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INTERNAL STRUCTURE OF DYNAMIC PHASE-TRANSITION FRONTS IN A FLUID WITH TWO COMPRESSIBLE OR INCOMPRESSIBLE PHASES

HEINRICH FREISTÜHLER[1,a] AND MATTHIAS KOTSCHOTE[2,b]

This paper is dedicated to Tai-Ping Liu on the occasion of his 70th birthday

[1]Department Mathematics and Statistics, University Konstanz, Fach 199, 78457 Konstanz, Germany.
[a]E-mail: Heinrich.Freistuehler@uni-konstanz.de
[2]Department Mathematics and Statistics, University Konstanz, Fach D 193, D-78457 Konstanz, Germany.
[b]E-mail: Matthias.Kotschote@uni-konstanz.de

Abstract

The framework of this article is the Navier-Stokes-Allen-Cahn system for the dynamics of a fluid whose two phases can transform into each other. It studies traveling waves that describe the internal structure of moving interfaces between the phases. A general result on the existence and bifurcation of these waves is detailed for fluids with (1) two compressible phases, (2) one incompressible and one compressible phase, (3) two incompressible phases, and (4) associated limits in which one or both of the two phases are almost incompressible.

1. A General Result on the Existence and Bifurcation of Phase-Transition Fronts

This paper considers families of *isothermal Navier-Stokes-Allen-Cahn* systems

$$\partial_t\rho+\nabla\cdot(\rho\mathbf{u}) = 0,$$
$$\partial_t(\rho\mathbf{u})+\nabla\cdot(\rho\mathbf{u}\otimes\mathbf{u}+p\mathbf{I}) = \nabla\cdot\left(\mu(\nabla\mathbf{u}+(\nabla\mathbf{u})^T)+(\lambda\nabla\cdot\mathbf{u})\mathbf{I}-\delta\rho\nabla c\otimes\nabla c\right), \tag{1.1}$$

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$$\partial_t(\rho c)+\nabla\cdot(\rho c\,\mathbf{u}) = \delta^{-1/2}(\rho q+\nabla\cdot(\delta\rho\nabla c)).$$

These equations model the spatiotemporal behaviour of a compressible viscous or inviscid fluid which is assumed to be a locally homogeneous mixture of two components such that its local thermodynamic state is completely described by its density ρ (or, equivalently, by its specific volume $\tau = 1/\rho$) and the mass fraction c of one of the components. Besides the 3-velocity $\mathbf{u}$, the other dependent variables in (1.1) are the pressure p and the phase transformation rate q; the coefficients δ and μ, λ reflect the fluid's capillarity and viscosity. We suppose that the fluid has a constant temperature θ and the equations derive from an extended Gibbs potential

$$G(c,p,\theta,|\nabla c|) \;=\; G^0(c,p,\theta)+\frac{1}{2}\delta|\nabla c|^2 \tag{1.2}$$

via

$$\tau(c,p,\theta) \;=\; G^0_p(c,p,\theta), \qquad q(c,p,\theta) = -G^0_c(c,p,\theta). \tag{1.3}$$

Model (1.1) derives from the fully *non-isothermal Navier-Stokes-Allen-Cahn* system

$$\begin{aligned}
\partial_t\rho + \nabla\cdot(\rho u) &= 0,\\
\partial_t(\rho u) + \nabla\cdot(\rho u\otimes u - \mathbf{T}) &= 0,\\
\partial_t\mathcal{E} + \nabla\cdot((\mathcal{E}\mathbf{I}-\mathbf{T})u) &= \nabla\cdot(\beta\nabla\theta),\\
\partial_t(\rho\chi) + \nabla\cdot(\rho\chi u) - J &= 0
\end{aligned} \tag{1.4}$$

by assuming that the heat conductivity β is infinite. (In (1.4), $\mathcal{E}, \mathbf{T}, J$ are total energy, total Cauchy stress, and extended transformation rate. Cf. [3, 9, 11] for details). In contrast to (1.4), the temperature enters (1.1) only as a parameter. This paper focusses on an interesting bifurcation that can happen in dependence on the value θ of this parameter.

We discuss traveling-wave solutions of (1.1),

$$(c(\mathbf{x},t),p(\mathbf{x},t),\mathbf{u}(\mathbf{x},t)) = \varphi(x), \quad x\equiv \mathbf{x}\cdot\mathbf{n}-st,$$

that are heteroclinic,

$$\varphi(-\infty)\neq\varphi(+\infty).$$

Such a solution is called a front, $s \in \mathbb{R}$ and $\mathbf{n} \in S^2$ are its speed and its direction of propagation. The quantity

$$m = \rho(\mathbf{u} \cdot \mathbf{n} - s),$$

obviously independent of x, is the associated mass flux. We exemplarily concentrate on a prototypical situation in which a class of such fronts, of small amplitude and small flux, arise during a bifurcation at a critical temperature θ_*.

The following two facts have been established in [6] under certain assumptions on G.[1]

Property 1 (Maxwell states and no-flux phase boundaries)**.** *With $\tilde{\theta} < \theta_*$ sufficiently close to θ_*, the following holds for every $\theta \in (\tilde{\theta}, \theta_*]$. There are locally uniquely determined fluid states $(\underline{c}_0.p_0), (\overline{c}_0, p_0)$, depending continuously on θ, such that* (i)

$$q(\underline{c}_0, p_0) = q(\overline{c}_0, p_0) = 0$$

with

$$\underline{c}_0 = \overline{c}_0 \quad \textit{if} \quad \theta = \theta_*,$$

and (ii) *if $\theta < \theta_*$, then*

$$\tau(\underline{c}_0, p_0) > \tau(\overline{c}_0, p_0)$$

and system (1.1) *admits a no-flux* $(m = 0)$ *phase boundary*

$$(\overrightarrow{c}(x), \overrightarrow{p}(x), 0) \textit{ with } (\overrightarrow{c}(-\infty), \overrightarrow{p}(-\infty)) = (\underline{c}_0, p_0), (\overrightarrow{c}(\infty), \overrightarrow{p}(\infty)) = (\overline{c}_0, p_0)$$

and (*equivalently via $x \mapsto -x$*) *a no-flux phase boundary*

$$(\overleftarrow{c}(x), \overleftarrow{p}(x), 0) \textit{ with } (\overleftarrow{c}(-\infty), \overleftarrow{p}(-\infty)) = (\overline{c}_0, p_0), (\overleftarrow{c}(\infty), \overleftarrow{p}(\infty)) = (\underline{c}_0, p_0).$$

Property 2 (Phase boundaries with non-zero mass flux)**.** *For sufficiently small $m \neq 0$,*

[1] In [6], Theorems 1 and 2 were phrased in terms of ρ and the Helmholtz potential F, which is Legendre conjugate to G, cf. Sec. 2.1 below. Under the assumptions of [6], the two formulations are equivalent.

(i) *the (left endstate, profile, right endstate) triple*

$$(\underline{c}_0, p_0, 0), (\overrightarrow{c}, \overrightarrow{p}, 0), (\overline{c}_0, p_0, 0)$$

perturbs regularly to a (left endstate, profile, right endstate) triple

$$(\overrightarrow{c}_m^-, \overrightarrow{p}_m^-, \overrightarrow{u}_m^-), (\overrightarrow{c}_m, \overrightarrow{p}_m, \overrightarrow{u}_m), (\overrightarrow{c}_m^+, \overrightarrow{p}_m^+, \overrightarrow{u}_m^+),$$

corresponding to a traveling-wave phase boundary that is densifying if $m > 0$ *and rarefying if* $m < 0$;

(ii) *the (left endstate, profile, right endstate) triple*

$$(\overline{c}_0, p_0, 0), (\overleftarrow{c}, \overleftarrow{p}, 0), (\underline{c}_0, p_0, 0)$$

perturbs regularly to a (left endstate, profile, right endstate) triple

$$(\overleftarrow{c}_m^-, \overleftarrow{p}_m^-, \overleftarrow{u}_m^-), (\overleftarrow{c}_m, \overleftarrow{p}_m, \overleftarrow{u}_m), (\overleftarrow{c}_m^+, \overleftarrow{p}_m^+, \overleftarrow{u}_m^+)$$

corresponding to a traveling-wave phase boundary that is rarefying if $m > 0$ *and densifying if* $m < 0$.

A proof of the following is given in [8] and sketched below.

Theorem 1. *Assume there exists a point* (c_*, p_*, θ_*) *at which* G *satisfies*

$$G_c = G_{cc} = G_{ccc} = 0, \quad G_{cccc} > 0, \quad G_{cc\theta} > 0, \quad G_{cp} \neq 0. \tag{1.5}$$

Then, Properties 1 *and* 2 *hold near that point.*

Sketch of proof. For all traveling waves, we will assume $\partial_t = 0$, i. e., we work in the rest frame of the wave. It suffices to consider traveling waves with zero mass flux, $m = 0$, cf. [6]. In the rest frame, these have

$$\mathbf{u} \cdot \mathbf{n} = 0$$

and are governed by the ordinary differential equations

$$0 = p' + (\delta\rho y^2)' \tag{1.6}$$

$$0 = \rho q + (\delta\rho y)' \tag{1.7}$$

$$c' = y. \tag{1.8}$$

It is easy to show (cf. Lemma 1 in [6]) that $G(c,p,\theta,y)$ is a first integral of (1.6)-(1.8). After integrating (1.6) and using the outcome

$$p+\delta\rho y^2=\pi, \quad \pi \text{ a constant of integration,}$$

in equations (1.7), (1.8), these latter reduce to a planar system in c and y, in which θ and π play the role of parameters. As the rest points of this system are precisely the points (c,y) with $y=0$ and

$$G^0_c(c,\pi,\theta)=0,$$

this system is easily understood along the lines of [6] by analyzing the local extrema of the elements of

$$\{G^0(.,p,\theta): \quad (p,\theta) \text{ near } (p_*,\theta_*)\}. \tag{1.9}$$

According to singularity theory [4], assumptions (1.5) mean that locally near c_*, the set (1.9) constitutes a universal unfolding of $G^0(.,p_*,\theta_*)$ and there exists a diffeomorphism from a neighborhood of (c_*,p_*,θ_*) in $\mathbb{R}^3$ to a neigborhood of $(0,0,0)$ in $\mathbb{R}^3$, with

$$(c,p,\theta)\mapsto(\tilde{c},\tilde{p},\tilde{\theta})\equiv(C(c,p,\theta),P(p,\theta),\Theta(p,\theta)),$$

such that locally

$$G^0(c,p,\theta)=\tilde{c}^4+\tilde{\theta}\tilde{c}^2+\tilde{p}\tilde{c}\equiv\tilde{G}(\tilde{c},\tilde{p},\tilde{\theta}).$$

Following Thom, this is called the *cusp catastrophe*, cf. [4]. p. 147. Now, $\tilde{G}(.,\tilde{p},\tilde{\theta}):\mathbb{R}\to\mathbb{R}$ has one local extremum (a mimimum) or three local extrema (two mimima with a maximum in between) according to whether

$$-8\tilde{\theta}^3<27\tilde{p}^2 \quad \text{or} \quad -8\tilde{\theta}^3>27\tilde{p}^2.$$

In the latter case the two minima of $\tilde{G}(.,\tilde{p},\tilde{\theta})$ occur with identical values if and only if $\tilde{p}=0$. The situation thus corresponds to the one displayed in Figures 3 and 4 of [6]. Concretely speaking, heteroclinic saddle-saddle connections exist if and only if $\tilde{\theta}<0$ and $\tilde{p}=0$. □

For the rest of the paper, we will assume that the fluid satisfies the assumption[2]

$$\text{(R)} \qquad G^0(c,p,\theta) = cG^1(p,\theta) + (1-c)G^2(p,\theta) + W(c,\theta). \tag{1.10}$$

Here, $G^1(p_1,\theta)$ and $G^2(p_2,\theta)$ denote the Gibbs potentials of the individual phases, and their individual pressures

$$p_1 = p_2 \tag{1.11}$$

have the same value p. Note (by differentiation w. r. t. p) that for the individual specific volumes τ_1, τ_2 of the phases, (R) amounts to the natural immiscibility condition

$$c\tau_1 + (1-c)\tau_2 = \tau. \tag{1.12}$$

For this still very general situation we find

Corollary 1. *Assume there exists a state (c_*,θ_*) at which the mixing energy W satisfies*

$$W_{cc} = W_{ccc} = 0, \quad W_{cccc} > 0, \quad W_{cc\theta} > 0. \tag{1.13}$$

If there exists a pressure value p_* such that

$$(G^2 - G^1)(p_*,\theta_*) = W_c(c_*,\theta_*) \quad \textit{while} \quad (G^2_p - G^1_p)(p_*,\theta_*) \neq 0, \tag{1.14}$$

Properties 1 *and* 2 *hold near the point (c_*,p_*,θ_*).*

Remark 1. (i) Conditions (1.13) simply means that, near $c = c_*$, the family

$$W(.,\theta)$$

undergoes a generic transition from convex ("one-well") for $\theta > \theta_*$ to convex-concave-convex ("double-well") for $\theta < \theta_*$.

(ii) The inequality in (1.14) means that the individual specific volumes of the two phases are different at the critical state (c_*,p_*,θ_*).

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[2] (R) is sometimes called Raoult's law. There are other natural settings that we do not consider here, for example Dalton's law $G^0(c,p,\theta) = cG_1(cp,\theta) + (1-c)G_2((1-c)p,\theta) + W(c,\theta)$. Cf. [9].

2. Compressibility versus Incompressibility

We will look at three classes of fluids according to whether one or both of the phases are compressible or incompressible, and conclude by commenting on incompressible limits. While we have intentionally formulated Theorem 1 for a much more general situation, it is for clarity's sake that we now restrict attention beyond the rule (R) by assuming additionally that the Gibbs energies G^1, G^2 of both phases themselves do not depend on the temperature. For all examples below, the classical part of the Gibbs potential thus reads

$$G^0(c,p,\theta) = cG^1(p) + (1-c)G^2(p) + W(c,\theta). \tag{2.1}$$

2.1. Both phases compressible

Assuming that both phases are compressible amounts to requiring

$$d^2G^1(p)/dp^2 < 0 \quad \text{and} \quad d^2G^2(p,\theta)/dp^2 < 0.$$

As this case is covered by the results in [6], we restrict its discussion to explaining the connection.

The Helmholtz potentials F^1, F^2, and F^0 of phase 1, phase 2, and the mixture are related to the respective Gibbs potentials through Legendre transforms,

$$F^1(\tau_1)=G^1(p_1)-\tau_1 p_1, \quad F^1(\tau_2)=G^1(p_2)-\tau_1 p_2, \; F^0(c,\tau,\theta)=G^0(c,p,\theta)-\tau p,$$

with

$$\tau_1 = \frac{dG^1(p_1)}{dp_1}, \quad \tau_2 = \frac{dG^2(p_2)}{dp_2}, \qquad \tau = \frac{\partial G^0(c,p,\theta)}{\partial p}.$$

The Helmholtz potential of the mixture thus is

$$F^0(c,\tau,\theta) \;=\; cF_1(T_1(c,\tau)) + (1-c)F_2(T_2(c,\tau)) + W(c,\theta),$$

with

$$\tau_j = T_j(c,\tau) \quad j=1,2,$$

found by solving (1.12) together with the relation

$$\frac{dF_1(\tau_1)}{d\tau_1} = \frac{dF_2(\tau_2)}{d\tau_2}$$

that expresses the equality (1.11) of partial pressures.

Note that the treatment of the phase-transition fronts by means of Gibbs potentials given in the present paper (and in its announcement [7]) is more convenient also in this case than the treatment via Helmholtz potentials in [6].

2.2. One phase incompressible, the other compressible

Assuming that phase 1 is incompressible and phase 2 is compressible means requiring

$$d^2G^1(p)/dp^2 = 0 \quad \text{and} \quad d^2G^2(p,\theta)/dp^2 < 0.$$

While Corollary 1 just holds immediately, we illustrate the occurrence of Property 1 in the prototypical case

$$G^1(p) = \tau_1 p \quad \text{with constant } \tau_1 > 0, \quad G^2(p) = 1 + \log p.$$

The considerations in the proof of Property 1 amount to studying the level sets of

$$\Gamma^{\theta,\pi}(c,y) \equiv \hat{G}(P^\pi(c,y),c) + W(c,\theta) + \frac{1}{2}y^2,$$

where

$$\hat{G}(p,c) = cG^1(p) + (1-c)G_2(p) = cp\tau_1 + (1-c)(1+\log p)$$

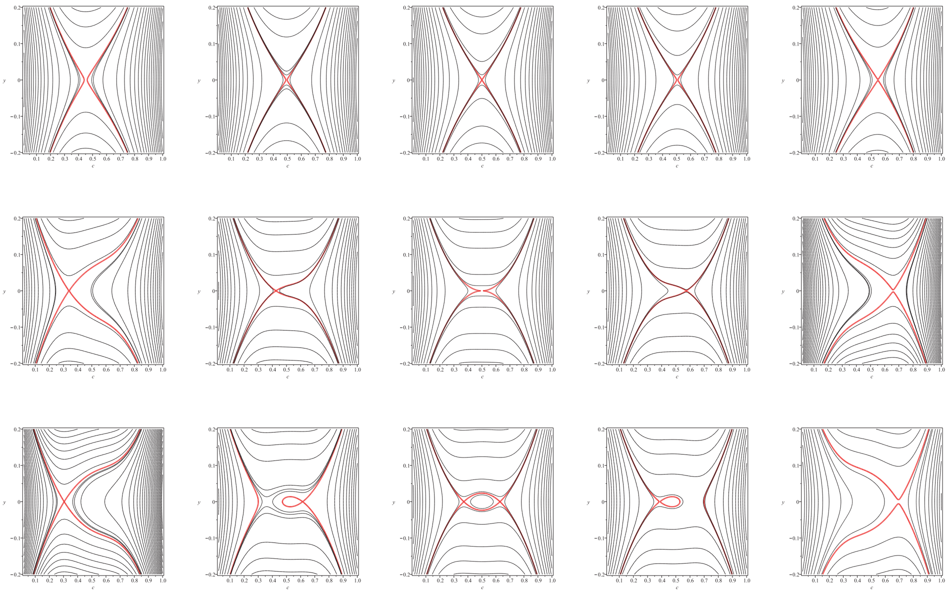
is $G^0 - W$ and $P^\pi(c,y)$ the unique positive root p of

$$0 = (p-\pi)(c\tau_1 p + (1-c)) + y^2 p.$$

The critical pressure is $p = p_*$, the unique solution < 1 of

$$G_c(p,c) = \tau_1 p - \log p - 1 = 0.$$

For (θ,π) near (θ_*,p_*), the level landscape of $\Gamma^{\theta,\pi}$ undergoes a transition from one saddle (for $\theta > \theta_*$) to a saddle-maximum-saddle configuration (for $\theta < \theta_*$ and certain π). In the latter case, the two saddles are at the same level and thus connected by two heteroclinic orbits (that together surround the maximum point) if π assumes a unique value $\pi_*(\theta)$.



Figure[3]**:** Level lines of $\Gamma^{\theta,\pi}$ for $\tau_1 = 0.5$ and $W(c,\theta) = (c-0.5)^4 + (\theta - \theta_*)(c-0.5)^2$. Top to bottom: $\theta - \theta_* = 0.16, 0.00, -0.08$. Left to right: $\pi - p_* = -0.010, -0.001, 0.000, 0.001, 0.010$.

2.3. Both phases incompressible

Assuming that both phases are incompressible means requiring

$$d^2G^1(p)/dp^2 \;=\; 0 \quad \text{and} \quad d^2G_2(p,\theta)/dp^2 = 0,$$

i.e.,

$$G^1(p) \;=\; \tau_1 p, \quad G^2(p) = \tau_2 p$$

with constant specific volumes $\tau_1, \tau_2 > 0$. Corollary 1 applies if one assumes the specific volumes to satisfy

$$\tau_* \equiv \tau_1 - \tau_2 \neq 0. \tag{2.2}$$

However, we have something deeper to report on this case, connected to the Navier-Stokes-Korteweg equations.

[3]We thank J. Höwing for producing these contour plots.

The *Navier-Stokes-Korteweg* equations are given by

$$\begin{aligned} \partial_t\rho + \nabla\cdot(\rho u) &= 0, \\ \partial_t(\rho\mathbf{u}) + \nabla\cdot(\rho\mathbf{u}\otimes\mathbf{u} + \bar{p}\mathbf{I}) &= \nabla\cdot\big(\mu(\nabla\mathbf{u} + (\nabla\mathbf{u})^T) + (\lambda\nabla\cdot\mathbf{u})\mathbf{I} + \mathbf{K}\big), \end{aligned} \tag{2.3}$$

Based on Korteweg's classical idea [10, 5], capillarity is reflected here in the fluid's Helmholtz energy

$$\bar{F}(\rho, \nabla\rho) = \check{\bar{F}}(\rho, |\nabla\rho|^2), \tag{2.4}$$

by its dependence on $\nabla\rho$, and the extended pressure $\bar{p}$ and the Korteweg tensor $\mathbf{K}$ derive from $\bar{F}$ as

$$\bar{p} \;=\; \rho^2\partial_\rho\bar{F} \tag{2.5}$$

and

$$\mathbf{K} \;=\; \rho\nabla\cdot\big(\partial_{\nabla\rho}(\rho\bar{F})\big)\mathbf{I} - \nabla\rho\otimes\partial_{\nabla\rho}(\rho\bar{F}). \tag{2.6}$$

Theorem 2. *In the case of two molecularly immiscible incompressible phases of different specific volumes,* (2.1), (2.2), *the Navier-Stokes-Allen-Cahn equations* (1.1) *can be written as the Navier-Stokes-Korteweg system*

$$\begin{aligned} \partial_t\rho + \nabla\cdot(\rho u) &= 0, \\ \partial_t(\rho\mathbf{u}) + \nabla\cdot(\rho\mathbf{u}\otimes\mathbf{u} + \bar{p}\mathbf{I}) &= \nabla\cdot\big(\mu(\nabla\mathbf{u} + (\nabla\mathbf{u})^T) + (\lambda_*\nabla\cdot\mathbf{u})\mathbf{I} + \mathbf{K}\big), \end{aligned} \tag{2.7}$$

with $\bar{p}, \mathbf{K}$ *deriving via* (2.5),(2.6) *from the induced Helmholtz energy*

$$\bar{F}(\rho, \nabla\rho) = W(\chi(\rho), \theta) + \frac{1}{2}[\chi'(\rho)]^2|\nabla\rho|^2 \quad \textit{with} \quad \chi(\rho) := \frac{1/\rho - \tau_2}{\tau_*}$$

and with the modified bulk viscosity

$$\lambda_* = \lambda + \Delta\lambda \quad \textit{where} \quad \Delta\lambda \equiv \frac{\delta^{1/2}}{\rho\tau_*^2}. \tag{2.8}$$

Theorem 2 is a corollary of a corresponding result for the non-isothermal case that has been stated and proven as Theorem 3.1 in [9]. The crucial point is the simple fact that the volume-addition law (1.12) amounts to the constraint

$$c = \chi(\rho).$$

The theorem shows that for fluids consisting of two immiscible incompressible phases of different specific volumes, the PDE theory of the Navier-Stokes-Korteweg system [12, 13] is an alternative to a conceivable "quasi-incompressible" description one might think of building analogously to how Lowengrub and Truskinovsky [14] and Abels et al. [1] treat two-phase fluids without phase transformation ("Cahn-Hilliard" case).

Returning to the issue of traveling waves, we note that our Theorem 1 thus recovers findings of Benzoni-Gavage [2] and others.

2.4. One or either phase almost incompressible

Certain fluids have one or two almost incompressible phases – an example is given by water, whose liquid phase is almost incompressible. This corresponds to limits

$$G^j_\epsilon \to G^j \text{ as } \epsilon \to 0 \quad \text{with} \quad \frac{dG^j_\epsilon}{dp} < 0 \text{ while } \frac{dG^j}{dp} = 0$$

for $j = 1$ or $j = 2$. We conclude by remarking that such limits are regular as regards the approach to traveling waves taken in this paper. I. e., Theorem 1 and Corollary 1 simply hold uniformly for small $\epsilon \geq 0$.

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