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The singular limit of the Cahn-Hilliard equation with a nonlocal term

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Let us consider the Landau-Ginzburg energy with an additional nonlocal term $F_\epsilon(u) :=$

$$\int_\Omega \left(\frac{\epsilon}{2}|\nabla u|^2 + \frac{1}{\epsilon}W(u)\right) + \sigma \int_\Omega \left((-\Delta_N^{-1})(u - \frac{1}{|\Omega|}\int_\Omega u)\right)(u - \frac{1}{|\Omega|}\int_\Omega u) \ ,$$

where $W(z) := (z^2-1)^2$ is the usual double-well potential, Δ_N^{-1} is the inverse of the Laplace operator with respect to homogeneous Neumann boundary data and ϵ and σ are small positive parameters. When minimizing F_ϵ on the affine subspace of $H^{1,2}(\Omega)$ which prescribes fixed mean value, then the first part $E_\epsilon(u) := \int_\Omega \left(\frac{\epsilon}{2}|\nabla u|^2 + \frac{1}{\epsilon}W(u)\right)$ of the functional wants the minimizer to take values $+1$ or -1 while minimizing the interface area (the area where the minimizer takes values strictly between $+1$ and -1), however the nonlocal term $N_\sigma(u) := \sigma \int_\Omega \left((-\Delta_N^{-1})(u - \frac{1}{|\Omega|}\int_\Omega u)\right)(u - \frac{1}{|\Omega|}\int_\Omega u)$ wants the minimizer to oscillate.

This leads to microstructures: according to numerical results the 'phase' $\{u < 0\}$ forms laminar structures when the mean value of u is close to 0, however other, for example sieve-like structures (in two dimensions) appear for values far from 0. The arising question whether global minimizers are periodic has been positively answered by S. Müller for mean value $= 0$ in one space dimension ([Mu]); for the case of mean values different from 0 and other boundary conditions see ([NiWe]). In higher dimensions however the

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question of periodicity presents a very hard problem, but steps in this direction (like estimating the frequency of minimizers) are done in a joint work with S. Müller.
Periodicity (in the time-dependent case) is interesting for other reasons, too, since it makes it possible to rescale the case $\sigma = O(\frac{1}{\epsilon})$ to the case $\sigma = O(1)$ (see [NiOh]).
The present paper is concerned with the *singular limit* as $\epsilon \to 0$ in the latter case, i.e. the singular limit of the gradient flow in $H^{-1}(\Omega)$ with respect to the functional F_ϵ. This gradient flow has been used in [OhKa] and [NiOh] to model the micro-phase separation of di-block copolymers where the parameter σ is inversely proportional to the square of the copolymers' total chain length.
In the stationary case one can prove that F_ϵ converges to

$$F_0(v) := \int_\Omega |\nabla\zeta(v)| + I_0(v) + \int_\Omega \left((-\Delta_N^{-1})(v - \frac{1}{|\Omega|}\int_\Omega v)\right)(v - \frac{1}{|\Omega|}\int_\Omega v)$$

in the sense of Γ-convergence in $L^1(\Omega)$ (here $\zeta(z) := \sqrt{2}\int_0^z \sqrt{W(s)}ds$ and

$$I_0(v) := \left\{ \begin{array}{ll} 0 & , v \in \{-1,+1\} \text{ a.e.} \\ +\infty & , \text{otherwise} \end{array} \right),$$

which leads to the conjecture that the solution (u_ϵ, v_ϵ) of the time-dependent ϵ-problem

$$\partial_\epsilon u + u_\epsilon - \frac{1}{|\Omega|}\int_\Omega u_\epsilon = \Delta v_\epsilon \text{ in }]0,T[\times\Omega ,$$

$$v_\epsilon = -\epsilon\Delta u_\epsilon + \frac{1}{\epsilon}W'(u_\epsilon) \text{ in }]0,T[\times\Omega ,$$

$$\nabla u_\epsilon \cdot \nu = \nabla v_\epsilon \cdot \nu = 0 \text{ on }]0,T[\times\partial\Omega ,\ u_\epsilon(0,\cdot) = u_\epsilon^0(\cdot)$$

converge to a solution (u, v) of

$$u \in \{-1,+1\} \text{ a.e. in } \Omega ,$$

$$\partial_t u + u - \frac{1}{|\Omega|}\int_\Omega u \;=\; \Delta v \text{ in }]0,T[\times\Omega \text{ in the distributional sense },$$

$$\text{the first variation of } \int_\Omega (|\nabla\zeta(\phi)| \;-\; v\phi) \text{ vanishes in } \phi = u(t) \text{ for a.e. } t\ ,$$

$$\nabla v\cdot\nu = 0 \text{ on }]0,T[\times\partial\Omega\ ,\ u(0,\cdot) = u^0(\cdot)\ .$$

Without the nonlocal term this system is known as Hele-Shaw system or Mullins-Sekerka equation: Xinfu Chen showed global existence of a solution in two dimensions in the case where the initial interface is close to a sphere ([Che]), and Luckhaus and Sturzenhecker ([LuSt]) considered an implicit time-discretization (assuming a Dirichlet condition for v) and proved existence of a weak solution provided that no energy loss occurs in the limiting process.

Regarding the above singular limit problem (still without our nonlocal term) Alikakos, Bates and Xinfu Chen ([AlBaCh]) showed that *if* the limit problem admits a unique smooth solution, then the E_ϵ-gradient flow converges to the limit problem.

However (bearing in mind the dumbbell-shaped interface appearing in mean curvature flow, the second order counterpart of the Mullins-Sekerka equation) one cannot expect existence of a smooth solution in general (not to speak of uniqueness), and because of the fourth-order situation viscosity methods may not be applied.

For our purpose we chose the approach of S. Luckhaus (see [Lu], [LuSt], [PlSt] and [Sch]), and our result is the following:

suppose $n \le 3, \partial\Omega \in C^{1,1}, u^{0\epsilon} \to u^0$ in $L^1(\Omega)$ and $\sup_{\epsilon>0} E_\epsilon(u^{0\epsilon}) < \infty$; then there exists a solution (u^ϵ, v^ϵ) of the ϵ-equation (with respect to initial data $u^{0\epsilon}$) satisfying the following:

there exists $(u,v) \in L^\infty(]0,T[;BV(\Omega)) \times L^2(]0,T[;H^{1,2}(\Omega))$ where u takes only values -1 and $+1$ and there exists a subsequence $\epsilon \to 0$ such that $u_\epsilon \to u$ in $L^2(]0,T[\times\Omega)$ and $v_\epsilon \to v$ in $L^2(]0,T[;H^{1,2}(\Omega))$;

furthermore, if there is no loss in the total energy when proceeding to the *limit in* ϵ *, i.e. if*

$$\limsup_{\epsilon\to 0} \int_0^T E_\epsilon(u_\epsilon(t))\,dt \le \int_0^T E_0(u(t))\,dt ,$$

then (u,v) *is a solution in the following sense:*

$$\int_0^T\int_\Omega \left[-\partial_t\eta\,(u-u_0) + \eta\,(u - \frac{1}{|\Omega|}\int_\Omega u) + \nabla\eta\cdot\nabla u\right] = 0$$

for any $\eta \in L^2(]0,T[;H^{1,2}(\Omega))$ *s.t.* $\eta(T)=0$ *, and*

$$\frac{1}{\mu}\int_\Omega u(t)\,div\,(v(t)\xi) = \int_\Omega (D\xi(\nu)(\nu) - div\,\xi)\,d|\nabla u|$$

for any $\xi \in C^1(\bar\Omega;\mathbf{R}^n)$ *s.t.* $\xi\cdot\nu_{\partial\Omega}=0$ *and a.e.* $t\in]0,T[$ *(here* $\nu_{\partial\Omega}$ *means the outer normal on* $\partial\Omega$ *,* $|\nabla u|$ *is the total variation of the measure* ∇u *,* $\nu = \frac{\nabla u}{|\nabla u|}$ *is the Radon-Nikodym derivative and* $\mu := \sqrt{2}\int_{-1}^{1}\sqrt{W(s)}\,ds$*).*

Before giving a sketch of proof let us remark three things:
First, that no energy loss occurs in the limiting process may be interpreted in the way that no phase-inner boundaries are allowed to appear, and thereby it represents a condition which makes physical sense.
Next, the condition may be verified numerically.
Last, the above notion of solution is rather strong since the interface is the boundary of an open set of finite perimeter and the second equation is already written as an equation on the interface.

Sketch of proofs (the detailed proofs will be given in the fourthcoming paper [NiWe]):
We pass up the construction of the solution for the ϵ-problem satisfying the following bounds:

$$\sup_{t\in]0,T[} E_\epsilon(u_\epsilon(t)) + \int_0^T\int_\Omega |\nabla v_\epsilon|^2 \le C_1 ,$$

$$\|u_\epsilon(t) - u_\epsilon(t-s)\|_{H^{-1}(\Omega)} \leq C_2\sqrt{s} \text{ and}$$
$$u_\epsilon \text{ bounded in } L^2(]0,T[;H^{-1}(\Omega)) \ .$$

Using results of Simon ([Si]), precompactness of u_ϵ in $L^2(]0,T[\times\Omega)$ follows, and the boundedness of the energy assures that any limit u takes values in $+1$ and -1 only.

Now we proceed as in [LuMo], [PlSt] and [Sch]:

using the assumptions and elliptic regularity theory, it is easy to show that $u_\epsilon(t) \in H^{2,2}(\Omega)$ for a.e. $t \in]0,T[$. Next, taking $\xi \cdot \nabla u$ (for ξ as in the assumption) as test function for the equation of u_ϵ , we obtain after some calculation

$$0 = \int\limits_\Omega \left[\partial_i\xi_j\partial_i u_\epsilon\partial_j u_\epsilon \ - \ \frac{1}{2}\left(\epsilon|\nabla u_\epsilon|^2 + \frac{1}{\epsilon}W(u_\epsilon)\right) \text{ div } \xi \ + \ u_\epsilon \operatorname{div}(v_\epsilon\xi)\right] \ . \tag{1}$$

Using the lower semicontinuity of the perimeter as well as the assumption that no energy loss occurs, we get

$$\limsup_{\epsilon\to 0} \int\limits_0^T |E_\epsilon(u_\epsilon(t) - E_0(u(t))| \ = \ 0 \ , \tag{2}$$

therefore it is easy to deal with the second term of the sum in (1). In order to handle the first term of the sum in (1), which is nonlinear in ∇u_ϵ , let us remark that using the convergence of the energy in (2) in can be proved that

$$\|\sqrt{\frac{\epsilon}{2}}|\nabla u_\epsilon| \ - \ \frac{1}{\sqrt{\epsilon}}\sqrt{W(u_\epsilon(t))}\|_{L^2(\Omega)} \ \to 0 \text{ and}$$

$$\||\nabla\zeta(u_\epsilon(t))| \ - \ \left(\frac{\epsilon}{2}|\nabla u_\epsilon(t)|^2 + \frac{1}{\epsilon}W(u_\epsilon(t))\right)\|_{L^1(\Omega)} \ \to 0$$

for a.e. $t \in]0,T[$ as $\epsilon \to 0$.

Therefore we may replace $\int\limits_\Omega D\xi(\nabla u_\epsilon(t))(\nabla u_\epsilon(t))$ first by

$$\int\limits_\Omega D\xi\left(\frac{\nabla\zeta(u_\epsilon(t))}{|\nabla\zeta(u_\epsilon(t))|}\right)\left(\frac{\nabla\zeta(u_\epsilon(t))}{|\nabla\zeta(u_\epsilon(t))|}\right) \ \epsilon^2 \ |\nabla u_\epsilon(t)|^2$$

and then by

$$\int_\Omega D\xi\left(\frac{\nabla\zeta(u_\epsilon(t))}{|\nabla\zeta(u_\epsilon(t))|}\right)\left(\frac{\nabla\zeta(u_\epsilon(t))}{|\nabla\zeta(u_\epsilon(t))|}\right)\sqrt{2}\sqrt{W(u_\epsilon(t))}\,|\nabla u_\epsilon(t)|\,,$$

which converges by Reshetnyak's theorem for a.e. $t\in]0,T[$ to

$$\int_\Omega D\xi\left(\frac{\nabla\zeta(u(t))}{|\nabla\zeta(u(t))|}\right)\left(\frac{\nabla\zeta(u(t))}{|\nabla\zeta(u(t))|}\right)d|\nabla\zeta(u(t))|\,.$$

Last, notice that, since $\left(\frac{1}{|\Omega|}\int_\Omega v_\epsilon(t)\right)\int_\Omega (u_\epsilon(t)\ \mathrm{div}\ \xi)$ is by (1) bounded in $L^\infty(0,T)$ and since $u_\epsilon \to u \in \{+1,-1\}$ strongly in $L^2(]0,T[\times\Omega)$, $\frac{1}{|\Omega|}\int_\Omega v_\epsilon(t)$ has to be bounded in $L^\infty(0,T)$, which makes it possible to handle the last term of the sum in (1).

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