

Droplet shrinkage in phase-field approaches: A comparison of the Allen-Cahn and the Cahn-Hilliard models

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Diffuse interface methods for multiphase flow simulations often exhibit nonphysical droplet or bubble shrinkage, particularly when based on the Cahn-Hilliard equation. This well-known artifact introduces a critical radius below which droplets vanish, thereby limiting the fidelity of simulations involving small-scale structures. In this study we examine a conservative Allen-Cahn model and demonstrate, through both analytical and numerical investigations, that it inherently avoids this shrinkage behavior. We show that the conservative Allen-Cahn model enforces an exact local balance of interfacial terms, enabling the stable preservation of droplets with radii larger than the interface thickness, regardless of the initial droplet size or domain geometry. Our analysis also provides a different theoretical treatment of the shrinkage phenomenon in the Cahn-Hilliard equation, distinguishing itself from earlier works by providing a rigorous explanation of why conservative Allen-Cahn models avoid this problem. The analysis reveals that conservative Allen-Cahn formulations achieve exact cancellation of curvature-driven terms through a local geometric force balance, while Cahn-Hilliard models exhibit systematic shrinkage due to unbalanced curvature effects that create driving forces for mass transport. Theoretical and numerical findings show that there is a shrinkage relation between interface radius r_I and time t in the form of $r_I^3(t) \sim -t$, which leads to a power law $t_f \propto r_0^3$ for the disappearance time t_f versus initial radius r_0 . Numerical experiments across a wide range of droplet sizes corroborate the theoretical predictions. These results position the conservative Allen-Cahn model as a robust and accurate phase-field approach, particularly well suited for applications demanding the resolution of fine features or long-time integration, such as multiphase transport in porous media.

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I. INTRODUCTION

Multiphase flows involving dynamic interfaces between immiscible phases arise in a wide range of natural and engineering systems. Accurately simulating such flows remains challenging due to the complexity of interfacial dynamics and the need for robust numerical techniques that can capture topological changes and fine-scale structures. Among the various approaches, diffuse interface methods have emerged as powerful tools over the past few decades [1,2]. These methods replace sharp interfaces with finite-thickness transition regions, enabling natural treatment of complex geometries, interfacial phenomena, and phase connectivity without explicit interface tracking.

Phase-field methods are computational tools for simulating interfacial phenomena in multiphase systems. These methods employ a diffuse interface approach where the sharp interface between phases is replaced by a thin transition region characterized by rapid but continuous variations of an order

parameter (also known as volume fraction or phase field). The evolution of this field is governed by partial differential equations derived from thermodynamic considerations, most notably the Cahn-Hilliard (CH) equation [3] and the Allen-Cahn (AC) equation [4].

A well-documented limitation of the CH equation is the spontaneous nonphysical shrinkage of droplets or bubbles. This phenomenon, intrinsic to the CH formulation rather than a numerical artifact, has been extensively analyzed by Yue *et al.* [5] and Zheng *et al.* [6]. Their studies demonstrate that droplets below a critical radius vanish over time, even in the absence of any imposed flow or external forcing. This imposes significant limitations on simulations involving small-scale features or systems characterized by multiple length scales, such as multiphase flow in porous media [7].

Numerous strategies have been proposed to mitigate droplet shrinkage in CH-based models. These include global mass and volume correction techniques [8,9], adaptive mesh refinement [10], and interface reinitialization schemes [11]. However, such approaches often introduce additional computational complexity, reliance on heuristic parameters, and reduced robustness.

The AC equation, initially developed for modeling grain boundary motion in alloys [4], was later reformulated for multiphase systems within the phase-field framework by Sun and Beckermann [12] and refined by Chiu and Lin [13] into the conservative Allen-Cahn (CAC) model. This model

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preserves mass conservation and has been widely applied in the context of pore-scale simulations of multiphase flow [7,14–18]. Haghani *et al.* [17] recently established a connection between the CAC model and the widely used color-gradient lattice Boltzmann method [19].

Unlike the CH model, simulations based on the CAC equation have consistently shown the ability to preserve small droplets and bubbles, including those with radii on the order of the interface thickness in different multiphase systems [15,16]. In this work we provide a theoretical foundation for this observation and demonstrate, through analytical derivation and numerical validation, that the CAC model inherently suppresses the curvature-driven shrinkage mechanism. Specifically, we show that the CAC model enforces a local geometric force balance at the interface, independent of surface tension terms that characterize the CH model. This balance ensures that droplets with radii larger than the interface thickness remain stable, regardless of their initial size or the computational domain.

Furthermore, we revisit the CH shrinkage problem from a different theoretical perspective, complementing the analyses of Yue *et al.* [5] and Zheng *et al.* [6], and elucidate the fundamental differences between the CH and CAC formulations.

The remainder of the paper is organized as follows. Section II introduces the CH and CAC phase-field models. Section III presents an alternative theoretical treatment of the CAC model and a detailed analysis of the shrinkage behavior in the CH model, including a power-law scaling for the shrinkage. Section IV provides numerical validation of the theoretical predictions. Section V summarizes the findings and outlines future research directions.

II. PHASE-FIELD EQUATIONS

Modeling multiphase flows with diffuse-interface (phase-field) methods involves capturing a smooth but steep transition zone between immiscible phases using a scalar order parameter. In the following, two widely used formulations in this context are briefly described, each with distinct mathematical properties and physical interpretations.

A. Conservative Allen-Cahn model

The CAC equation for a binary phase system is given by [13]

$$\frac{\partial \phi}{\partial t} + \mathbf{u} \cdot \nabla \phi = \nabla \cdot \left[M \left(\nabla \phi - \frac{4\phi(1-\phi)}{\xi} \mathbf{n} \right) \right]. \quad (1)$$

Here ϕ denotes the order parameter which smoothly varies between phases (e.g., $\phi = 1$ in one phase and $\phi = 0$ in the other), t represents time, and $\mathbf{u}$ is the velocity field. The mobility M is treated as both constant and degenerate in this study (Sec. IV B 3). The parameter ξ characterizes the interface thickness, and the unit normal vector to the interface is defined as

$$\mathbf{n} = \frac{\nabla \phi}{|\nabla \phi|}. \quad (2)$$

The right-hand side (RHS) of Eq. (1) can be decomposed into two terms; the first term represents isotropic diffusion,

while the second term acts as a compression mechanism that maintains interface sharpness during advection.

B. Cahn-Hilliard model

The CH equation is derived from the minimization of a free-energy functional and can be written as [2]

$$\frac{\partial \phi}{\partial t} + \mathbf{u} \cdot \nabla \phi = \nabla \cdot (M \nabla \mu), \quad (3)$$

where μ is the chemical potential and is supposed to be constant at the equilibrium. The variational derivative of the total free energy to the order parameter defines the chemical potential

$$\mu = \frac{\delta \mathcal{F}}{\delta \phi} = \frac{\partial F_0}{\partial \phi} - \kappa \nabla^2 \phi, \quad (4)$$

where the free-energy functional $\mathcal{F}$ for a binary system Ω is

$$\mathcal{F} = \int_{\Omega} \left(F_0(\phi) + \frac{\kappa}{2} |\nabla \phi|^2 \right) d\Omega, \quad (5)$$

with $F_0(\phi)$ the bulk free energy which is typically modeled as a double-well potential $F_0(\phi) = \beta \phi^2 (1 - \phi)^2$ for a $\phi \in [0, 1]$ system. In these equations $\beta = 12\sigma/\xi$ and the gradient energy coefficient $\kappa = 3\sigma\xi/2$, with σ the surface tension between the two phases.

Comparing the RHSs of Eqs. (1) and (3), we observe that the two formulations are governed by fundamentally different mechanisms. In particular, the CH equation involves higher-order spatial derivatives, resulting in different mathematical properties compared to the CAC equation.

III. DROPLET SHRINKAGE ANALYSIS

Yue *et al.* [5] were the first to systematically analyze droplet shrinkage within the CH phase-field model. For a quiescent circular droplet, they derived the initial change in droplet radius as

$$\frac{\delta r}{r_0} = -\frac{1}{48} \left(\frac{V}{V_0} \right) \left(\frac{\xi}{r_0} \right), \quad (6)$$

where r denotes the droplet radius, with subscript 0 indicating the initial value, $V_0 = \pi r_0^2$ is the initial droplet volume in a two-dimensional (2D) domain, and V is the total volume of the computational domain. They also identified a critical radius r_c below which droplets are predicted to vanish completely over time:

$$r_c = \left(\frac{\sqrt{3}}{16\pi} \xi V \right)^{1/3}. \quad (7)$$

Zheng *et al.* [6] investigated the same phenomenon in the context of the lattice Boltzmann method for nonideal gases, which exhibits dynamics similar to those of the CH model. For a quiescent circular droplet with initial radius r_0 in a domain of volume V , they demonstrated that energy minimization leads to droplet shrinkage consistent with the analysis of Yue *et al.* [5].

As discussed in Refs. [5,6], droplet shrinkage in the CH model originates from its thermodynamic structure. In a finite domain, the system can reduce its total free energy by

slightly shrinking the interface (reducing interfacial energy) while incurring only a small penalty in bulk free energy due to slight deviations in the phase-field variable from equilibrium values. This trade-off leads to a nonzero shrinkage rate, which increases with the ratio of the interface thickness to the droplet radius (ξ/r_0) and the domain-to-droplet volume ratio (V/V_0).

In this study, we demonstrate mathematically that a curvature term present in the Laplacian term in the chemical potential term in Eq. (4) primarily drives this shrinkage. In contrast, in the free curvature-driven AC equation [12,13], this curvature-driven term is exactly canceled out by a term embedded in the normal vector term [last term on the RHS of Eq. (1)], eliminating the shrinkage behavior.

Since the primary focus of this study is on droplet shrinkage, we formulate our analysis by assuming a circular interface and adopting a polar coordinate system to exploit the geometric symmetry of the problem. This approach simplifies the mathematical treatment while preserving the essential physics of interface dynamics. The analysis can be extended to Cartesian coordinates if needed. Furthermore, angular variations are neglected, assuming axisymmetry. Under these assumptions, the Laplacian operator, which appears in both the CAC and CH models, takes the following form in polar coordinates:

$$\nabla^2 \phi = \frac{\partial^2 \phi}{\partial r^2} + \frac{1}{r} \frac{\partial \phi}{\partial r}. \quad (8)$$

The second term ($1/r)(\partial\phi/\partial r)$ serves as a curvature-induced driving force, as will be shown in the following. This term also appears in axisymmetric equations and becomes more pronounced for smaller radii, which continuously results in mass violation even in conservative phase-field models [20].

For the analysis, we consider a circular droplet with a phase-field profile approximated by a hyperbolic tangent

$$\phi(r) = \frac{1}{2} \left[1 - \tanh \left(\frac{2(r - r_I)}{\xi} \right) \right], \quad (9)$$

where $\phi = 1$ inside the droplet and $\phi = 0$ outside. The interface location r_I is decided where $\phi = 1/2$. This interface profile emerges as a natural solution to the equilibrium equations and has been widely utilized in the phase-field method [2]. Considering the above interface profile, we compute the derivatives required in the Laplacian operator (8). Defining $\chi = 2(r - r_I)/\xi$, the first derivative is

$$\frac{\partial \phi}{\partial r} = -\frac{1}{\xi} \text{sech}^2(\chi) \quad (10)$$

and its second derivative is

$$\frac{\partial^2 \phi}{\partial r^2} = \frac{4}{\xi^2} \text{sech}^2(\chi) \tanh(\chi). \quad (11)$$

At the interface $r = r_I$, we obtain $\partial\phi/\partial r = -1/\xi$ and $\partial^2\phi/\partial r^2 = 0$. Substituting into Eq. (8), the Laplacian at the interface simplifies to

$$\nabla^2 \phi(r_I) = \frac{\partial^2 \phi}{\partial r^2} \Big|_{r_I} + \frac{1}{r_I} \frac{\partial \phi}{\partial r} \Big|_{r_I} = -\frac{1}{r_I \xi}. \quad (12)$$

This term was also observed in studies such as [21,22], however, then in the context of changes to solid structures, e.g., alloy solidification and crystal growth.

This curvature-driven term, which is nonzero and inversely proportional to the droplet radius, is the primary driver of droplet shrinkage in the CH model. In contrast, the CAC formulation precisely cancels this term through the contribution of the normal vector, thereby stabilizing the droplet's shape and size. As will be demonstrated below, when using the interface profile given in Eq. (9), the RHS of Eq. (1) vanishes for all r values.

A. CAC model

The CAC equation is given in Eq. (1). For a circular interface without variation in the angular direction $\mathbf{n} = \pm \hat{r}$, where $\hat{r}$ is the unit normal vector in the radial direction. The sign depends on whether ϕ increases or decreases with r , which, for the present study, with the convention $\phi = 1$ inside and $\phi = 0$ outside, the normal vector is given by $\mathbf{n} = -\hat{r}$. Assigning $\phi = 1$ outside the droplet (and $\phi = 0$ inside the droplet) does not affect the results.

It should be noted that, unlike the CH model, the CAC model does not involve the minimization of a free-energy functional. Nevertheless, similar to the RHS of the CH equation, the CAC equation includes a second-order gradient of ϕ , which can be interpreted as arising from a pseudochemical potential. However, to prevent potential misinterpretations of its physical significance, we refer to it as the effective source term, defined as

$$S_{\text{eff}} = -\nabla \cdot \left(\nabla \phi - \frac{4\phi(1-\phi)}{\xi} \mathbf{n} \right). \quad (13)$$

With this source term, the CAC equation (1) can be rewritten as

$$\frac{\partial \phi}{\partial t} + \mathbf{u} \cdot \nabla \phi = -MS_{\text{eff}}. \quad (14)$$

The negative sign in the above definition is chosen to match the sign of the Laplacian term in the CH model, ensuring consistency for comparison purposes.

For a circular interface with a phase field given by Eq. (9), the effective source term in the polar coordinate system becomes

$$S_{\text{eff}} = -\left(\frac{\partial^2 \phi}{\partial r^2} + \frac{1}{r} \frac{\partial \phi}{\partial r} \right) - \frac{4}{\xi} (1 - 2\phi) \frac{\partial \phi}{\partial r} - \frac{4\phi(1-\phi)}{\xi} \frac{1}{r}, \quad (15)$$

where $\nabla \phi \cdot \mathbf{n} = -\partial\phi/\partial r$ and $\nabla \cdot \mathbf{n} = -1/r$ have been taken into account. At the interphase region (where $\phi \approx 1/2$), we have $1 - 2\phi \approx 0$ and $\phi(1-\phi) \approx 1/4$. Substituting these values and considering $\partial\phi/\partial r \approx -1/\xi$ and $\partial^2\phi/\partial r^2 \approx 0$ at $r = r_I$ for the equilibrium profile of Eq. (9), we have

$$S_{\text{eff}}(r_I) \approx -\frac{\partial^2 \phi}{\partial r^2} \Big|_{r_I} + \frac{1}{r_I} \left(-\frac{\partial \phi}{\partial r} \Big|_{r_I} - \frac{1}{\xi} \right) = 0. \quad (16)$$

The evaluation at $r = r_I$ is motivated by the fact that droplet shrinkage is driven by interfacial dynamics rather than bulk behavior. As will be demonstrated in Sec. IV, there is no driving force for shrinkage in the bulk regions.

This result shows that the normal vector term [last term in Eq. (1)] introduces the correction term $\nabla \cdot \mathbf{n}$ that exactly cancels the curvature term in the Laplacian term which resembles

the standard Laplace pressure (proportional to $1/r_I$) as will be shown later. Appendix A shows that the RHS of the above equation for the interface profile given by Eq. (9) is equal to zero at any r . In contrast, the curvature contribution embedded in the Laplacian term remains present in the CH model, as demonstrated below.

It should be noted that the above discussion is still valid in 3D domains. For spherical droplets, the Laplacian becomes $\nabla^2\phi = \partial^2\phi/\partial r^2 + (2/r)\partial\phi/\partial r$, with the curvature factor of 2 [vs 1 for two dimensions as seen in Eq. (8)]. The phase-field profile is the same as a circular one, i.e., Eq. (9). As such, $\nabla \cdot \mathbf{n} = -2/r$ and $S_{\text{eff}}(r_I) = 0$ for a spherical interface.

B. CH model

In the CH equation, the equilibrium profile of an interface, e.g., a droplet, is determined such that the energy (5) is minimized. The chemical potential (4) is given in polar coordinates as [2]

$$\mu = \frac{\partial F_0}{\partial \phi} - \kappa \left(\frac{\partial^2 \phi}{\partial r^2} + \frac{1}{r} \frac{\partial \phi}{\partial r} \right). \quad (17)$$

As will be shown in Sec. IV, the chemical potential is zero in the bulk and nonzero in the interface. Therefore, we define an average equilibrium chemical potential

$$\mu_{\text{eq}} = \int_0^1 \mu d\phi = - \int_{r_I-\varepsilon}^{r_I+\varepsilon} \mu \frac{\partial \phi}{\partial r} dr, \quad (18)$$

where μ_{eq} is in the interphase region, i.e., from $r = r_I - \varepsilon$ (where $\phi \approx 1$) to $r = r_I + \varepsilon$ (where $\phi \approx 0$), and ε is of the order of the interface thickness. Considering the equilibrium condition, by multiplying Eq. (17) with $\partial\phi/\partial r$ and integrating it from $r_I - \varepsilon$ to $r_I + \varepsilon$, we have

$$-\mu_{\text{eq}} = \int_{r_I-\varepsilon}^{r_I+\varepsilon} \frac{\partial F_0}{\partial \phi} \frac{\partial \phi}{\partial r} dr - \kappa \int_{r_I-\varepsilon}^{r_I+\varepsilon} \left(\frac{\partial^2 \phi}{\partial r^2} + \frac{1}{r} \frac{\partial \phi}{\partial r} \right) \frac{\partial \phi}{\partial r} dr. \quad (19)$$

The first term on the RHS becomes

$$\int_{r_I-\varepsilon}^{r_I+\varepsilon} \frac{\partial F_0}{\partial \phi} \frac{\partial \phi}{\partial r} dr = - \int_0^1 \frac{\partial F_0}{\partial \phi} d\phi = F_0(0) - F_0(1) = 0 \quad (20)$$

as F_0 is zero in the bulk regions. The second term on the RHS of Eq. (19) is composed of two parts. The first part is

$$\kappa \int_{r_I-\varepsilon}^{r_I+\varepsilon} \frac{\partial^2 \phi}{\partial r^2} \frac{\partial \phi}{\partial r} dr = \frac{\kappa}{2} \int_{r_I-\varepsilon}^{r_I+\varepsilon} \frac{\partial}{\partial r} \left(\frac{\partial \phi}{\partial r} \right)^2 dr = 0 \quad (21)$$

due to the symmetry of $\partial\phi/\partial r$ around r_I as given by Eq. (10). The second part is

$$\kappa \int_{r_I-\varepsilon}^{r_I+\varepsilon} \frac{1}{r} \left(\frac{\partial \phi}{\partial r} \right)^2 dr \approx \frac{\kappa}{r_I} \int_{r_I-\varepsilon}^{r_I+\varepsilon} \left(\frac{\partial \phi}{\partial r} \right)^2 dr, \quad (22)$$

where we approximated $1/r$ to be constant as $\varepsilon \ll r_I$. The above equation is similar to the definition of surface tension σ in the phase-field model. For a planar interface, it is defined as [2]

$$\sigma = \kappa \int_{-\infty}^{\infty} \left(\frac{\partial \phi}{\partial r} \right)^2 dr \approx \kappa \int_{r_I-\varepsilon}^{r_I+\varepsilon} \left(\frac{\partial \phi}{\partial r} \right)^2 dr, \quad (23)$$

where the last term is the approximation for a curved interface.

Combining Eqs. (20)–(23), Eq. (19) reduces to

$$\mu_{\text{eq}} = \frac{\kappa}{r_I} \int_{r_I-\varepsilon}^{r_I+\varepsilon} \left(\frac{\partial \phi}{\partial r} \right)^2 dr = \frac{\sigma}{r_I}. \quad (24)$$

As can be seen, at equilibrium the value of μ_{eq} resembles the Laplace pressure ($\Delta p_{\text{CH}} = \sigma/r_I$). This term directly arises from the curvature term $(1/r)(\partial\phi/\partial r)$ in the Laplacian operator (8) during the derivation, without any other assumptions. This derivation establishes a direct link between curvature-induced pressure and droplet shrinkage, which emerge from the free energy $\mathcal{F}$.

The complete balance in the RHS of the CAC model explains why this model prevents droplet shrinkage: The key mathematical insight is that in CH models, the curvature term $(1/r)(\partial\phi/\partial r)$ creates a chemical potential gradient proportional to $1/r$ that is a driving force for shrinkage. In contrast, the CAC model possesses a normal vector term that generates a contribution exactly equal and opposite to this curvature effect, resulting in zero net driving force for shrinkage. Therefore, with a similar analysis to the CH model, one can say that the net pressure difference caused by the CAC model across the interface becomes zero, i.e., $\Delta p_{\text{CAC}} = 0$, regardless of droplet radius.

This cancellation in the CAC model is local and theoretically exact. It also does not depend on the size of the domain V or interface thickness ξ . Also, since there is no driving force for shrinkage in the CAC model, there is no critical radius in the same sense as in the CH model. Droplets of any size above the interface resolution limit can be stably maintained due to the local fundamental balance mechanism rather than the global one, which creates a pointwise cancellation of the curvature-induced pressure at every point along the interface. This is consistent with our observation in Refs. [15–17], where small droplets and bubbles with radii comparable to the interface thickness do not shrink. The only practical limitation with a minimum radius in the CAC model is the need to adequately resolve the interface. As shown in the next section, to have the theoretical bulk values of the order parameter across the interface, a minimum radius comparable to the interface thickness should be considered.

Power-law scaling of shrinkage

As established above, the chemical potential gradient at the interface creates a curvature-driven flux that leads to the droplet shrinkage. In this section we derive the temporal evolution of the droplet radius. We will show that this temporal evolution leads to a scaling law for the droplet shrinkage.

Starting from the CH equation (3), for a quiescent droplet ($\mathbf{u} = 0$) we have

$$\frac{\partial \phi}{\partial t} = M \nabla^2 \mu. \quad (25)$$

The total mass of the droplet is defined as (considering the droplet density is $\rho = 1$)

$$m(t) = \int_{\Omega} \phi dV. \quad (26)$$

Taking the time derivative, invoking Eq. (25), and applying the divergence theorem yields

$$\frac{dm}{dt} = \int_{\Omega} \frac{\partial \phi}{\partial t} dV = M \int_{\partial \Omega} \frac{\partial \mu}{\partial r} dA. \quad (27)$$

The chemical potential gradient at the interface can be obtained based on Eq. (B3). For a circular droplet with the initial radius of r_0 , we have

$$\left. \frac{\partial \mu}{\partial r} \right|_{r_I} \approx -C \frac{\sigma}{3r_I^2}, \quad (28)$$

where C is a constant to account for the mismatch in thermodynamic driving force between two phases [23] when $r_0 < r_c$, which is different from the equilibrium one when $r_0 > r_c$. The value of C will be determined through numerical simulations, with its equilibrium value predicted to be $9/2$ based on Eq. (B13). The derivation of the above relation is shown in Appendix B. This relation reveals that the shrinkage rate is inversely proportional to the droplet radius, implying that smaller droplets dissolve faster.

Considering that $\phi = 1$ inside the droplet, the mass of the droplet is $m = \pi r_I^2 \rho$ and $\partial \Omega = 2\pi r_I$ in 2D domains, and with $\rho = 1$ Eq. (27) simplifies to

$$2\pi r_I \frac{dr_I}{dt} = M \frac{\partial \mu}{\partial r} 2\pi r_I. \quad (29)$$

Invoking Eq. (28) in the above equation yields

$$r_I^3(t) = r_0^3 - CM\sigma t \quad (30)$$

or equivalently

$$r_I(t) = \sqrt[3]{r_0^3 - CM\sigma t}. \quad (31)$$

In contrast to the classical d^2 law observed in quasisteady evaporation in which $r_I(t) = \sqrt{r_0^2 - C't}$ [24], the present system follows a shrinkage exponent of $1/3$, which we call a d^3 law in this study. The droplet completely vanishes when $r_I(t_f) = 0$, giving the final dissolution time

$$t_f = \frac{r_0^3}{CM\sigma}. \quad (32)$$

Unlike the initial shrinkage [Eq. (6)] and the critical radius [Eq. (7)], the shrinkage rate depends on the mobility M and the surface tension σ . Increasing either parameter accelerates the disappearance. This dependence provides a physical basis for understanding how material properties influence the severity of the shrinkage problem in practical simulations.

In the following section, some comments on the values of C will be made.

IV. NUMERICAL VALIDATION

In this section we investigate our analysis for the CH and CAC models using two benchmarks.

A. Theoretical interface

In the first benchmark, to verify the analysis presented in Sec. III, the distribution of the RHS of both phase-field models is evaluated using identical interfaces in the r direction: a circular droplet with radius $r_0 = 10$ with interface thickness

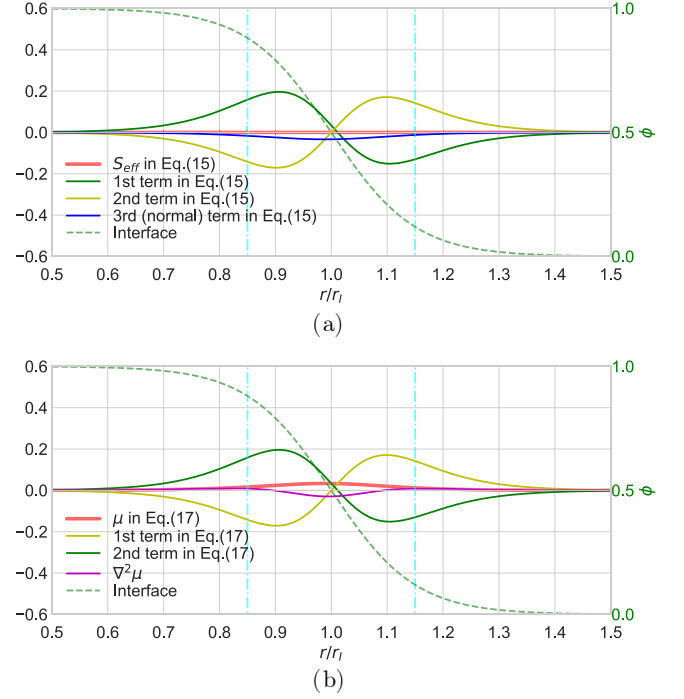


FIG. 1. Radial profiles of the RHS terms of the phase-field equations for (a) the CAC model and (b) the CH model, evaluated using the same input interface. Two cyan vertical lines correspond to $1 \pm \xi/2r_0$.

$\xi = 3$ and $M = 1$. The interface profile is defined by Eq. (9). The other parameter is selected as $\sigma = 2/9$ to make the coefficient of the Laplacian term for both models the same (κ becomes unity for the CH model).

Figure 1 presents the radial distribution of the RHS terms in both the CAC model [Eq. (15)] and the CH model [Eq. (17)]. The Laplacian of the chemical potential, $\nabla^2 \mu$, for the CH model is also shown, as derived in Appendix B. As evident from the figure, the sum of all RHS terms in the CAC model vanishes across the entire domain (red line), indicating the absence of any net driving force for droplet shrinkage. This behavior persists regardless of the droplet radius r_0 or the interface thickness ξ , thereby validating both the theoretical predictions and numerical results.

In contrast, the CH model exhibits a nonuniform profile in the sum of the RHS terms (red line), consistent with Eq. (24). The curvature of the interface generates a nonzero gradient in the chemical potential near the interfacial region, which acts as a driving force for droplet shrinkage. Notably, in the CH model, the two dominant contributions (represented by the yellow and green lines) largely cancel each other in the bulk but not near the interface, where curvature effects dominate. A similar partial cancellation is observed in the CAC model. However, the CAC formulation includes an additional correction term (shown by the blue line), which precisely compensates for the curvature-induced imbalance in the interfacial region.

This comparison highlights the fundamental difference between the two models: While the CH model evolves toward thermodynamic equilibrium via curvature-driven diffusion,

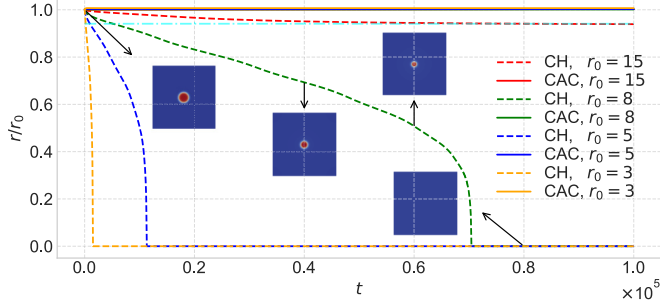


FIG. 2. Time evolution of the dimensionless droplet radius for the CAC and CH models at different initial radii r_0 . The simulation parameters are $\xi = 3$, $L_0 = 100$, and $r_c = 10.33$. Insets represent the droplet with the initial radius of $r_0 = 8$ at different times for the CH model. The cyan horizontal dash-dotted line corresponds to $\delta r/r_0 = 0.059$ based on Eq. (6) for $r_0 = 15$.

the CAC model enforces a local geometric force balance that stabilizes the interface.

B. Droplet shrinkage

1. Comparing CH and CAC models

In this section we employ two lattice Boltzmann (LB) models to solve the CAC [Eq. (1)] and CH [Eq. (3)] equations. Details of these LB implementations can be found in Refs. [17, 25] for the CAC and CH models, respectively, and are not repeated here for the sake of brevity.

Simulations are performed in a square domain of size $L_0 \times L_0$ with $L_0 = 100$. Droplets with different initial radii r_0 are initialized using the phase-field profile given by Eq. (9). The interface thickness is set to $\xi = 3$, and based on Eq. (7), the critical radius is approximately $r_c \approx 10.11$. Periodic boundary conditions are applied in all directions. Other parameters are $M = 0.02/\beta$ and $\sigma = 0.001$. Figure 2 plots the time evolution of the dimensionless droplet radius for both models.

The numerical results corroborate our analytical findings on the fundamental distinctions between the two models. The CH model exhibits the expected shrinkage behavior, in correspondence with the results of Yue *et al.* [5] and Zheng *et al.* [6]. This phenomenon originates from the curvature-dependent term in the chemical potential. For a droplet with $r_0 > r_c$ (case of $r_0 = 15$), an initial shrinkage happens and the droplet reaches a different equilibrium radius as $r_0 - \delta r$, with $\delta r/r_0 = 0.059$ computed by Eq. (6), shown by the horizontal cyan line in Fig. 2. When droplets are initialized with $r_0 < r_c$ (cases of $r_0 = 8, 5$, and 3), the system evolves toward complete dissolution (the green, blue, and yellow lines, respectively).

In contrast, the CAC simulations demonstrate strong stability, maintaining the droplet radius over time regardless of the initial size. This behavior confirms that a term embedded in the normal vector correction term effectively cancels the curvature-driven component of the Laplacian term. As a result, no driving force forms across the interface, and mass flux is suppressed. This balance leads to conservation of droplet shape and volume over extended simulation times.

We extended the analysis to smaller droplets with radii $r_0 = 2$ and 1 and observed that the droplets remained stable

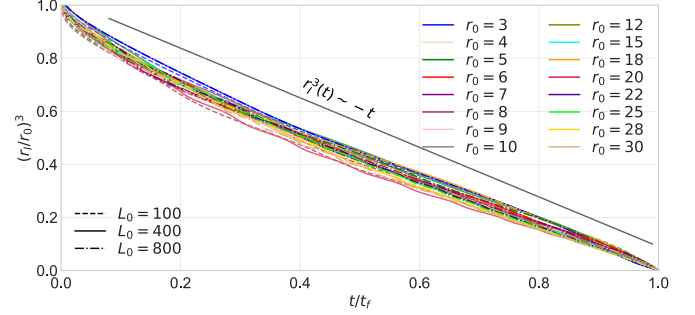


FIG. 3. Comparison of the theoretical prediction (solid line) with the numerical simulation results of Fig. 2 (dashed lines) for droplet radius evolution for the CH model. The theoretical curve is based on Eq. (31).

over time. This verifies the theoretical prediction that the CAC model does not impose a critical radius for droplet stability, in contrast to the CH model. As illustrated in Fig. 1, the order parameter ϕ retains values close to its bulk limits (0 and 1) at positions $r = r_0 \pm \xi/2$ (shown by two vertical cyan lines), indicating that the interface remains almost well defined even for small droplets with the radii equal to the interface thickness. However, when the droplet radius becomes smaller than the interface thickness, the transition region dominates the domain, and the bulk value of the order parameter deviates significantly from its theoretical limits of 0 or 1 for the inside of the interface. This effect is particularly evident for very small droplets, where the interface essentially spans the entire droplet. The hyperbolic tangent function is close to 1 at values larger than 2 and, equivalently, close to -1 at values smaller than -2 . From Eq. (9) we see that the order parameter ϕ retains values close to its bulk limits (0 and 1) when $|2(r - r_l)/\xi| \geq 2$; thus ϕ is close to its bulk values of 0 and 1 when $r = r_l \pm \xi$. This affects the minimum number of grid points needed to resolve the interface. Its value could be affected by the chosen numerical solvers. This constraint ensures a clear separation between bulk and interfacial regions and preserves the physical interpretation of the order parameter.

2. Radius-time scaling of shrinkage

To further validate the droplet shrinkage mechanism in the CH model, we compare the numerical simulation results (Fig. 2) with the theoretical prediction $r_l^3(t) \propto -t$ derived in Sec. III B 1.

Figure 3 presents a direct comparison between theoretical prediction [Eq. (31)] and numerical simulation results for droplets with initial radii below the critical radius within domains of different sizes: $L_0 = 100$ (with critical radius of $r_c \approx 10.11$), $L_0 = 400$ ($r_c \approx 25.48$), and $L_0 = 800$ ($r_c \approx 40.44$). For each case, the disappearance time t_f is determined as the time at which the droplet radius becomes zero. As shown in Fig. 3, fair agreement is observed between the theoretically predicted form of $r_l^3(t) \sim -t$ and the simulation results throughout the entire shrinkage process. This confirms that the curvature-driven diffusion mechanism, originating from the Laplacian term in Eq. (8), is indeed the dominant driving force for droplet shrinkage in the CH model. We observe some discrepancies with the power law in Fig. 3, particularly during

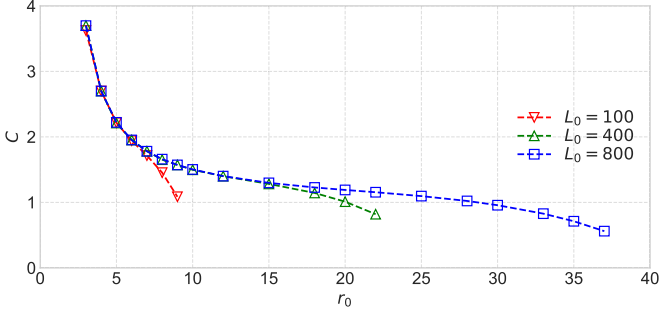


FIG. 4. Variation of the proportionality constant C in the radius-time scaling relation (32) for three different domain sizes. The interface thickness is $\xi = 3$ for all cases. As can be seen, for all droplets with $r_0 < r_c$, there is a droplet disappearance time.

early times. The phase-field initialization induces an initial period of rapid shrinkage. This artifact parallels observations in other physical systems, such as the d^2 law in evaporating droplets [24]. Additionally, the theoretical derivation assigns $\phi = 1$ uniformly within the droplet, while the numerical simulations inherently feature a diffuse interface with continuous ϕ variations near the interface and characteristic overshooting and undershooting in the bulk regions [26]. The finite computational domain, combined with discretization errors in both spatial and temporal dimensions, further contributes to deviations from the idealized theoretical predictions.

Figure 4 presents the variation of C as a function of initial droplet radius for three different domain sizes. The interface thickness is fixed at $\xi = 3$ for all cases. Several important trends emerge from this analysis.

Different values for C are primarily due to the resolution. For example, for the case with $r_0 = 3$, the interface thickness ($\xi = 3$) is comparable to the radius (high Cahn number $Cn = \xi/r_0$), while through the theoretical derivation, a sharp interface with a uniform value of ϕ inside the droplet is assumed. As r_0 increases, the interface becomes sharper (smaller Cn) and C approaches a limiting value which is in the range from 1 to 1.5. By approaching the initial radius to the stability threshold r_c , the droplet experiences a diminished thermodynamic driving force, which is reflected in smaller C values (higher t_f).

In summary, for sufficiently large r_0 (but still below r_c), the curves show a tendency toward horizontal asymptotes, suggesting that C approaches a domain-independent constant value when $Cn \ll 1$. The observed trends confirm that droplet shrinkage kinetics in the CH model are influenced by both geometric factors (ξ/r_0) and thermodynamic factors (domain-to-droplet volume ratio V/V_0). The former affects the accuracy of the sharp-interface approximation, while the latter determines the magnitude of the thermodynamic driving force.

3. Constant versus degenerate mobilities

To investigate whether the choice of mobility function affects the fundamental shrinkage behavior observed in the CH model, we performed additional simulations where we replaced the constant mobility term $M = M_0$ with a degenerate mobility of the form $M_\phi = 4M_0|\phi||1 - \phi|$ as proposed by Ref. [27]. The constant of 4 is to ensure that its

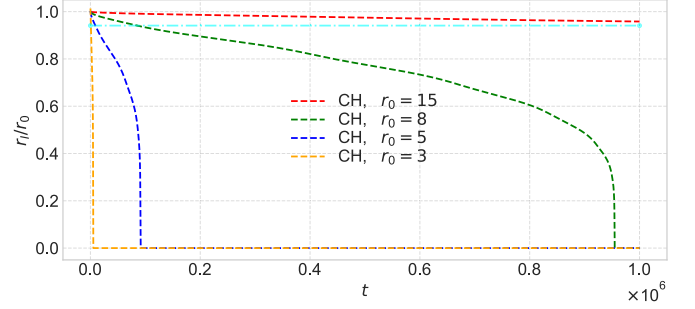


FIG. 5. Time evolution of the dimensionless droplet radius for the CH model with the degenerate mobility M_ϕ at different initial radii r_0 . The simulation parameters are $\xi = 3$, $L_0 = 100$, and $r_c = 10.33$. The cyan horizontal dash-dotted line corresponds to $\delta r/r_0 = 0.059$ based on Eq. (6) for $r_0 = 15$. Compared to Fig. 2, the degenerate form significantly extends the timescale but does not prevent eventual disappearance.

maximum value is identical to M_0 . This degenerate form, used in phase-field simulations [27,28], ensures that diffusion is suppressed in the bulk phases (where $\phi \approx 0$ or 1) and is active primarily near the interface (where $\phi \approx 1/2$). Figure 5 presents the time evolution of the dimensionless droplet radius for four initial radii ($r_0 = 3, 5, 8$, and 15) using the degenerate mobility M_ϕ . The simulation parameters are identical to those used in Fig. 2, yielding the same critical radius of $r_c \approx 10.11$ from Eq. (7).

Similar to the previous results for the constant mobility, we expect that for the radii less than the critical value, the shrinkage happens regardless of the mobility function. As can be seen in Fig. 5, the degenerate mobility significantly slows the mass redistribution process, extending the dissolution timescale by approximately one order of magnitude for the case. This behavior can be understood through the energy dissipation equation. Multiplying the CH equation (3) by μ and employing the divergence theorem and integrating over the domain yields

$$\frac{d\mathcal{F}}{dt} = - \int_{\Omega} M_\phi |\nabla \mu|^2 d\Omega \leq 0. \quad (33)$$

The negative sign ensures that the free energy $\mathcal{F}$ decreases toward its minimum. The mobility determines the rate of this energy dissipation (i.e., how fast the system approaches the equilibrium) but does not alter the equilibrium state itself. Therefore, the critical radius r_c and the initial shrinkage δr derived in Refs. [5,6] remain valid for any positive mobility function, whether constant or degenerate.

Comparing Eq. (17) with Eq. (15), one may add a term to the RHS of Eq. (17) to counteract the additional term appearing in the Laplacian term. While this could suppress the shrinkage behavior, it will interfere with the physics of the free energy.

4. Effect of solid boundaries

The analysis presented in the previous sections focused on interfaces suspended in bulk phase domains. In many practical applications, however, droplets and bubbles rest on solid surfaces, raising the question of how the presence of solid

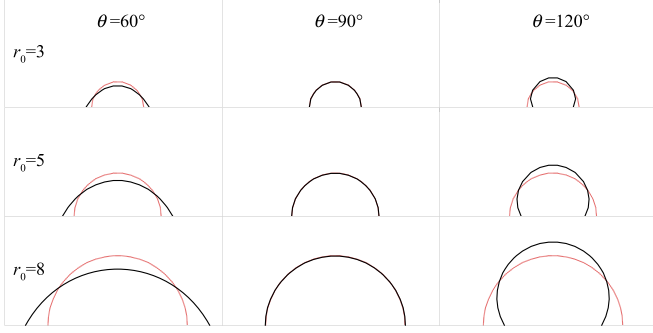


FIG. 6. Interface profile of a sessile droplet at $t = 0$ (red dashed line) and $t = 10^5$ (black solid line) for the CH model with different contact angles $\theta = 60^\circ$ (left column), $\theta = 90^\circ$ (middle column), and $\theta = 120^\circ$ (right column). The initial radii are $r_0 = 3$ (top row), $r_0 = 5$ (middle row), and $r_0 = 8$ (bottom row).

boundaries affects the shrinkage behavior. In the present study we extend our analysis to interfaces in contact with solid boundaries for the CAC model with various contact angles and initial droplet radii. It should be noted that the effects of the solid boundaries on the shrinkage for the CH model are investigated by Zheng *et al.* [6] and are not repeated for the sake of brevity. That study showed that the effects of the contact angle are only on the initial volume, while the shrinkage δr and critical radius r_c are still valid and similar to Eqs. (6) and (7).

For a sessile droplet on a solid surface, the geometry differs from a complete circular droplet, but the fundamental physics remains unchanged. Consider a 2D droplet on a horizontal solid surface with contact angle θ (measured through the liquid phase). The droplet forms a circular segment with the radius of the curvature r_0 and the base width $2r_0 \sin \theta$. The key insight is that a sessile droplet is simply a section of a circular droplet, bounded by the solid surface. Therefore, the interfacial profile along the radial direction still follows Eq. (9). The sessile droplet volume is now given by

$$V_0 = r_0^2 \left(\theta - \frac{\sin(2\theta)}{2} \right), \quad (34)$$

with θ given in radians. The effective source term given by Eq. (15) remains valid along any radial direction away from the solid surface as the local curvature-driven mechanism is unchanged. At the interphase we therefore still have $S_{\text{eff}}(r_I) \approx 0$.

To validate these theoretical predictions, we perform simulations of sessile droplets with contact angles $\theta = 60^\circ$, 90° , and 120° for the CAC model. The computational domain is $L_0 \times L_0/2$ with $L_0 = 100$. The rest of the parameters are the same as those of Fig. 2. The solid surface is located at the bottom and top boundaries with a no-flux condition for the phase field and appropriate wetting boundary conditions to maintain the prescribed contact angle. The side boundaries are treated as periodic. Details on the wetting boundary conditions can be found in Ref. [29]. Initially, a half droplet with initial radii of $r_0 = 3$, 5 , and 8 is placed on a solid surface with its center at $(1, L_0/2)$. The initial contact angle is therefore 90° .

Figure 6 presents snapshots of the droplet at the initial and equilibrium states. The CAC simulations demonstrate that

droplets keep their volume over extended simulation times regardless of the contact angle and initial radius, confirming that the local balance mechanism in Eq. (16) prevents shrinkage. This represents a significant practical advantage of understanding the local balance mechanism, as it provides confidence that CAC models will maintain their antishrinkage properties even in complex geometries with solid contacts, which are ubiquitous in real applications such as multiphase flow in porous media.

V. CONCLUSION

In this paper we analyzed the conservative Allen-Cahn model for phase-field simulations and demonstrated its ability to overcome the droplet shrinkage problem that affects the Cahn-Hilliard models. The CAC equation offers significant advantages over the CH equation for multiphase flow simulations involving numerous interfaces with varying curvatures, such as multiphase fluid flow in porous media. The CAC model preserves droplets of any size above the interface thickness through a local geometric balance at the interface. Unlike the CH model, where droplet shrinkage is proportional to $(V/V_0)(\xi/r_0)$ with a critical radius $r_c \propto (\xi V)^{1/3}$, the CAC model maintains original droplet size without radius limitations. In CH models, the curvature term $(1/r)(\partial\phi/\partial r)$ creates a chemical potential gradient, causing shrinkage. In the CAC model, however, the $\mathbf{V} \cdot \mathbf{n}$ term counterbalances this curvature effect, resulting in no driving force for shrinkage. We also considered the effects of degenerate mobility. Our simulations confirm that droplet shrinkage in the CH model is a fundamental consequence of the underlying thermodynamic energy functional. The mobility function governs the kinetics of interface evolution, but does not alter the equilibrium predictions.

It was shown that for the droplets below the critical radius, the droplet radius follows a d^3 law of the form $r_I^3(t) = r_0^3 - CM\sigma t$, with the disappearance time scaling cubically with the initial radius, i.e., $t_f \propto r_0^3$. This scaling has significant implications for multiscale simulations, as droplets spanning different length scales will disappear at different rates. Also, for interfaces in contact with solid surfaces, the same findings are still valid for the CAC model, and droplets with different initial radii and contact angles do not shrink over time, a property essential in the simulation of multiphase fluid flows in porous media. As part of future work, a remedy is being developed based on the findings of this study to mitigate the droplet shrinkage issue inherent to the CH model. This also includes extending the analysis and simulations to 3D domains to assess the robustness and applicability of the proposed remedy in more realistic geometries.

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DATA AVAILABILITY

The data that support the findings of this article are openly available [30].

APPENDIX A: EVALUATION OF RHS OF EQ. (15)

To show that the RHS of (15) is always equal to zero, we sum all terms on the RHS considering the interface profile is given by Eq. (9), where the first and second gradients are calculated in Eqs. (10) and (11), respectively. By inserting them into Eq. (15), we have

$$S_{\text{eff}} = -\left(\frac{4}{\xi^2} \text{sech}^2(\chi) \tanh(\chi) - \frac{1}{r} \frac{1}{\xi} \text{sech}^2(\chi)\right) - \frac{4}{\xi} [\tanh(\chi)] \left(-\frac{1}{\xi} \text{sech}^2(\chi)\right) - \frac{1}{\xi} \frac{1}{r} [1 - \tanh(\chi)][1 + \tanh(\chi)] = 0, \quad (\text{A1})$$

considering $\tanh^2(\chi) + \text{sech}^2(\chi) = 1$.

APPENDIX B: DERIVATION OF EQ. (28)

In this appendix, the RHS of the CH equation (3) is derived based on the interface profile given by Eq. (9). For a polar coordinate system with the origin at the droplet center, we have no changes in the angle direction, so the Laplacian of the chemical potential is

$$\nabla^2 \mu = \frac{\partial^2 \mu}{\partial r^2} + \frac{1}{r} \frac{\partial \mu}{\partial r}, \quad (\text{B1})$$

with μ defined in Eq. (4). If we model F_0 as the double-well potential $F_0(\phi) = \beta \phi^2(1 - \phi)^2$, then $\partial F_0 / \partial \phi = 2\beta \phi(1 - \phi)(1 - 2\phi)$ and Eq. (4) becomes

$$\mu = 2\beta \phi(1 - \phi)(1 - 2\phi) - \kappa \nabla^2 \phi. \quad (\text{B2})$$

Breaking Eq. (B1) down into components, we have

$$\frac{\partial \mu}{\partial r} = \frac{\partial}{\partial r} [2\beta \phi(1 - \phi)(1 - 2\phi)] - \kappa \frac{\partial}{\partial r} (\nabla^2 \phi), \quad (\text{B3})$$

with the first term as

$$\frac{\partial}{\partial r} [2\beta \phi(1 - \phi)(1 - 2\phi)] = 2\beta \frac{\partial \phi}{\partial r} (1 - 6\phi + 6\phi^2) \quad (\text{B4})$$

and the second term as

$$\begin{aligned} \frac{\partial}{\partial r} (\nabla^2 \phi) &= \frac{\partial}{\partial r} \left(\frac{\partial^2 \phi}{\partial r^2} + \frac{1}{r} \frac{\partial \phi}{\partial r} \right) \\ &= \frac{\partial^3 \phi}{\partial r^3} - \frac{1}{r^2} \frac{\partial \phi}{\partial r} + \frac{1}{r} \frac{\partial^2 \phi}{\partial r^2}. \end{aligned} \quad (\text{B5})$$

The second derivative of the chemical potential is

$$\frac{\partial^2 \mu}{\partial r^2} = \frac{\partial^2}{\partial r^2} [2\beta \phi(1 - \phi)(1 - 2\phi)] - \kappa \frac{\partial^2}{\partial r^2} (\nabla^2 \phi), \quad (\text{B6})$$

with the first term

$$\begin{aligned} &\frac{\partial^2}{\partial r^2} [2\beta \phi(1 - \phi)(1 - 2\phi)] \\ &= 2\beta \left[\frac{\partial^2 \phi}{\partial r^2} (1 - 6\phi + 6\phi^2) + \left(\frac{\partial \phi}{\partial r} \right)^2 (-6 + 12\phi) \right] \end{aligned} \quad (\text{B7})$$

and the second term

$$\frac{\partial^2}{\partial r^2} (\nabla^2 \phi) = \frac{\partial^4 \phi}{\partial r^4} + \frac{1}{r} \frac{\partial^3 \phi}{\partial r^3} - \frac{2}{r^2} \frac{\partial^2 \phi}{\partial r^2} + \frac{2}{r^3} \frac{\partial \phi}{\partial r}. \quad (\text{B8})$$

Finally, the complete expression for the Laplacian of μ in polar coordinates is

$$\begin{aligned} \nabla^2 \mu &= 2\beta \left[\frac{\partial^2 \phi}{\partial r^2} (1 - 6\phi + 6\phi^2) + \left(\frac{\partial \phi}{\partial r} \right)^2 (-6 + 12\phi) \right] \\ &\quad - \kappa \left(\frac{\partial^4 \phi}{\partial r^4} + \frac{1}{r} \frac{\partial^3 \phi}{\partial r^3} - \frac{2}{r^2} \frac{\partial^2 \phi}{\partial r^2} + \frac{2}{r^3} \frac{\partial \phi}{\partial r} \right) \\ &\quad + \frac{1}{r} \left[2\beta \frac{\partial \phi}{\partial r} (1 - 6\phi + 6\phi^2) \right. \\ &\quad \left. - \kappa \left(\frac{\partial^3 \phi}{\partial r^3} - \frac{1}{r^2} \frac{\partial \phi}{\partial r} + \frac{1}{r} \frac{\partial^2 \phi}{\partial r^2} \right) \right]. \end{aligned} \quad (\text{B9})$$

The above derivative terms on the RHS can be easily computed using Eqs. (10) and (11) and

$$\frac{\partial^3 \phi}{\partial r^3} = \frac{8}{\xi^3} [\text{sech}^4(\chi) - 2\text{sech}^2(\chi) \tanh^2(\chi)], \quad (\text{B10})$$

$$\frac{\partial^4 \phi}{\partial r^4} = \frac{64}{\xi^4} \text{sech}^2(\chi) \tanh(\chi) [\tanh^2(\chi) - 2\text{sech}^2(\chi)]. \quad (\text{B11})$$

To obtain the relation in Eq. (28), we evaluate the $\partial \mu / \partial r$. Inserting the terms in Eqs. (B4) and (B5) into the gradient of the chemical potential in Eq. (B3), we have

$$\begin{aligned} \frac{\partial \mu}{\partial r} &= \frac{\partial}{\partial r} [2\beta \phi(1 - \phi)(1 - 2\phi)] - \kappa \frac{\partial}{\partial r} (\nabla^2 \phi) \\ &= 2\beta \frac{\partial \phi}{\partial r} (1 - 6\phi + 6\phi^2) - \kappa \left(\frac{\partial^3 \phi}{\partial r^3} - \frac{1}{r^2} \frac{\partial \phi}{\partial r} + \frac{1}{r} \frac{\partial^2 \phi}{\partial r^2} \right). \end{aligned} \quad (\text{B12})$$

At the interface, i.e., $r = r_I$, we have $\phi \simeq 1/2$ and $\chi = 0$. Based on Eqs. (10), (11), (B10), and (B11), at $r = r_I$ ($\chi = 0$), different gradient orders of the phase field are $\partial \phi / \partial r = -1/\xi$, $\partial^2 \phi / \partial r^2 = 0$, $\partial^3 \phi / \partial r^3 = 8/\xi^3$, and $\partial^4 \phi / \partial r^4 = 0$, respectively. As such, by inserting these terms in the gradient of the chemical potential of Eq. (B12) and using $\beta = 12\sigma/\xi$ and $\kappa = 3\sigma\xi/2$, we have

$$\begin{aligned} \left. \frac{\partial \mu}{\partial r} \right|_{r_I} &= 2 \frac{12\sigma}{\xi} \left(-\frac{1}{\xi} \right) \left(-\frac{1}{2} \right) - \frac{3\sigma\xi}{2} \left(\frac{8}{\xi^3} + \frac{1}{r_I^2} \frac{1}{\xi} \right) \\ &= -\frac{3}{2} \frac{\sigma}{r_I^2} = -\frac{9}{2} \frac{\sigma}{3r_I^2}. \end{aligned} \quad (\text{B13})$$

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