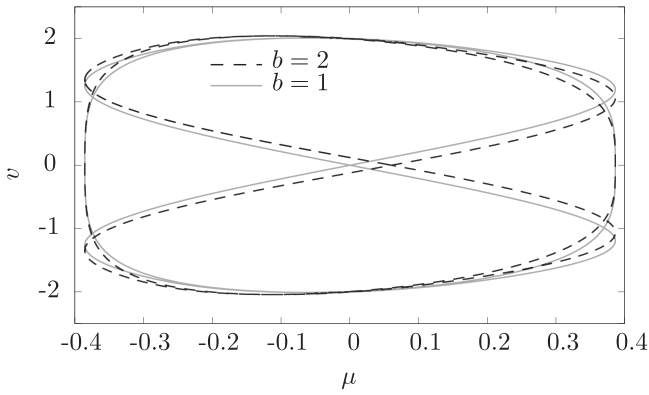


FIG. 7. Comparison of bifurcation diagrams for the variational cubic AC equation with $b = 1$ (gray solid) and the nonvariational cubic AC equation (17) with $b = 2$ (black dashed). The shift in velocity v_1 for a front propagating from ϕ^+ into ϕ^- at $\mu = 0$ for $\epsilon = 0.2$ is consistent with the analytical result.

vertical when approaching μ_{c1} from above where the structured front between ϕ_s^+ and ϕ_u^- decays into several fronts between ϕ_s^+ , ϕ_u^+ , ϕ_s^0 , and ϕ_u^- that exist for $\mu \leq \mu_{c1}$.

III. ACTIVE SYSTEMS

So far, we have examined front motion described by variational AC equations, i.e., systems that can be written as nonconserved gradient dynamics. They describe systems that ultimately approach thermodynamic equilibrium. Next, we consider active systems where this is not the case. In particular, we consider two different examples of nonvariational extensions of the cubic AC equation.

A. Nonvariational cubic Allen-Cahn equation

In the first considered example of a nonvariational AC equation, a term g_{nv} is added to (2) that breaks its gradient dynamics form. The resulting equation is¹⁹

$$\frac{\partial \phi}{\partial t} = \frac{\partial^2 \phi}{\partial \tilde{x}^2} + \phi - \phi^3 + \mu + \epsilon g_{nv} \left(\phi, \frac{\partial \phi}{\partial \tilde{x}}, \frac{\partial^2 \phi}{\partial \tilde{x}^2} \right)$$

with $g_{nv} \left(\phi, \frac{\partial \phi}{\partial \tilde{x}}, \frac{\partial^2 \phi}{\partial \tilde{x}^2} \right) = \left(\frac{\partial \phi}{\partial \tilde{x}} \right)^2 + 2b\phi \frac{\partial^2 \phi}{\partial \tilde{x}^2}$. (17)

Note that the complete equation becomes variational for $b = 1$. Again, we are interested in the velocities of fronts and their dependence on the external driving strength μ . Following Ref. 19, we use a front solutions of the variational Eq. (5) [i.e., Eq. (17) with $\epsilon = 0$] as a reference solution ϕ_F and employ the ansatz $\phi(\tilde{x}, t) = \phi_F(\tilde{x} - vt) + u(\tilde{x} - vt, \epsilon t)$. Here, $v \approx v_0 - \epsilon v_1$ with v_0 being the velocity of the reference front, i.e., $\phi_F(\tilde{x} - v_0 t) := \phi_F(x)$.

One multiplies Eq. (17) by $\partial \phi / \partial x$, integrates in x , employing the point symmetry $\phi_F(x) = -\phi_F(-x)$, and expands in ϵ (see the Appendix for details). Then, for linear order, one can write the

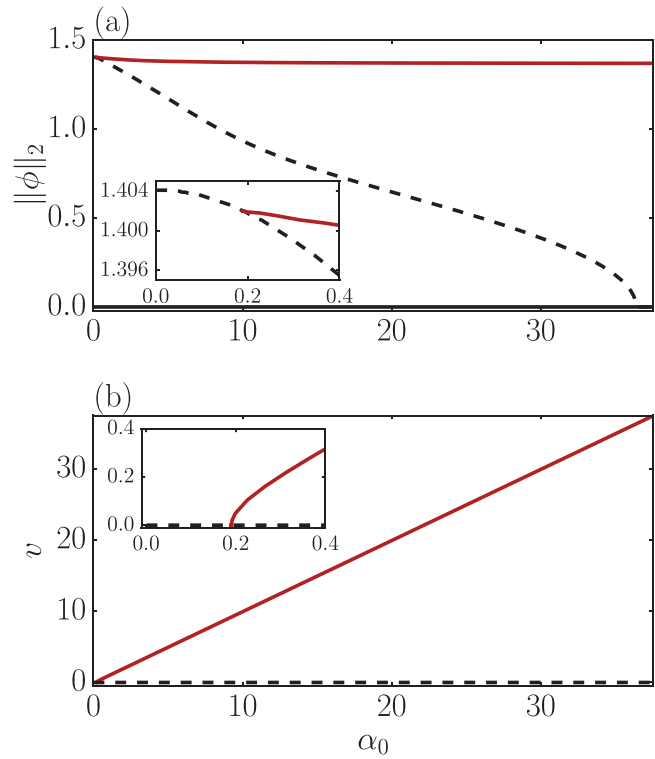


FIG. 8. Bifurcation diagram for resting and moving fronts for the active cubic AC Eq. (19) at $\mu = 0$. Panels (a) and (b) show the norm $\|\phi\|_2$ and the front velocity v in dependence of activity α_0 , respectively. The resting and moving fronts are given as black dashed and red solid lines, respectively. The insets focus on the region where the drift pitchfork bifurcation occurs. The black solid line represents the homogeneous solution branch.

nonvariational contribution as¹⁹

$$v_1 = \frac{\int_{-\infty}^{\infty} g_{nv} \left(\phi_F, \frac{\partial \phi_F}{\partial x}, \frac{\partial^2 \phi_F}{\partial x^2} \right) \partial_x \phi_F dx}{\int_{-\infty}^{\infty} (\partial_x \phi_F)^2 dx} \tag{18}$$

We notice that v_1 in contrast to v_0 not only depends on the difference in energy densities f but also on the nonvariational part g_{nv} and the shape of the reference front $\phi_F(\mu)$. Figure 7 gives the corresponding numerically obtained bifurcation diagram of front solutions to Eq. (17) for a nonvariational case with $b = 2$ and relatively small $\epsilon = 0.2$ (black dashed line) in comparison to the variational case with $b = 1$ (gray solid line). Because g_{nv} breaks the $\phi \rightarrow -\phi$ symmetry, the $\mu \rightarrow -\mu$ symmetry is broken.

Inserting ϕ_F into (18) and solving the integrals for $\mu = 0$, where $v_0 = 0$ yields $v_1 = \frac{2\sqrt{2}}{5}$, i.e., in the nonvariational case, the front moves even without external driving. The shift in velocity for the chosen ϵ coincides on the scale of Fig. 7 with the numerical result. At larger strength ϵ of the nonvariational term, linear considerations do not suffice anymore (not shown). Note that the point of zero velocity for the fronts connecting ϕ^- and ϕ^+ is with increasing

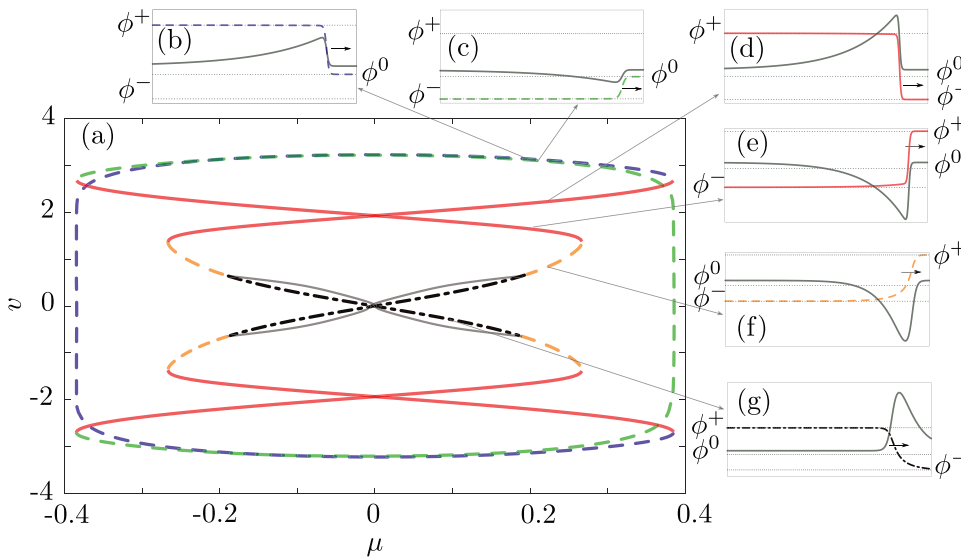


FIG. 9. (a) Bifurcation diagram of front states described by the active Allen–Cahn model (19). Shown is the front velocity as a function of the external driving strength μ at fixed activity $\alpha_0 = 1.9951$. There are various fronts between the two stable states ϕ^- and ϕ^+ , namely, the red solid, black dot-dashed, gray solid, and orange dashed lines. The blue and green dashed lines correspond to fronts propagating into the unstable state ϕ^0 . The gray solid line corresponds to a branch of time-periodic oscillating fronts. Panels (b)–(g) show selected front profiles $\phi(x)$ in colors equal to the corresponding branch in panel (a) at $\mu \approx 0.2$. The accompanying polarization profiles $P(x)$ are given in gray. For completeness, we also indicate the steady homogeneous states ϕ^- , ϕ^0 , and ϕ^+ as dotted horizontal lines. Note, however, that the solution panels are differently scaled on the ϕ, P axes as the polarization profiles differ in magnitudes.

ϵ shifted toward positive μ . It may be seen as the out-of-equilibrium coexistence point of the two states connected by the front.

B. Cubic Allen–Cahn equation coupled to polarization field

As the second and final example of the nonvariational AC equation, we consider a cubic AC equation coupled in a simple way to the linear dynamics of a polarization field. Here, we focus on the one-dimensional case, where P describes the local strength of directional order and employ the same coupling between order parameter field ϕ and P as employed in the active phase-field-crystal (PFC) model.^{24,25,52,53} The system of equations then reads

$$\begin{aligned} \frac{\partial \phi}{\partial t} &= -\frac{\delta \mathcal{F}}{\delta \phi} - \alpha_0 \frac{\partial P}{\partial x}, \\ \frac{\partial P}{\partial t} &= D_T \frac{\partial^2}{\partial x^2} \frac{\delta \mathcal{F}}{\delta P} - D_r \frac{\delta \mathcal{F}}{\delta P} - \alpha_0 \frac{\partial \phi}{\partial x}, \end{aligned} \quad (19)$$

with $\mathcal{F}[\phi, P] = \mathcal{F}_{AC}[\phi] + \mathcal{F}_P[P]$,

where

$$\mathcal{F}_{AC} = \int dx \left[\frac{1}{2} \left(\frac{\partial}{\partial x} \phi \right)^2 - \frac{1}{2} \phi^2 + \frac{1}{4} \phi^4 - \mu \phi \right] \quad (20)$$

is the energy for the cubic passive AC equation as used before,

$$\mathcal{F}_P = \int dx \frac{1}{2} P^2, \quad (21)$$

is the energy of the polarization P that favors a state of random orientation ($P = 0$) and does not allow for spontaneous polarization. Both coupling terms have a strength α_0 (called “activity”) and their form represents the simplest possible form to couple the scalar ϕ and the “vector” P . Furthermore, D_T and D_r are positive translational and rotational diffusivities, respectively. Note that the coupling terms break the gradient dynamics structure.

In analogy to the active PFC model, we expect that steady states of the passive model ($\alpha_0 = 0$) remain at rest until they undergo a drift pitchfork bifurcation at a critical activity where they start to move. We determine an analytical criterion for the onset of motion in analogy to the derivation for the active PFC model in Ref. 25. It reads

$$0 = \|\partial_x \phi_s\|^2 - \|\partial_x P_s\|^2 \quad (22)$$

and allows us to determine the critical values of the activity parameter α_0 . Here, ϕ_s and P_s denote steady state profiles whose L_2 -norm is taken. Note that the specific criterion differs from the one in Ref. 25 as there the order parameter field ϕ follows a conserved dynamics while here the dynamics is nonconserved. This is further discussed in Ref. 54.

Figure 8 presents results of continuation runs following front solutions of Eq. (19) at $\mu = 0$ using the activity α_0 as a control parameter. The black dashed line corresponds to resting fronts connecting ϕ^- and ϕ^+ . These resting fronts become shallower with increasing α_0 , and the branch terminates on the branch of trivial homogeneous states at about $\alpha_0 = 36.3$. However, already at rather small $\alpha_0 \approx 0.19$, a drift pitchfork bifurcation occurs [see the inset of Fig. 8(a)], where a branch of steadily moving fronts (red solid line)

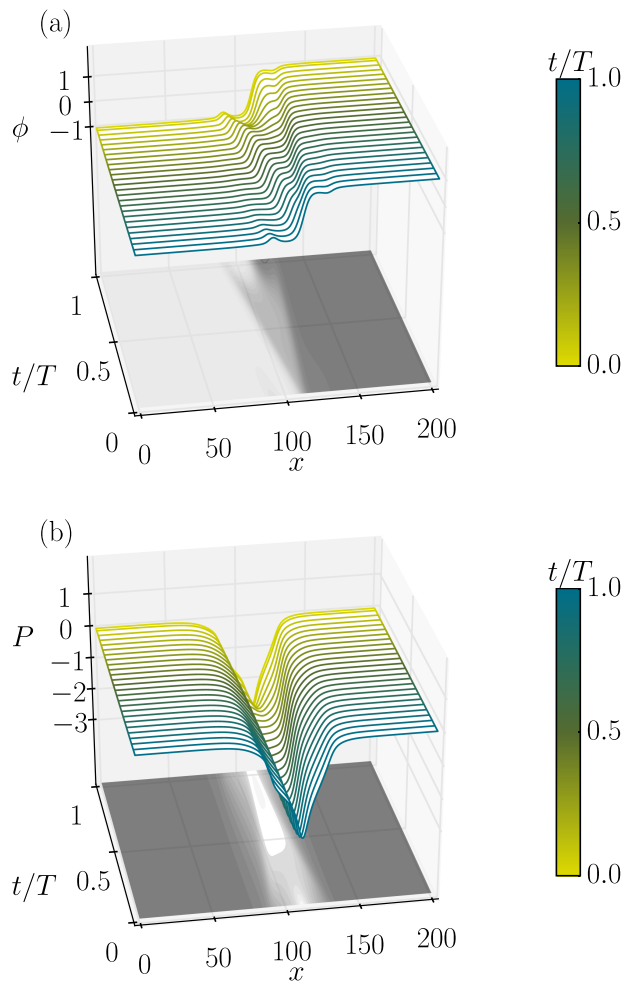


FIG. 10. Space-time plots for a periodically modulated front solution of Eq. (19). Shown are (top) the concentration profile and (bottom) the polarization profile at $\mu = 0.2$ in the frame moving with their mean velocity $v = 0.15$. The different colors of the contour indicate time scaled by the period $T \approx 14.5$. Furthermore, a projection of the profiles is shown on the x - t plane as gray-scale contour plot.

emerges from the branch of resting fronts. The numerical results confirm criterion (22). In the limit of large activity, we find $v = \alpha_0$, as depicted in Fig. 8(b). This agrees with analogous results in Ref. 25 where an analytical argument is also given.

Next, we take a moving front at a particular value of activity ($\alpha_0 = 1.9951$) from Fig. 8 and perform a continuation in μ to obtain a bifurcation diagram in analogy to Fig. 1 for the passive cubic AC equation. The result is presented in Fig. 9(a). Panels (b)–(g) show selected front profiles $\phi(x)$ in colors equal to the corresponding branch in panel (a). The accompanying polarization profiles $P(x)$ are given in gray. For completeness, we also indicate the steady homogeneous states ϕ^- , ϕ^0 , and ϕ^+ as dotted horizontal lines. Note that the front location is off center in the computational domain as the spatial relaxation toward the homogeneous states can be very asymmetric.

The fronts on the red solid and black dot-dashed branches at $\mu = 0$ correspond to the moving and resting front in Fig. 8. Increasing μ , the symmetry of the potential in ϕ is broken and two red branches emerge. Both of them undergo saddle-node bifurcations at respective critical values $\mu = 0.26$ and $\mu = 0.38$. The larger one is identical to μ_c in Sec. II B as the homogeneous steady states do not depend on activity (in contrast to their stability). The smaller one can not be obtained from an analysis of the local equilibrium potential $f(\phi) - \mu$.

Another interesting feature are fronts that do not move steadily but are modulated in a time-periodic manner. They are found on the gray solid branches in Fig. 9(a) and emerge with finite oscillation period of about $T = 12.5$ from a Hopf bifurcation where the orange dashed and the black dot-dashed branch connect. The branch continues toward smaller μ with a monotonically increasing period (up to about $T = 14.5$ at $\mu = 0$). Typical changes in the moving solution profiles over one period of time are depicted in Fig. 10.

Overall, one can state that the coupling of a simple AC dynamics to a linear dynamics of a polarization field introduces a number of additional unstable front solutions all connecting ϕ^+ and ϕ^- . Hence, the structure of the bifurcation diagram strongly changes from the passive case in Fig. 1(a) and the active case in Fig. 9(a). Note that due to the coupling, the marginal stable fronts propagating into the unstable state also become unstable in the active model.

IV. CONCLUSION

In the present work, we have investigated front solutions in a number of passive and active Allen–Cahn (AC) equations employing continuation techniques. We have focused on the dependency of front velocities on an external driving μ , e.g., a chemical potential or external field. The results have been presented in the form of bifurcation diagrams. First, we have reviewed the widely available analytical results for the simple cubic AC equation and have introduced the concepts of pulled and pushed fronts employing linear and nonlinear marginal stability analysis. We have highlighted that there exist fronts that change their character from pulled to pushed as the driving μ is increased across a threshold.

Next, we have extended the analysis to the cubic–quintic AC equation that allows for more homogeneous steady states and, in consequence, for more fronts connecting them. We have presented a rather involved bifurcation diagram, employing again the driving μ as control parameter. It shows the various front solutions connecting up to five homogeneous steady states. In general, our results allow one to better understand how the different fronts are related and how they transform with increasing driving strength. To understand substructures of the diagram, it has been helpful to discuss symmetries and how parts of the cubic–quintic potential resemble the cubic potential.

The considered model is similar to the one studied in Ref. 18 in the context of the creation of metastable phases in crystallization processes. In particular, they investigate how double-fronts emerge that first create a metastable phase before it is transformed into the stable phase. Their main control parameter is the order parameter value corresponding to one of the thermodynamic phases, while here we have kept the energy functional fixed and employed the chemical potential (external field) as a control parameter. We have

shown how fronts and transitions similar to the ones discussed in Ref. 18 are embedded into the full bifurcation diagram of front states. As Ref. 55 extends the discussion of Ref. 18 to systems where two order parameter fields are coupled, in the future, it may also be interesting to revisit such more complicated two- or multi-field models employing continuation techniques.

After considering the cubic and cubic–quintic AC equations that represent gradient dynamics models, we have considered non-variational extensions. First, we have analyzed a cubic AC equation with the addition of a standard nonvariational chemical potential (see, e.g., classification in the introduction of Ref. 16). We have found that main symmetries of the bifurcation diagram are broken, however, occurring front types and overall topology of the diagram remain the same as in the passive case. Our numerical results agree at small strength of the nonvariational influence ϵ with the approximate analytical results of Ref. 19 but show some deviations at larger ϵ . In the future, it will be interesting to extend our present investigation of the variational cubic–quintic AC equation toward the nonvariational case either by adding nonvariational terms to the cubic–quintic AC equation studied here or by considering the equation recently introduced in Ref. 56 as a model for a liquid crystal light valve experiment with optical feedback.

Changes with respect to the passive case are more dramatic in the second nonvariational model that couples a cubic AC equation with a linear equation of a polarization field, similar to such couplings in more involved models of active matter. In this case, we have encountered additional fronts between stable states that move due to activity even at zero external driving. They emerge in a drift pitchfork bifurcation similar to the onset of motion in active phase-field-crystal²⁵ and active Cahn–Hilliard models.⁵⁴ This then implies a much richer bifurcation diagram that even contains oscillating front states that emerge at a Hopf bifurcation of steady fronts. We believe future comparative studies that analyze the front motion and its emergence in a larger class of systems would be highly valuable.

APPENDIX: NONVARIATIONAL CUBIC ALLEN–CAHN EQUATION

As in the literature,¹⁹ the derivation of Eq. (18) is only sketched, and we find it instructive to reproduce and, here, reproduce it in greater detail. The aim is to determine an analytical expression for the velocity of moving fronts that are solutions of nonvariational AC Eq. (17) and to discuss its dependence on the strength of the nonvariational influence.

We introduce the ansatz

$$\begin{aligned} \phi(\tilde{x}, t) &= \phi_F(\tilde{x} - vt) + u(\tilde{x} - vt, \epsilon t), \\ v &= v_0 - \epsilon v_1, \end{aligned} \tag{A1}$$

where ϕ_F is a solution to (5) with velocity v_0 , i.e., $\phi_F(\tilde{x} - v_0 t) := \phi_F(x)$ as the velocity changes due to the nonvariational term. Moreover, we add a small adjustment function u also of order ϵ . For the ansatz (A1), we introduce $\xi = \tilde{x} - vt = x + \epsilon v_1 t$. Linearizing $\phi_F(\xi)$ around x yields

$$\phi_F(\xi) = \phi_F(x) + \epsilon v_1 \left. \frac{\partial \phi_F}{\partial \xi} \right|_{\xi=x} + \mathcal{O}(\epsilon^2). \tag{A2}$$

Inserting the ansatz (A1) into (17) using (A2) and linearizing in ϵ yields

$$\begin{aligned} & -\epsilon v_1 v_0 \left. \frac{\partial^2 \phi_F}{\partial \xi^2} \right|_{\xi=x} + \epsilon v_1 \left. \frac{\partial \phi_F}{\partial \xi} \right|_{\xi=x} - v_0 \frac{\partial u}{\partial \xi} \\ & = \epsilon v_1 \left. \frac{\partial^3 \phi_F}{\partial \xi^3} \right|_{\xi=x} + \epsilon v_1 \left. \frac{\partial \phi_F}{\partial \xi} \right|_{\xi=x} - 3\epsilon v_1 \phi_F^2 \left. \frac{\partial \phi_F}{\partial \xi} \right|_{\xi=x} \\ & + \frac{\partial^2 u}{\partial \xi^2} + u - 3\phi_F(x)^2 u(\xi)^2 u + \epsilon g_{nv} \left(\phi_F(\xi), \frac{\partial \phi_F}{\partial \xi}, \frac{\partial^2 \phi_F}{\partial \xi^2} \right) \Big|_{\xi=x}. \end{aligned} \tag{A3}$$

By deriving (5) with respect to x

$$-v_0 \frac{\partial}{\partial x} \frac{\partial \phi_F(x)}{\partial x} = \frac{\partial}{\partial x} \frac{\partial^2 \phi_F(x)}{\partial x^2} + \frac{\partial \phi_F(x)}{\partial x} - 3\phi_F(x)^2 \frac{\partial \phi_F(x)}{\partial x} \tag{A4}$$

and introducing the linear operator

$$L = -v_0 \frac{\partial}{\partial x} - \frac{\partial^2}{\partial x^2} - 1 + 3\phi_F(x)^2, \tag{A5}$$

we obtain

$$L^\dagger \left(\frac{\partial}{\partial x} \phi_F(-x) \right) = 0, \tag{A6}$$

where L^\dagger is the adjoint of L . Next, we identify the linear operator (A5) in (A3)

$$\epsilon v_1 \left. \frac{\partial \phi_F}{\partial \xi} \right|_{\xi=x} + \epsilon v_1 L \left(\frac{\partial}{\partial x} \phi_F \right) + Lu = \epsilon g_{nv} \Big|_{\xi=x}. \tag{A7}$$

With (A6), (A7) simplifies to

$$Lu = \epsilon g_{nv} \left(\phi_F, \frac{\partial \phi_F}{\partial x}, \frac{\partial^2 \phi_F}{\partial x^2} \right) - \epsilon v_1 \frac{\partial \phi_F}{\partial x}. \tag{A8}$$

According to the Fredholm alternative,⁵⁷ (A8) is only solvable if

$$\left\langle \epsilon g_{nv} \left(\phi_F, \frac{\partial \phi_F}{\partial x}, \frac{\partial^2 \phi_F}{\partial x^2} \right) - \epsilon v_1 \frac{\partial \phi_F}{\partial x} \Big| \frac{\partial}{\partial x} \phi_F \right\rangle = 0 \tag{A9}$$

because (A6) has a nontrivial solution.

DATA AVAILABILITY

The data that support the findings of this study are openly available in www.zenodo.org at <https://doi.org/10.1063/5.0003271> in Ref. 58.

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