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MATHEMATICAL ANALYSIS OF TWO-PHASE FIELD MODEL WITH SURFACE TENSION EFFECT

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ABSTRACT. In this short note, we give some preliminary materials and huristic descriptions of our recent results [HT] on two-phase field model.

Let $\Omega\subset \mathbb{R}^{n}$ be a bounded domain with smooth boundary, $n\geq 2$, and suppose that Ω is filled with some fluid which has two stable phases, say, phase A and phase B. Let $W:\mathbb{R}\to \mathbb{R}^{+}$ be a certain potential function with zeros at ± 1 and one local maximum on the interval $(-1, +1)$. One may regard W as a kind of (phenomenological) Ginzburg-Landau free energy, or Helmholtz free energy in the classical thermodynamics. To describe the local macroscopic state of the fluid, we introduce the order parameter function $u:\Omega\to \mathbb{R}$. We interprete u as the indication of local ratio of the two phases: i.e. if at $x\in\Omega$, $u(x)\approx 1$, it indicates that phase A occupies mostly around x and similarly for $u(x)\approx-1$, and if $u(x)\approx 0$, that phase A and phase B coexist locally at the same ratio around x. Given a suitable constraint such as $\int_{\Omega}u=m$, we consider the variational problem of minimizing

$$E(u)=\int_{\Omega}W(u(x))$$

with the given constraint. Here, the minimum of E may be obtained (and $=0$) for a suitable u taking values ± 1 only and having a suitable volume ratio so that $\int_{\Omega}u=m$. What is determined by this minimization is simply the volume ratio of the two phases, and the configuration of how they separate is completely arbitrary as far as E is concerned. This is caused by ignoring the surface tension energy of the phase boundary, which would have the effect of avoiding unnecessary interface as desirable configurations. Thus we instead consider a normalized free energy

$$E_{\varepsilon}(u)=\int_{\Omega}\varepsilon\frac{|\nabla u|^{2}}{2}+\frac{W(u)}{\varepsilon}.$$

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To get some insight into this energy, let's consider the one-dimensional case with $\Omega = \mathbb{R}$,

$$E_\varepsilon(u) = \int_{-\infty}^{\infty} \varepsilon\frac{(u')^2}{2} + \frac{W(u)}{\varepsilon}.$$

The (unconstraint) Euler-Lagrange equation for E_ε is

$$-\varepsilon u'' + \frac{W'(u)}{\varepsilon} = 0.$$

By the change of variable $x = \varepsilon\tilde{x}$, the equation is

$$-u'' + W'(u) = 0,$$

where $u'' = \frac{d^2u}{d\tilde{x}^2}$. Multiply the equation by u' and integrate from $\tilde{x} = a$ to $\tilde{x} = b$, then

$$0 = \int_a^b \frac{d}{d\tilde{x}}\left\{W(u) - \frac{(u')^2}{2}\right\} = W(u) - \frac{(u')^2}{2}\Big|_a^b.$$

Thus we have $\frac{(u')^2}{2} \equiv W(u)$ on $\mathbb{R}$ for the solution. Furthermore, this leads to $u' = \sqrt{2W(u)}$, which is a first-order ODE. It is not difficult to find a travelling wave solution with $u(-\infty) = -1$ and $u(+\infty) = 1$, with $u' > 0$ on $\mathbb{R}$. By rescaling back $\tilde{x} = x/\varepsilon$, we see that this travelling wave solution satisfies

$$\varepsilon\frac{(u')^2}{2} \equiv \frac{W(u)}{\varepsilon}$$

on $\mathbb{R}$ and the transition from -1 to $+1$ occurs within the ε-order length. The energy of the solution is

$$E_\varepsilon(u) = \int_{-\infty}^{\infty} 2\sqrt{\frac{W}{\varepsilon}}\sqrt{\frac{\varepsilon}{2}}u' = \int_{-1}^{1} \sqrt{2W(s)}\,ds \equiv 2\sigma,$$

where we changed the variable by $s = u(x)$. The constant 2σ may be considered as a unit surface energy contribution.

If we turn to the multi-dimensional problem, one may, by analogy, make various conjectures on the geometry of the interface for the critical points of the energy E_ε as well as how the energy may be determined. For example, it is natural to guess that, for ε small,

$$E_\varepsilon(u) \approx \text{ area of interface} \times 2\sigma$$

if u is a critical point of E_ε. One would wonder if $\frac{\varepsilon|\nabla u|^2}{2} \approx \frac{W(u)}{\varepsilon}$ in some appropriate sense. Also, since E_ε is expected to measure the area of interface, it may be expected that critical points of E_ε may have interfaces which are critical points of area energy: namely, the interfaces may be close to constant mean curvature hypersurfaces in some appropriate sense. These issues are first considered and answered for energy minimizing solutions by Modica [M1], Sternberg [S] and Luckhaus-Modica [LM]. With some technical assumptions on W,

Theorem *Suppose $\{u_\varepsilon\}_{\varepsilon>0}$ minimize E_ε with a given volume constraint, i.e.,*

$$E_\varepsilon(u_\varepsilon) = \min_{\int v=m} E_\varepsilon(v).$$

Then there exists a subsequence $\{u_{\varepsilon_i}\}_{i=1}^\infty$ with $\varepsilon_i \to 0$ and $u_0 \in BV(\Omega)$ such that
(i) $u_0 = \pm 1$ L^n a. e. on Ω,
(ii) $u_{\varepsilon_i} \to u_0$ in $L^1(\Omega)$,
(iii) $2\sigma \cdot Per(\partial\{u_0 = 1\} \cap \Omega) = \lim_{i\to\infty} E_{\varepsilon_i}(u_{\varepsilon_i})$,
(iv) $\lim_{i\to\infty} \int_\Omega \left| \frac{\varepsilon_i}{2}|\nabla u_{\varepsilon_i}|^2 - \frac{W(u_{\varepsilon_i})}{\varepsilon_i} \right| = 0$,
(v) $Per(\partial\{u_0 = 1\} \cap \Omega) = \min_{v=\pm 1 \text{ a.e. }, \int v=m} Per(\partial\{v = 1\} \cap \Omega)$,
(vi) the mean curvature of $\partial\{u_0 = 1\}$ is $\frac{\lambda}{\sigma}$, where $\lambda = \lim_{i\to\infty} \lambda_i$ and λ_i satisfies

$$-\varepsilon_i \Delta u_{\varepsilon_i} + \frac{W'(u_{\varepsilon_i})}{\varepsilon_i} = \lambda_i, \qquad i = 1, 2, \cdots .$$

The meaning of the above statements is: (iii) says that the energy E_ε approximates the area of interface times 2σ, and (v) says that the boundary of $\{u_0 = 1\}$ in Ω minimizes the area with the given volume constraint. By the well known regularity theory, $\partial\{u_0 = 1\} \cap \Omega$ is a regular hypersurface (with a possible closed singular set of Hausdorff dimension less than or equal to $n-8$). The mean curvature of the limit interface is constant, and is given as the limit of Lagrange multipliers for u_{ε_i}. The important observation is that, by defining

$$\Phi(t) = \int_0^t \sqrt{W(s)/2}\, ds$$

and $v_\varepsilon = \Phi(u_\varepsilon)$, one has

$$\int_\Omega |\nabla v_\varepsilon| = \int_\Omega \sqrt{W(u_\varepsilon)/2}|\nabla u_\varepsilon| \le \frac{1}{2} \int \frac{\varepsilon}{2}|\nabla u_\varepsilon|^2 + \frac{W(u_\varepsilon)}{\varepsilon}.$$

Note that the right-hand side is uniformly bounded for the minimization problem. Thus, (with appropriate assumptions on W which give L^∞ uniform bound on u_ε) BV-norm of $\{v_\varepsilon\}$ is uniformly bounded. The standard compactness theorem shows that there exist a L^1 converging subsequence $\{v_{\varepsilon_i}\}$ and the limit v_0 which is also a.e. pointwise limit.

Define $u_0 = \Phi^{-1}(v_0)$. The sequence $\{u_{\varepsilon_i}\}$ converges to u_0 a.e. pointwise, hence by Fatou's lemma,

$$\int_\Omega W(u_0) = \int_\Omega \liminf W(u_{\varepsilon_i}) \leq \liminf \int_\Omega W(u_{\varepsilon_i}) \to 0.$$

This shows that $u_0 = \pm 1$ a.e. on Ω, and $u_0 \in BV(\Omega)$ as well. To show that $\partial\{u_0 = 1\} \cap \Omega$ minimizes area with the given volume constraint, one constructs a sequence of functions which have phase boundaries of some area-minimizing boundary. Here, one shows that, if

$$Per(\partial\{u_0 = 1\} \cap \Omega) > \min_{v=\pm 1 \text{ a.e.}, \int v = m} Per(\partial\{v = 1\} \cap \Omega),$$

then one would reach a contradiction due to such construction. The energy minimality is an essential point of the argument.

To understand general critical points of the energy functional with finite energy which may not be energy minimizing, we use the Euler-Lagrange equation. The approach is through the famous monotonicity formula which holds in a number of variational problems and which originated in the study of minimal surfaces via measure-theoretic approach: define, for $r > 0$,

$$f(r) = \frac{1}{r^{n-1}} \mathcal{H}^{n-1}(M \cap B_r(x)),$$

where $M \subset \mathbb{R}^n$ is a minimal hypersurface, $\mathcal{H}^{n-1}$ the $(n-1)$-dimentional Hausdorff measure and $x \in M$. It is well-known that $f(r)$ is a non-decreasing function of r. Since the interface of the critical points of E_ε should behave like a minimal hypersurface (or constant mean curvature hypersurface, to be more precise), and since the energy $\left(\frac{\varepsilon}{2}|\nabla u|^2 + \frac{W}{\varepsilon}\right) dx$ as a measure concentrates only around the interface, it is naturally expected that, via analogy,

$$f(r) = \frac{1}{r^{n-1}} \int_{B_r(x)} \left(\frac{\varepsilon}{2}|\nabla u|^2 + \frac{W}{\varepsilon}\right)$$

may be non-decreasing for all sufficiently small ε for the critical point of E_ε. By using the Euler-Lagrange equation (see [HT, Section 3]) one computes

$$f'(r) = \frac{1}{r^n} \int_{B_r} \left(\frac{W}{\varepsilon} - \frac{\varepsilon}{2}|\nabla u|^2\right) + \frac{\varepsilon}{r^{n+1}} \int_{\partial B_r} (x \cdot \nabla u)^2,$$

where $B_r = B_r(0)$. The second term is non-negative, while the first term does not have a definite sign. Intuitively, the first term arises due to the scaling difference of the two terms under consideration: without ε, $|\nabla u|^2\, dx$ scales like r^{n-2}, $W\, dx$ like r^n, while we are scaling them by r^{n-1} which is the middle of the two. The fact that there exist a constant $c = c(n, \tilde{U}, W)$ independent of ε with

$$\sup_{\tilde{U}} \left(\frac{\varepsilon}{2}|\nabla u|^2 - \frac{W}{\varepsilon} \right) \le c$$

([HT, Proposition 3.3]) is the key point which shows that $f' \ge -c$. In all purposes this is good enough to controll the local behavior of the measure concentration. The above estimate is motivated by the earlier work of Modica [M2]: if $u \in C^2(\mathbb{R}^n) \cap L^\infty(\mathbb{R}^n)$ satisfies

$$\Delta u = W'(u) \quad \text{on } \mathbb{R}^n$$

(where W may not be double-well function at all), then

$$\frac{1}{2}|\nabla u|^2 - W(u) \le 0 \quad \text{on } \mathbb{R}^n.$$

Our problem, after rescaling by $\tilde{x} = x/\varepsilon$, becomes

$$-\Delta u + W'(u) = \lambda\varepsilon \quad \text{on } \varepsilon^{-1}\Omega,$$

where $\varepsilon^{-1}\Omega \to \mathbb{R}^n$ as $\varepsilon \to 0$. Thus, our result may be considered as a certain perturbation result from the entire solution case. On the other hand, the proof crucially depends on the fact that W has the double-well shape: so far we do not see how to prove the similar estimate for wider class of functions W. Once the monotonicity of the energy is established, the rectifiability of the limit interface and the equi-distribution of the energy

$$\int_{\tilde{U}} \left| \frac{\varepsilon}{2}|\nabla u|^2 - \frac{W}{\varepsilon} \right| \to 0$$

follows via some measure theoretic argument as well as some known results from Allard's paper [A] on varifolds. Thus, the limit interface measure $||V|| = \lim \frac{\varepsilon}{2}|\nabla u|^2 \, dx$ has a weak tangent plane a.e. $\mathcal{H}^{n-1}$ on the support of $||V||$ in particular. One expects that, at around (not necessarily unit density) points where a weak tangent plane exists, the converging phase boundary looks like a multi-layered one-dimensional travelling wave solution discussed at the beginning. Using in an essential manner the varifold convergence (rather than the convergence of measure in $\mathbb{R}^n$), we show that the density of $||V||$ are a.e. integer multiples of σ. Our analysis also shows that, at around the regular unit density point, the convergence of interfaces is in fact $C^{1,\alpha}$: that is, the indivisual level sets $\{u_\varepsilon = t\}$, $|t| < 1$, converge to the support of $||V||$ as a graph in the $C^{1,\alpha}$ norm for any $\alpha < 1$. It is a standard habit of PDE specialists to bootstrap at this point and obtain C^k estimates for any k. But here, it seems to us that it is difficult to obtain C^2

estimate due to a certain degeneracy of the equation that one must consider. This begs somewhat subtle but interesting question about the phase field theory: how close is it to the limiting sharp interface model? The formal asymptotic analysis often assumes that the level set of the phase boundary to be smooth. Of course, it often gives satisfactory answers when higher regularity is not a issue. It can be an important issue in the analysis of certain related dynamical problems such as the Cahn-Hilliard equation.

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