An Allen-Cahn type problem with curvature modification *

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Abstract

A two component system driven by both interface area and interface curvature is studied with a new phase field model. The Euler-Lagrange equation derived from the free energy functional of the system is a fourth order nonlinear partial differential equation. Formal asymptotic analysis shows that if the curvature impact in the system is strong, there exists a bubble profile in each space dimension. A bubble profile describes a pattern of an inner core of one component surround by an outer membrane of the other component. There are four distinct cases for dimension equal to 1, 2, 3, or 4 and larger. Outlines of the rigorous proofs of the existence theorems are given, based on the formal asymptotic analysis.

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1 Introduction

In a two component system of a condensed matter, when the conformation of the two components is solely determined by the area of the interfaces separating the two components, the free energy of the system is often described by the Allen-Cahn model [1]

$$I_{ac}(u) = \int_D [\frac{\epsilon^2}{2}|\nabla u|^2 + F(u)]\,dx, \tag{1.1}$$

where F is a balanced double well potential such as $F(u) = \frac{1}{4}u^2(1-u)^2$, and D is a region in R^n. The equilibria of I_{ac} are solutions of the second order nonlinear PDE

$$-\epsilon^2\Delta u(x) + f(u(x)) = 0, \quad x \in D, \quad \partial_\nu u(x) = 0, \quad x \in \partial D \tag{1.2}$$

where ∂_ν is the outward normal derivative on ∂D. The parameter ϵ is positive and small. The nonlinear function f is the derivative of F, such as $f(u) = u(u-1/2)(u-1)$ if F is the example given above.

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If $u(x)$ is close to 0, then the first component occupies x; if $u(x)$ is close to 1, then the second component occupies x. These two regions are separated by a transitional region where $u(x)$ is somewhat greater than 0 and less than 1. We may call the set $\{x \in D : u(x) = 1/2\}$, which is usually an $n-1$ dimensional surface, or a union of several surfaces, in R^n, the interface. Given a configuration $u(x)$ with x on the interface, we may roughly interpret $-\epsilon^2 \Delta u + f(u)$ as the mean curvature of the interface at x. The equation (1.2) then states that at an equilibrium state, the mean curvature of the interface must be everywhere equal to 0.

In such an interface area driven system, it is difficult for the two components to co-exist. Casten and Holland [3] (and Matano [10] independently) showed that when D is bounded and convex, any non-constant solution of (1.2) must be unstable.

More recently in the study of polymer blends (see Tang and Freed [18]) an additional molecular weight dependent curvature term is found to contribute to the free energy. In this case one observes two immiscible homopolymers, one forming an outer membrane and the other constituting an inner core.

This morphology pattern may be explained phenomenologically by a very simple model. Suppose that the two homopolymers are separated by a closed curve Γ in R^2. We propose that the free energy I_c of the system is given by

$$I_c(\Gamma) = \int_\Gamma \kappa^2 \, ds + \gamma \int_\Gamma ds, \tag{1.3}$$

where s is the length element, κ is the curvature and $\gamma > 0$ is a parameter. If we assume that Γ is a circle of radius ρ, then the curvature is everywhere $\frac{1}{\rho}$ and (1.3) becomes

$$\frac{2\pi}{\rho} + 2\pi\gamma\rho, \tag{1.4}$$

A stable configuration is obtained by minimizing (1.4) with respect to ρ. One finds that

$$\rho = \frac{1}{\sqrt{\gamma}}. \tag{1.5}$$

In this paper we study a more sophisticated phase field version of (1.3). As in the Allen-Cahn approach we let u be the phase field variable of a two component system. Again $u(x) \approx 0$ means that x is taken by one component; $u(x) \approx 1$ means that x is taken by the other component. The free energy of the system is now

$$I(u) = \frac{1}{2} \int_D |\Delta u - f(u)|^2 \, dx + \gamma \int_D [\frac{1}{2}|\nabla u|^2 + F(u)] \, dx. \tag{1.6}$$

Here $\Delta u - f(u)$ plays the role of curvature and $\frac{1}{2}|\nabla u|^2 + F(u)$ plays the role of length element. The constant $1/2$ in front of the first integral is put there for simplicity later. Also note that γ is the only parameter in I. It gives the relative weights of the two parts in I. There is no ϵ in (1.6) because one can always scale out ϵ by changing the x variable.

The connection between I and I_c is not very clear at the moment. There is a well know relationship between I_{ac} and $\int_\Gamma ds$, i.e. I_c without the curvature part: $\int_\Gamma ds$ is the Gamma-limit of I_{ac} to as $\epsilon \to 0$. See De Giorgi [6], Modica and Mortola [12], Modica [11], Kohn and Sternberg [9], etc, for this theory. We do not know if a Gamma-convergence theory between I and I_c is available. The curvature part of I_c, i.e. $\int_\Gamma \kappa^2\, ds$, is known as the Willmore functional [19] (also see Simon [17]). There are some partial results regarding the convergence of

$$\int_D [-\epsilon^2 \Delta u + f(u)]^2\, dx \tag{1.7}$$

to the Willmore functional (see Moser [13]).

We will study (1.6) in the general case of n dimensions, i.e. $D \subset R^n$ with n being a positive integer. Although in (1.3) we have assumed that γ is positive when $n = 2$, here we allow γ to be negative if $n \geq 3$. We are only interested in the situation where (1.6) is sufficiently different from (1.1), so we assume that $|\gamma|$ is small.

The Euler-Lagrange equation of (1.6) is a fourth order partial differential equation

$$\Delta(\Delta u - f(u)) - f'(u)(\Delta u - f(u)) - \gamma(\Delta u - f(u)) = 0. \tag{1.8}$$

If D has a boundary, then we impose the Neumann boundary conditions

$$\frac{\partial u}{\partial \nu} = \frac{\partial(\Delta u - f(u))}{\partial \nu} = 0 \text{ on } \partial D. \tag{1.9}$$

If we introduce a new variable $v = \Delta u - f(u)$, then (1.8) may be written as a system

$$\Delta u - f(u) - v = 0, \quad \Delta v - f'(u)v - \gamma v = 0 \text{ in } D. \tag{1.10}$$

If D has a boundary, then u and v both should satisfy the Neumann boundary condition there.

We are interested in the outer membrane/inner core pattern mentioned earlier, in the phase field model (1.6). More specifically we seek a radially symmetric solution of (1.8). The domain D is the entire space R^n. We require that the solution $u = u(|x|) = u(r)$ satisfy the conditions

$$u(0) > 0, \quad \lim_{r\to\infty} u(r) = 0. \tag{1.11}$$

We often call such a solution a bubble profile. Recall that γ is either positive or negative, but $|\gamma|$ is sufficiently small. This means that the curvature term in the free energy (1.6) is significant and the problem is very different from the Allen-Cahn problem (1.1). Note that the Allen-Cahn problem does not have a bubble profile solution.

In this paper we give a detailed description of the profile in each dimension using formal asymptotic analysis. The reader will see from our intuitive argument how the radius of a bubble profile is determined by the parameter γ in (1.6).

It turns out that our asymptotic analysis is very sensitive to the dimension n of the underlying space. The $n = 2$ and $n \geq 4$ cases are easier because one needs only to track quantities that are of algebraically small orders, measured by the bubble radius ρ. The results one obtains can be guessed from I_c. However in the $n = 1$ and $n = 3$ cases, one must study quantities that are exponentially small in terms of ρ. One can not derive any useful information from I_c. We study $n = 2$ case in Section 2, $n \geq 4$ case in Section 3, $n = 1$ case in Section 4, and $n = 3$ case in Section 5.

The formal asymptotic analysis leads to rigorous proofs of the existence of bubble profiles by Ren and Wei [14]. Bubble profiles exist in 1-dimension and 2-dimensions if γ is positive and sufficiently small. Bubble profiles exist, in $n = 3$ and $n \geq 4$ dimensions if γ is negative and sufficiently close to 0. In Section 6 we outline some key steps used in [14]. Many of the intricate constructions there are motivated by the formal study given here.

2 $n = 2$

Let (u, v) be a solution of (1.10). With u and v being radial in R^n the system (1.10) becomes

$$u'' + \frac{(n-1)u'}{r} - f(u) = v \tag{2.1}$$

$$v'' + \frac{(n-1)v'}{r} - f'(u)v = \gamma v \tag{2.2}$$

where u and v are now functions of $r = |x| \in (0, \infty)$. There are boundary conditions at $r = 0$:

$$u'(0) = 0 \tag{2.3}$$

$$v'(0) = 0. \tag{2.4}$$

One important quantity to analyze is the location of the interface of u. Define the interface location $\rho \in (0, \infty)$ to be the point where

$$u(\rho) = \frac{1}{2}. \tag{2.5}$$

In this section we consider the case $n = 2$. It turns out that it suffices to study the behavior of u and v near the interface point ρ. The leading order approximation of u near ρ is the function H which is the solution of

$$-H'' + f(H) = 0 \ \text{ in } R; \ \ H(-\infty) = 1, \ H(\infty) = 0, \ H(0) = \frac{1}{2}. \tag{2.6}$$

In the special case $f(H) = H(H - 1/2)(H - 1)$, H is known explicitly,

$$H(y) = \frac{1}{2}[\tanh(-\frac{y}{2\sqrt{2}}) + 1]. \tag{2.7}$$

We define a constant τ which is often called the surface tension from H:

$$\tau = \int_R (H'(y))^2 \, dy. \tag{2.8}$$

Therefore the first approximation of u is found:

$$u(\rho + y) = H(y) + \ldots. \tag{2.9}$$

In the next step we use H for u in (2.2) and look for the leading order approximation of v which we denote by v_1:

$$v(\rho + y) = \frac{v_1(y)}{\rho} + \ldots \tag{2.10}$$

Then v_1 must satisfy the following equation.

$$v_1'' - f'(H)v_1 = 0. \tag{2.11}$$

This implies that

$$v_1(y) = c_1 H'(y) \tag{2.12}$$

where c_1 is to be determined.

Now the next order approximation of u is sought. Write

$$u(\rho + y) = H(y) + \frac{u_1(y)}{\rho} + ... \tag{2.13}$$

Use $v_1 = c_1 H'$ for v in (2.1) to find the equation for u_1:

$$u_1'' - f'(H)u_1 + H' = c_1 H', \quad u_1(0) = 0. \tag{2.14}$$

Here $u_1(0) = 0$ since $u(\rho) = H(0) = 1/2$. If one multiplies the last equation by H' and integrates over $(-\infty, \infty)$, then integration by parts yields that

$$c_1 = 1, \tag{2.15}$$

and $u_1 = c_2 H'$. Therefore because $u_1(0) = 0$ and $H'(0) \neq 0$,

$$u_1 = 0. \tag{2.16}$$

With $c_1 = 1$ one also derives that

$$v_1(y) = H'(y). \tag{2.17}$$

We move to the next order by setting

$$v = \frac{H'}{\rho} + \frac{v_2}{\rho^2} + ... \tag{2.18}$$

With u set to be H in (2.2) one finds the equation for v_2:

$$v_2'' - f'(H)v_2 + H'' = \gamma_1 H' \tag{2.19}$$

where γ_1 is the leading order approximation of γ:

$$\gamma = \frac{\gamma_1}{\rho} + ... \tag{2.20}$$

Multiplying (2.19) by H' and integrating over $(-\infty, \infty)$ show that

$$\gamma_1 = 0 \tag{2.21}$$

and v_2 satisfies

$$v_2'' - f'(H)v_2 + H'' = 0. \tag{2.22}$$

The last equation can be solved to give

$$v_2 = -\frac{yH'}{2} + c_3 H' \tag{2.23}$$

where c_3 is to be determined. The expansion for u is now

$$u = H' + \frac{u_2}{\rho^2} + ... \tag{2.24}$$

The equation for u_2 is

$$u_2'' - f'(H)u_2 - yH' = v_2. \tag{2.25}$$

Multiplying (2.25) by H' and integrating show that the constant c_2 in (2.23) must vanish and

$$v_2 = -\frac{yH'}{2}. \tag{2.26}$$

Then (2.25) becomes

$$u_2'' - f'(H)u_2 = \frac{yH'}{2}. \tag{2.27}$$

We now come to the last order. Let

$$v = \frac{H'}{\rho} - \frac{yH'}{2\rho^2} + \frac{v_3}{\rho^3} + ... \tag{2.28}$$

The equation for v_3 is

$$v_3'' - f'(H)v_3 - yH'' + v_2' - f''(H)u_2H' = \gamma_2 H' \tag{2.29}$$

where γ_2 is the second order approximation of γ:

$$\gamma = \frac{\gamma_2}{\rho^2} + ... \tag{2.30}$$

Multiplying by H' and integrating yield that

$$-\int_R yH''H' + \int_R v_2'H' - \int_R f''(H)(H')^2 u_2 = \gamma_2 \int_R (H')^2 \tag{2.31}$$

Differentiating the equation (2.27) for u_2 leads to

$$u_2''' - f'(H)u_2' - f''(H)H'u_2 = \frac{1}{2}(H' + yH''). \tag{2.32}$$

Multiplying by H' and integrating show that

$$-\int_R f''(H)(H')^2 u_2 = \int_R \frac{1}{2}(H' + yH'')H'. \tag{2.33}$$

Substituting (2.33) back to (2.31) yields

$$\gamma_2 \int_R (H')^2 = -\int_R yH''H' + \int_R v_2'H' + \frac{1}{2}(\int_R (H')^2 + \int_R yH'H''). \tag{2.34}$$

Note that

$$\int_R yH''H' = -\frac{1}{2}\int_R (H')^2 = -\frac{\tau}{2} \tag{2.35}$$

for integration by parts shows that

$$\int_R yH'H'' = \int_R yH'dH' = -\int_R H'(H' + yH'') = -\int_R (H')^2 - \int_R yH'H''. \tag{2.36}$$

Moreover

$$\int_R v_2' H' = \int_R -(\frac{yH'}{2})' H' = -\frac{1}{2}\int_R (H' + yH'')H' = -\frac{1}{4}\int_R (H')^2 = -\frac{\tau}{4} \tag{2.37}$$

We find from (2.34) that

$$\gamma_2 = \frac{1}{2}. \tag{2.38}$$

There is enough information now about the presumed solution. Particularly we know that

$$\gamma = \frac{1}{2\rho^2} + ... \tag{2.39}$$

The last equation should be read backwards so that

$$\rho = \frac{1}{\sqrt{2\gamma}} + ... \tag{2.40}$$

This tells us where the interface of the solution should be. Note that γ must be a positive number.

In two dimensions, the phase field problem (1.6) is consistent with the simple model (1.3). We have the following existence theorem.

Theorem 2.1 ([14]) *When γ is positive and sufficiently small, there exists a bubble profile. The radius of the bubble is $\frac{1}{\sqrt{2\gamma}} + o(\gamma^{-1/2})$.*

3 $n \geq 4$

The asymptotic analysis of a radial solution of (1.8) in the case $n \geq 4$ is similar to that in the case $n = 2$. Again near ρ we can expand u, v and γ to

$$u(\rho + y) = H(y) + \frac{u_1}{\rho} + \frac{u_2}{\rho^2} + ... \tag{3.1}$$

$$v(\rho + y) = \frac{v_1(y)}{\rho} + \frac{v_2(y)}{\rho^2} + \frac{v_3(y)}{\rho^3} + ... \tag{3.2}$$

$$\gamma = \frac{\gamma_1}{\rho} + \frac{\gamma_2}{\rho^2} .... \tag{3.3}$$

Similar calculations show that

$$v_1 = (n-1)H';\ u_1 = 0;\ \gamma_1 = 0;\ v_2 = -\frac{(n-1)^2 yH'}{2}; \tag{3.4}$$

the equation for u_2 is

$$u_2'' - f'(H)u_2 = \frac{(n-1)(3-n)}{2} yH', \quad u_2(0) = 0; \tag{3.5}$$

and the equation for v_3 is

$$v_3'' - f'(H)v_3 - (n-1)^2 yH'' + (n-1)v_2' - (n-1)f''(H)H'u_2 = (n-1)\gamma_2 H'. \tag{3.6}$$

From the last equation and the equation for u_2' derived by differentiating (3.5) one finds

$$\gamma_2 = \frac{(n-1)(3-n)}{2}. \tag{3.7}$$

Note that in this case γ_2 is negative. Reading the equation (3.7) backwards we deduce that

$$\rho = \sqrt{\frac{(n-1)(n-3)}{-2\gamma}} + \ldots. \tag{3.8}$$

The outcome of our analysis is consistent with (1.3) for $n \geq 4$. With Γ being a $n-1$ dimensional sphere,

$$I_c(\Gamma) = \omega_{n-1}\rho^{n-3} + \omega_{n-1}\gamma\rho^{n-1} \tag{3.9}$$

where ω_{n-1} is the area of the $n-1$ dimensional unit sphere. It is clear that if $\gamma > 0$, the right side is increasing in ρ. Only if $\gamma < 0$, there exists a critical point, but this critical point is a maximum. It is (3.8) up to a multiplicative constant.

The existence theorem in the $n \geq 4$ case for the phase field model is the following.

Theorem 3.1 ([14]) *When γ is negative and sufficiently close to 0, there exists a bubble profile. The radius of the bubble is $\sqrt{\frac{(n-1)(n-3)}{-2\gamma}} + o(\gamma^{-1/2})$.*

4 $n = 1$

When $n = 1$, the phase field problem is far more complex than (1.3). A zero dimensional sphere is just the union of two points in R, and ρ is half the distance between the two points. This sphere has no curvature. Hence

$$I_c(\Gamma) = 2\gamma, \tag{4.1}$$

a constant independent of ρ. No conclusion can be drawn from (4.1). For the phase field problem, we can still carry out an asymptotic analysis. However we must analyze the effect of the point $x = 0$ very carefully.

A little more information from H (2.6) is needed. The derivative of H, $H'(y)$, decays to 0 exponentially fast as $|y| \to \infty$. More precisely we have $a > 0$ and $k < 0$ such that

$$H'(y) = ke^{-a|y|} + O(e^{-2a|y|}). \tag{4.2}$$

Necessarily

$$a^2 = f'(1) = f'(1). \tag{4.3}$$

In the special case $f(H) = H(H-1/2)(H-1)$,

$$a = \frac{1}{\sqrt{2}}, \quad k = -\frac{1}{\sqrt{2}}.$$

The leading order approximation of u is still H near ρ. But we need to include a correction due to the boundary condition $u'(0) = 0$. To have this boundary condition satisfied let

$$u(x) = H(x-\rho) + \frac{H'(-\rho)}{a}e^{-ax} + \ldots. \tag{4.4}$$

The leading order approximation of v near ρ is v_1,

$$v(\rho + y) = v_1(y) + ... \tag{4.5}$$

where v_1 satisfied

$$v_1'' - f'(H)v_1 = 0. \tag{4.6}$$

Hence

$$v_1(y) = dH'(y) \tag{4.7}$$

for some d to be determined. For v_1 we must also add a correction so that it satisfies the boundary condition $v'(0) = 0$:

$$v(\rho + y) = d(H'(y) + \frac{H''(-\rho)}{a}e^{-a(\rho+y)}) + ... \tag{4.8}$$

We turn to the next order approximation of u near ρ:

$$u(\rho + y) = H(y) + \frac{H'(-\rho)}{a}e^{-a(\rho+y)} + u_1(y) + ... \tag{4.9}$$

where u_1 satisfies the equation

$$u_1'' - f'(H)u_1 + \frac{H'(-\rho)}{a}e^{-a(\rho+y)}(f'(1) - f'(H)) = dH', \quad u_1(0) = -\frac{H'(-\rho)}{a}e^{-a\rho}. \tag{4.10}$$

Multiplying by H' and integrating over $(-\infty, \infty)$ yield that

$$d = \frac{1}{\tau}\int_R \frac{H'(-\rho)}{a}e^{-a(\rho+y)}(f'(1) - f'(H))H'\,dy. \tag{4.11}$$

This constant d is of order $O(e^{-2a\rho})$. The integral in (4.11) may be calculated as in (4.18). One sees that $u_1 = O(e^{-2a\rho})$, and $v_1 = O(e^{-2a\rho})$.

The next order approximation of v near ρ is denoted v_2:

$$v(\rho + y) = d(H'(y) + \frac{H''(-\rho)}{a}e^{-a(\rho+y)}) + v_2(y) + ... \tag{4.12}$$

where $v_2(y)$ satisfies

$$v_2'' - f'(H)v_2 + d\frac{H''(-\rho)}{a}e^{-a(\rho+y)}(f'(1) - f'(H)) - df''(H)H'(\frac{H'(-\rho)}{a}e^{-a(\rho+y)} + u_1) = \gamma_1 dH' \tag{4.13}$$

where γ_1 is the leading order approximation of γ:

$$\gamma = \gamma_1 + ... \tag{4.14}$$

Differentiation of (4.10) implies

$$u_1''' - f'(H)u_1' - f''(H)H'u_1 - H'(-\rho)e^{-a(\rho+y)}(f'(1) - f'(H)) - \frac{H'(-\rho)}{a}e^{-a(\rho+y)}f''(H)H' = dH''. \tag{4.15}$$

Let $w = v_2 - du_1'$. Then w satisfies

$$w'' - f'(H)w + d(\frac{H''(-\rho)}{a} + H'(-\rho))e^{-a(\rho+y)}(f'(1) - f'(H)) = \gamma_1 dH' - d^2H''. \tag{4.16}$$

Multiplying by H' and integrating find that

$$\gamma_1\tau = (\frac{H''(-\rho)}{a} + H'(-\rho)) \int_R e^{-a(y+\rho)}(f'(1) - f'(H))H'\,dy. \tag{4.17}$$

To calculate the integral in (4.17) note that $H''' - f'(H)H' = 0$ by differentiating (2.6). Then

$$\begin{aligned}\int_R e^{-ay}(f'(1) - f'(H))H'\,dy &= \int_R (f'(1)H' - H''')e^{-ay}\,dy \\ &= [-H''(y)e^{-ay} - aH'(y)e^{-ay}]_{-\infty}^{\infty} \\ &= 2ak.\end{aligned} \tag{4.18}$$

This implies that

$$\gamma_1 = \frac{1}{\tau}(\frac{H''(-\rho)}{a} + H'(-\rho))e^{-a\rho}2ak \approx \frac{4ak^2e^{-2a\rho}}{\tau}. \tag{4.19}$$

One can see that $v_2 = O(e^{-4a\rho})$.

With the leading order term of γ determined the structure of the solution is rather clear. The formula (4.19) is read backwards to give the location of the interface:

$$\rho = \frac{1}{2a}\log\frac{1}{\gamma} + ... \tag{4.20}$$

Note in this case γ must be positive. As γ tends to 0, ρ approaches ∞, but very slowly. The following existence theorem is proved in [14].

Theorem 4.1 ([14]) *When γ is positive and sufficiently small, there exists a bubble profile. The radius of the bubble is $\frac{1}{2a}\log\frac{1}{\gamma} + o(\log\frac{1}{\gamma})$.*

5 $n = 3$

When $n = 3$, for a sphere $\kappa = \frac{1}{\rho}$ and $\int_\Gamma \kappa^2\,ds = \frac{1}{\rho^2}4\pi\rho^2 = 4\pi$. Hence

$$I_c(\Gamma) = 4\pi + 4\pi\gamma\rho^2, \tag{5.1}$$

which has no critical point for positive ρ. The phase field problem is again very different.

In the three dimensional case it is often more convenient to consider

$$\tilde{v}(r) = rv(r) \tag{5.2}$$

instead of v. Then $\tilde{v}$ satisfies the equation

$$\tilde{v}'' - f'(u)\tilde{v} = \gamma\tilde{v}, \quad \tilde{v}(0) = 0. \tag{5.3}$$

The first approximation of u, taking the condition $u'(0) = 0$ into account, is

$$u(r) = H(r-\rho) + \frac{H'(-\rho)}{a} e^{-ar} .... \tag{5.4}$$

The leading order approximation of $\tilde{v}$ which we denote by $\tilde{v}_1$ satisfies the equation

$$\tilde{v}_1'' - f'(H)\tilde{v}_1 = 0 \tag{5.5}$$

near ρ. This implies that

$$\tilde{v}_1(y) = dH'(y) \tag{5.6}$$

where d is to be determined. To have the boundary condition $\tilde{v}(0) = 0$ satisfied we add a correction term so that

$$\tilde{v}(r) = d(H'(r-\rho) - H'(-\rho)e^{-ar}) + ... \tag{5.7}$$

Let

$$u(r) = H(r-\rho) + \frac{H'(-\rho)}{a} e^{-ar} + u_1(r-\rho) + ... \tag{5.8}$$

where $u_1(y)$ satisfies

$$u_1'' - f'(H)u_1 + \frac{H'(-\rho)}{a} e^{-a(\rho+y)}(f'(1) - f'(H)) = \frac{d-2}{\rho} H', \quad u_1(0) = -\frac{H'(-\rho)}{a} e^{-a\rho}. \tag{5.9}$$

Multiplying the equation by H' and integrating yield

$$\frac{(d-2)\tau}{\rho} = \frac{H'(-\rho)}{a} \int_R (f'(1) - f'(H))H' e^{-a(\rho+y)}\, dy = \frac{H'(-\rho)}{a} e^{-a\rho} 2ak = 2kH'(-\rho)e^{-a\rho}, \tag{5.10}$$

where we have used (4.18). One sees that $u_1 = O(e^{-2a\rho})$. This also implies that $\tilde{v}_1 = O(1)$.

The next order approximation of $\tilde{v}$ is denoted by $\tilde{v}_2(y)$ so that

$$\tilde{v}(r) = d(H'(r-\rho) - H'(-\rho)e^{-ar}) + \tilde{v}_2(r-\rho) + ... \tag{5.11}$$

The equation for $\tilde{v}_2$ is

$$\tilde{v}_2'' - f'(H)\tilde{v}_2 - 2H'(-\rho)e^{-ar}(f'(1) - f'(H)) - 2f''(H)H'(\frac{H'(-\rho)}{a} e^{-ar} + u_1) = 0. \tag{5.12}$$

Comparing this with the equation for u_1', which is

$$u_1''' - f'(H)u_1' - f''(H)H'u_1 - H'(-\rho)e^{-ar}(f'(1) - f'(H)) - \frac{H'(-\rho)}{a} e^{-ar} f''(H)H' = \frac{d-2}{\rho} H'', \tag{5.13}$$

we find that the difference $w = \tilde{v}_2 - 2u_1'$ satisfies

$$w'' - f'(H)w = -\frac{2(d-2)}{\rho} H''. \tag{5.14}$$

The equation (5.14) can be solve to yield

$$w = -\frac{d-2}{\rho} yH' + eH', \tag{5.15}$$

where the constant e is to be determined. Hence

$$\tilde{v}_2 = 2u_1' - \frac{d-2}{\rho} yH' + eH'. \tag{5.16}$$

In this case we have to expand to one more order. Let

$$u = H + \frac{H'(-\rho)}{a} e^{-ar} + u_1 + u_2 ... \tag{5.17}$$

where u_2 satisfies

$$u_2'' - f'(H)u_2 = -\frac{d-2}{\rho^2} yH' + \frac{\tilde{v}_2 - 2u_1'}{\rho}, \quad u_2(0) = 0. \tag{5.18}$$

Multiplying by H' and integrating show that

$$0 = \int_R \frac{\tilde{v}_2 - 2u_1'}{\rho} H' = \frac{e}{\rho} \int_R (H')^2. \tag{5.19}$$

Therefore

$$e = 0 \tag{5.20}$$

and

$$\tilde{v}_2 = 2u_1' - \frac{d-2}{\rho} yH'. \tag{5.21}$$

Here we see that $u_2 = O(\frac{e^{-2a\rho}}{\rho})$ and $\tilde{v}_2 = O(e^{-2a\rho})$.

Introduce $\tilde{v}_3$ so that

$$v(\rho + y) = d(H'(y) - H'(-\rho)e^{-a(\rho+y)}) + 2u_1' - \frac{d-2}{\rho} yH' + \tilde{v}_3 + ... \tag{5.22}$$

The new function $\tilde{v}_3(y)$ satisfies

$$\tilde{v}_3'' - f'(H)\tilde{v}_3 - 2f''(H)H'u_2 = 2\gamma_1 H' \tag{5.23}$$

where γ_1 is the leading order approximation of γ. Multiplying by H' and integrating yield

$$\gamma_1 \tau = -\int_R f''(H)(H')^2 u_2 \tag{5.24}$$

To compute the integral in (5.24) we differentiate the equation for u_2 to obtain

$$u_2''' - f'(H)u_2' - f''(H)H'u_2 = -\frac{d-2}{\rho^2}(yH')' + (\frac{\tilde{v}_2 - 2u_1'}{\rho})'. \tag{5.25}$$

Multiplying by H' and integrating show that

$$\begin{aligned}
-\int_R f''(H)(H')^2 u_2 &= -\frac{d-2}{\rho^2} \int_R (yH')'H' + \frac{1}{\rho} \int_R w'H' \\
&= -\frac{d-2}{\rho^2} \int_R (yH')'H' + \frac{1}{\rho} \int_R (-\frac{d-2}{\rho} yH')'H' \\
&= -\frac{2(d-2)}{\rho^2} \int_R (yH')'H' \\
&= -\frac{(d-2)\tau}{\rho^2}
\end{aligned}$$

where we have used (2.35). This and (5.10) show that

$$\gamma_1 = -\frac{d-2}{\rho^2} = -\frac{2kH'(-\rho)e^{-a\rho}}{\tau\rho} \approx -\frac{2(H'(-\rho))^2}{\tau\rho} \approx -\frac{2k^2e^{-2a\rho}}{\tau\rho}. \tag{5.26}$$

One also sees that $\tilde{v}_3 = O(\frac{e^{-2a\rho}}{\rho})$.

Note that this γ_1 is negative. To read (5.26) backwards, let $l(s)$ be the inverse function of

$$\rho \to -\frac{2k^2e^{-2a\rho}}{\tau\rho}. \tag{5.27}$$

Here $l : (-\infty, 0) \to (0, \infty)$. As s tends to 0, $l(s)$ grows to ∞, but more slowly than $-\frac{1}{2a}\log(-s)$ does, i.e. more slowly than in the $n = 1$ case. The interface ρ is at

$$\rho = l(\gamma) + ... \tag{5.28}$$

In this case the existence theorem is the following.

Theorem 5.1 ([14]) *When γ is negative and sufficiently close to 0, there exists a bubble profile. The radius of the bubble is $l(\gamma) + o(l(\gamma))$.*

6 Localized energy method

The rigorous proofs of Theorems 2.1, 3.1, 4.1 and 5.1 are given in [14]. We used the so-called localized energy method which is a combination of the Lyapunov-Schmidt reduction argument and variational techniques. In this section we list some key steps in this method.

Let ρ be the location of the interface of bubble profile u in the sense that $u(\rho) = 1/2$. Near ρ, u has a rather particular shape. This shape is mostly described by the function H given in (2.6). When r is much less than ρ, $u(r)$ is close to 1; when r is much larger than ρ, $u(r)$ is close to 0. The proofs of the existence theorems are very much about locating ρ. As $\gamma \to 0$, $\rho \to \infty$. The construction is divided into two steps: in the first step, we fix ρ large and solve a nonlinear problem with an orthogonal condition. In the next step, we locate ρ by finding a critical point for a reduced energy function involving ρ only. For the localized energy method used in other problems, see [2, 4, 5, 7, 8, 16, 15].

n = 2. Let us first consider the case $n = 2$. The operator on the left side of (1.8) is denoted by S, i.e.

$$S(u) = (\Delta - f'(u) - \gamma)[\Delta u - f(u)] \tag{6.1}$$

For each $\rho \in (\frac{1}{2\sqrt{2\gamma}}, \frac{2}{\sqrt{2\gamma}})$, we construct an approximate solution w to (1.8) of the form

$$w(r; \rho) = H(r - \rho) + \beta(r; \rho) \tag{6.2}$$

where

$$\beta(r; \rho) = c_{1,\rho}e^{-ar} + c_{2,\rho}re^{-ar}. \tag{6.3}$$

The constants $c_{1,\rho}$ and $c_{2,\rho}$ are so chosen that $w'(0) = w'''(0) = 0$, which ensures that $S(w)$ is regular at $r = 0$. More explicitly

$$c_{1,\rho} = \frac{H'(-\rho)}{a} + \frac{1}{2a}(H'(-\rho) - \frac{H'''(-\rho)}{a^2}), \quad (6.4)$$

$$c_{2,\rho} = \frac{1}{2}(H'(-\rho) - \frac{H'''(-\rho)}{a^2}). \quad (6.5)$$

In the case $n = 2$, the exact form of β is not too important. The main role played by β is to have the boundary conditions at $r = 0$ satisfied.

We define an approximate kernel

$$h(r;\rho) = H'(r-\rho) + b_{1,\rho}e^{-ar} + b_{2,\rho}re^{-ar} \quad (6.6)$$

where $b_{1,\rho} = O(e^{-a\rho})$ and $b_{2,\rho} = O(e^{-a\rho})$ are constants so chosen that $h'(0) = h'''(0) = 0$.

Let π_ρ be the projection operator to the subspace perpendicular to h:

$$\pi_\rho g = g - \frac{< g, h >}{\|h\|_2^2} h. \quad (6.7)$$

Here $\langle g, h\rangle$ is the $L^2(R^2)$ inner product of g and h, and $\|h\|_2$ is the $L^2(R^2)$ norm of h. We view

$$M = \{w(\cdot;\rho) : \frac{1}{2\sqrt{2\gamma}} < \rho < \frac{2}{\sqrt{2\gamma}}\} \quad (6.8)$$

as a one-dimensional submanifold in $H_r^4(R^2)$. The space $H_r^4(R^2)$ is the collection of radial H^4 functions on R^2. At each $w(\cdot;\rho)$ we define an approximate normal subspace

$$F_\rho = \{\phi \in H_r^4(R^2) : \phi \perp h(\cdot;\rho)\}. \quad (6.9)$$

It turns out that in each F_ρ there exists $\phi(\cdot;\rho)$ so that

$$\pi_\rho S(w(\cdot;\rho) + \phi(\cdot;\rho)) = 0. \quad (6.10)$$

The free energy of $w + \phi$ is close to the free energy of w. One can show that

$$I(w + \phi) = I(w) + O(\gamma^{1.5}). \quad (6.11)$$

The free energy of w can be calculated:

$$I(w) = 2\pi\tau(\frac{1}{2\rho} + \gamma\rho) + O(\gamma^{1.5}). \quad (6.12)$$

Therefore we conclude that

$$I(w(\cdot;\rho) + \phi(\cdot;\rho)) = 2\pi\tau(\frac{1}{2\rho} + \gamma\rho) + O(\gamma^{1.5}). \quad (6.13)$$

If we minimize $I(w(\cdot;\rho) + \phi(\cdot;\rho))$ with respect to ρ, then a minimum is found at

$$\rho = \rho_\gamma = \frac{1}{\sqrt{2\gamma}} + o(\gamma^{-1/2}). \quad (6.14)$$

One can show that at this ρ_γ

$$S(w(\cdot;\rho_\gamma)+\phi(\cdot;\rho_\gamma))=0, \tag{6.15}$$

i.e. (1.8) is exactly solved.

$\mathbf{n \geq 4}$. The case $n \geq 4$ is very similar. We use the same approximate solution w. The main difference occurs in the last step:

$$I(w+\phi)=\omega_{n-1}\tau\Big(\frac{(n-1)^2\rho^{n-3}}{2}+\gamma\rho^{n-1}\Big)+o(\gamma^{(3-n)/2}) \tag{6.16}$$

where ω_{n-1} is the area of the $n-1$ dimensional unit sphere. If $\gamma<0$, the above quantity has a *maximum* at

$$\rho_\gamma=\sqrt{\frac{(n-1)(n-3)}{-2\gamma}}+o(\gamma^{-1/2}).$$

This gives a solution $w(\cdot;\rho_\gamma)+\phi(\cdot;\rho_\gamma)$ of (1.8).

$\mathbf{n = 1}$. The case $n=1$ is more complex. Let

$$\rho\in\Big(\frac{1}{4a}\log\frac{1}{\gamma},\frac{1}{a}\log\frac{1}{\gamma}\Big). \tag{6.17}$$

For each ρ satisfying (6.17) we define an approximate solution w. Compared to the $n=2$ and $n\geq 4$ cases, the construction of w is more involved. We let

$$\alpha(x;\rho)=c_{0,\rho}e^{-ax},\ \text{ where } c_{0,\rho}=\frac{H'(-\rho)}{a},\ \text{ so that } H'(-\rho)+\alpha'(0)=0. \tag{6.18}$$

Now we define a function $g(y;\rho)$ on $(-\infty,\infty)$ which is the solution of

$$g''-f'(H)g+\alpha(y+\rho)(f'(1)-f'(H))=d_\rho H',\ \ g(0)=-\alpha(\rho). \tag{6.19}$$

Note that g is motivated by u_1 in Section 4. In (6.19) the constant d_ρ is chosen so that

$$d_\rho\int_R (H')^2\,dy=\int_R \alpha(y+\rho)(f'(1)-f'(H(y)))H'(y)\,dy. \tag{6.20}$$

This ensures that (6.19) is solvable. The condition $g(0)=-\alpha(\rho)$ gives a unique solution. We calculate the right side of (6.20):

$$\begin{aligned}
&\int_R \alpha(y+\rho)(f'(1)-f'(H(y)))H'(y)\,dy\\
&= \alpha(\rho)\int_R e^{-ay}(f'(1)H'-H''')\,dy\\
&= \alpha(\rho)[-e^{-ay}H''(y)-ae^{-ay}H'(y)]|_{y=-\infty}^{y=\infty}\\
&= \alpha(\rho)\lim_{y\to-\infty}[e^{-ay}H''(y)+ae^{-ay}H'(y)]\\
&= 2ak\alpha(\rho) \ = \ 2k^2e^{-2a\rho}+o(e^{-2a\rho}).
\end{aligned}$$

Therefore

$$d_\rho = \frac{2k^2 e^{-2a\rho}}{\tau} + o(e^{-2a\rho}). \tag{6.21}$$

We include g in the construction of w. One last term is β which is given as

$$\beta(x;\rho) = c_{1,\rho} e^{-ax} + c_{2,\rho} x e^{-ax} + \frac{f''(1)c_{0,\rho}^2}{6a^2} e^{-2ax}. \tag{6.22}$$

It is a solution of

$$(D^2 - f'(1))^2 \beta = (D^2 - f'(1)) \frac{f''(1)\alpha^2}{2}. \tag{6.23}$$

The constants $c_{1,\rho}$ and $c_{2,\rho}$ are chosen so that

$$\beta'(0) = -H'(-\rho) - \alpha'(0) - g'(-\rho) = -g'(-\rho), \tag{6.24}$$

$$\beta'''(0) = -H'''(-\rho) - \alpha'''(0) - g'''(-\rho). \tag{6.25}$$

Here

$$c_{1,\rho} = O(e^{-2a\rho}), \quad c_{2,\rho} = O(e^{-2a\rho}). \tag{6.26}$$

Now we set

$$w(x;\rho) = H(x-\rho) + \alpha(x;\rho) + g(x-\rho;\rho) + \beta(x;\rho). \tag{6.27}$$

Our choice of β ensures that $w'(0) = w'''(0) = 0$. Note that this β is different from the one (6.3) used in the $n = 2$ case.

As in the proof of the $n = 2$ case one can find ϕ so that

$$\pi_\rho S(w + \phi) = 0. \tag{6.28}$$

The free energy of $w + \phi$ is

$$I(w+\phi) = I(w) + o(\gamma^2) = \frac{4k^4 e^{-4a\rho}}{\tau} + \gamma(2\tau - \frac{2k^2 e^{-2a\rho}}{a}) + o(\gamma^2). \tag{6.29}$$

We minimize $I(w(\cdot;\rho) + \phi(\cdot;\rho))$ with respect to ρ and find that $I(w+\phi)$ is minimized at some

$$\rho_\gamma = -\frac{1}{2a} \log \frac{\gamma\tau}{4ak^2} + o(\log \frac{1}{\gamma}). \tag{6.30}$$

At this ρ_γ,

$$S(w(\cdot;\rho_\gamma) + \phi(\cdot;\rho_\gamma)) = 0. \tag{6.31}$$

$\mathbf{n = 3}$. Recall the function l in Section 5, We let

$$\rho \in (\frac{l(\gamma)}{2}, 2l(\gamma)). \tag{6.32}$$

We define a family of approximate solutions

$$w(r;\rho) = H(r-\rho) + \beta(r;\rho) \tag{6.33}$$

where β is the same as the one (6.3) used in the $n = 2$ case. Here β plays a more important role than in the $n = 2$ case. One can again find ϕ so that $\pi_\rho S(w + \phi) = 0$ and calculations show that

$$I(w + \phi) = 4\pi[2\tau - \frac{2k^2 e^{-2a\rho}}{a} + \gamma\tau\rho^2] + O(\gamma^{1+\delta}) \tag{6.34}$$

for some $\delta > 0$ independent of ρ and γ. We now maximize the above with respect to ρ to find a particular ρ_γ at which the equation (1.8) is solved.

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