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GRADIENT THEORY OF PHASE TRANSITIONS WITH GENERAL SINGULAR PERTURBATIONS*

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1. Introduction. In this article we shall discuss some recent results concerning the gradient theory of phase transitions in a Van der Waals fluid. In particular, we shall be interested in singular perturbations of the free energy of a more general form than $\varepsilon^2|\nabla u|^2$, which has been studied in detail in [**4, 10** and **14**].

In the Van der Waals theory of phase transitions, the equilibrium states of the system are given by the minimizers of the total free energy $I(u) = \int_\Omega W(u)\,dx$, where $\Omega \subseteq \mathbf{R}^n$ is bounded and open, and $u : \Omega \to \mathbf{R}$ is the density of the fluid. The function $W : (0, \infty) \to \mathbf{R}$ is the free-energy per unit volume. We shall assume that W satisfies the following conditions

$W : (0, \infty) \to [0, \infty)$ is C^3,

$W(\tau) \to \infty$ as $\tau \to 0, \infty$,

$W(\tau) = 0$ if and only if $\tau = a, b$, where $0 < a < b < \infty$,

$W''(a) > 0$, $W''(b) > 0$.

Hence, W is a nonconvex function with two minima of equal heights at $u = a, b$. (For the case where the free-energy W has two local minima of different heights, we consider the integrand $W(\tau) - (\alpha\tau + \beta)$, for some $\alpha, \beta \in \mathbf{R}$.) We refer to a and b as the phases of the fluid.

We shall look for minimizers of I in the class of functions satisfying the constraint

$$\int_\Omega u(x)\,dx = M; \tag{1}$$

that is, the total mass of the fluid is specified. If $M \in (a|\Omega|, b|\Omega|)$, where $|\Omega|$ is the measure of Ω, then the minimizers of I subject to (1)

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are the piecewise constant functions

$$\hat{u}(x) = \begin{cases} a & x \in A, \\ b & x \in B, \end{cases}$$

where A, B are any disjoint measurable sets such that $A \cup B = \Omega$, $A \cap B = \phi$ and $|A| = (b|\Omega| - M)\backslash(b-a)$, $|B| = (M - a|\Omega|)\backslash(b-a)$. Clearly, there are infinitely many such minimizers.

One method to resolve this nonuniqueness is to select as admissible functions those which are limits of the minimizers, u_ε, of the perturbed energy functional,

$$I_\varepsilon(u) = \int_\Omega \{W(u) + \varepsilon^2|\nabla u|^2\}\, dx, \tag{2}$$

as the parameter ε goes to zero. The extra term $\varepsilon^2|\nabla u|^2$ represents interfacial energy; its effect is to smooth the minimizers of I and penalize large changes in u.

In the case $n = 1$, the pointwise limits of u_ε as $\varepsilon \to 0$ have been determined in [**4**]. In the case $n > 1$, there is a slightly weaker result:

Theorem 1 [**10**, **14**]. *Suppose $u_\varepsilon \in W^{1,1}(\Omega)$ is a minimizer of I_ε subject to* (1) *and suppose $u_\varepsilon \overset{L^1(\Omega)}{\to} u_0$ as $\varepsilon \to 0$. Then u_0 is a solution of the minimal surface problem*

$$\textit{Minimize } Per_\Omega\{u = a\} \quad \textit{for } u \in BV(\Omega), W(u(x)) = 0 \textit{ a.e.}$$
$$\textit{and} \quad \int_\Omega u dx = M.$$

Here, $BV(\Omega)$ is the space of functions of bounded variation on Ω and $Per_\Omega \Delta = \int_\Omega |\nabla \chi_\Delta|$. If $\partial\Delta$ is smooth, then $\int_\Omega |\nabla \chi_\Delta| = H^{n-1}(\partial\Delta \cap \Omega)$ where H^{n-1} is the $n-1$ dimensional Hausdorff measure. (For further details on functions of bounded variation see [**6**].) This theorem shows that the effect of the $\varepsilon^2|\nabla u|^2$ perturbation is to pick out the minimizers of I which have minimal surface area between the phases.

A natural question to consider is whether or not the same theorem is true for a more general perturbation. By a more "general perturbation" we shall mean replacing the integrand in I_ε by $f(u, \varepsilon\nabla u)$ where f is a smooth function satisfying $f(u,0) = W(u)$ and $f(u,p)$ is a convex function of p (precise hypotheses will be given in the next section). Two examples of general perturbations are

(i) $f(u, \varepsilon\nabla u) = W(u) + \varepsilon^2|\nabla u|^2 + \varepsilon^4|\nabla u|^4$,

(ii) $f(u, \varepsilon\nabla u) = W(u) + \varepsilon^2\langle A\nabla u, \nabla u\rangle$, where A is a positive definite $n \times n$ matrix.

It turns out that the resulting variational problems that u_0 satisfies for each of these examples are quite different. This is because in example (i) the perturbation just depends on the magnitude of ∇u, whereas in example (ii) the direction of ∇u is also considered. Thus, for example (ii) we expect the limit problem to depend on the orientation of the interfaces. We shall call a perturbation *isotropic* if it can be written in the form $f(u, \nabla u) = \hat{f}(u, |\nabla u|)$. Otherwise, we shall call the perturbation *anisotropic*.

The general problem of determining a limit functional of a sequence of functionals is part of the theory of Γ-convergence of nonlinear functionals developed by De Giorgi. We refer to [**1**] (where Γ-convergence is called "epi-convergence") for further information on Γ-convergence.

2. General perturbations. We shall consider singularly perturbed functionals of the form

$$J_\varepsilon(u) = \int_\Omega f(u, \varepsilon\nabla u)\, dx,$$

where f satisfies:

H1 $f(u,p) : (0,\infty) \times \mathbf{R}^n \to [0,\infty)$ is C^3,

H2 $f(u,0) = W(u)$, $\forall u \in (0,\infty)$,

H3 $f_{p_i}(u,0) = 0$, $\forall u \in (0,\infty)$, $i = 1, 2, \ldots, n$,

H4 $f_{p_i p_j}(u,p)\eta_i\eta_j > 0$, $\forall u \in (0,\infty)$, $\forall p \in \mathbf{R}^n$, $\forall \eta \in \mathbf{R}^n \backslash \{0\}$,

H5 There exists $k_1 > 0$ such that

$$f(u,p) \geq k_1|p|^2 \qquad \forall u \in (0,\infty),\ \forall p \in \mathbf{R}^n,$$

H6 There exists $N > 0$, $k_2 > 0$ and $q_0 \geq 2$ such that

$$f(u,p) \leq W(u) + k_2|p|^{q_0} \qquad \forall u \in (0,\infty),\ \forall p \in \mathbf{R}^n \text{ such that } |p| > N.$$

Note, by H2 and H3, a Taylor expansion of $f(u, \varepsilon\nabla u)$ about $(u, 0)$ gives

$$f(u, \varepsilon\nabla u) \approx W(u) + \frac{1}{2} f_{p_i p_j}(u, 0)\varepsilon^2 u_{,x_i} u_{,x_j},$$

(cf. (2)).

Since f is convex in its highest derivative (H4) it follows by the direct method of the Calculus of Variations that there exists a minimizer of J_ε in the class of functions $W^{1,1}(\Omega)$ satisfying the constraint (1). We shall denote minimizers of J_ε subject to the constraint (1) by u_ε.

Suppose $u_\varepsilon \overset{L^1(\Omega)}{\to} u_0$ as $\varepsilon \to 0$. In order to determine what limit problem u_0 satisfies we need to construct two new functions as follows: Let $\nu \in S^{n-1} = \{y \in \mathbf{R}^n : |y| = 1\}$. By H5, the algebraic equation

$$r\nu_i f_{p_i}(u, r\nu) - f(u, r\nu) = 0 \tag{3}$$

can be solved for $r \in [0, \infty)$; that is, there exists a function $\bar{r}$: $(0, \infty) \times S^{n-1} \to [0, \infty)$ such that $r = \bar{r}(u, \nu)$ solves (3). Furthermore, the function $\bar{r}$ is continuous and

$$\bar{r}(a, \nu) = \bar{r}(b, \nu) = 0, \qquad \bar{r}(u, \nu) > 0 \quad \forall u \in (a, b), \forall \nu \in S^{n-1}.$$

Let $p \in \mathbf{R}^n \backslash \{0\}$ and $s \in [0, \infty)$. By the convexity of $f(u, \cdot)$,

$$f(u, s\hat{p}) \geq f(u, \bar{r}(u, \hat{p})\hat{p}) + \hat{p} \cdot f_p(u, \bar{r}(u, \hat{p})\hat{p})(s - \bar{r}(u, \hat{p})),$$

where $f_p = \nabla_p f(u, p)$ and $\hat{p} = p/|p|$. Setting $s = |p|$ and using the definition of $\bar{r}(u, \hat{p})$ gives

$$f(u, p) \geq p \cdot f_p(u, \bar{r}(u, \hat{p})\hat{p}) = (f(u, \bar{r}(u, \hat{p})\hat{p}) \backslash \bar{r}(u, \hat{p}))|p|. \tag{4}$$

Let

$$G(u, p) = \begin{cases} (f(u, \bar{r}(u, \hat{p})\hat{p}) \backslash \bar{r}(u, \hat{p}))|p| & u \neq a, b \text{ and } p \neq 0, \\ 0 & \text{otherwise.} \end{cases}$$

It is reasonably straightforward to show that G is continuous, and $G(u, \cdot)$ is convex and positively homogeneous of degree 1.

From (4), we see that $G(u, p)$ is just the tangent cone to f whose vertex is at the origin.

3. The isotropic case. In this section we shall consider the isotropic perturbation $f(u,p) = \hat{f}(u,|p|)$. It follows that the functions $\bar{r}$ and G, defined in the previous section, can now be written as $\bar{r}(u,\nu) = \bar{r}(u)$ and $G(u,p) = (f(u,\hat{r}(u))\backslash\hat{r}(u))|p|$.

The following result shows that for isotropic perturbations, the limit function u_0 solves a simple geometry problem:

Theorem 2 [**11**]. *If $f(u,p)$ is isotropic, then u_0 solves*

$$\textit{Minimize } Per_\Omega\{u = a\} \quad \textit{for } u \in BV(\Omega),\ f(u(x),0) = 0 \ \textit{a.e.}$$
$$\textit{and} \quad \int_\Omega u\,dx = M.$$

Comparing this result with Theorem 1 we see that u_0 satisfies the same geometry problem. Hence, for isotropic perturbations there is no loss of generality in just considering the simplest perturbation $\varepsilon^2|\nabla u|^2$.

The first step in the proof of Theorem 2 is to scale and extend the functional J_ε. Define

$$F_\varepsilon(u) = \begin{cases} \int_\Omega \varepsilon^{-1}\hat{f}(u,\varepsilon|\nabla u|)\,dx & u \in W^{1,1}(\Omega),\ \int_\Omega u\,dx = M, \\ +\infty & \text{otherwise,} \end{cases}$$

and

$$F_0(u) = \begin{cases} K Per_\Omega\{u = a\} & u \in BV(\Omega), f(u(x),0) = 0 \text{ a.e.,} \\ & \int_\Omega u\,dx = M, \\ +\infty & \text{otherwise,} \end{cases}$$

where $K = \int_a^b f(\tau,\hat{r}(\tau))\backslash\hat{r}(\tau)\,d\tau$.

The functionals F_ε and F_0, which are both defined on L^1, are related in the following way:

(A) For each $v \in L^1(\Omega)$ and for each sequence $\{v_\varepsilon\}$ in $L^1(\Omega)$ such that $v_\varepsilon \overset{L^1(\Omega)}{\to} v$ as $\varepsilon \to 0$,

$$\varliminf_{\varepsilon\to 0} F_\varepsilon(v_\varepsilon) \geq F_0(v)$$

(B) For each $w \in L^1(\Omega)$, there exists a sequence $\{w_\varepsilon\}$ in $L^1(\Omega)$ such that $w_\varepsilon \overset{L^1(\Omega)}{\to} w$ as $\varepsilon \to 0$ and

$$\lim_{\varepsilon\to 0} F_\varepsilon(w_\varepsilon) = F_0(w).$$

In terms of the convergence of functionals, (A) and (B) are equivalent to saying that F_0 is the Γ-limit of F_ε as $\varepsilon \to 0$ ([**1**]).

Theorem 2 follows immediately from (A) and (B) since if $\{w_\varepsilon\}$ and w are chosen as in (B), then

$$F_0(w) = \underline{\lim}_{\varepsilon\to 0} F_\varepsilon(w_\varepsilon) \geq \underline{\lim}_{\varepsilon\to 0} F_\varepsilon(u_\varepsilon) \geq F_0(u_0),$$

where the last inequality follows by (A). The result follows since w is arbitrary.

We give now a sketch of the proof of (A). Without loss of generality, suppose $\{v_\varepsilon\} \subset W^{1,1}(\Omega)$, $\int_\Omega v_\varepsilon\, dx = M$ and $a \leq v_\varepsilon \leq b$, $\forall \varepsilon > 0$. Furthermore, suppose $v_\varepsilon \overset{L^1(\Omega)}{\to} v$, where $v \in BV(\Omega)$ satisfies $\int_\Omega v\, dx = M$ and $f(v(x), 0) = 0$ a.e. By (4) and the homogeneity of G,

(5)
$$F_\varepsilon(v_\varepsilon) \geq \int_\Omega \varepsilon^{-1} G(v_\varepsilon, \varepsilon\nabla v_\varepsilon)\, dx = \int_\Omega G(v_\varepsilon, \nabla v_\varepsilon)\, dx = \int_\Omega |\nabla\phi(v_\varepsilon)|\, dx,$$

where $\phi(s) = \int_a^s (f(\tau, \hat{r}(\tau))\backslash\hat{r}(\tau))\, d\tau$. By dominated convergence it follows that $\phi(v_\varepsilon) \overset{L^1(\Omega)}{\to} \phi(v)$, so that lower semicontinuity of the total variation ([**6**]) and (5) imply

$$\underline{\lim}_{\varepsilon\to 0} F_\varepsilon(v_\varepsilon) \geq \underline{\lim}_{\varepsilon\to 0} \int_\Omega |\nabla\phi(v_\varepsilon)|\, dx \geq \int_\Omega |\nabla\phi(v)|\, dx.$$

Part (A) now follows since

$$\phi(v(x)) = \begin{cases} 0 & \{v = a\}, \\ K & \{v = b\}, \end{cases}$$
$$= K\chi_{\{v=b\}}.$$

4. The anisotropic case. When the perturbation depends on the direction of ∇u, the Γ-limit will no longer be a simple geometry problem. Instead, the limit problem will be weighted in the sense that there will be certain preferred directions for the normal to the interface.

In some recent work with P. Sternberg the limit problem for the anisotropic case has been determined:

Theorem 3 [**12**]. *If f is anisotropic, then u_0 satisfies*

$$\text{Minimize } H_0(u) \quad \text{for } u \in L^1(\Omega), \tag{6}$$

where

$$H_0(u) = \begin{cases} \frac{1}{b-a}\int_\Omega \int_a^b G(s, \frac{d\mu(x)}{d|\mu|})\, ds\, d|\mu|(x) & u \in BV(\Omega), f(u(x), 0) = 0, \\ & \int_\Omega u\, dx = M, \\ +\infty & \textit{otherwise.} \end{cases}$$

Here, μ is the derivative measure of u, $|\mu|$ is the total variation of μ and $d\mu(x)/d|\mu|$ is the associated Radon-Nikodym derivative (roughly speaking, $d\mu(x)/d|\mu|$ lies in the normal direction to the boundary of $\{u = a\}$).

One application of this theorem is to determine the existence and structure of local minimizers of J_ε using the results of Kohn and Sternberg [**9**] (see also the article by Peter Sternberg in this volume).

Some idea of the structure of solutions to (6) is given by the following example in two dimensions. Let $\Omega = [0,1] \times [0,1]$ and consider the perturbation

$$f(u, \varepsilon\nabla u) = W(u) + \varepsilon^2(4u_{,x_1}^2 + u_{,x_2}^2).$$

Clearly, f satisfies H1–H6. The functions $\bar{r}$ and G are given by

$$\bar{r}(u,\nu) = \left[\frac{W(u)}{4\nu_1^2 + \nu_2^2}\right]^{1/2}, \qquad G(u, r\nu) = 2[W(u)(4\nu_1^2 + \nu_2^2)]^{1/2}, \quad \nu \in S^{n-1}.$$

Hence,

$$H_0(u) = \begin{cases} \left(\frac{2}{b-a}\int_a^b W(s)^{1/2}\, ds\right) \int_\Omega (4v_1^2(x) + v_2^2(x))^{1/2}\, d|\mu|(x) \\ \qquad u \in BV(\Omega), f(u(x), 0) = 0, \int_\Omega u\, dx = M, \\ +\infty \quad \text{otherwise} \end{cases}$$

where $v = d\mu/d|\mu|$. Under the change of variables $y_1 = x_1/2$, $y_2 = x_2$, minimization of H_0 reduces to solving the geometry problem:
(7)

$$\text{Minimize } |\mu|(\Omega') \quad \text{for } u \in BV(\Omega'),\ u \in \{a,b\} \text{ and } \int_{\Omega'} u\, dy = \mu\backslash 2,$$

where $\Omega' = [0, \frac{1}{2}] \times [0,1]$. Depending on the value of M, the boundary of $\{u = a\}$ will either be a line segment or a quarter-circle for a solution of (7). Transforming back to x-coordinates shows that the minimum of H_0 will have either a line segment or an ellipse as its interface. This should be compared with an example of Gurtin's [**7**] for the isotropic perturbation $W(u) + \varepsilon^2|\nabla u|^2$, where the interface is either a line segment or a quarter-circle. Other examples are discussed in [**12**].

As in the isotropic case, the proof of Theorem 3 follows immediately from showing that the rescaled functionals

$$H_\varepsilon(u) = \begin{cases} \int_\Omega \varepsilon^{-1} f(u, \varepsilon\nabla u)\, dx & u \in W^{1,1}(\Omega),\ \int_\Omega u\, dx = M, \\ +\infty, & \text{otherwise,} \end{cases}$$

converge, in the sense of Γ-convergence, to H_0. We shall give a brief sketch of the proof of the lower semicontinuity property (A) of Γ-convergence. Details of the proof of (A) and (B) can be found in [**12**]. (The proof in [**12**] is actually for the case where $f(u, \varepsilon\nabla u)$ is defined for all $u \in \mathbf{R}$ and there is no integral constraint on u; it is straightforward to adapt the proof to the case considered here.) Suppose the sequence $\{v_\varepsilon\} \subset W^{1,1}(\Omega)$ and $v_0 \in L^1(\Omega)$ are such that $v_\varepsilon \overset{L^1(\Omega)}{\to} v_0$ and $H_\varepsilon(v_\varepsilon)$, $H_0(v_0)$ are finite. By (4) and the homogeneity of G,

$$H_e(v_\varepsilon) \geq \int_\Omega G(v_\varepsilon, \nabla v_\varepsilon)\, dx.$$

Since $G(u, \cdot)$ is convex and homogeneous of degree one, we can apply a representation result of Dal Maso [**5**, Theorem 3.4] to show that the greatest L^1-lower semicontinuous which is less than or equal to $\int_\Omega G(u, \nabla u)\, dx$ is H_0. Hence,

$$\varliminf_{\varepsilon\to 0} H_\varepsilon(v_\varepsilon) \geq \varliminf_{\varepsilon\to 0} \int_\Omega G(v, \nabla v_\varepsilon)\, dx \geq H_0(v).$$

In [**12**], nonhomogeneous perturbations of the form $f(x, u, \varepsilon\nabla u)$ are also considered. In this case, the limit problem is weighted spatially in addition to the directional dependence.

Finally, we remark that it would be interesting to extend the method of singular perturbations of nonconvex variational problems to the theory of phase transformations in elastic solids. In elasticity theory, the unknown $u : \Omega \to \mathbf{R}^n$ is the displacement of the solid from some reference state and the behavior of the solid is determined through the stored-energy density function $\Phi(Du)$, where $Du = \left(\frac{\partial u^i}{\partial x_j}\right)$. The functions Φ that are of interest in phase transformations are those which fail to be rank-one convex. (See [**2**] for a discussion of rank-one convexity.) In this situation, the minimizer of $\int_\Omega \Phi(Du)\,dx$ will not exist in a classical sense. However, the minimizing sequences of $\int_\Omega \Phi(Du(x))\,dx$ indicate that equilibrium deformations of the solid consist of fine bands of different phases. One possible way to determine the geometric structure of these bands is to consider the perturbed functional $\int_\Omega \{\Phi(Du) + \varepsilon^2 |D^2 u|^2\}\,dx$, for which a minimizer exists. For further details on phase transformations in solids see [**3,7,8** and [**13**].

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