Positivity of the Temperature for Phase Transitions with Micro-Movements

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**Abstract.** We focus on the thermodynamic consistency of a class of phase change models recently proposed by M. Frémond. By establishing a maximum principle, we prove that, under rather weak assumptions on data, the temperature remains almost everywhere strictly positive. This general result applies to all dissipative models of this class that have been taken into account in the literature.

**Key words:** phase transition – microscopic movements – maximum principle

1 Introduction

The present analysis is concerned with the thermodynamic consistency of a novel class of solid-liquid phase transition models recently proposed by M. Frémond [1]. The main feature of this modelization relies in taking into account the *microscopic movements* of particles by including their effect on the macroscopic behavior of the body. Although the substance that undergoes the phase transition may often be macroscopically regarded as a *rigid continuum*, it is actually clear that, in order the phase transition to occur, no rigidity can be assumed at the microscopic level. In fact, the phase transition is, heuristically speaking, the effect of some structural rearrangement or reorganization of the microscopic components of the substance.

In the framework of Frémond’s theory, one still considers that the mechanical effect of the microscopic rearrangements of particles is *negligible* at the macro-scales, where it is assumed that the latter movements are somehow averaged out. Nevertheless, one admits that the microscopic movements of particles might give rise to some thermal macroscopic effect which influences the overall energy balance of the body.

A brief derivation of this class of models in the setting of Continuum Thermo-Mechanics is given in the forthcoming Section 2. As it will appear clearly later on, at the derivation level the absolute temperature of the body is obviously assumed to be strictly positive in the space-time domain. As we shall see below, this in particular entails the validity of the Second Principle of Thermodynamics in the form of the Clausius-Duhem inequality. On the other hand, as soon as one faces the (mathematical) PDE problem arising from such a physical modeling, the crucial proof of the positivity of the temperature for all times (starting from a positive initial datum) turns out to be a non-trivial question, which seems to have been positively solved only in specific situations (see [2–4]) by means of various types of *ad hoc* maximum principle arguments. Indeed, up to now, no general result on the positivity of the temperature (and, a posteriori, on the thermodynamic consistency of the models) was available.

The main result of this paper is that of providing a general positivity and hence thermodynamic consistency proof for a large class of models that have been taken into account in the literature. Namely,
by assuming some dissipation in the model (see (3.1)), we prove that any temperature \( \theta \) solving the problem (in a sense that will be later specified) remains almost everywhere uniformly separated from zero as the evolution occurs from a uniformly positive datum. The strategy of the proof is quite classical and relies on providing a uniform bound on the inverse of the temperature \( 1/\theta \). In particular, we carefully exploit the dissipative character of the system in order to handle its nonlinearities. Finally, it is worth mentioning that this argument works for solutions enjoying the natural regularity properties without strong smoothness assumptions.

This is the plan of the paper. In Section 2 we recall the derivation of the model. Then, the statement of our main result is given in Section 3 while its proof is detailed in Section 4.

2 Modeling

This section is devoted to the general derivation of Frémond’s models of phase transitions with micro-movements. The reader is obviously referred to [1] for further details on this procedure, as well as on the general physical framework. Here, we just aim to present a basic physical motivation of the concrete situations to which our result will be applied.

Assume we are given a regular domain \( \Omega \subset \mathbb{R}^n \) (\( n = 1, 2, 3 \)), connected, with a smooth boundary \( \Gamma := \partial \Omega \), and filled with a substance which may undergo a two-phase transformation. We aim to study the evolution of the system in a fixed time interval \([0, T]\) where \( T > 0 \) is a final reference time. In order to describe the process, we will focus on the two state variables \( \theta \) and \( \chi \). Namely, the first variable \( \theta \) will stand for the absolute temperature of the body, hence it is assumed for the purposes of this section to be strictly positive (which will turn out to be our main theorem later on). On the other hand, \( \chi \) represents an order parameter and might be interpreted as a local proportion between the different phases.

Let us now come to the main novelty of Frémond’s approach. Indeed, we assume that, although in the rigid-body framework, the micro-movements of particles give rise to macroscopic effects. To this end, let us postulate from the very beginning that the proper quantities describing such micro-movements are \( \dot{\chi} \) and \( \nabla \dot{\chi} \), where the dot denotes differentiation in time, while \( \nabla \) is the usual gradient with respect to spatial variables (as it is customary, at this stage we assume that all the quantities occurring in the analysis are as smooth as needed in order to go through the differentiations).

In this context, it seems convenient to regard the vector \((u, \dot{\chi})\) (where \( u = u(x, t) \) is the (macroscopic) velocity of the material point \( x(t) \)) as an actual rigid velocity vector. Moreover, let us assume that there exists a linear space of rigid body velocities \( R \) (see [1] for a full discussion). Finally, we suppose that, for all times \( t \in [0, T] \), the virtual power of the internal forces of the body with respect to the generic subdomain \( D \subset \Omega \) and virtual velocities \((v, c) \in R \) is

\[
P_{\text{internal}}(D, v, c) := - \int_D (Bc + \mathbf{H} \cdot \nabla c) \, dx.
\]

In the latter relation the two quantities \( B \) and \( \mathbf{H} \) come into play. Indeed, an obvious dimensional argument entails that they shall be regarded as energy densities. In particular, \( B \) represents and energy density per units of \( \chi \), while \( \mathbf{H} \) may be considered as a density of energy flux. The term \( \int_D \sigma : \varepsilon(v) \) where \( \sigma \) is the (macroscopic) stress and \( \varepsilon(v) \) is the symmetric gradient does not appear above as an effect of our overall rigid body assumption. However, we shall remark that the above derivation can be easily extended to the situation when the macroscopic dynamics is not negligible.

We now introduce the virtual power of the external forces as

\[
P_{\text{external}}(D, v, c) := \int_D (f \cdot v + Ac) \, dx + \int_{\partial D} (T \cdot v + ac) \, dS^{n-1}.
\]

Here, the terms involving \( v \) are quite classical and \( f \) represents an action density at distance (body force) while \( T \) is an action density at contact (traction). On the other hand, the quantity \( A \) is a volume density of energy supplied to the material per units of \( \chi \) by microscopic actions without macroscopic motions. One may think, for instance, to chemical or radioactive actions. Moreover, the quantity \( a \) represents the surface density of energy per units of \( \chi \) supplied to the body.
Finally, as for the virtual power of acceleration forces we set
\[ P_{\text{acceleration}}(D, \mathbf{v}, c) := \int_D \rho \gamma \cdot \mathbf{v} \, dx + \int_D \rho_0 \gamma_0 \, c \, dx, \]
where \( \gamma = \ddot{\mathbf{u}} \) is the macroscopic acceleration and \( \rho \) is the material density. On the other hand, the second term takes into account the micro-accelerations. In particular, \( \rho_0 \gamma_0 \) represents the inertia forces of the microscopic-motions (although it of course has the dimension of an energy density). In particular \( \gamma_0 = \ddot{x} \) and \( \rho_0 \) represents a mass density of microscopic links between molecules or grains in the substance (see [5]).

**Equation of motion.** By recalling the Virtual Power Principle [6], choosing arbitrarily the regular and connected domain \( D \) and the field \( c \), and letting \( \mathbf{v} = \mathbf{0} \) we easily obtain that
\[
\rho_0 \ddot{x} + B - \text{div} \mathbf{H} = A \quad \text{in} \quad \Omega \times (0,T), \tag{2.1}
\]
\[
\mathbf{H} \cdot \nu = a \quad \text{on} \quad \Gamma \times (0,T), \tag{2.2}
\]
where \( \nu \) stands for the unit normal vector field pointing outward \( \Gamma \). Of course (2.1) reduces to a balance of micro-motions since the body is rigid at the macroscopic scale.

**Energy balance.** Letting \( e \) denote the internal energy density of the body, \( q \) the heat flux, and supposing that the system is insulated from the exterior we can follow [1, Sec. 3.2] and deduce that, in our situation, the energy balance is expressed by
\[
\dot{e} + \text{div} \, q = B \ddot{x} + \mathbf{H} \cdot \nabla \dot{x} \quad \text{in} \quad \Omega \times (0,T), \tag{2.3}
\]
\[
q \cdot \nu = 0 \quad \text{on} \quad \Gamma \times (0,T). \tag{2.4}
\]
In particular, we note that the right hand side of (2.3) differs from zero and takes into account the contribution to the energy balance provided by the microscopic movements.

**Constitutive relations.** The next step is to define the quantities \( e, q, B, \mathbf{H} \) in terms of the state variables in such a way that the Second Principle of Thermodynamics, in the form of the Clausius-Duhem inequality, is fulfilled. In particular, the latter reduces in our case to
\[
\int_\Omega (s + \text{div} \left( \frac{q}{\theta} \right)) \, dx \geq 0 \quad \forall t \in (0,T], \tag{2.5}
\]
where \( s \) is the entropy of the system. In order to accomplish the above requirement we will exploit the Ginzburg-Landau theory by introducing the free energy density function \( \psi = \psi(\theta, \chi, \nabla \chi) \) and define\[
s := -\frac{\partial \psi}{\partial \theta}, \quad e := \psi + \theta s, \tag{2.6}
\]
As for the heat flux we choose the standard Fourier law
\[
q := -k \nabla \theta,
\]
where \( k \) is a positive conductivity coefficient.

Moreover, we will introduce a pseudo-potential of dissipation [1,7] \( \phi = \phi(\theta, \dot{x}, \nabla \dot{x}) \) such that, for all \( \theta \), the function \( \phi(\theta, \cdot, \cdot) \) is convex, non-negative, proper, and vanishes as \( \dot{x} \) and \( \nabla \dot{x} \) are both zero, and define
\[
B := \frac{\partial \psi}{\partial x} + \frac{\partial \phi}{\partial x}, \quad \mathbf{H} := \frac{\partial \psi}{\partial (\nabla \chi)} + \frac{\partial \phi}{\partial (\nabla \chi)}.
\tag{2.7}
\]
The above choices split both terms \( B \) and \( \mathbf{H} \) into a non-dissipative and a dissipative part, respectively, and are inspired by thermodynamic considerations (see below). Moreover, the latter notion of derivative is intended to be properly generalized in case \( \phi, \psi \) are non-smooth functions.

**Choice for \( \psi \).** We now come to our actual choice of \( \psi \). In particular, we let
\[
\psi(\theta, \chi, \nabla \chi) = -c_s \theta \ln \theta - \frac{L}{\theta_c} (\theta - \theta_c) \chi + w(\chi, \nabla \chi).
\]
In the latter expression, the first term is purely caloric and \( c_s \) represents a specific heat density, while the second term stands for the phase-temperature interaction, \( L \) is a latent heat density, and \( \theta_c \) is the phase transition temperature. The last term represents a general potential on \( \chi \) and \( \nabla \chi \). One may have for instance \( w(\chi, \nabla \chi) = \frac{\gamma}{2} |\nabla \chi|^2 \) representing a density of surface energy. Alternatively, one could
consider a double well potential \( w(\chi, \nabla \chi) = (1 - \chi^2)^2 \) or a constraining term \( w(\chi, \nabla \chi) = I_{[-1,1]}(\chi) \) where \( \pm 1 \) denote the pure configurations or phases and the indicator function of the non-empty and closed interval \( K \) in \( \mathbb{R} \) is defined as
\[
I_K(x) := \begin{cases} 0 & \text{if } x \in K, \\ +\infty & \text{otherwise.} \end{cases}
\]
We remark that all these choices, or combinations, are physically motivated and have been considered in the literature.

**Model.** Moving from the above positions, one exploits (2.1) and (2.3) in order to get the full system of solid-liquid phase transitions with micro-movements
\[
c_s \dot{\theta} + L \dot{\chi} - k \Delta \theta = -\frac{L}{\theta_c} (\theta - \theta_c) \dot{\chi} + \left( \frac{\partial \phi}{\partial \chi}, \frac{\partial \phi}{\partial \nabla \chi} \right) \cdot (\dot{\chi}, \nabla \dot{\chi}),
\]
\[
\rho_0 \ddot{\chi} + B - \text{div } H = A.
\]

**Relations with classic models.** We aim to show that a variety of classic phase transition models can be obtained in the framework of the general full system (2.8)-(2.9) by suitably choosing functionals and parameters. In particular, one might observe that we are in the position of revisiting and unifying the proofs of the thermodynamic consistency of some known models.

*Stefan.* Whenever we make the choices \( \phi = 0, \) and \( w(\chi, \nabla \chi) = I_{[-1,1]}(\chi), \) the system (2.8)-(2.9) reduces to
\[
c_s \dot{\theta} + L \dot{\chi} - k \Delta \theta = -\frac{L}{\theta_c} (\theta - \theta_c) \dot{\chi},
\]
\[
\dot{\theta} I_{[-1,1]}(\chi) \equiv \frac{L}{\theta_c} (\theta - \theta_c).
\]
Here of course \( \dot{\theta} \) is the usual subdifferential of Convex Analysis. Hence \( \chi \in \text{sign} (\theta - \theta_c) \) where \( \text{sign} (r) = \{ -1 \} \) if \( r < 0, \) \( \text{sign} (0) = [-1,1], \) and \( \text{sign} (r) = \{ 1 \} \) otherwise, and we readily have that \( \dot{\chi} \neq 0 \) only if \( \theta = \theta_c. \) Thus, we conclude that (2.10)-(2.11) entail
\[
c_s \dot{\theta} + L \dot{\chi} - k \Delta \theta = 0,
\]
\[
\chi \in \text{sign} (\theta - \theta_c),
\]
which corresponds to the weak formulation of a classical two-phase Stefan problem. Let us however mention that our positivity result does not apply to this situation.

*Phase relaxation.* The choices \( \phi(\theta, \dot{\chi}, \nabla \dot{\chi}) = \mu \dot{\chi}^2 / 2 \) for some \( \mu > 0, \) and \( w(\chi, \nabla \chi) = I_{[-1,1]}(\chi), \) correspond to the system
\[
c_s \dot{\theta} + L \dot{\chi} - k \Delta \theta = \mu \dot{\chi}^2 - \frac{L}{\theta_c} (\theta - \theta_c) \dot{\chi},
\]
\[
\mu \ddot{\chi} + \dot{\theta} I_{[-1,1]}(\chi) \equiv \frac{L}{\theta_c} (\theta - \theta_c).
\]
It suffices now to take the product of (2.15) with \( \dot{\chi} \) in order to deduce that (2.14)-(2.15) is indeed equivalent to the system
\[
c_s \dot{\theta} + L \dot{\chi} - k \Delta \theta = 0,
\]
\[
\mu \ddot{\chi} + \dot{\theta} I_{[-1,1]}(\chi) \equiv \frac{L}{\theta_c} (\theta - \theta_c),
\]
which is of course the analogue (in this setting) of the phase relaxation model [8,9]. Actually, this model is included in our discussion. Namely, we are in the position of proving that, whenever we start from a uniformly positive initial temperature, \( \theta \) remains positive for all times \( t > 0. \)

*Penrose-Fife phase relaxation.* The choices \( \phi(\theta, \dot{\chi}, \nabla \dot{\chi}) = \mu \theta \dot{\chi}^2 / 2 \) and \( w(\chi, \nabla \chi) = I_{[-1,1]}(\chi) \) lead to the system
\[
c_s \dot{\theta} + \frac{L}{\theta_c} \theta \dot{\chi} - k \Delta \theta = \mu \theta \dot{\chi}^2,
\]
\[
\mu \theta \ddot{\chi} + \dot{\theta} I_{[-1,1]}(\chi) \equiv \frac{L}{\theta_c} (\theta - \theta_c),
\]
and, whenever $\theta > 0$, we get that
\[
c_\theta \dot{\theta} + L \dot{x} - k \Delta \theta = 0,
\]
\[
\mu \dot{x} + \partial I_{[-1,1]}(x) \ni L \left( \frac{1}{\theta_c} - \frac{1}{\theta} \right),
\]
which is the standard Penrose-Fife phase-relaxation problem [10-12]. This situation is also covered by our result.

*Quasi-stationary phase-field-like models.* The general system (2.8)-(2.9) along with the choices $\phi = 0$, and $w(x, \nabla x) = (1 - x^2)^2/4$, reduces to the model
\[
c_\theta \dot{\theta} + \frac{L}{\theta_c} \theta \dot{x} - k \Delta \theta = 0, \quad (2.18)
\]
\[
-\nu \Delta x + x^3 - x \ni \frac{L}{\theta_c} (\theta - \theta_c). \quad (2.19)
\]
The latter system is a possible generalization of the quasi-stationary standard Caginalp phase-field model to the situation where $\theta$ can go far from the equilibrium temperature. Indeed, linearizing around $\theta \sim \theta_c$, (2.18) reduces to (2.12) and the above system is the typical model of Caginalp type [13]. Unfortunately, our result does not apply directly to this case where the potential $\phi$ turns out to be degenerate.

**Thermodynamic Consistency.** Let us go back to (2.3), exploit (2.6)-(2.7), and compute that
\[
0 = \frac{d}{dt} (\psi + \theta s) + \text{div } q - B \dot{x} - H \cdot \nabla \dot{x}
\]
\[
= \theta \dot{s} + \text{div } q - \frac{\partial \phi}{\partial x} \dot{x} - \frac{\partial \phi}{\partial (\nabla x)} \nabla \dot{x} \leq \theta \dot{s} + \text{div } q,
\]
where we used the properties of the pseudo-potential $\phi$. Hence, as the Fourier law holds, the Clausius-Duhem inequality (2.5) easily *follows from the positivity of $\theta$. As a consequence, the general positivity proof detailed below entails the thermodynamic consistency of the whole class of models.*

**Survey on the literature.** Before closing this section, we aim to briefly relate our result to the current literature on the mathematical treatment of models of phase transitions with micro-movements. As stated above, our uniform positivity result applies to almost all the modeling situations that have been taken into account so far from the point of view of the well-posedness analysis. In particular, we shall mention that the available existence results for phase transitions with micro-movements often refer to different notions of solvability (weak vs. strong, local vs. global). In this regard, let us stress that the regularity requirements of our main positivity result turn out to cover all these different situations.

In particular, we are in the position of sharpening the non-negativity results of the papers [5,14-17] by providing a novel uniform lower bound for the temperature. Moreover, we recover in an independent and unified fashion the lower bounds for the temperature of the papers [2-4].

3 **Positivity**

Let us start by fixing some assumptions.

(A1) $\Omega$ is a bounded and connected domain in $\mathbb{R}^n$ ($n \in \mathbb{N}$) with a smooth boundary $\Gamma = \partial \Omega$.

The vector $\nu$ stands for the outward unit normal to $\Gamma$, $\theta_c, \theta_c^* > 0$, $k, h \geq 0$ are constants, $\theta_c \in L^2(\Gamma)$, and $\theta_c \geq \theta_c^* > 0$ almost everywhere in $\Gamma$.

For the sake of convenience let us introduce some notations setting $Q_t := \Omega \times (0, t)$, $\Sigma_t := \Gamma \times (0, t)$ for $t \in (0, T]$, and $Q := Q_T$, $\Sigma := \Sigma_T$. Let us refer the reader at once to [18] for definitions and properties of function spaces and denote by $(H^1(\Omega))^\prime$ the dual of $H^1(\Omega)$ and by $\langle \cdot, \cdot \rangle$ the respective duality pairing.
(A2) \( \phi : \mathbb{R} \times \mathbb{R} \times \mathbb{R}^n \to [0, +\infty] \) such that for all \( \theta \in \mathbb{R} \) the function \( \phi(\theta, \cdot, \cdot) \) is convex, proper, lower semicontinuous, and \( \phi(\theta, 0, 0) = 0 \). Moreover,
\[
\phi(\theta, \xi, \eta) \geq \mu|\theta|^\beta |\xi|^\alpha \quad \forall (\theta, \xi, \eta) \in \mathbb{R} \times \mathbb{R} \times \mathbb{R}^n
\]
and for some \( \mu > 0, \beta \in [0, 1], \) and \( \alpha > 1 \).

In particular, our framework, where we remark once more that degeneration in \( \xi \) is not allowed, includes, for instance, the following classic cases:

- phase relaxation: \( \phi(\theta, \tilde{x}, \nabla \tilde{x}) := \mu \tilde{x}^2 \),
- irreversible phase relaxation: \( \phi(\theta, \tilde{x}, \nabla \tilde{x}) := \mu \tilde{x}^2 + I_{[0, +\infty]}(\tilde{x}) \),
- viscous phase relaxation: \( \phi(\theta, \tilde{x}, \nabla \tilde{x}) := \mu \tilde{x}^2 + \delta \nabla \tilde{x}^2 \) for \( \delta > 0 \),
- Penrose-Fife phase relaxation: \( \phi(\theta, \tilde{x}, \nabla \tilde{x}) := \mu |\theta| \tilde{x}^2 \),

as well as, of course, suitable combinations of the latter. Let us point out that the term irreversibility above refers to the situation where \( \tilde{x} \) is constrained to be non-negative (such as in glue hardening or food cooking [8]) and it is used with no explicit relation with the notion of irreversibility in Thermodynamics.

As for the initial datum we ask

(A3) \( \theta_0 \in L^2(\Omega) \) and \( \theta_0 \geq \theta_0^* > 0 \) almost everywhere in \( \Omega \) for some constant \( \theta_0^* \).

**Theorem 1.** Under assumptions (A1)-(A3) let
\[
\theta \in H^1(0, T; (H^1(\Omega))') \cap L^2(0, T; H^1(\Omega)),
\]
\[
\chi \in H^1(0, T; H^1(\Omega)),
\]
\[
(d_1, d_2) \in L^2(Q) \times (L^2(Q))^n,
\]
fulfill \( \theta(0) = \theta_0 \) a.e. in \( \Omega \), \( |\theta|^\beta |\chi|^\alpha \in L^1(\Omega) \) and
\[
c_s \int_0^T \langle \theta_t, \zeta \rangle + L \int_{\Omega_t} \chi_t \zeta \, dx + k \int_{\Omega_t} \nabla \theta \cdot \nabla \zeta \, dx + h \int_{\Gamma_t} (\theta - \theta_c) \zeta \, d\Gamma_t = -\frac{L}{\theta_c} \int_{\Omega_t} (\theta - \theta_c) \chi_t \zeta
\]
\[
+ \int_{\Omega_t} (d_1, d_2) \cdot (\chi_t, \nabla \chi_t) \zeta \quad \forall \zeta \in L^2(0, T; H^1(\Omega)) \cap L^\infty(Q), \forall t \in [0, T],
\]
\[
(\theta, \tilde{x}, \nabla \tilde{x}) < +\infty \quad \text{a.e. in } Q \text{ and}
\]
\[
(d_1, d_2) \cdot (\tilde{x} - \xi, \nabla \tilde{x} - \eta) \geq \phi(\theta, \tilde{x}, \nabla \tilde{x}) - \phi(\theta, \xi, \eta) \quad \text{a.e. in } Q
\]
for all \( (\xi, \eta) \in L^2(Q) \times (L^2(Q))^n \) such that \( \phi(\theta, \xi, \eta) < +\infty \) a.e. in \( Q \).

Then, there exists a constant \( \theta^* > 0 \) depending on \( \theta_c, h, \theta_0^*, \mu, \beta, \theta_0^*, c_s, L, |\Gamma|, |\Omega|, \) and \( T \), such that
\[
\theta \geq \theta^* \quad \text{a.e. in } Q.
\]

In the latter statement \( |\Gamma| \) and \( |\Omega| \) stand for the surface measure of \( \Gamma \) and the volume of \( \Omega \), respectively.

Equation (3.2) is a suitable variational formulation of the following system
\[
c_s \theta_t + L \chi_t + k D\theta = -\frac{L}{\theta_c} (\theta - \theta_c) \chi_t + (d_1, d_2) \cdot (\chi_t, \nabla \chi_t) \quad \text{a.e. in } Q,
\]
\[
k \partial_\nu \theta + h (\theta - \theta_c) = 0 \quad \text{a.e. on } \Sigma.
\]
In particular, relation (3.5) is nothing but the former (2.8) and \( (d_1, d_2) \) represent the dissipative components of the quantities \( B \) and \( H \), respectively, in the case of a (possibly) non-smooth convex potential \( \phi \) (see (2.7)).

Theorem 1 may be easily adapted to even more general situations. First of all let us observe that our proof basically relies on an ODE argument. Hence, the result holds in any space dimension and some different (even degenerate) choices for the heat flux \( q \) could be considered. Moreover, our choice of boundary conditions (3.6) includes at once homogeneous Neumann as well as third-type conditions. On the other hand we could easily state the result for suitable Dirichlet conditions as well.
Secondly, we could easily take into account some additional terms in the energy balance equations and, in particular, we could discuss the presence of thermal effects due to macroscopic deformations. More generally, our result applies to the situation where an additional term \( \lambda \theta \), with \( \lambda \in L^2(0,T; L^p(\Omega)) \cap L^1(0,T; L^\infty(\Omega)) \) being a datum, appears in the right hand side of (3.5) (in this case we however require \( q \) to be the standard Fourier flux in order to obtain some control on space derivatives). Moreover, we might include the discussion of a source term in (3.5) of the form \( f(x,t,\theta, \lambda) \) along with suitable smoothness and sign assumptions. Again, it is clear that we could also deal with a wider class of modeling choices for \( \phi \) without particular intricacy.

Finally, the regularity assumptions in Theorem 1 are intended simply to justify notations in (3.2)-(3.3) and could be weakened in many directions. In particular, let us point out that the regularity requirements on \( \chi \) could be weakened to \( \chi \in H^1(0,T; L^2(\Omega)) \) whenever \( d_2 = 0 \), i.e. the pseudopotential \( \phi \) is independent of \( \nabla \chi \). We prefer to stick to the situation of (3.2)-(3.3) for simplicity since it contains all the models with micro-movements referred above and seems to present all the mathematical difficulties that we aim to solve.

4 Proof of Theorem 1

The strategy of the proof consists in obtaining a bound on \( 1/\theta \) in \( L^\infty(\Omega \times (0,T)) \) by proving bounds in \( L^\infty(0,T; L^p(\Omega)) \) which are independent of \( p \).

We start by introducing a suitable truncation of \( \theta \). Namely, for all \( \varepsilon \in (0,\theta_0) \) one defines

\[
\theta_\varepsilon := (\theta - \varepsilon)^+ + \varepsilon = \max\{\theta, \varepsilon\}.
\]

In particular, let us stress that \( \theta_\varepsilon(0) = \theta_0 \) almost everywhere in \( \Omega \). Moreover, we set

\[
\gamma := (\alpha - \beta)/(\alpha - 1),
\]

and recall that (A2) entails \( \gamma \geq 1 \).

Let us consider (3.1) and make use of (3.3) with the choice \( (\xi, \eta) = (0,0) \) in order to deduce from (3.2) that

\[
c_s \int_0^t \langle \theta_\varepsilon, \zeta \rangle + L \int \nabla \theta_\varepsilon : \nabla \zeta + \mu \int \theta_\varepsilon \zeta + \int \Sigma_t (\theta - \theta_\varepsilon) \zeta \geq -\frac{L}{\theta_0} \int (\theta - \theta_\varepsilon) \chi_\varepsilon + \mu \int \theta_\varepsilon |\chi_\varepsilon|^2 \zeta \|
\]

\[
\forall \zeta \in L^2(0,T; H^1(\Omega)) \cap L^\infty(\Omega), \forall t \in (0,T].
\]

We now choose

\[
z = -\theta_\varepsilon^{-p} \in L^2(0,T; H^1(\Omega)) \cap L^\infty(\Omega)
\]

for some \( p > \gamma \) and obtain

\[
\frac{c_s}{p-1} \int \Theta_{\varepsilon}^{1-p}(t) + k p \int \theta_\varepsilon^{-1-p} |\nabla \theta_\varepsilon|^2 + h \int \Sigma_t \theta_\varepsilon \theta_\varepsilon + \mu \int \theta_\varepsilon |\chi_\varepsilon|^2 \theta_\varepsilon^{-p} \leq \frac{c_s}{p-1} \int \Theta_{\varepsilon}^{1-p} + h \int \Theta_{\varepsilon}^{1-p} + \frac{L}{\theta_\varepsilon} \int \Theta_{\varepsilon} \chi_\varepsilon \theta_\varepsilon^{-p},
\]

where we made use of the the following facts

\[
\theta \leq \theta_\varepsilon \quad \nabla \theta : \nabla \theta_\varepsilon = |\nabla \theta_\varepsilon|^2 \quad \text{a.e. in } Q.
\]

Moreover, we also made use of the following inequality

\[
- \int_0^t \langle \theta_1, \theta_{\varepsilon}^{-p} \rangle \geq \frac{1}{p-1} \int \Theta_{\varepsilon}^{1-p}(t) - \frac{1}{p-1} \int \Theta_{\varepsilon}^{1-p},
\]

whose proof is not completely trivial. First of all one establishes (4.2) for functions \( \theta \in H^1(0,T; L^2(\Omega)) \cap L^2(0,T; H^1(\Omega)) \) such that \( \theta(0) = \theta_0 \) almost everywhere. Then, the same relation is extended to functions \( \theta \in H^1(0,T; (H^1(\Omega))^\prime) \cap L^2(0,T; H^1(\Omega)) \) by means of a singular perturbation argument (see, e.g., [19, Appendix]).
Our next aim is now to deal with the right hand side of (4.1). As for the boundary term we simply apply the standard Young inequality

\[ ab \leq \frac{(\delta a)^q}{q} + \frac{1}{q} \left( \frac{b}{\delta} \right)^{q'} \quad \forall a, b \geq 0, \delta > 0, q, q' > 1, \frac{1}{q} + \frac{1}{q'} = 1, \quad (4.3) \]

with the choices

\[ a = \theta^1_{e^{-p}}, \quad b = 1, \quad \delta = \left( \frac{\theta^*_p}{p - 1} \right)^\frac{q-1}{p-1}, \quad q = \frac{p}{p - 1}, \]

and obtain that

\[ h \int_{\Sigma_t} \theta^1_{e^{-p}} \leq h\theta^*_{p} \int_{\Sigma_t} \theta^*_{p} + \frac{1}{p} h |\Gamma| t(\theta^*_p)^{1-p}. \quad (4.4) \]

Let us now turn our attention to the last term in the right hand side of (4.1). By exploiting again (4.3) with the choices

\[ a = (\alpha \mu)^\frac{q}{p} |\partial \Omega| \theta^*_{e^{-p}}, \quad b = \frac{L}{\theta^*_e(\alpha \mu)^\frac{q}{p}} |\theta^*_{e^{-p}} - \theta^*_{e^{-p}}|, \quad \delta = 1, \quad q = \alpha, \]

where the prime stands for the usual notation for the conjugate exponent, we readily get that

\[ \frac{L}{\theta^*_e} \int_{Q_t} \theta^*_{e^{-p}} \leq \mu \int_{Q_t} |\theta^*_{e^{-p}} x_{\theta^*_{e^{-p}}} + \frac{1}{\alpha} \left( \frac{L}{\theta^*_e(\alpha \mu)^\frac{q}{p}} \right) \int_{Q_t} \theta^*_{e^{-p}}. \quad (4.5) \]

Here we simply made use of the fact that, since \( \theta \leq \theta^*_e \) almost everywhere and \( \alpha > \beta \), one has that \( \theta^* \leq \theta^*_e \) almost everywhere. Moreover, the definition of \( \gamma \) entails that

\[ \left( 1 - \frac{\beta}{\alpha} - \frac{p}{\alpha'} \right) \alpha' = \left( \alpha' - \frac{\alpha}{\alpha'} \beta - \alpha - p \right) = \left( \frac{\alpha}{\alpha - 1} \left( 1 - \frac{\beta}{\alpha} \right) - p \right) \gamma - p. \]

Next, owing to (4.4)-(4.5), relation (4.1) entails

\[ c_s \int_{Q_t} \theta^*_{e^{-p}} \leq c_s \int_{Q_t} \theta^*_{e^{-p}} + \frac{p - 1}{p} h |\Gamma| t(\theta^*_p)^{1-p} + \frac{p - 1}{p} \left( \frac{L}{\theta^*_e(\alpha \mu)^\frac{q}{p}} \right) \int_{Q_t} \theta^*_{e^{-p}}. \quad (4.6) \]

Let us now focus on the case \( \gamma > 1 \). By using (4.3) with the choices

\[ a = \theta^1_{e^{-p}}, \quad b = 1, \delta = 1, \quad q = (1 - p)/(\gamma - p), \]

one obtains that

\[ c_s \int_{Q_t} \theta^1_{e^{-p}} \leq c_s \int_{Q_t} \theta^1_{e^{-p}} + \frac{p - 1}{p} h |\Gamma| t(\theta^*_e)^{1-p} + \frac{p - 1}{p} \left( \frac{L}{\theta^*_e(\alpha \mu)^\frac{q}{p}} \right) \int_{Q_t} \theta^1_{e^{-p}} + \left( \frac{L}{\theta^*_e(\alpha \mu)^\frac{q}{p}} \right) \int_{Q_t} \theta^1_{e^{-p}} |\Omega| t. \quad (4.7) \]

Since all the constants in the latter estimate are independent of \( \varepsilon \) we readily exploit the monotone convergence theorem and, by letting \( C_1 \) be a suitable positive constant depending only on \( c_s, h, |\Gamma|, |\Omega|, T, \gamma, L, \theta^*_e, \alpha, \) and \( \mu \), but independent of \( p \), we deduce from (4.7) that

\[ \int_{Q_t} \theta^1_{e^{-p}} \leq C_1 \left( 1 + (\theta^*_e)^{1-p} + (\theta^*_e)^{1-p} + (p - \gamma) \int_{Q_t} \theta^1_{e^{-p}}(s)ds \right). \quad (4.8) \]

Finally, an application of Gronwall’s lemma entails that

\[ \|\theta^{-1}(t)\|_{L^{p-1}(\Omega)} \leq C_1^{1/(p-1)} (1 + (\theta^*_e)^{-1} + (\theta^*_e)^{-1}) \exp \left( C_1 \frac{p - \gamma}{p - 1} t \right) \leq (1 + C_1)(1 + (\theta^*_e)^{-1} + (\theta^*_e)^{-1}) \exp (C_1 T). \]

Since the above right hand side is independent of \( p \), the assertion of the theorem easily follows.

In the case \( \gamma = 1 \) the computation is even simpler since we may directly use (4.6) in order to conclude as above.

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References