Global Solution to the Penrose-Fife Phase-Field Model With Zero Interfacial Energy and Fourier Law

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Abstract

In this paper we study a system of field equations of Penrose-Fife type governing the dynamics of phase transitions with a nonconserved order parameter. In many recent contributions on this subject, the heat flux law has been assumed in the form $\mathbf{q} = \nabla(1/\theta)$. In contrast to that, here we consider the (more realistic) case of the Fourier law when $\mathbf{q}$ is proportional to the negative gradient $-\nabla\theta$ of the (absolute) temperature θ. The assumption of Fourier heat conduction presents particular difficulties in the framework of the Penrose-Fife model, since then the field equation representing the balance of internal energy does not seem to have a maximum principle from which the positivity of θ could be derived. In this connection, we recall that the main difficulty in proving existence for phase-field systems of Penrose-Fife type is the proof of the positivity of θ. It is shown in this paper that in the case without interfacial energy, that is, when the free energy does not contain a quadratic gradient term of the order parameter, there exists a comparatively easy way to conclude the positivity of θ under rather weak and quite natural conditions on the data of the system. Having established this result, the existence of a weak solution is readily obtained using known results on general phase-field systems.

1 Introduction

In this paper we study the initial-boundary value problem

$$(\theta + \lambda(\chi))_t(x,t) - \Delta\theta(x,t) = g(x,t,\theta(x,t),\chi(x,t)) \quad \text{for a. e. } (x,t) \in Q\,, \tag{1.1}$$

$$\chi_t + \partial I(\chi) + \sigma'(\chi) \ni -\lambda'(\chi)/\theta \quad \text{a. e. in } Q\,, \tag{1.2}$$

$$\frac{\partial\theta}{\partial\nu} = 0 \quad \text{a. e in } \Sigma\,, \tag{1.3}$$

$$\theta(\,\cdot\,,0) = \theta_0\,, \quad \chi(\,\cdot\,,0) = \chi_0 \quad \text{a. e. in } \Omega\,. \tag{1.4}$$

Here, $\Omega \subset \mathbb{R}^N$ $(N \geq 1)$ denotes some bounded domain with smooth boundary $\partial\Omega$, $\partial/\partial\nu$ is the outward normal derivative to $\partial\Omega$, and we have set $Q := \Omega \times (0,T)$, $\Sigma := \partial\Omega \times (0,T)$, where $T > 0$ stands for some final time. In addition, σ, λ, g are smooth functions, θ_0, χ_0 are given data, and ∂I denotes the subdifferential of the indicator function I of the interval $[0,1]$. Namely, we have that $I(\chi) = 0$ if $\chi \in [0,1]$, $I(\chi) = +\infty$ otherwise, and consequently

$$\xi \in \partial I(\chi) \quad \text{if and only if} \quad \chi \in [0,1] \ \text{ and } \ \xi \begin{cases} \in (-\infty, 0] & \text{for } \chi = 0 \\ = 0 & \text{for } 0 < \chi < 1\,. \\ \in [0,+\infty) & \text{for } \chi = 1 \end{cases}$$

The nonlinear system (1.1–2) constitutes the system of field equations arising from the Penrose-Fife phase-field model of phase transitions for a nonconserved order parameter χ and the absolute temperature θ when no diffusive effect is assumed for the phase transition, the heat flux obeys the Fourier law, and the free energy has the (nonsmooth) normalized form

$$F(\theta,\chi) = \theta - \theta \log\theta + \theta\,(I(\chi) + \sigma(\chi)) + \lambda(\chi)\,. \tag{1.5}$$

Then equation (1.1) yields the balance of internal energy, while (1.2) describes the evolution of the order parameter (where all physical constant are normalized to unity). For details of the Penrose-Fife model we refer the reader either to the original papers [22, 23] or to the monograph [5] (cf. especially Chapter 4). The presence of the singular factor $1/\theta$ in the right hand side of (1.2) and of a nonlinear function $\lambda(\chi)$ in (1.1) distinguishes the above system from the standard phase-field model [6, 13], which can be viewed as a linearization of (1.1–2) around some equilibrium temperature. In fact, the advantage of the actual system (1.1–2) is that it is consistent with the Second Law of Thermodynamics, as the Clausius-Duhem inequality is satisfied, and (1.1) and (1.2) have been tailored with exactly this purpose. Moreover, since the quadratic gradient term for χ is missing in the free energy expression (1.5), the Clausius-Duhem inequality holds not only in integrated form but locally in space (and time). In this respect, notice that the inclusion (1.2) can be equivalently rewritten as a pointwise variational inequality, namely

$$\begin{gathered} 0 \le \chi(x,t) \le 1 \quad \text{for a.e. } (x,t) \in Q\,, \\ \chi_t\,(\chi - r) \le -\,(\sigma'(\chi) + \lambda'(\chi)/\theta)\,(\chi - r) \quad \text{a.e. in } Q\,, \quad \forall\, r \in [0,1]\,. \end{gathered} \tag{1.6}$$

Clearly, (1.6) forces the order parameter χ to attain only values in $[0,1]$, that is, χ may for instance be regarded as the volume fraction of one of the two phases between which the phase transition occurs.

Typical nonlinearities λ and σ in the case of a *solid-liquid phase transition* are given by

$$\lambda(\chi) = \int_{1/2}^{\chi} \ell(\xi)\,d\xi\,, \quad \sigma(\chi) = -\frac{\lambda(\chi)}{\theta_c} + 4\,a\,\chi\,(1-\chi)\,, \tag{1.7}$$

where $\ell(\chi) > 0$ represents the (possibly constant) latent heat of the phase transition, $\theta_c > 0$ the critical (melting or freezing) temperature, and $a > 0$ the maximum value of the function $4\,a\,\chi\,(1-\chi)$, attained at the midpoint $\chi = 1/2$ and measuring the depth of the potential wells corresponding to the different phases. Notice that this choice of λ and σ turns out to provide the *double obstacle potential* considered for instance in [3, 4]. We point out that by (1.7) one point between 0 and 1 is always preferred as minimum provided $\theta \neq \theta_c$. Another interesting form for the free energy is obtained with the choice

$$\lambda(\chi) = 4\,b\,\chi\,(1-\chi)\,, \quad \sigma(\chi) = \frac{b}{\theta_c}\,(1 - 2\,\chi)^2\,, \tag{1.8}$$

which corresponds to the *Ising model of ferromagnetism* if the configurational entropy $k\,\chi\log(\chi) + k\,(1-\chi)\log(1-\chi)$ considered in [22 , 23] (k denotes a constant factor) is replaced by the expression $I(\chi) + \sigma(\chi)$. Here, the parameter b is analogous with a, while θ_c plays the role of the Curie temperature. This situation is rather different from the previous one, since here the free energy may assume either two absolute minima with the same value (two symmetric phase variants) if $\theta < \theta_c$ or just one absolute minimum in the midpoint if $\theta > \theta_c$.

The main novelty of this paper lies in the use of the standard Fourier law of heat conduction in (1.1) in the framework of the Penrose-Fife model. Until now (up to the paper [21] where a very particular case was considered), no global existence results could be derived for Penrose-Fife phase-field systems with Fourier law. Instead, the heat flux $\mathbf{q}$ was always assumed in the singular form

$$\mathbf{q} = \nabla(1/\theta)\,, \tag{1.9}$$

or in a generalized form thereof which was still singular in θ for $\theta \searrow 0$. In this connection, the reader is referred to [8 , 9 , 11 , 15–17 ,19, 20, 24, 25].

The reason for the lack of conclusions under the Fourier law lies in the presence of the inverse temperature $1/\theta$ in (1.2). The occurrence of this singular term renders the evolution equation for χ singular, so that earlier existence results for phase relaxation systems (cf. [1 , 2 , 7 , 12 , 14 , 26 , 27], for instance) do not apply. However, once that a positive lower bound for θ has been found, it becomes a standard matter to show global existence, due to the Lipschitz continuity of the reduced nonlinearity. Therefore, the proof of the positivity of θ constitutes the main step in any existence proof for the system (1.1–4). However, while a maximum principle turned out to be hidden in the balance of internal energy for the heat flux law (1.9) (the related balance law then reads

$$(\theta + \lambda(\chi))_t + \Delta(1/\theta) = g \quad \text{a.e. in } Q\,, \tag{1.10}$$

in place of (1.1)), this did not seem to be true for the Fourier law.

We will demonstrate in this note that, under both simple and quite natural conditions on the form of the nonlinearities λ and σ, a uniform lower bound for θ can be constructed. While in the case of the heat flux (1.9) (treated in [11]) the corresponding maximum principle proof is based on technically difficult Moser-type iterations applied to (1.10) (following an argument devised in [25]), our proof for the case of the Fourier law is comparatively easy. Its main idea is to combine (1.1) with the phase relaxation law (1.2) instead of discussing (1.1) by itself. The general scheme behind this approach is motivated by physics: in a system of phase-field equations complying with the Second Principle of Thermodynamics the positivity of temperature should be hidden somewhere. However, in general one cannot expect to extract it by considering the balance of internal energy alone; after all, the latter reflects the First Principle of Thermodynamics and not the Second Principle. Therefore, to obtain full information about the behaviour of θ, one will usually have to invoke the whole system of field equations.

Then, determining a lower bound for θ allows us to deduce existence of solutions to the initial-boundary value problem (1.1-4). We should point out another advantage of our technique: it is noteworthy that it does not require to assume λ to be a *convex* function as in the corresponding papers [11 , 17 , 24] that deal with equation (1.10).

The rest of the paper is organized as follows. In Section 2, we formulate the general assumptions and the main existence and uniqueness result. Section 3 brings the detailed proof of this result and, in particular, of the positivity of temperature.

2 Statement of Problem and Existence

In this section we give a complete statement of the problem and formulate the existence result which will be proved in Section 3. To this end, let us consider the system (1.1–4). We make the following general assumptions on the data λ, σ, g, θ_0, χ_0.

(A1) $\lambda\,,\,\sigma\in C^{1,1}[0,1]\,.$

(A2) g is a Carathéodory function satisfying $g(\cdot\,,\cdot\,,\varphi,r)\in L^2(Q)$ for all pairs $(\varphi,r)\in\mathbb{R}\times[0,1]$, and there exists some constant $C_g>0$ such that

$$|g(x,t,\varphi_1,r_1)\,-\,g(x,t,\varphi_2,r_2)|\,\le\,C_g\,(|\varphi_1-\varphi_2|\,+\,|r_1-r_2|) \quad \text{for a.e. } (x,t)\in Q\,,\quad \forall\,\varphi_1\,,\,\varphi_2\in\mathbb{R}\,,\quad \forall\,r_1\,,\,r_2\in[0,1]\,. \tag{2.1}$$

(A3) $\theta_0\in H^1(\Omega)\,,\quad \chi_0\in L^2(\Omega)\,,\quad \theta_0>0$ and $0\le\chi_0\le 1$ a.e. in $\Omega\,.$

Now, we may define our notion of solution to the system (1.1–4).

Definition 2.1 A pair (θ,χ) is said to be a solution to (1.1–4) if

$$\theta\in H^1(0,T;L^2(\Omega))\cap C^0([0,T];H^1(\Omega))\cap L^2(0,T;H^2(\Omega))\,, \tag{2.2}$$

$$\chi\in H^1(0,T;L^2(\Omega))\cap L^\infty(Q)\,, \tag{2.3}$$

$$\theta>0 \ \text{ a.e. in } Q\,,\quad \frac{1}{\theta}\in L^1(Q)\,, \tag{2.4}$$

and the equations (1.1–4) are satisfied in the sense specified there.

Observe that in our setting all terms in (1.1) belong to $L^2(Q)$ and that, by virtue of **(A1)** and (2.4), $\lambda'(\chi)/\theta\in L^1(Q)$, whence (1.2) and (1.6) are meaningful.

For the proof of positivity of the temperature θ the next assumption will be crucial.

(A4) There exists some constant $\theta_* > 0$ such that the following three conditions are fulfilled at the same time,

$$\theta_0 \geq \theta_* \quad \text{a.e. in } \Omega\,, \tag{2.5}$$

$$g(x,t,\varphi,r) \geq 0 \quad \text{for a.e. } (x,t) \in Q\,, \quad \forall\, \varphi \leq \theta_*\,, \quad \forall\, r \in [0,1]\,, \tag{2.6}$$

$$|\lambda'(r)|^2 + \sigma'(r)\,\lambda'(r)\,\theta_* \geq 0 \quad \forall\, r \in [0,1]\,. \tag{2.7}$$

We remark that (2.5) and (2.6) are rather natural constraints for the initial (absolute) temperature and the heat supply, respectively, while (2.7) holds if either $\sigma'\,\lambda'$ has the right sign or if $|\sigma'|$ is not too large when compared with $|\lambda'|$. Note that both the physically interesting nonlinearities mentioned in (1.7) and (1.8) satisfy **(A4)** provided that $\theta_* > 0$ is chosen small enough.

We have the following existence and uniqueness result.

Theorem 2.2 *Suppose that the assumptions* **(A1–4)** *hold. Then the system* (1.1–4) *has a unique solution* (θ,χ) *(in the sense of Definition 2.1). Moreover, it turns out that* $\chi_t \in L^\infty(Q)$ *and*

$$\theta \geq \theta_* \quad \textit{a.e. in } Q\,. \tag{2.8}$$

The proof of this result will be given in the next section.

The following additional statement yields a sufficient condition for the boundedness of temperature from above.

Proposition 2.3 *Let* **(A1–4)** *be satisfied and let* $\theta_0 \in L^\infty(\Omega)$. *Besides, assume that there is some* $p > 1 + n/2$ *such that*

$$g_0 := g(\cdot,\cdot,0,0) \in L^p(Q). \tag{2.9}$$

Then we have $\theta \in L^\infty(Q)$.

Note that Theorem 2.2, (2.1), and (2.9) entail

$$\begin{aligned} |-(\lambda(\chi))_t + g(x,t,\varphi,r)| \;&\leq\; |g_0(x,t)| + C_g|\varphi| + C_1 \\ &\text{for a.e. } (x,t) \in Q\,, \quad \forall\, \varphi \in \mathbb{R}\,, \quad \forall\, r \in [0,1], \end{aligned} \tag{2.10}$$

for some constant C_1 depending only on $\|\lambda'\|_{L^\infty(0,1)}$, $\|\chi_t\|_{L^\infty(Q)}$, and C_g. Hence, arguing on (1.1) and (1.3–4), it is not difficult to check that Proposition 2.3 is just a consequence of [18, Theorem V.2.1]. The proof is essentially based on a maximum principle procedure, which can be reproduced directly on (1.1) with minor effort.

3 Proof of the Theorem

In order to show the assertion of Theorem 2.2, we first verify that (2.8) must hold for any solution of (1.1–4). The simple argument used in the proof of the following lemma constitutes the main new idea of this paper.

Lemma 3.1 *Let* (θ, χ) *be a solution to* (1.1–4) *in the sense specified in Definition 2.1, and suppose that* **(A1–4)** *hold. Then* (2.8) *is satisfied.*

Proof. We multiply (1.1) by the function

$$-(\theta-\theta_*)^- := \min\{\theta-\theta_*\,,\,0\} \in L^2(0,T;H^1(\Omega))\,,$$

and integrate over $\Omega \times (0,t)$ (where $t \in [0,T]$) and by parts. Owing to (2.5), we obtain that

$$\frac{1}{2}\,\|(\theta-\theta_*)^-(\cdot\,,t)\|^2_{L^2(\Omega)} \;+\; \int_0^t\!\int_\Omega |\nabla((\theta-\theta_*)^-)|^2 \;=\; I_1(t) \;+\; I_2(t)\,, \tag{3.1}$$

where, thanks to (2.6),

$$I_1(t) := -\int_0^t\!\int_\Omega g(x,s,\theta(x,s),\chi(x,s))\,(\theta-\theta_*)^-(x,s)\,dx\,ds \;\le\; 0\,, \tag{3.2}$$

and where

$$I_2(t) := \int_0^t\!\int_\Omega \lambda'(\chi)\,(\theta-\theta_*)^-\,\chi_t\,. \tag{3.3}$$

Now, we notice that the integrand of $I_2(t)$ may only differ from 0 in the set

$$A_t := \{\,(x,s)\in\Omega\times(0,t)\;|\;0<\chi(x,s)<1 \quad\text{and}\quad \theta(x,s)<\theta_*\,\}\,. \tag{3.4}$$

Indeed, since $\chi \in H^1(0,T;L^2(\Omega))$, we have $\chi_t = 0$ in both the sets $\{\chi=0\}$ and $\{\chi=1\}$, so that $\lambda'(\chi)\,(\theta-\theta_*)^-\,\chi_t = 0$ a. e. in $(\Omega\times(0,t))\setminus A_t$. Moreover, from (1.6) we infer that

$$\chi_t = -\,\sigma'(\chi) \;-\; \lambda'(\chi)/\theta \quad \text{a. e. in } A_t\,, \tag{3.5}$$

since we may take both values $r>\chi$ and $r<\chi$ as test numbers. Therefore, $I_2(t)$ reduces to the expression

$$I_2(t) = \int\!\!\int_{A_t} -\,\frac{(\theta-\theta_*)^-}{\theta}\,\Big(\theta\,\sigma'(\chi)\,\lambda'(\chi) \;+\; |\lambda'(\chi)|^2\Big)\,, \tag{3.6}$$

and we can deduce from (2.4) and (2.7) that $I_2(t) \le 0$. Indeed, it follows that $\theta\,\sigma'(\chi)\,\lambda'(\chi) \;\ge\; \theta_*\,\sigma'(\chi)\,\lambda'(\chi)$ whenever $\theta<\theta_*$ and $\sigma'(\chi)\,\lambda'(\chi) < 0$, and that $\theta\,\sigma'(\chi)\,\lambda'(\chi) \ge 0$, otherwise.

In conclusion, on account of (3.1) we realize that $\|(\theta-\theta_*)^-(\cdot\,,t)\|_{L^2(\Omega)} = 0$ for all $t\in[0,T]$, whence the assertion follows. □

Remark 3.2 The argumentation in the proof of Lemma 3.1 is similar to that used by the authors in [10] to show the positivity of temperature in the so-called *Frémond model for shape memory alloys.* The details, however, were quite different there. Nevertheless, we suspect that the scheme of our proof, namely to play with the variational inequality for the order parameter, should be applicable in much more general situations. From the physical point of view, the method consists in making full use of the Second Principle of Thermodynamics.

We are now in the position to prove Theorem 2.2.

Proof of Theorem 2.2. We use a "cut-off"-argument. To this end, we consider the initial-boundary value problem (1.1) + (3.7) + (1.3–4), in which the evolution equation (1.2) for the order parameter is replaced by

$$\chi_t + \partial I(\chi) + \sigma'(\chi) \ni -\lambda'(\chi)\,\rho(\theta) \quad \text{a.e. in } Q\,, \tag{3.7}$$

with the cut-off function $\rho \in C^{0,1}(\mathbb{R})$ defined by

$$\rho(\varphi) = \begin{cases} 1/\theta_* & \text{if } \varphi \le \theta_* \\ 1/\varphi & \text{if } \varphi > \theta_* \end{cases} . \tag{3.8}$$

Apparently, the function ρ is bounded, and hence the right-hand side of (3.7) is Lipschitz continuous with respect to both variables. In addition, **(A1–3)** are satisfied. Using these facts, it is not difficult to verify that the abstract result contained in [7, Theorem 1] can be suitably adapted to yield the existence of a unique pair (θ, χ) satisfying $\theta \in H^1(0,T;L^2(\Omega)) \cap C^0([0,T];H^1(\Omega))$, (2.3–4), (3.7), (1.4), and (1.1) and (1.3) in some weaker sense. Moreover, by comparison in equation (1.1), and using standard elliptic estimates, we find that $\theta \in L^2(0,T;H^2(\Omega))$ as well. Since $\chi \in H^1(0,T;L^2(\Omega))$, we can conclude that $\chi_t = 0$ a.e. in the set $A := \{\chi = 0\} \cup \{\chi = 1\}$ and, with the help of the variational inequality corresponding to (3.7), that

$$\chi_t = -\sigma'(\chi) - \lambda'(\chi)\,\rho(\theta) \quad \text{a.e. in } Q \setminus A\,. \tag{3.9}$$

Hence, by **(A1)** and the boundedness of ρ, it turns out that $\chi_t \in L^\infty(Q)$.

Next, we show that (θ, χ) solves (1.1–4). To this end, it suffices to check that $\theta \ge \theta_*$ a.e. in Q. But this can be performed by repeating the argument in the proof of Lemma 3.1 and just remarking that $\rho(\theta) = 1/\theta_*$ in A_t (indeed, estimating $I_2(t)$ is even simpler than before because of (2.7)). Thus, we achieve that $\rho(\theta) = 1/\theta$ a.e. in Q, and (θ, χ) satisfies also (1.2), i.e. it is a solution to (1.1–4). On the other hand, Lemma 3.1 implies that any solution to (1.1–4) also fulfils (3.7). Then, since the problem (1.1) + (3.7) + (1.3–4) admits at most one solution, it follows that (θ, χ) is uniquely determined. This completes the proof of Theorem 2.2. □

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