Bubbles Interactions in the Cahn-Hilliard Equation

H. Calisto,[2] M. Clerc,[1] R. Rojas,[2,3] and E. Tirapegui[4]

[1]Institut Non Linéaire de Nice, UMR 6618 CNRS-UNSA, 1361 Route des lucioles, F-065600 Valbonne, France
[2]Centro de Física No Lineal y Sistemas Complejos de Santiago, Casilla 27122 Correo 27, Santiago, Chile
[3]Facultad de Ciencias Físicas y Matemáticas, Departamento Ingeniería Matemáticas, Universidad de Chile, Casilla 487-3, Santiago, Chile
[4]Facultad de Ciencias Físicas y Matemáticas, Departamento Físicas, Universidad de Chile, Casilla 487-3, Santiago, Chile

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We study the dynamics of bubbles in the one dimensional Cahn-Hilliard equation. For a gas of diluted bubbles we find ordinary differential equations describing their interaction which permits us to describe the ulterior dynamics of the system in very good agreement with numerical simulations.

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The spatiotemporal evolution of macroscopic systems can be described by partial differential equations (PDE). A successful strategy to study PDE is to look for particle or defectlike types of solutions [1–7] which have the property of being localized in space. If after some transient a solution consisting of a certain number of these localized solutions is established, we can describe the ulterior dynamics of the system through the evolution of these solutions due to their mutual interactions, and this evolution turns out to be determined in many cases by ordinary differential equations (ODE) [2,3]. We see then that in this way we can have a simplified description with ODE of the physical phenomenons occurring in the system [1–7]. We shall use here this strategy to study the dynamics of the one dimensional Cahn-Hilliad equation [8] which describes the dynamics of phase separation in conservative systems. Some examples are binary alloys [8], crystal growth between two competing thermodynamic phases [9], and the facets dynamics of the Ising wall in liquid crystals [10]. Our aim will be to identify the particlelike solutions of the one dimensional Cahn-Hilliard equation and to study their interactions in order to describe the ulterior dynamics of the system.

The universal equation which describes in two spatial dimensions the interface between two symmetric states is a simple diffusion equation. However, when the diffusion coefficient ε becomes small, positive or negative, one has to consider other kinds of terms and the equation becomes [10]

$$\partial_t P = \varepsilon P_{xx} + 3P_x^2 P_{xx} - P_{xxxx}, \tag{1}$$

where $P(x,t)$ is the curve representing the interface, x is the variable which parametrizes the interface, $P_x^2 P_{xx}$ is a nonlinear diffusion, and the last term can be interpreted as a hyperdiffusion. The signs in (1) have been chosen to saturate the instability, and from now on we shall be interested in the case $\varepsilon < 0$. Equation (1) is a continuity equation which expresses the conservation of the area under the curve $P(x,t)$, a property which is a consequence of the fact that the interface connects two symmetric states. Moreover, one has that Eq. (1) is variational, i.e., it can be written in the form

$$\partial_t P = -\frac{\delta \mathcal{F}}{\delta P},$$
$$\mathcal{F}[P] = \int dx \left\{ \varepsilon \frac{P_x^2}{2} + \frac{P_x^4}{4} + \frac{P_{xx}^2}{2} \right\}, \tag{2}$$

where the "free energy" $\mathcal{F}$ depends only on the derivatives of P. We introduce the variable $u \equiv P_x$ which is a more classic order parameter ($u \ll 1$). In terms of $u(x,t)$, Eq. (1) is transformed in the Cahn-Hilliard equation [8]

$$\partial_t u = \partial_{xx}(\varepsilon u + u^3 - u_{xx}) = \partial_{xx} \frac{\delta \mathcal{F}[u]}{\delta u(x)}, \tag{3}$$

which is also a continuity equation with a Lyapunov functional $\mathcal{F}[u] \equiv \int dx[\varepsilon \frac{u^2}{2} + \frac{u^4}{4} + \frac{u_x^2}{2}]$. We recall now some well-known facts about particlelike solutions. These solutions appear as homoclinic or heteroclinic orbits of the spatial dynamical system. They correspond to inhomogeneous solutions in which the symmetry of space translation is broken in a small localized region of space [5] and they play a fundamental role in complex spatiotemporal dynamics [11,12]. Some examples are kink, pulses, localized structures [2–4]. The orbit of a spatial dynamical system which connects two different fixed points is a front or kink solution [2], and as a consequence of translation invariance it is possible to construct multikink solutions which describe the ulterior dynamics of the system through the interaction of kinks which give logarithmic growth of domains with time [6,7]. We shall see that this picture changes for conservative systems described by continuity equations which is the case of the Cahn-Hilliard equation. The stationary solutions of Eq. (3) satisfy

$$\lambda = \varepsilon u + u^3 - u_{xx}, \tag{4}$$

where λ is a parameter related to the initial condition that determines the conserved area under the curve $y = u(x,t)$ [10,13]. When the area of the initial condition vanishes

($\lambda = 0$) the system has kink type solutions

$$u_i(x, x_i) = \sqrt{|\varepsilon|}\tanh\left[\sqrt{\frac{|\varepsilon|}{2}}\,(x - x_i)\right]. \tag{5}$$

From these solutions it is possible to construct a bubble type solution (kink-antikink) when λ is small enough. In the nonconservative case these bubble type solutions are unstable due to the interaction between the kink and the antikink [7]. On the contrary, in the conservative case, this changes because the interaction between the kink and the antikink is not allowed since it violates the conservation of the area under the curve, and consequently the bubbles are stable stationary solutions of Eq. (3). This is easy to verify in the spatial dynamical system (4) since for small nonvanishing λ one has three fixed points, a center and two saddle points, and one of them has a homoclinic curve which is the bubble solution. The analytic expression of the bubble is

$$U(y \equiv x - x_0) = u_0 + \frac{2(3u_0^2 + \varepsilon)}{-2u_0 + \sqrt{2(|\varepsilon| - u_0^2)}\,[(\sqrt{(3u_0^2 + \varepsilon)}y)]}, \tag{6}$$

with

$$u_0 = -2\sqrt{\frac{|\varepsilon|}{3}}\sin\left\{\frac{1}{3}\left[\arctan\left(\sqrt{\frac{4|\varepsilon|^3}{27\lambda^2} - 1}\right) + \frac{\pi}{2}\right]\right\}, \quad \lambda \geq 0,$$

$$u_0 = 2\sqrt{\frac{|\varepsilon|}{3}}\cos\left[\frac{1}{3}\arctan\left(\sqrt{\frac{4|\varepsilon|^3}{27\lambda^2} - 1}\right)\right], \qquad \lambda < 0,$$

where x_0 is the position of the bubble, i.e., the value around which the bubble is centered (see Fig. 1). This particlelike solution is parametrized by a symmetry group characterized by two quantities x_0 and λ which determine the position and the area of the bubble. The parameter λ is related directly to the width Δ of the bubble defined as the distance between the two roots of the solution (cf. Fig. 1). The relation is $\Delta \approx \ln(8|\varepsilon|^{3/2}/|\lambda|)/\sqrt{2|\varepsilon|}$. For small and positive λ the previous solution takes the following form as a function of the position and the width:

$$\begin{aligned} U(x, x_0, \Delta) \approx & -\sqrt{|\varepsilon|} + \sqrt{|\varepsilon|}\tanh\left[\sqrt{\frac{|\varepsilon|}{2}}\left(x - x_0 + \frac{\Delta}{2}\right)\right] \\ & - \sqrt{|\varepsilon|}\tanh\left[\sqrt{\frac{|\varepsilon|}{2}}\left(x - x_0 - \frac{\Delta}{2}\right)\right] \\ & + O(\sqrt{|\varepsilon|}\,e^{-\sqrt{2|\varepsilon|}\Delta}). \end{aligned} \tag{7}$$

An important fact is that the bubble takes different asymptotic values when $x \to \pm\infty$ and the difference depends on the width of the bubble since it is due to the last term in the previous equation which is proportional to $(\exp -\sqrt{2|\varepsilon|}\Delta)$. We shall see later that this difference plays a central role in the interaction of the bubbles.

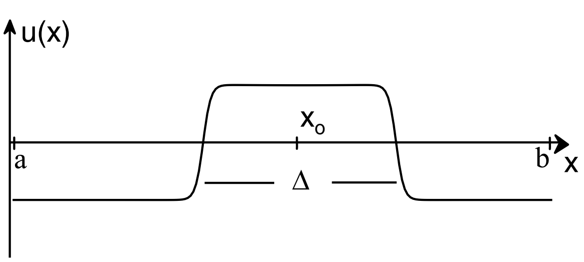

FIG. 1. Bubble solution obtained through numerical simulation of the Cahn-Hilliard equation for $\varepsilon = -0.25$. The position of the center of the bubble is x_0 and the width Δ is defined as the distance between the two zeros of the bubble.

We consider a system of finite size L, but with L much bigger than the width of the bubbles, i.e., we have $L \gg \Delta \gg 1/\sqrt{|\varepsilon|}$. In this case the bubble can have a nontrivial dynamic. In order to describe it we promote the parameters of the symmetry group (x_0, Δ) to functions of time $[x_0(t), \Delta(t)]$. We shall obtain now two equations directly from the Cahn-Hilliard equation: the first one corresponds to integrate between a and b, while for the second one we multiply first Eq. (3) by x and then we integrate between a and b. The result is

$$\begin{aligned} d_t \int_a^b u(x)\,dx &= \partial_x \frac{\delta \mathcal{F}}{\delta u}\bigg|_a^b, \\ d_t \int_a^b x u(x)\,dx &= x\partial_x \frac{\delta \mathcal{F}}{\delta u}\bigg|_a^b + \frac{\delta \mathcal{F}}{\delta u}\bigg|_b^a, \end{aligned} \tag{8}$$

where $\partial_x \frac{\delta \mathcal{F}}{\delta u}|_a^b = \partial_x \frac{\delta \mathcal{F}}{\delta u}|_b - \partial_x \frac{\delta \mathcal{F}}{\delta u}|_a$. The first equation is related to the evolution of the width of the bubble. If we associate the width of the localized solution with the "mass of the particle" we see that the second equation describes the motion of the center of mass. In the case of periodic boundary conditions Eqs. (8) reduce to

$$\begin{aligned} \partial_t \int_a^b u(x)\,dx &= 0, \\ \partial_t \int_a^b x u(x)\,dx &= (b - a)\,\partial_x \frac{\delta \mathcal{F}}{\delta u}\bigg|_b \end{aligned}$$

where the first equation expresses the conservation of the area under the curve $y = u(x)$. If $u(x)$ is a solution of Eq. (4) we have also $\partial_x \frac{\delta \mathcal{F}}{\delta u}|_b = 0$ and, consequently, the bubble is a stable stationary solution of the system and one can check that it is a minimum of the free energy $\mathcal{F}$ for periodic boundary conditions.

We consider now the boundary conditions $\partial_x u = \partial_{xx} u = 0$. Taking into account the dominant contribution to the integrals in Eqs. (8) we obtain

$$\begin{aligned} 2\sqrt{\varepsilon}\,d_t\Delta &= u_{xxx}|_b^a, \\ 2\sqrt{\varepsilon}\,d_t(x_o\Delta) &= \varepsilon u + u^3 + x u_{xxx}|_b^a, \end{aligned}$$

where we see that now the bubble changes its width, moves towards the nearest border, and finally disappears giving rise to a kink solution [14] which is the global minimum of the free energy $\mathcal{F}$ with these new boundary conditions for small λ.

The problem we address now is how the system evolves in the ulterior time, i.e., how the system arrives asymptotically to its global minimum. Before minimizing globally the free energy $\mathcal{F}$ the system will minimize locally the free energy in different regions of space yielding several bubbles. We shall consider then a gas of diluted bubbles, i.e., the separation of the bubbles is bigger than their widths. The ith bubble is characterized by the position x_i of its center (the middle point between the two zeros of the bubble) and its width Δ_i (see Fig. 2).

One can consider Eqs. (8), where a and b are two intermediate points between the bubbles (see Fig. 2). Using the fact that the intermediate region between the bubbles is well approximated by straight lines and taking into account the dominating terms in the integrals of Eqs. (8) and simplifying, the equations are reduced to

$$\begin{aligned} d_t\Delta_i &= \frac{1}{2\sqrt{|\varepsilon|}}\left[\partial_x \frac{\delta\mathcal{F}}{\delta u}\bigg|_b - \partial_x \frac{\delta\mathcal{F}}{\delta u}\bigg|_a\right], \\ d_t x_i &= \frac{1}{4\sqrt{|\varepsilon|}}\left[\partial_x \frac{\delta\mathcal{F}}{\delta u}\bigg|_b + \partial_x \frac{\delta\mathcal{F}}{\delta u}\bigg|_a\right]. \end{aligned} \tag{9}$$

We remark that these expressions do not depend explicitly on the choice of the integration limits (a and b). In order to estimate the right hand side of the previous expressions, we must consider the different asymptotic values of the bubbles which will allow us to evaluate the slope between the bubbles ($\partial_x \frac{\delta\mathcal{F}}{\delta u} \approx 2|\varepsilon| u_x$). The equations for the position and the width read

$$d_t\Delta_i = I_{i+1,i} - I_{i,i-1}, \qquad d_t x_i = \frac{I_{i+1,i} + I_{i,i-1}}{2}, \tag{10}$$

where

$$I_{l,k} = \frac{8|\varepsilon| \sinh[\sqrt{|\varepsilon|/2}\,(\Delta_l - \Delta_k)]}{(x_l - x_k - \frac{\Delta_l+\Delta_k}{2})} e^{-\sqrt{|\varepsilon|/2}\,(\Delta_l+\Delta_k)}.$$

The influence of each lateral bubble on the central bubble is to increase (decrease) its width and to diminish the distance of the bubble to the lateral bubble if this one is thinner (wider) than the central one (see Fig. 3). Therefore the larger bubbles increase as a consequence of the disappearance of their thin neighbors, and this in such a way that the global area is conserved for periodic boundary conditions ($d_t \sum \Delta_i = 0$). The interaction of the bubbles depend on the inverse of the distance between them, which is different from the interaction of the kinks forming the bubble which contribute with an exponential interaction $[\exp -\sqrt{|\varepsilon|/2}[x_i - x_{i-1} - (\Delta_i + \Delta_{i-1})/2]]$, as it is shown in Ref. [7]. This interaction is obtained through the study of the non-Hermitian operator associated to the perturbation of one bubble by the presence of others or by the study of an equivalent Hermitian operator through the inclusion of two functions related to the conservation of area and center of mass [7]. It is important to remark that these exponential terms are relevant when the distance between the bubbles is smaller than or equal to the average width of these ($\Delta_i/2 + \Delta_{i-1}/2$). When the bubbles are diluted ($x_i - x_{i-1} \gg \Delta_i + \Delta_{i-1}$) the dominating term of the interaction has its origin in the difference of the asymptotic values of each bubble which is given by the term $O(\sqrt{|\varepsilon|}e^{-\sqrt{2|\varepsilon|}\Delta})$ in Eq. (7) [the explicit form of this term is obtained expanding the exact expression (6)].

We have shown then that if one has several bubbles of different sizes the smaller bubbles begin to disappear and to give rise to bigger bubbles. Since we know that with periodic boundary conditions the global minimum of the system is given by one bubble we conclude that the previous stage before arriving to the stationary state will be described by the interaction of two bubbles. Let $\{x_1, \Delta_1\}$ and $\{x_2, \Delta_2\}$ be the position and width of these two bubbles. The dynamics will be given by

$$\begin{aligned} d_t(\Delta_1 + \Delta_2) &= 0, \\ d_t(x_1\Delta_1 + x_2\Delta_2) &= (b - a)I_{1,2}, \\ d_t\Delta_1 &= I_{2,1} - I_{1,2}, \\ d_t(x_2 - x_1) &= -|\varepsilon|^{-1/2}(I_{2,1} + I_{1,2})\frac{(\Delta_1 - \Delta_2)}{2\Delta_1\Delta_2}. \end{aligned} \tag{11}$$

The first equation expresses the conservation of the area in the dominating order. The second equation tells us that the global "center of mass" moves in the direction of the thinner bubble. From the third equation we deduce that the widest bubble increases its width while the other decreases. It is also simple to see that the case of symmetrical bubbles is an unstable stationary state ($\Delta_1 = \Delta_2$). The last equation indicates to us that the bubbles always attract themselves, i.e., the distance between them always

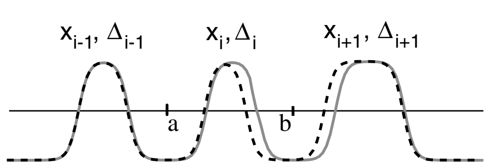

FIG. 2. Numerical simulation of the Cahn-Hilliard equation for $\varepsilon = -0.25$. The solid line is the initial condition and the dashed line represents the state of the system at a later time.

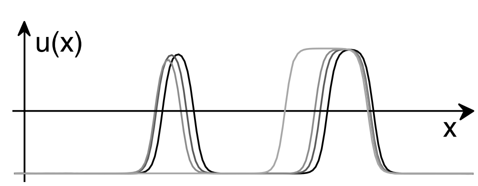

FIG. 3. Numerical simulation of the evolution of two bubbles in the Cahn-Hilliard equation for $\varepsilon = -0.25$. The bubble in the right increases its width while the other decreases it. Finally, the bubble in the left disappears and the remaining bubble is the stationary state of the system.

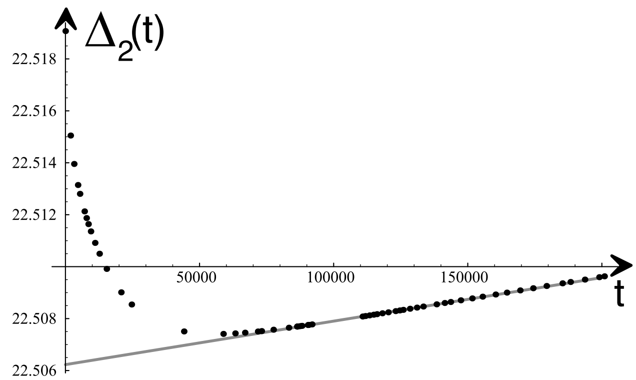

FIG. 4. Comparison of $\Delta_2(t)$ obtained directly from the Cahn-Hilliard equation (dashed line) with the analytical expression (solid line) which is obtained from the dominating terms of Eqs. (11).

decreases (the smallest one) and the law of interaction depends on the inverse of the distance (see the definition of $I_{1,2}$), but the intensity of this effect is $|\varepsilon|^{1/2}$ smaller than the evolution of the other quantities ($\Delta \sim 1/|\varepsilon|^{-1/2}$) since the dominating term vanishes as it is easy to see from Eq. (10). Therefore the bubbles interact mainly through their widths (see Fig. 3). As a consequence of the previous evolution the widest bubble increases towards the thinnest bubble and moves slightly. Numerical simulations show a complete agreement with this description (cf. Figs. 3 and 4). In Fig. 4 we compare the evolution of $\Delta_2(t)$ obtained from the Cahn-Hilliard equation with the evolution of $\Delta_2(t)$ obtained analytically from the preceding equations when one neglects the right hand side of the last equation $[d_t(x_2 - x_1) = 0]$. We remark that for short times the difference between the curves is related to the establishment of the bubble solution, which is typically of order ε^{-2}. From the analytical expression one can estimate the extinction time of the smallest bubble $\tau \sim t_0 + \varepsilon^{-3/2} \exp(\sqrt{\varepsilon/2}\Delta) \ln[\tanh(\sqrt{\varepsilon/8}\Delta)/\tanh(\sqrt{\varepsilon/8}\delta)]$, where $\Delta = \Delta_1(t_0) + \Delta_2(t_0)$, $\delta = \Delta_2(t_0) - \Delta_1(t_0)$, and t_0 is the time of order ε^{-2} needed for the establishment of the two bubbles. After this time τ the latter equations loose their validity.

Summarizing we have considered the universal equation which describes the interface between two symmetric states which is a Cahn-Hilliard type equation. This equation has localized structures which present themselves as bubbles solutions which are parametrized by two quantities: the position and the width. For a gas of diluted bubbles we have found a set of ordinary differential equations which describe the interactions between them and this has allowed us to give a simple description of the ulterior dynamics of the system in terms of the position and the width of the bubbles. In the case of two diluted bubbles with periodic boundary conditions we have also found a set of ordinary differential equations in which the dynamic occurs mainly through the width of the bubbles. The evolution given by the set of ordinary differential equations is in very good agreement with numerical simulations.

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