

THE CAHN-HILLIARD EQUATION AS DEGENERATE LIMIT OF THE PHASE-FIELD EQUATIONS

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Abstract. We show that the Cahn-Hilliard equation occurs as a special scaling limit of the phase-field equation.

Introduction and statement of the results. Within this paper we study the relationship between the Cahn-Hilliard equation and the phase-field model studied by Caginalp (1986). We recollect that the Cahn-Hilliard equation may be written as

$$\begin{aligned} \partial_t \varphi &= \Delta u, \\ u &= -\varepsilon \Delta \varphi + \frac{\sigma^2}{\varepsilon} f'(\varphi), \end{aligned} \tag{CH}$$

where $f(\varphi) = \frac{1}{2}(1 - \varphi^2)^2$ is a double well potential, σ a measure for surface tension, and ε a (mostly) small parameter measuring the width of the transition layer, where φ varies quickly from -1 to $+1$.

The phase-field equations we consider (see Caginalp 1989) have the form

$$\begin{aligned} \alpha \partial_t u + \partial_t \varphi - \Delta u &= 0, \\ \alpha \varepsilon \partial_t \varphi - \varepsilon \Delta \varphi + \frac{\sigma^2}{\varepsilon} f'(\varphi) - u &= 0. \end{aligned} \tag{PhF}$$

Formally we expect the Cahn-Hilliard equation as the limit α to zero (see Elliott 1989), and in fact it turns out that this is true rigorously under reasonable restrictions on the initial data.

Our assumptions are the following.

A) The functions $u, \varphi = u_\alpha, \varphi_\alpha \in C^\infty(\overline{\Omega_T})$ are solutions of (PhF) in some smooth space-time domain $\Omega_T := (0, T) \times \Omega$.

B) The boundary values $u_\alpha|_{\partial\Omega} =: u_D$ are independent of time and the parameter α and either the boundary values $\varphi_\alpha|_{\partial\Omega} =: \varphi_D$ are independent of time and the parameter α or $\nabla \varphi_\alpha \cdot \nu|_{\partial\Omega} = 0$.

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C) The initial data $u_\alpha(0, \cdot)$ and $\varphi_\alpha(0, \cdot)$ satisfy

$$\left(\frac{\varepsilon}{2} \int_\Omega |\nabla \varphi_\alpha|^2 dx + \frac{\sigma^2}{\varepsilon} \int_\Omega f(\varphi_\alpha) dx + \frac{\alpha}{2} \int_\Omega u_\alpha^2 dx \right) (0) \leq C,$$

$$\left(\frac{\alpha \varepsilon^2}{\sigma^2} \int_\Omega |\nabla u_\alpha|^2 dx + \frac{\varepsilon}{\sigma^2} \int_\Omega u_\alpha^2 dx + \frac{\varepsilon^3}{\sigma^2} \int_\Omega |\Delta \varphi_\alpha|^2 dx + \|\varphi_\alpha\|_{L^\infty(\Omega)} \right) (0) \leq C$$

with some constant C independent of α , and the initial data of the phase-field φ_α converge in $L^1(\Omega)$ to some $\varphi^0 \in H^{2,2}(\Omega)$.

As an example we may take smooth initial data independent of α .

All subsequently introduced constants C will depend implicitly only on the boundary values, the above constant C , the domain Ω and T , but not on the parameters ε , σ , and α .

The existence of such solutions of the phase-field equations has been shown by Elliott and Zheng (1989).

THEOREM 1. Under the above hypotheses a subsequence $(u_\alpha, \varphi_\alpha)$ converges to limiting functions (u, φ) with

$$u \in L^2(0, T; H^{1,2}(\Omega)) \quad \text{and} \quad \varphi \in L^\infty(0, T; H^{1,2}(\Omega)) \cap L^\infty(0, T; L^4(\Omega))$$

in the sense that, as $\alpha \rightarrow 0$,

$$u_\alpha, \nabla u_\alpha, \nabla \varphi_\alpha \rightarrow u, \nabla u, \nabla \varphi \quad \text{weakly in } L^2(\Omega_T),$$

$$\varphi_\alpha \rightarrow \varphi \quad \text{in } L^1(\Omega_T) \text{ and pointwise a.e.}$$

The limiting functions are weak solutions of the Cahn-Hilliard equation

$$\begin{aligned} \partial_t \varphi &= \Delta u, \\ u &= -\varepsilon \Delta \varphi + \frac{\sigma^2}{\varepsilon} f'(\varphi) \end{aligned} \tag{CH}$$

in Ω_T with boundary values

$$\begin{aligned} u|_{\partial\Omega} &= u_D, \\ \varphi|_{\partial\Omega} &= \varphi_D \quad (\nabla \varphi \cdot \nu|_{\partial\Omega} = 0, \text{ resp.}), \end{aligned}$$

and initial values $\varphi(0, \cdot) = \varphi^0$.

The weak formulation of (CH) does not allow one to resubstitute u by $-\varepsilon \Delta \varphi + \frac{\sigma^2}{\varepsilon} f'(\varphi)$ in the first equation of (CH). In order to obtain the usual Cahn-Hilliard equations we need higher regularity of the solution.

PROPOSITION 2. If $n \leq 3$, then the limiting phase-field φ belongs to $L^2(0, T; H^{3,2}(\Omega))$. If, in addition, the initial values satisfy the compatibility condition

$$\varphi^0 \in H^{4,2}(\Omega) \quad \text{and} \quad \begin{cases} -\varepsilon \Delta \varphi^0 + \frac{\sigma^2}{\varepsilon} f'(\varphi^0) = u_D, \\ \varphi^0 = \varphi_D \quad (\nabla \varphi^0 \cdot \nu = 0, \text{ resp.}) \end{cases} \quad \text{on } \partial\Omega,$$

then

$$\varphi \in H^{1,2}(0, T; L^2(\Omega)) \cap L^2(0, T; H^{4,2}(\Omega))$$

and φ is the unique solution of the Cahn-Hilliard equation

$$\partial_t \varphi + \Delta \left(\varepsilon \Delta \varphi - \frac{\sigma^2}{\varepsilon} f'(\varphi) \right) = 0 \quad \text{on } \Omega_T$$

with initial values φ^0 and Dirichlet boundary values φ_D (Neumann-0 boundary values, resp.) for φ and Dirichlet boundary values $(-\varepsilon \Delta \varphi + \frac{\sigma^2}{\varepsilon} f'(\varphi))|_{\partial \Omega} = u_D$.

In particular, the whole sequence φ_α converges to φ .

A priori bounds, compactness, and regularity. We start collecting some useful a priori estimates.

LEMMA 3. The sequence $(u_\alpha, \varphi_\alpha)$ satisfies

(i)

$$\begin{aligned} \alpha \varepsilon \int_0^T \int_\Omega |\partial_t \varphi_\alpha|^2 dx dt + \int_0^T \int_\Omega |\nabla u_\alpha|^2 dx dt \\ + \sup_{t \in [0, T]} \left(\varepsilon \int_\Omega |\nabla \varphi_\alpha|^2 dx + \frac{\sigma^2}{\varepsilon} \int_\Omega f(\varphi_\alpha) dx + \alpha \int_\Omega u_\alpha^2 dx \right) (t) \leq C, \end{aligned}$$

(ii)

$$\begin{aligned} \sup_{t \in [0, T]} \left(\alpha \varepsilon \int_\Omega |\partial_t \varphi_\alpha|^2 dx + \int_\Omega |\nabla u_\alpha|^2 dx \right) + \varepsilon \int_0^T \int_\Omega |\nabla \partial_t \varphi_\alpha|^2 dx dt \\ + \alpha \int_0^T \int_\Omega |\partial_t u_\alpha|^2 dx dt \leq \frac{C}{\alpha \varepsilon^2} \end{aligned}$$

with some constant C independent of α .

Proof. The first estimate (i) can be derived by multiplying the first of the phase-field equations (PhF) by $(u - u_D)$, the second by $\partial_t \varphi$, adding both results and integrating over Ω_T . Then hypothesis B on the boundary data and the first of the estimates of the initial data in C implies the result.

To obtain (ii) differentiate the second of the phase-field equations (PhF) with respect to t , multiply by $\partial_t \varphi$, multiply the first equation by $\partial_t u$, add the results and integrate. Note that $-f'' \leq 2$ to estimate the nonquadratic term, apply the first part of this lemma to estimate $\iint |\partial_t \varphi|^2$, and use the second estimate of hypothesis C to control the initial values.

Proof of Theorem 1. Since we deal with a nonlinear equation we have to show strong compactness of the sequence φ_α in $L^1(\Omega_T)$. Lemma 3 only furnishes estimates of derivatives in the x -direction, but no uniform bounds on time derivatives. Compactness follows from interpolating the fact that we know $\partial_t \varphi_\alpha \in L^2(0, T; H^{-1,2}(\Omega))$ and $\nabla \varphi_\alpha \in L^\infty(0, T; L^2(\Omega))$. We define the time differences

$$\chi_\alpha(t) := \varphi_\alpha(t+h) - \varphi_\alpha(t).$$

The differential equation

$$\partial_t \varphi_\alpha = -\alpha \partial_t u_\alpha + \Delta u_\alpha$$

immediately implies

$$\int_0^{T-h} \|\chi_\alpha(t)\|_{H^{-1,2}} dt \leq T^{\frac{1}{2}} h \left(\left(\int_0^T \int_\Omega |\nabla u_\alpha|^2 dx dt \right)^{\frac{1}{2}} + \alpha \left(\int_0^T \int_\Omega |\partial_t u_\alpha|^2 dx dt \right)^{\frac{1}{2}} \right).$$

The right-hand side can be estimated by Lemma 3 and we find

$$\int_0^{T-h} \|\chi_\alpha(t)\|_{H^{-1,2}} dt \leq C \cdot h.$$

We apply the following interpolation inequality, valid for all $w \in L^1(0, T; H^{1,1}(\Omega))$ and $\rho > 0$ (see Luckhaus 1990):

$$\int_0^T \int_\Omega |w| dx dt \leq \rho \int_0^T \int_\Omega |\nabla w| dx dt + \frac{C}{\rho} \int_0^T \|w(t)\|_{H^{-1,2}} dt + \int_0^T \int_{B_{2\rho}(\partial\Omega)} |w| dx dt.$$

We set $w = \chi_\alpha$, use the above estimate to obtain bounds for the right-hand side and arrive at

$$\int_0^{T-h} \int_\Omega |\varphi_\alpha(t+h, x) - \varphi_\alpha(t, x)| dt dx \leq \left(\rho + \frac{h}{\rho} + \rho^{1/2} \right).$$

Now choose $\rho = h^{1/4}$. This estimate, together with Lemma 3, then implies the compactness of φ_α in $L^1(\Omega_T)$ such that we can select a subsequence of φ_α converging in $L^1(\Omega_T)$ and pointwise almost everywhere to some limiting phase-field φ . Lemma 3 allows to assume that, for a further subsequence, $\nabla\varphi_\alpha$, ∇u_α , and u_α converge weakly in $L^2(\Omega_T)$ to $\nabla\varphi$, ∇u , and u (resp.). The uniform bounds from Lemma 3 carry over to the limits φ and u .

Now we pass to the limit in the phase-field equations (PhF). To this end multiply (PhF)₁ by a smooth test function ζ with $\zeta(T, \cdot) = 0$ and $\zeta(t, \cdot) \in C_0^\infty(\Omega)$ in the case of prescribed Dirichlet values and (PhF)₂ by a smooth test function η with $\eta(T, \cdot) = 0$:

$$\begin{aligned} & - \int_0^T \int_\Omega (\alpha u_\alpha + \varphi_\alpha) \partial_t \zeta dx dt - \int_\Omega (\alpha u_\alpha + \varphi_\alpha) \zeta(0, x) dx + \int_0^T \int_\Omega \nabla u_\alpha \cdot \nabla \zeta dx dt = 0, \\ \alpha \varepsilon \int_0^T \int_\Omega \varphi_\alpha \partial_t \eta dx dt - \alpha \varepsilon \int_\Omega (\varphi_\alpha \eta)(0, x) dx + \varepsilon \int_0^T \int_\Omega \nabla \varphi_\alpha \cdot \nabla \eta dx dt \\ & \qquad \qquad \qquad + \int_0^T \int_\Omega \left(\frac{\sigma^2}{\varepsilon} f'(\varphi_\alpha) - u_\alpha \right) \eta dx dt = 0. \end{aligned}$$

We note that αu_α and $\alpha \varphi_\alpha$ converge weakly to zero. Furthermore, $f'(\varphi_\alpha) = -2(\varphi_\alpha - \varphi_\alpha^3)$ converges in $L^1(\Omega_T)$, since it converges pointwise and $\varphi_\alpha \in L^4(\Omega_T)$ uniformly in α . All the other terms are linear and converge as a consequence of the weak convergence of the respective terms. We obtain

$$\begin{aligned} & - \int_0^T \int_\Omega \varphi \partial_t \zeta dx dt - \int_\Omega \varphi^0 \zeta(0) dx + \int_0^T \int_\Omega \nabla u \cdot \nabla \zeta dx dt = 0, \\ & \varepsilon \int_\Omega \nabla \varphi \cdot \nabla \eta dx + \int_\Omega \frac{\sigma^2}{\varepsilon} f'(\varphi) \eta dx - \int_\Omega u \eta dx = 0 \end{aligned}$$

for all $\zeta \in C_0^\infty([0, T] \times \Omega)$ and for all $\eta \in C_0^\infty(\Omega)$ ($\eta \in C^\infty(\Omega)$ resp.). This is a weak formulation of the Cahn-Hilliard equation.

Proof of Proposition 2. By elliptic and parabolic regularity theory, weak solutions of the Cahn-Hilliard equation (CH) as in Theorem 1 are in fact pointwise solutions: we first observe that, since $f''(\varphi) = 6\varphi^2 - 2 \in L^\infty(0, T; L^2(\Omega))$, we have

$$\nabla f'(\varphi) = f''(\varphi)\nabla\varphi \in L^\infty(0, T; L^1(\Omega)),$$

and thus by the Sobolev imbedding theorem

$$f'(\varphi) \in L^\infty(0, T; L^{n/(n-1)}(\Omega)).$$

We apply elliptic regularity theory to the second equation of (CH) and obtain (since $u \in L^2(\Omega_T)$)

$$\varphi \in L^2(0, T; H^{2, n/(n-1)}(\Omega)),$$

such that in return

$$-\varepsilon\Delta\varphi + \frac{\sigma^2}{\varepsilon}f'(\varphi) = u \quad \text{almost everywhere in } \Omega_T.$$

If $n \leq 3$ the Sobolev imbedding theorem yields for all $q < \infty$

$$\varphi \in L^2(0, T; L^q(\Omega)).$$

This implies for all $p < 2$

$$\nabla f'(\varphi) = f''(\varphi)\nabla\varphi \in L^1(0, T; L^p(\Omega)),$$

and together with $\nabla f'(\varphi) \in L^p(0, T; L^1(\Omega))$ that for all $m < 3/2$

$$\nabla f'(\varphi) \in L^m(0, T; L^m(\Omega)).$$

Then elliptic regularity theory implies (since $\nabla u \in L^2(\Omega_T)$)

$$\nabla\varphi \in L^m(0, T; H^{2, m}(\Omega))$$

and so

$$\varphi \in L^m(0, T; H^{3, m}(\Omega)) \subset L^m(0, T; H^{2, 3m/(3-m)}(\Omega)) \subset L^m(0, T; H^{1, 3m/(3-2m)}(\Omega)).$$

In addition since $\varphi \in L^\infty(0, T; H^{1, 2}(\Omega))$ we have $\varphi \in L^\infty(0, T; L^6(\Omega))$.

We substitute u by $-\varepsilon\Delta\varphi + \frac{\sigma^2}{\varepsilon}f'(\varphi)$ in the first equation of (CH) and obtain a weak formulation of

$$\partial_t\varphi + \varepsilon\Delta^2\varphi = \frac{\sigma^2}{\varepsilon}(f'''(\varphi)|\nabla\varphi|^2 + f''(\varphi)\Delta\varphi) =: g$$

with a right-hand side

$$g \in L^m(0, T; L^m(\Omega)).$$

For this calculate

$$\begin{aligned} \int_0^T \|f''(\varphi)\Delta\varphi\|_m^m(t) dt &\leq C \int_0^T (\|\varphi(t)\|_6^3 + 1) \|\Delta\varphi(t)\|_{2m}^m dt \\ &\leq C \sup_t (\|\varphi(t)\|_6^3 + 1) \int_0^T \|\Delta\varphi(t)\|_{2m}^m dt \end{aligned}$$

and

$$\begin{aligned}
 & \int_0^T \|f'''(\varphi)|\nabla\varphi|^2\|_m^m(t) dt \\
 & \leq C \int_0^T \|\nabla\varphi(t)\|_{3m/(3-2m)}^m \left(\int_{\Omega} (|\varphi|^m + 1)|\nabla\varphi|^m(t, x) dx \right)^{2m/3} dt \\
 & \leq C \int_0^T \|\nabla\varphi(t)\|_{3m/(3-2m)}^m \|\varphi(t)\|_6^m \|\nabla\varphi\|_2^m dt \\
 & \leq C \sup_t \|\varphi(t)\|_6^m \sup_t \|\nabla\varphi(t)\|_2^m \int_0^T \|\nabla\varphi(t)\|_{3m/(3-2m)}^m dt.
 \end{aligned}$$

Parabolic regularity theory together with the compatibility condition of the initial data then implies that

$$\varphi \in H^{1,m}(0, T; L^m(\Omega)) \cap L^m(0, T; H^{4,m}(\Omega));$$

such that in return

$$\partial_t \varphi + \Delta \left(\varepsilon \Delta \varphi - \frac{\sigma^2}{\varepsilon} f'(\varphi) \right) = 0 \quad \text{almost everywhere in } \Omega_T.$$

Elliott and Zheng proved (1986) that a solution of this class is unique.

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