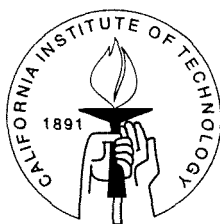


# Dynamics of phase transformations in thermoelastic solids

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# Abstract

The dynamical aspects of solid-solid phase transformations are studied within the framework of the theory of thermoelasticity. The main purpose is to analyze the role of temperature in the theory of phase transitions. This investigation consists of two parts: first, it is shown that by imposing a *kinetic relation* and a *nucleation criterion* it is possible to single out a *unique* solution to the Riemann problem for an adiabatic process. This extends to the thermomechanical case results previously found in a purely mechanical context. Secondly, based on an admissibility criterion for traveling wave solutions within the context of an *augmented* theory that includes viscosity, strain gradient and heat conduction effects, a special kinetic relation is *derived* using singular perturbation techniques.

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# Chapter 1 Introduction

Materials can exist in different solid phases which are characterized, at a microscopic level, by their underlying crystalline structure. A change in temperature, stress or other variables can induce a material to change from one solid phase to another. Phase changes are usually classified according to the main mechanism driving the transformation, viz., by diffusion of chemical species or by displacement, although these are not mutually exclusive (see CHRISTIAN [11]). The present work deals with the latter type in which the transition from one phase to another is characterized by a sudden change in the crystalline lattice, achieved without diffusion but rather via a cooperative movement of atoms.

One approach to analyze and predict this behavior is provided by the framework of solid state physics, which takes into account the microstructure of the material. Another viewpoint is to disregard the microstructure and consider the material as a continuum. This phenomenological approach, used in the present work, is the basis of theories like classical thermoelasticity and constitutes a useful framework to analyze phase transitions at a macroscopic level (see ABEYARATNE & KNOWLES[1]). It is worth noting that some continuum theories take into account the microstructure via the Cauchy-Born hypothesis which links the displacement of atoms with the (macroscopic) deformation of a solid (see, ERICKSEN [16], BALL & JAMES [7], BHATTACHARYA [8], JAMES & KINDERLEHRER [22]).

Inside a body, the interface between two distinct phases, known as a *phase boundary*, can be modeled as a surface of zero thickness across which the displacement is continuous but the deformation gradient suffers a jump. Other models, related to the Landau-Ginzburg theory, consider the interface as a transition layer of small but finite thickness where the deformation gradient varies rapidly but continuously (see, e.g., ERICKSEN [17], PENROSE & FIFE [26], TRUSKINOVSKY [31]). Implicit in the term “small” is the idea that the model has some kind of length scale. Some related

theories that incorporate separate balance principles associated with the motion of material particles and the motion of the phase boundary have also been proposed (see, FRIED & GURTIN [19], LUSK[24]).

Within the framework of classical thermoelasticity theory, the thermomechanical properties of a material can be described by a Helmholtz free energy density that depends smoothly on the deformation gradient and the temperature. In order to model a material that can exist in different solid phases —and hence analyze phase transitions— the Helmholtz potential, at some temperatures, exhibits multiple wells, each one of them associated to a distinct solid phase. The nonconvexity of the potential allows the existence of weak solutions to static and dynamic problems. In statics, such solutions are composed of regions throughout which the material is in one of the admissible phases (for a given temperature). These regions are separated by surfaces that correspond to coherent phase boundaries. In dynamics, it is possible to have *shock waves* —across which the deformation gradient is discontinuous but the material on each side of the surface of discontinuity is in the same phase— and propagating phase boundaries if on each side the material phases are different.

Phase transformations in solids have been studied in recent papers by ABEYARATNE & KNOWLES [1]-[4]. In particular, [4] deals with the *adiabatic* theory for a dynamically propagating phase boundary in a one-dimensional thermoelastic solid where an initial value problem of the Riemann type is analyzed. The phase boundary is modeled as a sharp interface. It is found that the solution to the Riemann problem, which involves initial data from two *distinct* phases, is not unique. In order to recover uniqueness, ABEYARATNE & KNOWLES propose the existence of an additional piece of constitutive information, a *kinetic relation*, which restricts the mobility of the phase boundary and singles out a unique solution for the Riemann problem. Following Onsager's formalism in thermodynamics (see, e.g., CALLEN [9], TRUESDELL [30]), the kinetic relation relates a *driving traction* (associated with a jump in entropy) to the speed of propagation of the phase boundary and to a state parameter, namely the temperature. The kinetic relation is introduced from the onset and represents an admissibility criterion for solutions to the Riemann problem.

One purpose of the present analysis is to investigate, within the context of the adiabatic theory, the Riemann problem involving initial data from the *same* phase. The results are qualitatively different from those in [4] in the sense that, in order to recover uniqueness, a *nucleation criterion* has to be enforced. This nucleation criterion signals the onset of a phase change and generalizes, for the thermoelastic case, the results found in [3] in the context of a purely mechanical theory.

As a second goal, a special kinetic relation is *derived* from an admissibility criterion related to a traveling wave problem in which an *augmented* theory is used. In the augmented (or *regularized*) theory, the sharp discontinuities are replaced by *transition layers* of finite thickness. By introducing dissipation and dispersion mechanisms associated with higher order derivatives of the strain (viscosity and strain gradient in this case), it is possible to simulate a region where the strain varies rapidly but continuously. The regularized theory also includes heat conduction in order to have a continuously varying temperature across the transition layer. In a sense, the sharp interface theory should be obtained from the regularized theory through a limit process where the dissipation and dispersion mechanisms and the heat conduction are removed. In this sense, the regularized theory can be viewed as a singular perturbation of the sharp interface theory.

In Chapter 2, the basic field equations and jump conditions are derived for the sharp interface theory and the results are specialized using a model for a thermoelastic material proposed in [2]. In Chapter 3, a Riemann problem for the thermoelastic material is analyzed and solved. It is shown that, under certain conditions, there exists a two-parameter family of solutions. Uniqueness is guaranteed by imposing a kinetic relation and a nucleation criterion. In Chapter 4, an augmented theory is introduced and some general features of solutions to the traveling wave problem are derived. In Chapter 5, a *reduced* problem, where viscosity and strain gradient are not present, is analyzed and solved. In this case, it is found that only supersonic traveling waves can be achieved. This reduced problem corresponds to the basic solution of a singularly-perturbed system which is analyzed in Chapter 6. It is shown that the admissibility criterion for the existence of a subsonic traveling wave in the

augmented theory provides an additional restriction on the data that can be casted as a kinetic relation. Finally, Chapter 7 contains some conclusions and recommendations for future work.

## Chapter 2 Sharp interface theory: adiabatic case

### 2.1 Basic equations.

Consider a bar that occupies the interval  $[-L, L]$  in a reference configuration. Consider longitudinal motions of the bar during a time interval  $[t_0, t_1]$ . Points in the reference configuration are denoted by  $(x, t) \in [-L, L] \times [t_0, t_1]$ . Assume that the particle  $x$  is mapped to the position  $y(x, t)$  at time  $t$ , (i.e.,  $y(x, t) = x + u(x, t)$ , where  $u$  is the displacement); assume that  $u \in C^0([-L, L] \times [t_0, t_1])$  and piecewise  $C^2([-L, L] \times [t_0, t_1])$ . Let  $\gamma = u_x$  and  $v = u_t$  be the strain and particle velocity (the subscript refers to partial differentiation). The restriction  $-1 < \gamma(x, t), \forall x, t$ , guarantees that the deformation  $y(x, t)$  is one-to-one. Let  $\rho$  be the *referential* mass density (assumed to be independent of  $x$ ),  $\sigma$ , the stress,  $\epsilon$ , the internal energy per unit mass and  $\eta$ , the entropy. Assume that  $\sigma$ ,  $\epsilon$  and  $\eta$  are piecewise  $C^1([-L, L] \times [t_0, t_1])$ . The balance of linear momentum, balance of energy and the Clausius-Duhem inequality for an *adiabatic thermomechanical process* in a one-dimensional bar are

$$[\sigma]_{x_1}^{x_2} = \frac{d}{dt} \int_{x_1}^{x_2} \rho v dx, \quad (2.1)$$

$$[\sigma v]_{x_1}^{x_2} = \frac{d}{dt} \int_{x_1}^{x_2} \rho \left( \epsilon + \frac{1}{2} v^2 \right) dx, \quad (2.2)$$

$$\Gamma(t) = \frac{d}{dt} \int_{x_1}^{x_2} \rho \eta dx \geq 0, \quad (2.3)$$

$\forall t \in [t_0, t_1]$  and  $\forall [x_1, x_2] \subseteq [-L, L]$ . Here,  $\Gamma(t)$  is the entropy production rate in the interval  $[x_1, x_2]$ . The local versions of (2.1), (2.2) and (2.3) at points where  $\sigma$ ,  $v$ ,  $\gamma$ ,  $\epsilon$

and  $\eta$  are smooth are

$$\sigma_x = \rho v_t , \quad (2.4)$$

$$(\sigma v)_x = \rho \left( \epsilon + \frac{1}{2} v^2 \right)_t , \quad (2.5)$$

$$\eta_t \geq 0 . \quad (2.6)$$

The compatibility equation is

$$v_x = \gamma_t . \quad (2.7)$$

Equation (2.5), with the use of (2.4), can be expressed as

$$\sigma \gamma_t = \rho \epsilon_t . \quad (2.8)$$

Let  $x = s(t)$  be a point in  $[x_1, x_2]$  across which some (or all) of the fields are discontinuous. Localization at  $x = s(t)$  of the compatibility equation (2.7) and the global balances (2.1)-(2.3) provide the corresponding jump conditions, viz.,

$$[[v]] + \dot{s} [[\gamma]] = 0 , \quad (2.9)$$

$$[[\sigma]] + \rho \dot{s} [[v]] = 0 , \quad (2.10)$$

$$[[\sigma v]] + \rho \dot{s} \left[ \epsilon + \frac{1}{2} v^2 \right] = 0 , \quad (2.11)$$

$$[[\eta]] \dot{s} \leq 0 , \quad (2.12)$$

where, for any function  $g$ ,

$$[[g]] \equiv g^+ - g^- , \quad g^- = \lim_{x \rightarrow s(t)^-} g(x, t) , \quad g^+ = \lim_{x \rightarrow s(t)^+} g(x, t) .$$

The superscript refers to one side of the moving discontinuity as follows: the “+” (“-”) side is the front (back) state if  $\dot{s} > 0$  or the back (front) state if  $\dot{s} < 0$ . Moving discontinuities are said to be *compressive* if the strain in the front state is higher than

in the back state and *expansive* otherwise.

The velocity jump can be eliminated from (2.10) by using equation (2.9), i.e.,

$$[[\sigma]] = \rho \dot{s}^2 [[\gamma]] . \quad (2.13)$$

Similarly, equation (2.11), with the use of (2.9) and (2.10), can also be expressed as

$$(\rho [[\epsilon]] - \langle \sigma \rangle [[\gamma]]) \dot{s} = 0 , \quad (2.14)$$

where, for any function  $g$ ,

$$\langle g \rangle \equiv \frac{1}{2} (g^+ + g^-) .$$

Some simple but useful identities are

$$\begin{aligned} [[gh]] &= [[g]] \langle h \rangle + \langle g \rangle [[h]] , \\ \langle g \rangle &= g^+ - \frac{1}{2} [[g]] = \frac{1}{2} [[g]] + g^- . \end{aligned}$$

Discontinuities are classified into two types, viz., classical *shock waves* and *phase boundaries*. The former are related to a discontinuity where the material on each side is in the *same* phase, whereas the latter refers to the case where different material phases exist on each side of the discontinuity. Moreover, in the adiabatic theory, a shock wave whose Lagrangian velocity  $\dot{s}$  is zero is referred to as a *contact discontinuity*. Specific jump conditions in each case are given in Section 2.6.

## 2.2 Thermoelastic material.

Classical thermodynamics for simple, single-component materials without memory is based on four different potentials, each one with two “natural” variables as shown

below:

$$\begin{array}{ccccc}
 \gamma & \longleftarrow & \psi & \longrightarrow & \theta \\
 \uparrow & & & & \uparrow \\
 \epsilon & & & & \mathcal{G} \\
 \downarrow & & & & \downarrow \\
 \eta & \longleftarrow & \mathcal{E} & \longrightarrow & \sigma
 \end{array}$$

where the potentials are  $\epsilon$  (internal energy),  $\psi$  (Helmholtz free energy),  $\mathcal{G}$  (Gibbs' potential) and  $\mathcal{E}$  (enthalpy) and the natural variables of each potential are indicated by the arrows on the side. One of these potentials is taken as a fundamental quantity that defines the material and the others can be obtained from it via a Legendre transformation. If certain invertibility requirements between variables are met, it is possible to express these potentials in terms of any combination of two variables. In order to specify which pair of variables is being used, the following notation is employed: a function of strain and temperature is denoted as  $\bar{g}$  and a function of strain and entropy is denoted as  $\tilde{g}$ . The value of the function is denoted as  $g$  or as  $\bar{g}(\gamma, \theta)$  or  $\tilde{g}(\gamma, \eta)$ . If  $\gamma$  and  $\theta$  are used as variables, then the stress and the entropy are viewed as functions of these variables.

As shown in subsequent sections, for the thermoelastic materials considered here—which are capable of phase transformations—the stress  $\bar{\sigma}$  is *not* a monotonic function of  $\gamma$  or  $\theta$  and the entropy  $\bar{\eta}$  is *not* a monotonic function of  $\gamma$ . Hence, in principle, they cannot be used as variables. Nevertheless, these functions are monotonic within a given phase. Therefore, in this restricted sense, they can be used as variables. In particular, it is assumed that the entropy is a monotonic function of the temperature, hence either  $(\gamma, \theta)$  or  $(\gamma, \eta)$  can be used as variables. *Throughout the present analysis, the preferred variables are  $\gamma$  and  $\theta$ .*

Let the Helmholtz potential be given by  $\psi = \bar{\psi}(\gamma, \theta)$ . This potential is related to the internal energy through

$$\psi = \epsilon - \theta\eta . \quad (2.15)$$



For a classical thermoelastic material, the stress  $\sigma$  and the entropy  $\eta$  are given by

$$\sigma = \bar{\sigma}(\gamma, \theta) = \rho \bar{\psi}_{\gamma}(\gamma, \theta) \quad (2.16)$$

and

$$\eta = \bar{\eta}(\gamma, \theta) = -\bar{\psi}_{\theta}(\gamma, \theta) . \quad (2.17)$$

The isothermal elastic modulus  $\mu$ , the specific heat at constant strain  $c$  and the coefficient of thermal expansion  $\alpha$  are defined by

$$\left. \begin{aligned} \mu &= \bar{\mu}(\gamma, \theta) = \bar{\sigma}_{\gamma}(\gamma, \theta) = \rho \bar{\psi}_{\gamma\gamma}(\gamma, \theta) , \\ c &= \bar{c}(\gamma, \theta) = \theta \bar{\eta}_{\theta}(\gamma, \theta) = -\theta \bar{\psi}_{\theta\theta}(\gamma, \theta) , \\ \alpha &= \bar{\alpha}(\gamma, \theta) = -\frac{\bar{\sigma}_{\theta}(\gamma, \theta)}{\bar{\sigma}_{\gamma}(\gamma, \theta)} = -\frac{\bar{\psi}_{\gamma\theta}(\gamma, \theta)}{\bar{\psi}_{\gamma\gamma}(\gamma, \theta)} . \end{aligned} \right\} \quad (2.18)$$

These material parameters are defined in the reference configuration, i.e., at a given particle  $x$  at time  $t$ , the value of a function  $\bar{g}$  is  $g(x, t) = \bar{g}(\gamma(x, t), \theta(x, t))$ . Alternatively, one can introduce the modified<sup>1</sup> Grüneisen coefficient (in the reference configuration) defined, in terms of the above quantities, as

$$G = \bar{G}(\gamma, \theta) = \frac{\bar{\psi}_{\gamma\theta}(\gamma, \theta)}{\theta \bar{\psi}_{\theta\theta}(\gamma, \theta)} = \frac{\alpha \mu}{\rho c} . \quad (2.19)$$

As a fundamental assumption, only materials with positive specific heat at constant strain and positive coefficient of thermal expansion are considered. Hence, it is assumed that  $\bar{G}(\gamma, \theta) \geq 0$ . Moreover, assuming that,

$$\bar{c}(\gamma, \theta) > 0 \quad \forall(\gamma, \theta) , \quad (2.20)$$

then, since  $\theta > 0$  and by (2.18)<sub>2</sub>,  $\bar{\eta}$  is a strictly increasing function of  $\theta$ . Hence, it is

---

<sup>1</sup>The Grüneisen coefficient is usually defined as  $(1 + \gamma)G$ , where  $G$  is given by (2.19). It turns out that (2.19) is a more convenient parameter. See CLIFTON [12].

possible to define an inverse function

$$\theta = \tilde{\theta}(\gamma, \eta) .$$

The natural variables for the internal energy are  $\gamma$  and  $\eta$ , (i.e.,  $\epsilon = \tilde{\epsilon}(\gamma, \eta)$ ). From equation (2.15), in terms of the Helmholtz potential,  $\tilde{\epsilon}$  is given by

$$\tilde{\epsilon}(\gamma, \eta) = \tilde{\psi}(\gamma, \tilde{\theta}(\gamma, \eta)) + \tilde{\theta}(\gamma, \eta)\eta . \quad (2.21)$$

Therefore, from (2.16) and (2.21), the stress can also be expressed as a function of  $\gamma$  and  $\eta$ , i.e.,

$$\sigma = \tilde{\sigma}(\gamma, \eta) = \rho \tilde{\epsilon}_{\gamma}(\gamma, \eta) .$$

Similarly, the temperature is given by

$$\theta = \tilde{\theta}(\gamma, \eta) = \tilde{\epsilon}_{\eta}(\gamma, \eta) .$$

The isentropic elastic modulus  $\mu_e$  is defined as

$$\mu_e = \tilde{\mu}_e(\gamma, \eta) = \tilde{\sigma}_{\gamma}(\gamma, \eta) = \rho \tilde{\epsilon}_{\gamma\gamma}(\gamma, \eta) .$$

Henceforth, though, from the invertibility of  $\eta$  and  $\theta$ , the internal energy  $\epsilon$  is to be considered as given by a function  $\bar{\epsilon}$  of  $\gamma$  and  $\theta$ , i.e.,

$$\epsilon = \bar{\epsilon}(\gamma, \theta) = \tilde{\epsilon}(\gamma, \bar{\eta}(\gamma, \theta)) .$$

This gives an interpretation for the specific heat at constant strain, i.e., from the above expression for  $\bar{\epsilon}$  and (2.18)<sub>2</sub>,

$$c = \bar{c}(\gamma, \theta) = \bar{\epsilon}_{\theta}(\gamma, \theta) .$$

In terms of  $\gamma$  and  $\theta$ , the isentropic elastic modulus can be expressed as

$$\mu_e = \bar{\mu}_e(\gamma, \theta) = \rho \left( \frac{\bar{\psi}_{\gamma\gamma}(\gamma, \theta)\bar{\psi}_{\theta\theta}(\gamma, \theta) - \bar{\psi}_{\gamma\theta}^2(\gamma, \theta)}{\bar{\psi}_{\theta\theta}(\gamma, \theta)} \right). \quad (2.22)$$

Using the material parameters defined by equation (2.18), it follows that

$$\mu_e = \mu + \frac{\theta\alpha^2\mu^2}{\rho c}. \quad (2.23)$$

The isothermal and the isentropic sound speeds are defined, when  $\mu, \mu_e > 0$ , as

$$\begin{aligned} a &= \bar{a}(\gamma, \theta) = \sqrt{\frac{\bar{\mu}(\gamma, \theta)}{\rho}}, \\ a_e &= \bar{a}_e(\gamma, \theta) = \sqrt{\frac{\bar{\mu}_e(\gamma, \theta)}{\rho}}. \end{aligned} \quad (2.24)$$

Therefore, from (2.23) and (2.24), the sound speeds are related by

$$a_e^2 = a^2 \left( 1 + \frac{\alpha^2 a^2}{c} \theta \right), \quad (2.25)$$

hence, if  $\mu, \mu_e > 0$  and since  $c > 0$ , then  $a_e^2 \geq a^2$ .

## 2.3 Entropy jump condition and driving traction.

Using equations (2.15), (2.16) and (2.17) in equation (2.8) provides an alternative expression for the energy equation, i.e.,

$$\eta_t = 0. \quad (2.26)$$

It follows that the dissipation inequality (2.6) is trivially satisfied at regular points. The rate of entropy production for a segment  $[x_1, x_2]$  of the bar which contains a

propagating discontinuity at  $x = s(t)$  can be expressed as

$$\Gamma(t) = \Gamma_b(t) + \Gamma_s(t) , \quad (2.27)$$

where

$$\Gamma_b(t) = \int_{x_1}^{x_2} \rho \eta_t dx , \quad (2.28)$$

$$\Gamma_s(t) = -\rho [[\eta]] \dot{s} . \quad (2.29)$$

Here,  $\Gamma_b$  represents the bulk entropy production and  $\Gamma_s$  corresponds to the entropy production due to the moving discontinuity. Equations (2.26) and (2.28) imply that

$$\Gamma_b = 0 , \quad (2.30)$$

hence the entropy production for a thermoelastic material under an adiabatic process occurs solely because of the presence of a moving discontinuity. Based on this entropy production, define the *driving traction* as

$$f = -\rho [[\eta]] \langle \theta \rangle . \quad (2.31)$$

For a discussion of the notion of driving traction, see ABEYARATNE & KNOWLES [1] and TRUSKINOVSKY [31]. From the energy jump condition (2.14), when  $\dot{s} \neq 0$ , it follows that

$$\rho [[\epsilon]] = \langle \sigma \rangle [[\gamma]] .$$

Moreover, since

$$[[\eta\theta]] = \langle \eta \rangle [[\theta]] + [[\eta]] \langle \theta \rangle ,$$

then (2.15) and (2.31) provide the following equivalent expression for the driving traction:

$$f = \rho [[\psi]] - \langle \sigma \rangle [[\gamma]] + \rho \langle \eta \rangle [[\theta]] . \quad (2.32)$$

For a thermoelastic material, (2.16), (2.17) and (2.32) give

$$f = \rho \{ \llbracket \bar{\psi} \rrbracket - \langle \bar{\psi}_\gamma \rangle \llbracket \gamma \rrbracket - \langle \bar{\psi}_\theta \rangle \llbracket \theta \rrbracket \} . \quad (2.33)$$

In terms of the driving traction, the dissipation inequality (2.12) can be expressed as

$$f \dot{s} \geq 0 . \quad (2.34)$$

Therefore, the jump conditions are given by (2.9)-(2.12) or, equivalently, by (2.9), (2.13), (2.14) and (2.34).

## 2.4 Hugoniot, Rayleigh and isentropic sets.

The jump conditions (2.9), (2.13), (2.14) and (2.34) are conditions that must be satisfied by the temperature, strain and velocity ahead and behind a discontinuity. These conditions are necessary but *not* sufficient to obtain a solution for phase transformation problems (see e.g., [31]). Let the superscripts + and – refer, respectively, to the conditions on the right side and the left side of a discontinuity. Suppose that the conditions on one side of the discontinuity, say  $(\gamma^+, \theta^+)$ , are known. For a thermoelastic material, since  $\epsilon = \bar{\epsilon}(\gamma, \theta)$  and  $\sigma = \rho \bar{\psi}_\gamma(\gamma, \theta)$ , the jump conditions (2.13) and (2.14) can be viewed as a (generally nonlinear) system of two equations and three unknowns (i.e.,  $\gamma^-$ ,  $\theta^-$  and  $\dot{s}$  are unknown). Moreover, for a *given*  $\dot{s}$ , it is important to know how many states  $(\gamma^-, \theta^-)$  (if any) satisfy (2.13) and (2.14).

The Rayleigh and Hugoniot sets, as defined below, are a convenient way to analyze the possible states on each side of a discontinuity. They also provide a geometrical interpretation of the system of equations arising from the jump conditions (2.13) and (2.14). Similarly, the isentropic set is introduced to analyze the entropy jump inequality (2.34). The slopes of the curves associated with these sets play an important role and their expressions are developed here. See also DUNN & FOSDICK [14].

The energy jump condition (2.14), when  $\dot{s} \neq 0$ , corresponds to

$$\rho \bar{\epsilon}(\gamma^-, \theta^-) - \rho \bar{\epsilon}(\gamma^+, \theta^+) - \frac{1}{2} (\bar{\sigma}(\gamma^-, \theta^-) + \bar{\sigma}(\gamma^+, \theta^+)) (\gamma^- - \gamma^+) = 0 .$$

Given a pair  $(\gamma_0, \theta_0)$ , define the Hugoniot function  $H$  as

$$H(\gamma, \theta; \gamma_0, \theta_0) \equiv \bar{\epsilon}(\gamma, \theta) - \epsilon_0 - \frac{1}{2\rho} (\bar{\sigma}(\gamma, \theta) + \sigma_0) (\gamma - \gamma_0) , \quad (2.35)$$

where  $\epsilon_0 = \bar{\epsilon}(\gamma_0, \theta_0)$  and  $\sigma_0 = \bar{\sigma}(\gamma_0, \theta_0)$ . To simplify the notation, the Hugoniot function will sometimes be expressed only as  $H(\gamma, \theta)$ , bearing in mind that it depends on a given generating point  $(\gamma_0, \theta_0)$ . The *Hugoniot set*  $\mathcal{H}$  in the  $\gamma$ - $\theta$  plane, generated by the point  $(\gamma_0, \theta_0)$ , is defined as

$$\mathcal{H} = \{(\gamma, \theta) \mid H(\gamma, \theta) = 0\} .$$

It is customary to choose the point  $(\gamma_0, \theta_0)$  as the state ahead of a moving discontinuity since in most problems these conditions are known a priori. Here, though, the point  $(\gamma_0, \theta_0)$  could also correspond to the conditions behind the discontinuity. Locally, at a point where  $H(\gamma, \theta) = 0$  and  $H_\theta(\gamma, \theta) \neq 0$ , it is possible to solve for the temperature in the equation  $H(\gamma, \theta) = 0$ , i.e.,

$$\theta = \theta^H(\gamma) .$$

Thus, the temperature that satisfies the energy jump condition can be determined uniquely from the corresponding strain for given conditions  $(\gamma_0, \theta_0)$  on one side of the discontinuity. Therefore,

$$H(\gamma, \theta^H(\gamma)) = \bar{\epsilon}(\gamma, \theta^H(\gamma)) - \epsilon_0 - \frac{1}{2\rho} (\bar{\sigma}(\gamma, \theta^H(\gamma)) + \sigma_0) (\gamma - \gamma_0) = 0 .$$

Differentiate this expression with respect to  $\gamma$  (i.e., along the Hugoniot curve) to get

$$(\bar{\epsilon}_\gamma + \bar{\epsilon}_\theta \theta_\gamma^H) - \frac{1}{2\rho} (\bar{\sigma}_\gamma + \bar{\sigma}_\theta \theta_\gamma^H) (\gamma - \gamma_0) - \frac{1}{2\rho} (\bar{\sigma} + \sigma_0) = 0 ,$$

where all the functions are evaluated at a point  $(\gamma, \theta^H(\gamma))$ . Expressing the internal energy  $\bar{\epsilon}$  and the stress  $\bar{\sigma}$  in terms of the Helmholtz potential  $\bar{\psi}$  provides the following relations:

$$\begin{aligned} \bar{\epsilon}_\gamma + \bar{\epsilon}_\theta \theta_\gamma^H &= \bar{\psi}_\gamma - \theta^H \bar{\psi}_{\gamma\theta} - \theta^H \bar{\psi}_{\theta\theta} \theta_\gamma^H , \\ \bar{\sigma}_\gamma + \bar{\sigma}_\theta \theta_\gamma^H &= \rho \bar{\psi}_{\gamma\gamma} + \rho \bar{\psi}_{\gamma\theta} \theta_\gamma^H . \end{aligned}$$

Therefore, the derivative of  $\theta^H$  (along the Hugoniot curve) is

$$\theta_\gamma^H = \frac{(\bar{\sigma} - \sigma_0)/\rho - \bar{\psi}_{\gamma\gamma}(\gamma - \gamma_0) - 2\theta^H \bar{\psi}_{\gamma\theta}}{\bar{\psi}_{\gamma\theta}(\gamma - \gamma_0) + 2\theta^H \bar{\psi}_{\theta\theta}} ,$$

or, in terms of the material parameters (2.18),

$$\theta_\gamma^H = \frac{-(\bar{\sigma} - \sigma_0)/\rho + a^2(\gamma - \gamma_0) - 2\alpha a^2 \theta^H}{\alpha a^2(\gamma - \gamma_0) + 2c} .$$

If  $H(\gamma, \theta) = 0$  and  $H_\gamma(\gamma, \theta) \neq 0$ , it is possible to express the Hugoniot set, locally, as

$$\gamma = \gamma^H(\theta) ,$$

in which case the slope is

$$\gamma_\theta^H = \frac{\alpha a^2(\gamma - \gamma_0) + 2c}{-(\bar{\sigma} - \sigma_0)/\rho + a^2(\gamma - \gamma_0) - 2\alpha a^2 \theta^H} .$$

**Remark:** Let  $\mathcal{H}_1$  be the Hugoniot set generated by  $(\gamma_1, \theta_1)$  and consider a state  $(\gamma_2, \theta_2) \in \mathcal{H}_1$ . Observe that the Hugoniot set  $\mathcal{H}_2$  generated by  $(\gamma_2, \theta_2)$  is *different* from  $\mathcal{H}_1$  but, necessarily,  $(\gamma_1, \theta_1) \in \mathcal{H}_2$ .  $\square$

The momentum jump condition (2.13) corresponds to

$$(\bar{\sigma}(\gamma^-, \theta^-) - \bar{\sigma}(\gamma^+, \theta^+)) - \rho \dot{s}^2 (\gamma^- - \gamma^+) = 0 .$$

Define the Rayleigh function  $R$ , for a given pair  $\gamma_0, \theta_0$  and a speed  $\dot{s}$ , as

$$R(\gamma, \theta; \gamma_0, \theta_0, \dot{s}) \equiv \frac{1}{\rho} (\bar{\sigma}(\gamma, \theta) - \sigma_0) - \dot{s}^2 (\gamma - \gamma_0) . \quad (2.36)$$

The Rayleigh function will be sometimes denoted only as  $R(\gamma, \theta)$  whenever the generating state and speed are given by the context. The *Rayleigh set*  $\mathcal{R}$  in the  $\gamma$ - $\theta$  plane, generated by the point  $(\gamma_0, \theta_0)$  and the speed  $\dot{s}$ , is defined as

$$\mathcal{R} = \{(\gamma, \theta) \mid R(\gamma, \theta) = 0\} .$$

Therefore,  $\mathcal{R}$  corresponds to the set of all points that satisfy the jump condition (2.13) for given conditions on one side of the discontinuity. If  $R(\gamma, \theta) = 0$  and  $R_\theta(\gamma, \theta) \neq 0$  (i.e., if  $\bar{\psi}_{\gamma\theta} \neq 0$ ), it is possible to express the Rayleigh set, locally, as

$$\theta = \theta^R(\gamma) .$$

It follows from this representation that

$$R(\gamma, \theta^R(\gamma)) = \frac{1}{\rho} [\bar{\sigma}(\gamma, \theta^R(\gamma)) - \sigma_0] - \dot{s}^2 (\gamma - \gamma_0) = 0 .$$

Differentiation of the above relation with respect to  $\gamma$  provides

$$\bar{\sigma}_\gamma + \bar{\sigma}_\theta \theta_\gamma^R = \rho \dot{s}^2 ,$$

where all the functions are evaluated at  $(\gamma, \theta^R(\gamma))$ . Expressing  $\bar{\sigma}$  in terms of the Helmholtz potential gives

$$\theta_\gamma^R = -\frac{\bar{\psi}_{\gamma\gamma} - \dot{s}^2}{\bar{\psi}_{\gamma\theta}} ,$$



or, in terms of the material parameters (2.18),

$$\theta_\gamma^R = \frac{a^2 - \dot{s}^2}{\alpha a^2} .$$

If  $R(\gamma, \theta) = 0$  and  $R_\gamma \neq 0$  (i.e., if  $\psi_{\gamma\gamma} - \dot{s}^2 \neq 0$ ), then one can express the Rayleigh set, locally, as

$$\gamma = \gamma^R(\theta) ,$$

in which case

$$\gamma_\theta^R = -\frac{\bar{\psi}_{\gamma\theta}}{\bar{\psi}_{\gamma\gamma} - \dot{s}^2} . \quad (2.37)$$

**Remark:** Let  $\mathcal{R}_1$  be the Rayleigh set generated by  $(\gamma_1, \theta_1)$  and a speed  $\dot{s}$  and let  $\mathcal{R}_2$  be the Rayleigh set generated by  $(\gamma_2, \theta_2)$  and the *same* speed  $\dot{s}$ . Hence, by definition,

$$\begin{aligned} (\gamma, \theta) \in \mathcal{R}_1 &\Rightarrow \sigma(\gamma, \theta) - \rho\dot{s}^2\gamma = \sigma(\gamma_1, \theta_1) - \rho\dot{s}^2\gamma_1 , \\ (\gamma, \theta) \in \mathcal{R}_2 &\Rightarrow \sigma(\gamma, \theta) - \rho\dot{s}^2\gamma = \sigma(\gamma_2, \theta_2) - \rho\dot{s}^2\gamma_2 . \end{aligned}$$

Suppose that  $(\gamma_2, \theta_2) \in \mathcal{R}_1$ , thus

$$\sigma(\gamma_2, \theta_2) - \rho\dot{s}^2\gamma_2 = \sigma(\gamma_1, \theta_1) - \rho\dot{s}^2\gamma_1 ,$$

and it follows that

$$\mathcal{R}_1 = \mathcal{R}_2 .$$

□

To analyze the entropy jump inequality (2.12), define the isentropic function  $I$  in the  $\gamma, \theta$ -plane, for a given point  $(\gamma_0, \theta_0)$ , as

$$I(\gamma, \theta; \gamma_0, \theta_0) = \bar{\eta}(\theta, \gamma) - \bar{\eta}(\gamma_0, \theta_0) . \quad (2.38)$$

Whenever it is clear by the context, the isentropic function will be denoted as  $I(\gamma, \theta)$ .

The *isentropes* (or, following the previous formalism, the *isentropic set*)  $\mathcal{I}$ , for a given point  $(\gamma_0, \theta_0)$ , is defined as

$$\mathcal{I} = \{(\gamma, \theta) \mid I(\gamma, \theta) = 0\} ,$$

i.e.,  $\mathcal{I}$  is simply the set of all points that have the same entropy as a given point  $(\gamma_0, \theta_0)$ .

If  $I(\gamma, \theta) = 0$  and  $I_\theta = -\psi_{\theta\theta} \neq 0$  then, locally, the isentrope can be expressed as

$$\theta = \theta^I(\gamma) .$$

Since  $I(\gamma, \theta^I(\gamma)) = 0$ , then

$$\bar{\eta}_\gamma + \bar{\eta}_\theta \theta_\gamma^I = 0 .$$

Expressing the entropy in terms of the Helmholtz potential gives

$$\theta_\gamma^I = -\frac{\bar{\psi}_{\gamma\theta}}{\bar{\psi}_{\theta\theta}} ,$$

or, in terms of the parameters of Section 2.2,

$$\theta_\gamma^I = -\frac{\alpha a^2}{c\theta^I} = -\frac{G}{\theta^I} .$$

Similarly, if  $I(\gamma, \theta) = 0$  and  $I_\gamma = -\psi_{\gamma\theta} \neq 0$  then, locally,

$$\gamma = \gamma^I(\theta) ,$$

and the slope is given by

$$\gamma_\theta^I = -\frac{c\theta^I}{\alpha a^2} = -\frac{\theta^I}{G} .$$

In view of the above definitions, the admissible states  $(\gamma^+, \theta^+)$  and  $(\gamma^-, \theta^-)$  are those that belong to the Rayleigh *and* Hugoniot sets generated at either  $(\gamma^+, \theta^+)$  or  $(\gamma^-, \theta^-)$  and also satisfy the entropy jump condition (2.34).

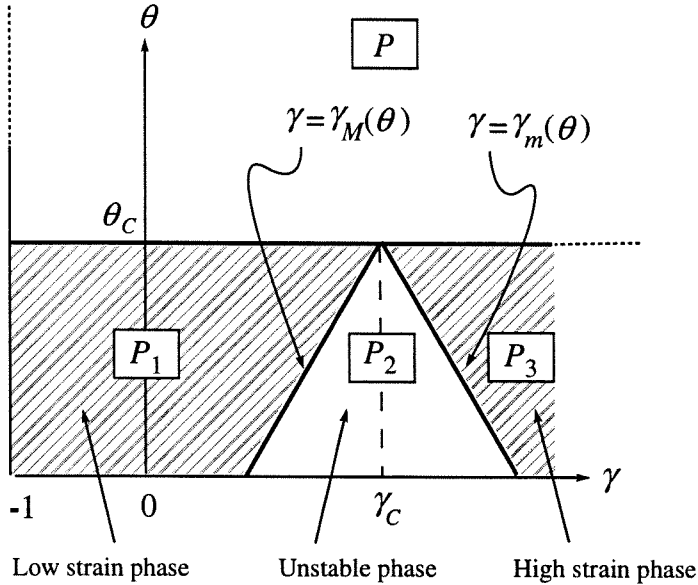


Figure 2.1: Material phases in the temperature-strain plane.

## 2.5 A specific thermoelastic material.

In order to obtain results in specific problems, consider a thermoelastic material introduced by ABEYARATNE & KNOWLES [2]. A phase diagram of this material in the  $\gamma, \theta$ -plane is shown in Figure 2.1. For temperatures below a critical temperature  $\theta_C$ , the material can exist in either a low strain phase  $P_1$  or a high strain phase  $P_3$ . These phases are metastable and are separated by an unstable phase  $P_2$ . Above the critical temperature the material can only exist in a stable phase  $P$ . Throughout this analysis, only transformations from or to the low and high strain phases are considered. A thorough description of the thermomechanical characteristics of this material can be found in [2]. The boundaries between the different phases are given by

$$\begin{aligned}\gamma_M(\theta) &= \gamma_C + M(\theta - \theta_C), \\ \gamma_m(\theta) &= \gamma_C + m(\theta - \theta_C),\end{aligned}\tag{2.39}$$

where  $\gamma_C > 0$ ,  $\theta_C > 0$ ,  $M$  and  $m$  are constants. The expression for the Helmholtz potential is given in each phase by

$$\bar{\psi}(\gamma, \theta) = \begin{cases} \frac{\mu}{2\rho}\gamma^2 - \frac{\alpha\mu}{\rho}\gamma(\theta - \theta_T) - c\theta \log\left(\frac{\theta}{\theta_T}\right) & \text{in } P_1, \\ \frac{\mu}{2\rho}\left[\gamma^2 - \frac{\gamma_T(\gamma - \gamma_M)^2}{\gamma_m - \gamma_M}\right] - \frac{\alpha\mu}{\rho}\gamma(\theta - \theta_T) - c\theta \log\left(\frac{\theta}{\theta_T}\right) & \text{in } P_2, \\ \frac{\mu}{2\rho}(\gamma - \gamma_T)^2 - \frac{\alpha\mu}{\rho}(\gamma - \gamma_T)(\theta - \theta_T) - c\theta \log\left(\frac{\theta}{\theta_T}\right) + \frac{\lambda_T}{\theta_T}(\theta - \theta_T) & \text{in } P_3, \end{cases} \quad (2.40)$$

where  $\theta_T$  is the transformation temperature,  $\gamma_T$  is the transformation strain,  $\lambda_T$  is the latent heat at  $\theta = \theta_T$  and  $\gamma_m = \gamma_m(\theta)$ ,  $\gamma_M = \gamma_M(\theta)$ . The remaining parameters were defined in Section 2.2 and are assumed constant. According to the model developed in [2], the material parameters must satisfy the following restrictions:

$$\left. \begin{aligned} \gamma_T &> (M - m)\theta_C > 0, \\ \gamma_C &= \frac{\gamma_T}{2} + \frac{1}{2}(M + m)(\theta_C - \theta_T), \\ M + m &= \frac{2\rho\lambda_T}{\mu\gamma_T\theta_T} + 2\alpha. \end{aligned} \right\} \quad (2.41)$$

The first restriction guarantees that there is no overlap between the two metastable phases in the  $\gamma, \theta$ -plane (hence, the stress is uniquely determined for a given temperature *and* strain). Restrictions (2.41)<sub>2,3</sub> are related to the fact that the metastable phases and the unstable phase coincide at the critical point  $(\gamma_C, \theta_C)$ . From (2.16) and

(2.40), the stress response function is given by

$$\bar{\sigma}(\gamma, \theta) = \begin{cases} \mu\gamma - \alpha\mu(\theta - \theta_T) & \text{in } P_1, \\ \mu \left[ \gamma - \frac{\gamma_T(\gamma - \gamma_M)}{\gamma_m - \gamma_M} \right] - \alpha\mu(\theta - \theta_T) & \text{in } P_2, \\ \mu(\gamma - \gamma_T) - \alpha\mu(\theta - \theta_T) & \text{in } P_3, \end{cases} \quad (2.42)$$

where, as before,  $\gamma_m = \gamma_m(\theta)$ ,  $\gamma_M = \gamma_M(\theta)$ . Observe that, for a fixed temperature, the stress-strain relation is linear in each phase. Hence, this material will be referred to as the *trilinear* material. The entropy response function, from (2.17) and (2.40), is given by

$$\bar{\eta}(\gamma, \theta) = \begin{cases} \frac{\alpha\mu}{\rho}\gamma + c \log \left( \frac{\theta}{\theta_T} \right) + c & \text{in } P_1, \\ \frac{\alpha\mu}{\rho}\gamma + c \log \left( \frac{\theta}{\theta_T} \right) + c \\ \quad + \frac{\mu}{2\rho} \frac{\gamma_T}{M - m} \left[ \frac{(\gamma - \gamma_C)^2}{(\theta - \theta_C)^2} - M^2 \right] & \text{in } P_2, \\ \frac{\alpha\mu}{\rho}(\gamma - \gamma_T) + c \log \left( \frac{\theta}{\theta_T} \right) + c - \frac{\lambda_T}{\theta_T} & \text{in } P_3, \end{cases} \quad (2.43)$$

where the explicit forms of  $\gamma_m$  and  $\gamma_M$  given by (2.39) were used. Moreover, from (2.15), (2.40) and (2.43), the corresponding internal energy as a function of  $\gamma$  and  $\theta$

is given by

$$\bar{\epsilon}(\gamma, \theta) = \begin{cases} \frac{\mu}{2\rho}\gamma^2 + \frac{\alpha\mu\theta_T}{\rho}\gamma + c\theta & \text{in } P_1, \\ \frac{\mu}{2\rho} \left\{ \gamma^2 + \frac{\gamma_T(2\theta - \theta_C)(\gamma - \gamma_C)^2}{(M - m)(\theta - \theta_C)^2} - \frac{M^2}{M - m}\gamma_T\theta_C \right. \\ \quad \left. - 2\frac{M}{M - m}\gamma_T(\gamma - \gamma_C) \right\} + \frac{\alpha\mu\theta_T}{\rho}\gamma + c\theta & \text{in } P_2, \\ \frac{\mu}{2\rho}(\gamma - \gamma_T)^2 + \frac{\alpha\mu\theta_T}{\rho}(\gamma - \gamma_T) + c\theta - \lambda_T & \text{in } P_3. \end{cases} \quad (2.44)$$

Observe that the specific heat at constant strain, using (2.18)<sub>2</sub>, is given by

$$\bar{c}(\gamma, \theta) = \begin{cases} c & \text{in } P_1, \\ c - \frac{\mu\gamma_T}{\rho} \left[ \frac{(\gamma - \gamma_C)^2}{M - m} \right] \left[ \frac{\theta}{(\theta - \theta_C)^3} \right] & \text{in } P_2, \\ c & \text{in } P_3. \end{cases}$$

Since  $(\theta - \theta_C)^3 < 0$ , then, in any phase,  $\bar{c}(\gamma, \theta) > 0$ . This fact guarantees the invertibility between entropy and temperature as mentioned in Section 2.2.

## 2.6 Specific jump conditions.

For the special material introduced in Section 2.5, the jump conditions take the following form:

### 2.6.1 Shock waves and contact discontinuities.

At a point of discontinuity where both sides are in the *same* phase, the jump conditions (2.9), (2.13), (2.14) and (2.34) become

$$\left. \begin{aligned} \llbracket v \rrbracket + \dot{s} \llbracket \gamma \rrbracket &= 0 , \\ (a^2 - \dot{s}^2) \llbracket \gamma \rrbracket - \alpha a^2 \llbracket \theta \rrbracket &= 0 , \\ (\alpha a^2 \langle \theta \rangle \llbracket \gamma \rrbracket + c \llbracket \theta \rrbracket) \dot{s} &= 0 , \\ \left( \alpha a^2 \llbracket \gamma \rrbracket + c \log \frac{\theta^+}{\theta^-} \right) \dot{s} &\leq 0 . \end{aligned} \right\} \quad (2.45)$$

There are two possible cases to consider, viz.,

**Shock waves:** if  $\dot{s} \neq 0$  then, from the jump conditions (2.45)<sub>2,3</sub>, the speed of propagation of the discontinuity is given by

$$\dot{s}^2 = a^2 \left( 1 + \frac{\alpha^2 a^2}{c} \langle \theta \rangle \right) , \quad (2.46)$$

and the rest of the jump conditions are

$$\left. \begin{aligned} \llbracket v \rrbracket + \dot{s} \llbracket \gamma \rrbracket &= 0 , \\ \alpha a^2 \langle \theta \rangle \llbracket \gamma \rrbracket + c \llbracket \theta \rrbracket &= 0 , \\ \left\{ \frac{\llbracket \theta \rrbracket}{\langle \theta \rangle} - \log \frac{\theta^+}{\theta^-} \right\} \dot{s} &\geq 0 , \end{aligned} \right\} \quad (2.47)$$

where (2.47)<sub>3</sub> was obtained from (2.45)<sub>4</sub>, (2.47)<sub>2</sub> and the fact that  $c > 0$ . The entropy jump inequality is equivalent to

$$\theta^- \geq \theta^+ , \quad \text{for } \dot{s} > 0 \quad \text{or} \quad \theta^- \leq \theta^+ , \quad \text{for } \dot{s} < 0 , \quad (2.48)$$

hence the temperature behind the shock wave increases. Observe that the entropy jump inequality (2.48) differs from (2.45)<sub>4</sub> in the sense that (2.48) holds only if the strain and the temperature are related through (2.47)<sub>2</sub>. From (2.25), the speed of

propagation can be written as

$$\dot{s}^2 = \langle a_e^2 \rangle, \quad (2.49)$$

i.e., the square of the velocity of propagation is an “average” of the square of the isentropic sound speed. Furthermore, from (2.47)<sub>2</sub>, it follows that  $[[\gamma]][[\theta]] \leq 0$ , i.e., the jumps in strain and temperature have opposite signs. In view of the entropy jump inequality (2.48) and the shock wave speed (2.49) and assuming  $\alpha \neq 0$ , it follows that

$$\begin{aligned} \text{if } \gamma^+ < \gamma^- &\Rightarrow \dot{s} < 0, \theta^+ > \theta^- \text{ and } a^2 < (a_e^-)^2 < \dot{s}^2 < (a_e^+)^2, \\ \text{if } \gamma^+ > \gamma^- &\Rightarrow \dot{s} > 0, \theta^+ < \theta^- \text{ and } a^2 < (a_e^+)^2 < \dot{s}^2 < (a_e^-)^2. \end{aligned}$$

This result is the special version for the trilinear material of the subsonic-supersonic condition for shock waves which holds for more general thermoelastic materials. This condition asserts that  $\dot{s}$  is bounded below by the isentropic sound speed of its front state and bounded above by the isentropic sound speed of its back state. Moreover, in either case, the strain in the front state is higher than in the back state, hence, as expected, only compressive shock waves are admissible.

**Remark:** Along with the subsonic-supersonic condition, other bounds for *structured, steady* shock waves (as defined in Chapter 4) were established by DUNN & FOSDICK [14] for general thermoelastic materials. In particular, the shock wave speed is bounded below by the *isothermal* sound speed and by the isentropic sound speed of the back state. For the specific thermoelastic material considered here and in the context of a non-structured adiabatic shock wave, this result agrees with the relations shown above. Another consequence of (2.46) is to rule out the occurrence of the so-called ultra slow shock waves as defined by DUNN & FOSDICK.  $\square$



**Contact discontinuities:** if  $\dot{s} = 0$ , then (2.45) becomes

$$\left. \begin{aligned} \llbracket v \rrbracket &= 0 , \\ \llbracket \gamma \rrbracket - \alpha \llbracket \theta \rrbracket &= 0 . \end{aligned} \right\} \quad (2.50)$$

## 2.6.2 Phase boundaries.

The jump conditions when the low strain phase is on the *right* of the phase boundary (and the high strain phase on its left) are, from (2.9), (2.13), (2.14), (2.34), (2.40), (2.42) and (2.43), given by

$$\left. \begin{aligned} \llbracket v \rrbracket + \dot{s} \llbracket \gamma \rrbracket &= 0 , \\ (a^2 - \dot{s}^2) \llbracket \gamma \rrbracket + a^2 \gamma_T - \alpha a^2 \llbracket \theta \rrbracket &= 0 , \\ \left\{ \alpha a^2 \langle \theta \rangle \llbracket \gamma \rrbracket + c \llbracket \theta \rrbracket + a^2 \gamma_T \left( \langle \gamma \rangle - \frac{\gamma_T}{2} \right) + \alpha a^2 \theta_T \gamma_T + \lambda_T \right\} \dot{s} &= 0 , \\ \left\{ \alpha a^2 (\llbracket \gamma \rrbracket + \gamma_T) + c \log \frac{\theta^+}{\theta^-} + \frac{\lambda_T}{\theta_T} \right\} \dot{s} &\leq 0 . \end{aligned} \right\} \quad (2.51)$$

Similarly, the jump conditions when the high strain phase is on the *right* of the phase boundary (and the low strain phase on its left) are given by

$$\left. \begin{aligned} \llbracket v \rrbracket + \dot{s} \llbracket \gamma \rrbracket &= 0 , \\ (a^2 - \dot{s}^2) \llbracket \gamma \rrbracket - a^2 \gamma_T - \alpha a^2 \llbracket \theta \rrbracket &= 0 , \\ \left\{ \alpha a^2 \langle \theta \rangle \llbracket \gamma \rrbracket + c \llbracket \theta \rrbracket - a^2 \gamma_T \left( \langle \gamma \rangle - \frac{\gamma_T}{2} \right) - \alpha a^2 \theta_T \gamma_T - \lambda_T \right\} \dot{s} &= 0 , \\ \left\{ \alpha a^2 (\llbracket \gamma \rrbracket - \gamma_T) + c \log \frac{\theta^+}{\theta^-} - \frac{\lambda_T}{\theta_T} \right\} \dot{s} &\leq 0 . \end{aligned} \right\} \quad (2.52)$$

For the special case of a *stationary* phase boundary (i.e.,  $\dot{s} = 0$ ), the entropy inequality and the energy jump conditions are trivially satisfied and the remaining jump

conditions are

$$\begin{aligned} [[v]] = 0, \quad [[\gamma]] - \alpha[[\theta]] + \gamma_T = 0 & \text{ right side: low strain,} \\ [[v]] = 0, \quad [[\gamma]] - \alpha[[\theta]] - \gamma_T = 0 & \text{ right side: high strain.} \end{aligned}$$

## 2.7 Nondimensional parameters.

It is convenient to introduce a set of nondimensional parameters for the trilinear material. Define the following parameters:

$$\left. \begin{aligned} T &= \frac{c\theta}{a^2\gamma_T^2}, \quad \delta = \frac{\gamma}{\gamma_T}, \quad \bar{v} = \frac{v}{a\gamma_T}, \\ l_T &= \frac{\lambda_T}{a^2\gamma_T^2}, \quad G = G\gamma_T, \\ v &= \frac{\dot{s}}{a}, \quad M = \frac{a^2\gamma_TM}{c}, \quad m = \frac{a^2\gamma_Tm}{c}. \end{aligned} \right\} \quad (2.53)$$

The variable  $\delta$  might be viewed as a “normalized” strain. The parameter  $G$  will also be called the (modified) Grüneisen coefficient. Nondimensional stress and entropy are defined as

$$\left. \begin{aligned} \tau &= \frac{\sigma}{\rho a^2 \gamma_T}, \\ s &= \frac{\eta}{c}. \end{aligned} \right\} \quad (2.54)$$

Other nondimensional parameters will be introduced as required. Observe that it is also possible to define nondimensional parameters using the coefficient of thermal expansion  $\alpha$  instead of the specific heat at constant strain  $c$ . Nevertheless, to analyze the limit case  $\alpha \rightarrow 0$ , it is more convenient to use the above nondimensional form. For future reference, the nondimensional form of some relations is recorded here. The

stress and the entropy are given by

$$\bar{\tau}(\delta, T) = \begin{cases} \delta - G(T - T_T) & \text{low strain phase,} \\ \left[ \delta - \frac{\delta - \delta_M}{\delta_m - \delta_M} \right] - G(T - T_T) & \text{unstable phase,} \\ (\delta - 1) - G(T - T_T) & \text{high strain phase,} \end{cases} \quad (2.55)$$

and

$$\bar{s}(\delta, T) = \begin{cases} G\delta + \left( 1 + \log \frac{T}{T_T} \right) & \text{low strain phase,} \\ G\delta + \left( 1 + \log \frac{T}{T_T} \right) \\ - \frac{1}{2(m - M)} \left[ \frac{(\delta - \delta_C)^2}{(T - T_C)^2} - M^2 \right] & \text{unstable phase,} \\ G(\delta - 1) + \left( 1 + \log \frac{T}{T_T} \right) - \frac{l_T}{T_T} & \text{high strain phase.} \end{cases} \quad (2.56)$$

The restrictions on the material parameters given by (2.41) become

$$\left. \begin{aligned} 1 > (M - m)T_C > 0, \\ \delta_C = \frac{1}{2} + \frac{1}{2}(M + m)(T_C - T_T), \\ \frac{M + m}{2} = \frac{l_T}{T_T} + G. \end{aligned} \right\} \quad (2.57)$$

The nondimensional isentropic sound speeds on each side of the moving discontinuity (i.e., their relative magnitude with respect to the isothermal sound speed) are

$$(\mathbf{a}_e^\pm)^2 = 1 + G^2 T^\pm.$$

The nondimensional forms of the jump conditions (2.51)<sub>2,3,4</sub>, where it is assumed that  $(\delta^+, T^+)$  is in the low strain phase, are given by

$$\left. \begin{aligned} (1 - v^2)[[\delta]] + 1 - G[T] &= 0, \\ \left\{ G\langle T \rangle [[\delta]] + [T] + \left( \langle \delta \rangle - \frac{1}{2} \right) + GT_T + l_T \right\} v &= 0, \\ \left\{ G([\delta] + 1) + \log \frac{T^+}{T^-} + \frac{l_T}{T_T} \right\} v &\leq 0, \end{aligned} \right\}$$

and the jump conditions (2.52)<sub>2,3,4</sub>, where it is assumed that  $(\delta^+, T^+)$  is in the high strain phase, are given by

$$\left. \begin{aligned} (1 - v^2)[[\delta]] - 1 - G[T] &= 0, \\ \left\{ G\langle T \rangle [[\delta]] + [T] - \left( \langle \delta \rangle - \frac{1}{2} \right) - GT_T - l_T \right\} v &= 0, \\ \left\{ G([\delta] - 1) + \log \frac{T^+}{T^-} - \frac{l_T}{T_T} \right\} v &\leq 0. \end{aligned} \right\} \quad (2.58)$$

Using (2.58)<sub>1</sub> in (2.58)<sub>2</sub> to eliminate  $[[\delta]]$  gives

$$r_1(v)[T]^2 - r_2(v, T^+)[T] + r_3(v, \delta^+, T^+) = 0, \quad (2.59)$$

where

$$\left. \begin{aligned} r_1(v) &= -\frac{G^2 v}{2(1 - v^2)}, \\ r_2(v, T^+) &= -v \left[ \frac{(a_e^+)^2 - v^2}{1 - v^2} \right], \\ r_3(v, \delta^+, T^+) &= \frac{v}{1 - v^2} \left[ GT^+ + \frac{1}{2} - (1 - v^2) \left( \delta^+ - \frac{1}{2} + GT_T + l_T \right) \right]. \end{aligned} \right\} \quad (2.60)$$

The dependence of  $r_2$  on  $T$  is implicit in the isentropic sound speed. Equivalently, equation (2.59) can be expressed as

$$r_1(v)[T]^2 + r_2(v, T^-)[T] + r'_3(v, \delta^-, T^-) = 0, \quad (2.61)$$

where

$$r'_3(v, \delta^-, T^-) = -\frac{v}{1-v^2} \left[ GT^- - \frac{1}{2} - (1-v^2) \left( \delta^- - \frac{1}{2} + GT_T + l_T \right) \right] .$$

## 2.8 Specific Hugoniot and Rayleigh sets.

The explicit form of the Hugoniot and Rayleigh sets for the specific thermoelastic material of Section 2.5 can be obtained for a shock wave or a phase boundary. Since the Hugoniot set depends on the generating point, it is useful to develop expressions for sets based at either the low strain or the high strain phase. Let  $\mathcal{R}_\pm$  be the Hugoniot sets generated at  $(\gamma^\pm, \theta^\pm)$  respectively. Without loss of generality, assume that  $(\gamma^+, \theta^+)$  is on the *high strain* phase and  $(\gamma^-, \theta^-)$  in the *low strain* phase. Moreover, let  $\mathcal{R}_\pm$  be the Rayleigh sets generated by  $(\gamma^+, \theta^+)$  and the speed  $\dot{s}$  and by  $(\gamma^-, \theta^-)$  and the same speed  $\dot{s}$ . To analyze phase boundaries it is convenient to think of  $(\gamma^\pm, \theta^\pm)$  as the states on each side of a moving discontinuity, although no *a priori* assumption is made regarding which one corresponds to the front or back state since ultimately this information is provided by the sign of  $\dot{s}$ . In view of the above remark, assume henceforth that  $(\gamma^-, \theta^-) \in \mathcal{R}_+$ , hence

$$\mathcal{R} = \mathcal{R}_+ = \mathcal{R}_- .$$

For given conditions on each side of the discontinuity, there is a *unique* velocity magnitude  $|\dot{s}|$  (as given by the momentum jump condition) that connects the states  $(\gamma^\pm, \theta^\pm)$ —the velocity itself being  $\dot{s}$  or  $-\dot{s}$ .

From (2.42), (2.44) and (2.35) (or, alternatively, from (2.51)<sub>3</sub>), solving the equation  $H(\gamma, \theta) = 0$  for e.g.,  $\theta$ , provides an expression for the Hugoniot set in the  $\gamma$ - $\theta$  plane generated at  $(\gamma^-, \theta^-)$ . In terms of the nondimensional parameters introduced

in Section 2.7, one has

$$T^H(\delta) = \begin{cases} \frac{[2 - G(\delta - \delta^-)] T^-}{2 + G(\delta - \delta^-)} & \text{for } \delta < \delta_M(T) , \\ \frac{2T^- - (GT^- - 1)(\delta - \delta^-) + h(\delta^-)}{2 + G(\delta - \delta^-)} & \text{for } \delta > \delta_m(T) , \end{cases} \quad (2.62)$$

where

$$h(\delta^-) = 2\delta^- - 1 + 2(l_T + GT_T) .$$

The restriction  $\delta < \delta_M(T)$  guarantees that the material is in the low strain phase and  $\delta > \delta_m(T)$  restricts the corresponding formula to the high strain phase. For the unstable phase, it is possible to solve numerically the equation  $H(\gamma, \theta) = 0$  in order to get the Hugoniot set, i.e.,

$$\frac{1}{2(m - M)} \left[ \frac{(\delta - \delta_C)[T_C(\delta^- - \delta_C) - T(\delta + \delta^- - 2\delta_C)]}{(T - T_C)^2} + M(\delta + \delta^- - 2\delta_C) + M^2 T_C \right] + \frac{1}{2} G(T + T^-)(\delta - \delta^-) + (T - T^-) = 0 .$$

Similarly, the Hugoniot set generated at  $(\delta^+, T^+)$  can be expressed as

$$T^H(\delta) = \begin{cases} \frac{2T^+ - (GT^+ + 1)(\delta - \delta^+) - h(\delta^+)}{2 + G(\delta - \delta^+)} & \text{for } \delta < \delta_M(T) , \\ \frac{[2 - G(\delta - \delta^+)] T^+}{2 + G(\delta - \delta^+)} & \text{for } \delta > \delta_m(T) , \end{cases} \quad (2.63)$$

where

$$h(\delta^+) = 2\delta^+ - 1 + 2(l_T + GT_T) ,$$

and, as before, the Hugoniot in the unstable phase is given implicitly by

$$\frac{1}{2(m - M)} \left[ \frac{(\delta - \delta_C)[T_C(\delta^+ - \delta_C) - T(\delta + \delta^+ - 2\delta_C)]}{(T - T_C)^2} + m(\delta + \delta^+ - 2\delta_C) + m^2 T_C \right] + \frac{1}{2} G(T + T^+)(\delta - \delta^+) + (T - T^+) = 0 .$$

From (2.42) and (2.36), the Rayleigh set in the  $\gamma$ - $\theta$  plane can be obtained by solving the equation  $R(\gamma, \theta) = 0$ . In terms of nondimensional parameters, this set is given by

$$T^R(\delta) = \begin{cases} \frac{1}{G}(1 - v^2)(\delta - \delta^-) + T^- & \text{for } \delta < \delta_M(T) , \\ \frac{1}{G}(1 - v^2)(\delta - \delta^-) + T^- - \frac{1}{G} & \text{for } \delta > \delta_m(T) . \end{cases} \quad (2.64)$$

For the unstable phase, it is easier to express the Rayleigh set as a function of the temperature, i.e.,

$$\delta^R(T) = \frac{\delta^- - \delta_C - M(T - T_C) + G(m - M)(T - T_C)(T - T^-)}{(1 - v^2)(m - M)(T - T_C) - 1} + \delta^- .$$

Recall that  $\mathcal{R}_+ = \mathcal{R}_-$ , so only one expression for the Rayleigh set is given.

If one works with strain and entropy as fundamental variables, the entropy jump condition (2.12) simply states that the entropy of the state *behind* of the moving discontinuity (shock wave or phase boundary) has to be greater or equal to the entropy of the *front* state, regardless of the strain. Nevertheless, if the variables used are strain and temperature, this condition becomes more difficult to visualize and, therefore, it is useful to develop an expression for the isentropic curves.

For a *phase boundary*, the entropy jump inequality is expressed either by (2.51)<sub>4</sub> if the high strain phase is to the left of the phase boundary or by (2.52)<sub>4</sub> if it is to the right. Henceforth, without loss of generality, consider the latter case (in nondimensional form). For a given state  $(\delta^-, T^-)$  in the *low strain* phase, from (2.56), the isentropic curve  $\bar{s}(\delta, T) = s^-$  can be expressed as

$$T^I(\delta) = \begin{cases} T^- \exp[-G(\delta - \delta^-)] & \text{for } \delta < \delta_M(T) , \\ T^- \exp\left[-G(\delta - 1 - \delta^-) + \frac{l_T}{T^-}\right] & \text{for } \delta > \delta_m(T) . \end{cases} \quad (2.65)$$

For the unstable phase, the isentropic curve is given implicitly by

$$G(\delta - \delta^-) + \log \frac{T}{T^-} - \frac{1}{2(m - M)} \left[ \frac{(\delta - \delta_C)^2}{(T - T_C)^2} - M^2 \right] = 0 .$$

Similarly, for a given state  $(\delta^+, T^+)$  in the *high strain* phase, the curve  $\bar{s}(\delta, T) = s^+$  can be expressed as

$$T^I(\delta) = \begin{cases} T^+ \exp \left[ -G(\delta - (\delta^+ - 1)) - \frac{l_T}{T_T} \right] & \text{for } \delta < \delta_M(T) , \\ T^+ \exp [-G(\delta - \delta^+)] & \text{for } \delta > \delta_m(T) , \end{cases}$$

and for the unstable phase, the isentropic curve is given implicitly by

$$G(\delta - \delta^+) + \log \frac{T}{T^+} - \frac{1}{2(m - M)} \left[ \frac{(\delta - \delta_C)^2}{(T - T_C)^2} - M^2 \right] + \left[ G + \frac{l_T}{T_T} \right] = 0 .$$

From the entropy jump inequality (2.12), expressed here as  $[\mathbf{s}]\mathbf{v} \leq 0$ , there are two situations to consider depending on the sign of  $\mathbf{v}$ . For a *given* state  $(\delta^+, T^+)$  in the high strain phase, the isentropic curve  $\bar{s}(\delta, T) = s^+$  in the  $\delta, T$ -plane divides the low strain region into a region of lower entropy than  $s^+$  and a region of higher entropy. The former corresponds to admissible *front* states  $(\delta^-, T^-)$  if  $\mathbf{v} < 0$  and the latter to admissible *back* states  $(\delta^-, T^-)$  if  $\mathbf{v} > 0$ .

Figure 2.2 shows a typical case of a Hugoniot and Rayleigh curves for a pair of states  $(\delta^\pm, T^\pm)$ . The isentropic lines  $\bar{s}(\delta, T) = s^-$  and  $\bar{s}(\delta, T) = s^+$  are also shown, with  $s^+ < s^-$ . Figure 2.3 shows the detailed behavior of the different curves close to the point  $(\delta^-, T^-)$ .

Notice that the state  $(\delta^+, T^+)$  lies in the region of admissible front states for a given  $(\delta^-, T^-)$  with  $\mathbf{v} > 0$ . Conversely, the state  $(\delta^-, T^-)$  lies in the region of admissible back states for a given  $(\delta^+, T^+)$  with  $\mathbf{v} > 0$ . Hence, in this case,  $(\delta^-, T^-)$  corresponds to the *back* state and  $(\delta^+, T^+)$  to the *front* state with  $\mathbf{v} > 0$ . Observe also that the Hugoniot and Rayleigh curves do not intersect in the unstable region.



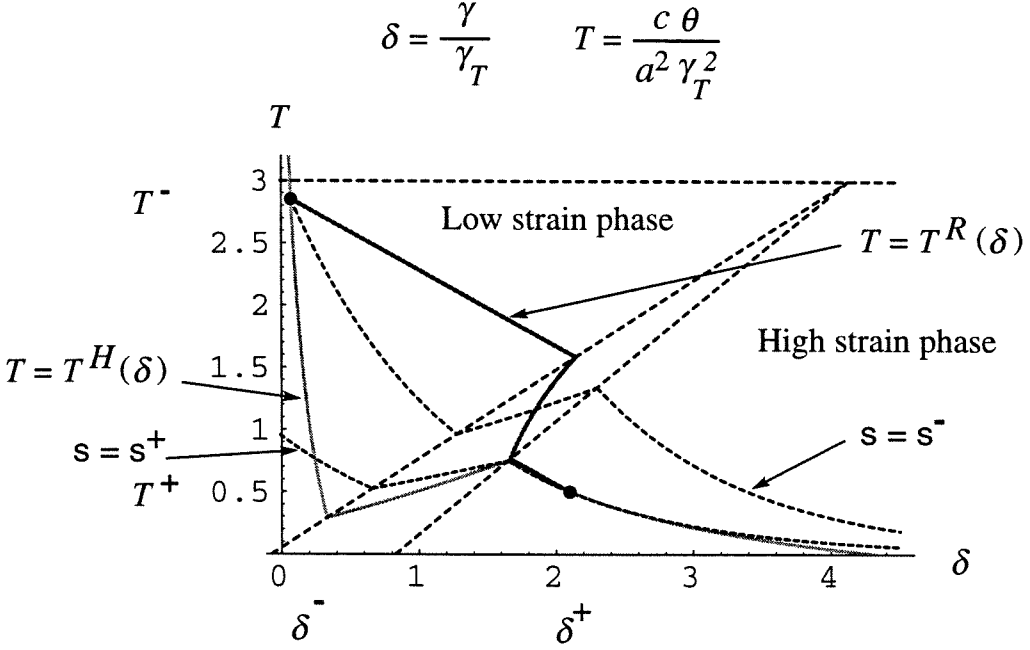


Figure 2.2: Rayleigh, Hugoniot and isentropic curves ( $m > 0$ ).

## 2.9 Small Grüneisen coefficient case.

In this section, it is assumed that the Grüneisen coefficient is small in the sense that the coefficient of thermal expansion is small but the specific heat  $c$  is finite (hence the nondimensional parameters of Section 2.7 are well defined). Suppose, for definiteness, that the material on the right side of a phase boundary is in the high strain phase. Thus, from the momentum jump condition (2.58)<sub>1</sub>, the jump in strain is given by

$$[[\delta]] = \frac{1}{1 - v^2} + O(G) .$$

Hence, if  $[[\delta]] > 0$  and up to  $O(G)$ , the phase boundary velocity is *subsonic* with respect to the isothermal sound speed (i.e.,  $v^2 < 1$ ). If  $[[\delta]] < 0$  then the phase boundary is *supersonic*. The energy jump condition (2.58)<sub>2</sub> gives, for small  $G$ ,

$$[[T]] = \langle \delta \rangle - \frac{1}{2} + l_T + O(G) .$$

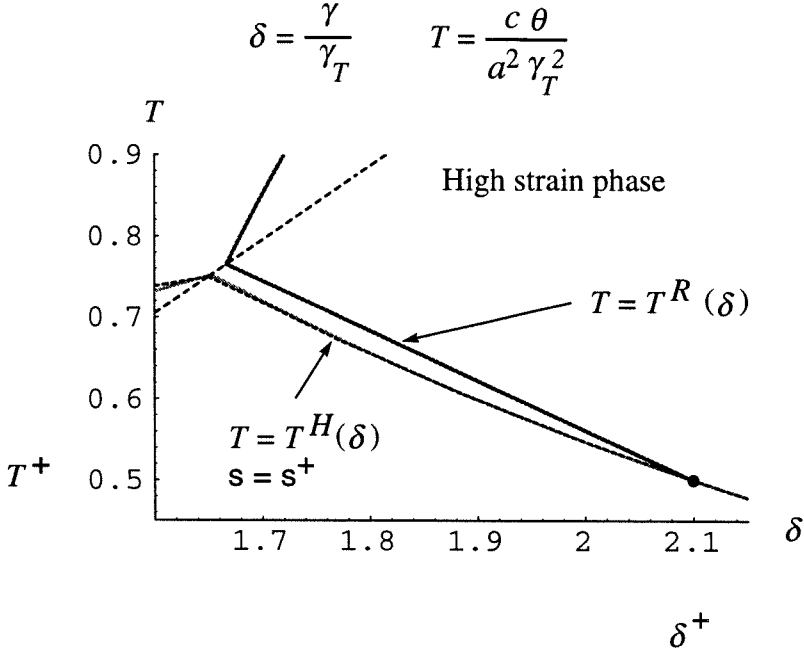


Figure 2.3: Hugoniot, Rayleigh and isentropic curves in the high strain region.

Observe that  $[[T]]$  could be either negative or positive. From the entropy inequality (2.58)<sub>3</sub>, if  $l_T \neq 0$  then, up to  $O(G)$ ,

$$\log \frac{T^+}{T^-} + l_T \mathbf{v} + O(G) \geq 0 .$$

If  $T^+ = T^-$ , the entropy inequality is satisfied as long as the latent heat and the speed of propagation  $\mathbf{v}$  have the same sign. Moreover, if  $l_T = 0$ , from (2.58)<sub>3</sub>, it follows that

$$\mathbf{v} \log \frac{T^+}{T^-} + O(G) \leq 0 ,$$

hence the temperature behind the phase boundary has to be greater than the temperature in the front state.

## 2.10 The strain-entropy representation.

Previous work in shock waves and phase transformation problems has been carried out using different basic thermodynamic variables. To be able to compare qualitatively

the predictions of different models, it is convenient to specify the trilinear material in other representations. For the strain-entropy representation, the phase diagram can be expressed as follows: for a given strain  $\delta$ ,

$$\begin{aligned} \text{low strain phase:} & \quad \mathbf{s} < \mathbf{s}_M(\delta) \text{ and } \mathbf{s} < \mathbf{s}_C(\delta) , \\ \text{unstable phase:} & \quad \mathbf{s}_M(\delta) < \mathbf{s} < \mathbf{s}_m(\delta) \text{ and } \mathbf{s} < \mathbf{s}_C(\delta) , \\ \text{high strain phase:} & \quad \mathbf{s} > \mathbf{s}_m(\delta) \text{ and } \mathbf{s} < \mathbf{s}_C(\delta) , \end{aligned}$$

where the phase boundaries are given by

$$\begin{aligned} \mathbf{s}_M(\delta) &= G\delta + \left[ 1 + \log \frac{1}{T_T} \left( \frac{\delta - \delta_C}{M} + T_C \right) \right] , \\ \mathbf{s}_m(\delta) &= G(\delta - 1) + \left[ 1 + \log \frac{1}{T_T} \left( \frac{\delta - \delta_C}{m} + T_C \right) \right] - \frac{l_T}{T_T} , \\ \mathbf{s}_C(\delta) &= \bar{\mathbf{s}}(\delta, T_C) . \end{aligned}$$

Define a nondimensional internal energy  $\mathbf{e}$ , as

$$\mathbf{e} = \frac{\epsilon}{a^2 \gamma_T^2} ,$$

then

$$\tilde{\mathbf{e}}(\delta, \mathbf{s}) = \begin{cases} \frac{\delta^2}{2} + GT_T \delta + T_T \exp [s - G\delta - 1] & \text{low strain phase,} \\ \frac{(\delta - 1)^2}{2} + GT_T (\delta - 1) - l_T \\ \quad + T_T \exp \left[ s - G(\delta - 1) + \frac{l_T}{T_T} - 1 \right] & \text{high strain phase.} \end{cases}$$

Since in the strain-entropy representation the temperature and the strain are related to the internal energy through

$$\tilde{\sigma}(\gamma, \eta) = \rho \tilde{\epsilon}_\gamma(\gamma, \eta), \quad \tilde{\theta}(\gamma, \eta) = \tilde{\epsilon}_\eta(\gamma, \eta),$$

then, in nondimensional form, these are given by

$$\bar{\tau}(\delta, s) = \begin{cases} \delta + GT_T \{1 - \exp [s - G\delta - 1]\} & \text{low strain phase,} \\ (\delta - 1) \\ \quad + GT_T \left\{ 1 - \exp \left[ s - G(\delta - 1) + \frac{l_T}{T_T} - 1 \right] \right\} & \text{high strain phase,} \end{cases}$$

and

$$\bar{T}(\delta, s) = \begin{cases} T_T \exp [s - G\delta - 1] & \text{low strain phase,} \\ T_T \exp \left[ s - G(\delta - 1) + \frac{l_T}{T_T} - 1 \right] & \text{high strain phase.} \end{cases}$$

For a given state  $(\delta_0, s_0)$  it is possible to obtain formulas, not displayed here, for the Rayleigh and Hugoniot sets.

## Chapter 3 A Riemann problem

### 3.1 Introduction.

Within the framework of the thermoelastic theory of Chapter 2, an initial value problem of the Riemann type for a one-dimensional bar is formulated. In Section 3.3, it is found that there exist two different kinds of solutions. One kind involves no phase transition, whereas the other kind involves a two-parameter family of solutions containing two propagating phase boundaries (the phase boundary velocities acting as parameters). In the latter case, a kinetic relation is used to obtain the phase boundary velocities and hence the structure of the solution is fully determined. It is also found that for some range of the initial data, it is possible to have either kind of solution (i.e., with or without phase boundaries). Therefore, a nucleation criterion is enforced to single out the unique solution to the problem from the two different kinds. Finally, in Section 3.5, the connection between the Riemann problem with uniform data and the nucleation criterion is investigated. In this chapter, for simplicity, the coefficient of thermal expansion is taken as zero. Consequently, the mechanical and thermal effects are decoupled in the differential equations. Nevertheless, a connection between the strain and the temperature remains in place via the jump conditions.

### 3.2 Field equations and jump conditions.

For the thermoelastic material introduced in Section 2.5, at points where the fields are smooth, (2.4), (2.7), (2.8) and (2.53) provide, with  $\alpha = 0$ ,

$$\gamma_t - v_x = 0 , \tag{3.1}$$

$$v_t - a^2 \gamma_x = 0 , \tag{3.2}$$

$$\theta_t = 0 . \tag{3.3}$$

The jump conditions (2.45), when  $\alpha = 0$  and in nondimensional form, are equivalent to either

$$\left\{ \begin{array}{l} \mathbf{v} = \pm 1, \\ \mathbf{v}[[\delta] + [\bar{v}]] = 0, \\ [[\delta]] \neq 0, \\ [[\bar{v}]] \neq 0, \\ [[T]] = 0, \end{array} \right. \quad \text{or} \quad \left\{ \begin{array}{l} \mathbf{v} = 0, \\ [[\delta]] = 0, \\ [[\bar{v}]] = 0, \\ [[T]] \neq 0. \end{array} \right. \quad (3.4)$$

The first case corresponds to a *shock wave* whereas the second is a *contact discontinuity*. Contact discontinuities are *stationary* in the the reference configuration (i.e., in the Lagrangian sense). If the high strain phase is on the *right* of the phase boundary, then the jump conditions (2.51), when  $\alpha = 0$  and in nondimensional form, are given by

$$\left. \begin{array}{l} \mathbf{v}[[\delta] + [\bar{v}]] = 0, \\ [[\delta]] - 1 + \mathbf{v}[[\bar{v}]] = 0, \\ \left\{ [[T]] - \left( \langle \delta \rangle - \frac{1}{2} \right) - l_T \right\} \mathbf{v} = 0, \\ \left\{ \log \frac{T^+}{T^-} - \frac{l_T}{T} \right\} \mathbf{v} \leq 0. \end{array} \right\} \quad (3.5)$$

If the high strain phase is on the *left* of the phase boundary, then the jump conditions (2.52) are given by

$$\left. \begin{array}{l} \mathbf{v}[[\delta] + [\bar{v}]] = 0, \\ [[\delta]] + 1 + \mathbf{v}[[\bar{v}]] = 0, \\ \left\{ [[T]] + \left( \langle \gamma \rangle - \frac{1}{2} \right) + l_T \right\} \mathbf{v} = 0, \\ - \left\{ \log \frac{T^-}{T^+} - \frac{l_T}{T} \right\} \mathbf{v} \leq 0. \end{array} \right\} \quad (3.6)$$

### 3.3 Riemann problem.

Consider the Riemann problem corresponding to an infinitely long bar composed of the thermoelastic material described in Section 2.5. This problem can be formulated as follows: *Find functions  $\delta(x, t)$ ,  $\bar{v}(x, t)$  and  $T(x, t)$  such that equations (3.1)-(3.3) are satisfied at points where the functions are sufficiently smooth and the corresponding jump conditions (3.4)-(3.6) are satisfied at points where the functions are discontinuous, subject to the following initial conditions:*

$$\delta(x, 0), \bar{v}(x, 0), T(x, 0) = \begin{cases} \delta_L, \bar{v}_L, T_L & \text{for } -\infty < x < 0, \\ \delta_R, \bar{v}_R, T_R & \text{for } 0 < x < \infty. \end{cases} \quad (3.7)$$

It is assumed that, initially, the bar is in the *low strain phase*, in which case

$$\begin{aligned} \delta_L &\in (-1, \delta_M(T_L)], \\ \delta_R &\in (-1, \delta_M(T_R)]. \end{aligned}$$

The structure of the solution, as shown by ABEYARATNE & KNOWLES [4], must necessarily involve either *no* phase boundaries (in which case all particles of the bar remain in the original phase at all times) or *two* phase boundaries moving in opposite directions (in which case the particles jump to the high strain phase). In the latter case, there is a two-parameter family of solutions.

#### 3.3.1 Solution with no phase boundary.

The solution with no phase boundary involves two shock waves (traveling along  $x/at = \pm 1$ ) and a contact discontinuity at  $x = 0$ . The bar remains in the low

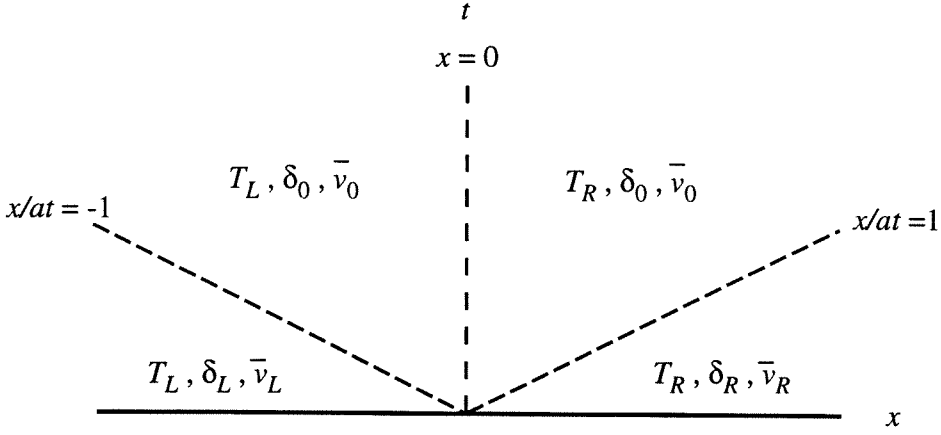


Figure 3.1: Solution with no phase boundary.

strain phase at all times. One seeks a solution of the form

$$\delta(x, t), \bar{v}(x, t), T(x, t) = \begin{cases} \delta_L, \bar{v}_L, T_L & \text{for } -\infty < x < -at, \\ \delta_0, \bar{v}_0, T_L & \text{for } -at < x < 0, \\ \delta_0, \bar{v}_0, T_R & \text{for } 0 < x < at, \\ \delta_R, \bar{v}_R, T_R & \text{for } at < x < \infty, \end{cases} \quad (3.8)$$

where  $\delta_0, \bar{v}_0$  are the only unknowns. Notice that the continuity of  $T$  across the shock waves and the continuity of  $\delta$  and  $\bar{v}$  across the contact discontinuity were enforced.

The solution is shown in Figure 3.1. Let

$$h = \frac{\delta_R + \delta_L}{2} + \frac{\bar{v}_R - \bar{v}_L}{2} \quad (3.9)$$

and

$$j = \frac{\delta_R - \delta_L}{2} + \frac{\bar{v}_R + \bar{v}_L}{2}$$

then, from the jump condition (3.4) it follows that

$$\delta_0 = h, \quad (3.10)$$

$$\bar{v}_0 = j.$$



It was assumed that the bar was initially in the low strain phase, then, for the whole bar to remain in the low strain phase at all times and from (3.8), it is required that  $-1 < \delta_0 < \min[\delta_M(T_L), \delta_M(T_R)]$ . Hence, from (3.10), there is a solution of the form (3.8) to the Riemann problem if and only if the initial datum  $h$  is such that

$$-1 < h \leq \min[\delta_M(T_L), \delta_M(T_R)] . \quad (3.11)$$

### 3.3.2 Solutions with two phase boundaries.

The solution with two phase boundaries involves two shock waves (traveling along  $x/at = \pm 1$ ), a contact discontinuity at  $x = 0$  and two phase boundaries at  $x/at = v < 0$  and  $x/at = v_* > 0$ . One seeks a solution of the form

$$\delta(x, t) , \bar{v}(x, t) , T(x, t) = \begin{cases} \delta_L , \bar{v}_L , T_L & \text{for } -\infty < x < -at , \\ \delta_0 , \bar{v}_0 , T_L & \text{for } -at < x < avt , \\ \delta_1 , \bar{v}_1 , T' & \text{for } avt < x < 0 , \\ \delta_1 , \bar{v}_1 , T'' & \text{for } 0 < x < av_*t , \\ \delta_2 , \bar{v}_2 , T_R & \text{for } av_*t < x < at , \\ \delta_R , \bar{v}_R , T_R & \text{for } at < x < \infty , \end{cases} \quad (3.12)$$

where  $\delta_0, \delta_1, \delta_2, \bar{v}_0, \bar{v}_1, \bar{v}_2, T'$  and  $T''$  are unknown. Notice that the continuity of  $T$  across the shock waves and the continuity of  $\delta$  and  $\bar{v}$  across the contact discontinuity were enforced. Here, as in the previous section, the bar is initially in the low strain phase. The form of the solution is shown in Figure 3.2. From the jump

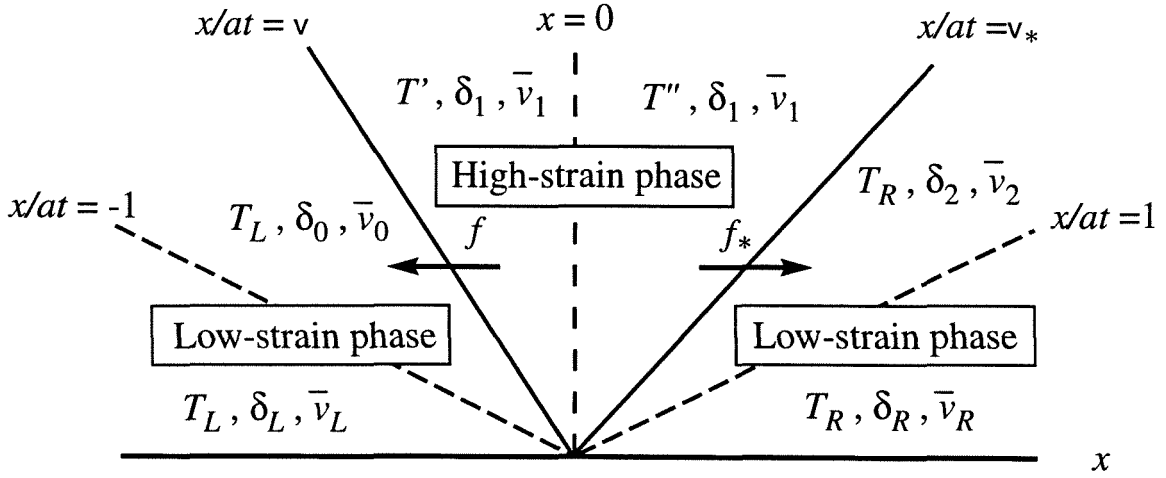


Figure 3.2: Two-phase solution.

conditions (3.4), (3.5)<sub>1,2</sub> and (3.6)<sub>1,2</sub>, one has

$$\begin{aligned}
 -(\delta_0 - \delta_L) + (\bar{v}_0 - \bar{v}_L) &= 0, \\
 v(\delta_1 - \delta_0) + (\bar{v}_1 - \bar{v}_0) &= 0, \\
 v_*(\delta_2 - \delta_1) + (\bar{v}_2 - \bar{v}_1) &= 0, \\
 (\delta_R - \delta_2) + (\bar{v}_R - \bar{v}_2) &= 0, \\
 (\delta_1 - \delta_0 - 1) + (\bar{v}_1 - \bar{v}_0)v &= 0, \\
 (\delta_2 - \delta_1 + 1) + (\bar{v}_2 - \bar{v}_1)v_* &= 0.
 \end{aligned}$$

Solving this system provides

$$\left. \begin{aligned}
 \delta_0 &= h + \frac{1}{2} \left( \frac{1}{1+v_*} - \frac{1}{1+v} \right), \\
 \delta_1 &= h + \frac{1}{2} \left( \frac{1}{1-v} + \frac{1}{1+v_*} \right), \\
 \delta_2 &= h + \frac{1}{2} \left( \frac{1}{1-v} - \frac{1}{1-v_*} \right),
 \end{aligned} \right\} \quad (3.13)$$

and

$$\left. \begin{aligned} \bar{v}_0 &= j + \frac{1}{2} \left( \frac{1}{1+v_*} - \frac{1}{1+v} \right) , \\ \bar{v}_1 &= j + \frac{1}{2} \left( \frac{1}{1+v_*} - \frac{1}{1-v} \right) , \\ \bar{v}_2 &= j + \frac{1}{2} \left( \frac{1}{1-v_*} - \frac{1}{1-v} \right) . \end{aligned} \right\} \quad (3.14)$$

Moreover, using the jump conditions (3.5)<sub>3</sub> and (3.6)<sub>3</sub> together with (3.12) yields

$$\begin{aligned} T' &= \frac{1}{2} (\delta_1 + \delta_0 - 1) + l_T + T_L , \\ T'' &= \frac{1}{2} (\delta_2 + \delta_1 - 1) + l_T + T_R . \end{aligned}$$

Furthermore, using (3.13) in the above equations provides

$$T' = T_L + r(v, v_*) , \quad (3.15)$$

$$T'' = T_R + r_*(v, v_*) , \quad (3.16)$$

where

$$r(v, v_*) = \left\{ h - \frac{1}{2} \left( \frac{v_*}{1+v_*} - \frac{v}{1-v^2} \right) \right\} + l_T , \quad (3.17)$$

$$r_*(v, v_*) = \left\{ h - \frac{1}{2} \left( \frac{v_*}{1-v_*^2} - \frac{v}{1-v} \right) \right\} + l_T . \quad (3.18)$$

Notice that

$$r_*(-v_*, -v) = r(v, v_*) .$$

It is important to remark that a solution of the form (3.12) is not unique. In fact, equations (3.13)-(3.18) represent a two-parameter family of solutions where the phase boundary velocities  $v$  and  $v_*$  can be used as such parameters. The uniqueness issue is addressed in Section 3.4 with the postulation of a kinetic relation which singles out an appropriate pair  $(v, v_*)$  to fully determine the solution with two phase boundaries.

### 3.3.3 Phase segregation conditions and entropy inequality.

From (3.11) it is clear that for suitable initial data there exists a solution to the Riemann problem with no phase boundary. The solution which involves two phase boundaries requires further analysis. One has to ensure that the solution satisfies the entropy inequalities (3.5)<sub>4</sub> and (3.6)<sub>4</sub> and that  $(\delta_0, T_L) \in P_1$ ,  $(\delta_1, T') \in P_3$ ,  $(\delta_1, T'') \in P_3$  and  $(\delta_2, T_R) \in P_1$ , i.e.,

$$\left. \begin{aligned} \delta_1 &\geq \delta_m(T') , \\ \delta_1 &\geq \delta_m(T'') , \\ \delta_0 &\in (-1, \delta_M(T_L)] , \\ \delta_2 &\in (-1, \delta_M(T_R)] , \\ T' &\in (0, T_C) , \\ T'' &\in (0, T_C) . \end{aligned} \right\} \quad (3.19)$$

Conditions (3.19) are referred to as the *phase segregation* conditions. From (3.13), (3.15), (3.16), (3.17), and (2.39), it follows that the restrictions (3.19) and the entropy inequalities (3.5)<sub>4</sub> and (3.6)<sub>4</sub> are equivalent to

$$\left. \begin{aligned} H_0(T_L, \mathbf{v}, \mathbf{v}_*) &\leq (1 - m)h , \\ H_1(T_R, \mathbf{v}, \mathbf{v}_*) &\leq (1 - m)h , \\ H_2(\mathbf{v}, \mathbf{v}_*) &< h &\leq H_3(T_L, \mathbf{v}, \mathbf{v}_*) , \\ H_4(\mathbf{v}, \mathbf{v}_*) &< h &\leq H_5(T_R, \mathbf{v}, \mathbf{v}_*) , \\ H_6(T_L, \mathbf{v}, \mathbf{v}_*) &\leq h &< H_7(T_L, \mathbf{v}, \mathbf{v}_*) , \\ H_8(T_R, \mathbf{v}, \mathbf{v}_*) &\leq h &< H_9(T_R, \mathbf{v}, \mathbf{v}_*) , \end{aligned} \right\} \quad (3.20)$$

where the functions  $H_i$  are defined for  $-1 < v \leq 0$ ,  $0 \leq v_* < 1$  by

$$\begin{aligned}
H_0(T_L, v, v_*) &= \delta_C + m(T_L - T_C) - \frac{1}{2}(1 - m) \left\{ \frac{1}{1 - v} + \frac{1}{1 + v_*} \right\} \\
&\quad - \frac{m}{2} \left\{ 1 + \frac{1}{1 - v^2} \right\} + ml_T , \\
H_1(T_R, v, v_*) &= \delta_C + m(T_R - T_C) - \frac{1}{2}(1 - m) \left\{ \frac{1}{1 - v} + \frac{1}{1 + v_*} \right\} \\
&\quad - \frac{m}{2} \left\{ 1 + \frac{1}{1 - v_*^2} \right\} + ml_T , \\
H_2(v, v_*) &= \frac{1}{2} \left\{ \frac{1}{1 + v} - \frac{1}{1 + v_*} \right\} - 1 , \\
H_3(T_L, v, v_*) &= \delta_C + 1 + M(T_L - T_C) + H_2(v, v_*) , \\
H_4(v, v_*) &= \frac{1}{2} \left\{ \frac{1}{1 - v_*} - \frac{1}{1 - v} \right\} - 1 , \\
H_5(T_R, v, v_*) &= \delta_C + 1 + M(T_R - T_C) + H_4(v, v_*) , \\
H_6(T_L, v, v_*) &= \left\{ T_L \left( e^{\frac{l_T}{T}} - 1 \right) - l_T \right\} + \frac{1}{2} \left\{ \frac{v_*}{1 + v_*} - \frac{v}{1 - v^2} \right\} , \\
H_7(T_L, v, v_*) &= \left\{ (T_C - T_L) - l_T \right\} + \frac{1}{2} \left\{ \frac{v_*}{1 + v_*} - \frac{v}{1 - v^2} \right\} , \\
H_8(T_R, v, v_*) &= \left\{ T_R \left( e^{\frac{l_T}{T}} - 1 \right) - l_T \right\} + \frac{1}{2} \left\{ \frac{v_*}{1 - v_*^2} - \frac{v}{1 - v} \right\} , \\
H_9(T_R, v, v_*) &= \left\{ (T_C - T_R) - l_T \right\} + \frac{1}{2} \left\{ \frac{v_*}{1 - v_*^2} - \frac{v}{1 - v} \right\} .
\end{aligned}$$

Notice the following symmetries:

$$\begin{aligned}
H_2(v, v_*) &= H_4(-v_*, -v) , \\
H_3(\cdot, v, v_*) &= H_5(\cdot, -v_*, -v) , \\
H_6(\cdot, v, v_*) &= H_8(\cdot, -v_*, -v) , \\
H_7(\cdot, v, v_*) &= H_9(\cdot, -v_*, -v) .
\end{aligned}$$

Equations (3.20)<sub>1,2,3,4</sub> are equivalent to (3.19)<sub>1,2,3,4</sub> respectively; the upper bounds in (3.20)<sub>5,6</sub> are equivalent to the upper admissible value of the temperature in (3.19)<sub>5,6</sub>, whereas the lower bounds in (3.20)<sub>5,6</sub> are equivalent to the entropy inequalities (3.5)<sub>4</sub>

and (3.6)<sub>4</sub> respectively. Notice that if the entropy inequalities are satisfied, then  $T' - T_L = r \geq 0$  at the phase boundary  $x/at = v$  and  $T'' - T_R = r_* \geq 0$  at the phase boundary  $x/at = v_*$ . Thus, necessarily, the conditions  $T' > 0$  and  $T'' > 0$  are satisfied.

The inequalities (3.20) determine, for fixed  $T_L, T_R$ , a region in the  $(v, v_*, h)$ -space where it is possible to have a two-parameter family of solutions of the form (3.12). For simplicity, consider the case when  $l_T = 0$  which corresponds to *twinning*. Furthermore, since it was assumed that  $\alpha = 0$ , (2.57) gives

$$\mathbf{M} = -\mathbf{m} > 0, \quad \delta_C = \frac{1}{2}, \quad \delta_C > \mathbf{M}T_C. \quad (3.21)$$

Under these assumptions, the functions  $H_1$  to  $H_9$  take the following form:

$$\begin{aligned} H_0(T_L, v, v_*) &= \mathbf{M}(T_C - T_L) - \frac{1}{2}(1 + \mathbf{M}) \left\{ \frac{1}{1-v} + \frac{1}{1+v_*} - 1 \right\} \\ &\quad + \frac{\mathbf{M}}{2} \left\{ \frac{1}{1-v^2} \right\}, \\ H_1(T_R, v, v_*) &= \mathbf{M}(T_C - T_R) - \frac{1}{2}(1 + \mathbf{M}) \left\{ \frac{1}{1-v} + \frac{1}{1+v_*} - 1 \right\} \\ &\quad + \frac{\mathbf{M}}{2} \left\{ \frac{1}{1-v_*^2} \right\}, \\ H_2(v, v_*) &= \frac{1}{2} \left\{ \frac{1}{1+v} - \frac{1}{1+v_*} \right\} - 1, \\ H_3(T_L, v, v_*) &= \frac{3}{2} - \mathbf{M}(T_C - T_L) + H_2(v, v_*), \\ H_4(v, v_*) &= \frac{1}{2} \left\{ \frac{1}{1-v_*} - \frac{1}{1-v} \right\} - 1, \\ H_5(T_R, v, v_*) &= \frac{3}{2} - \mathbf{M}(T_C - T_R) + H_4(v, v_*), \\ H_6(v, v_*) &= H_2(v, v_*) + \frac{3}{2} - \frac{1}{2} \left\{ \frac{1}{1-v^2} \right\}, \\ H_7(T_L, v, v_*) &= \{T_C - T_L\} + H_6(v, v_*), \\ H_8(v, v_*) &= H_4(v, v_*) + \frac{3}{2} - \frac{1}{2} \left\{ \frac{1}{1-v_*^2} \right\}, \\ H_9(T_R, v, v_*) &= \{T_C - T_R\} + H_8(v, v_*). \end{aligned}$$

Let

$$\bar{H}_0 \equiv \frac{H_0}{1 + M}, \quad \bar{H}_1 \equiv \frac{H_1}{1 + M}.$$

Notice that

$$H_6 > \bar{H}_0 \text{ if } v^2 > \frac{(MT_C - 1/2) - MT_L}{M(T_C - T_L)}.$$

But, from (3.21)<sub>3</sub>,  $(MT_C - 1/2) - MT_L < 0$ , hence  $H_6 > \bar{H}_0$  for all  $v$ . A similar analysis reveals that  $H_8 > \bar{H}_1$  for all  $v_*$ . Moreover, one has

$$\begin{aligned} H_2 &> H_4 \text{ if } v_*^2 < v^2, \\ H_6 &> H_8 \text{ if } v_*^2 < v^2, \\ H_2 &> H_6 \text{ if } v^2 > c_1^2, \\ H_4 &> H_8 \text{ if } v_*^2 > c_1^2, \end{aligned}$$

where

$$c_1^2 = \frac{2}{3}.$$

The lower bound for  $h$  is given by

$$\begin{aligned} \text{for } v^2 > v_*^2 \quad H_{\min} &= \begin{cases} H_6 & \text{for } 0 < v^2 < c_1^2, \\ H_2 & \text{for } c_1^2 < v^2 < 1, \end{cases} \\ \text{for } v_*^2 > v^2 \quad H_{\min} &= \begin{cases} H_8 & \text{for } 0 < v_*^2 < c_1^2, \\ H_4 & \text{for } c_1^2 < v_*^2 < 1. \end{cases} \end{aligned} \tag{3.22}$$

Henceforth, for definiteness, it is assumed that

$$T_R > T_L. \tag{3.23}$$

For the upper bound, one has to consider two cases for the given initial temperatures  $T_L$  and  $T_R$ . Only the first case is considered here: assume the given temperatures  $T_L$

and  $T_R$  satisfy

$$2(M+1)(T_R - T_L) < 1. \quad (3.24)$$

Under this assumption, it follows that  $H_7 < H_3$  and  $H_9 < H_5$  for all  $v^2$  and  $v_*^2$ . Moreover,

$$H_{\max} = \begin{cases} H_9 & \text{for } v_*^2 < 1 - \frac{1}{4(T_R - T_L) + 1/(1 - v^2)}, \\ H_7 & \text{for } v_*^2 > 1 - \frac{1}{4(T_R - T_L) + 1/(1 - v^2)}. \end{cases} \quad (3.25)$$

The lower and upper limits for  $h$  in the  $v^2, v_*^2$ -plane corresponding to the phase segregation conditions are shown in Figure 3.3. Notice that  $H_9 > H_8$  for any  $v^2, v_*^2$ , hence the admissible region is always non-empty. The values of  $v^2, v_*^2$  for which  $H_{\max} \geq H_{\min}$  correspond to the shaded region in Figure 3.4. Thus, the shaded region corresponds to the *projection* on the  $v^2, v_*^2$ -plane of the admissible region in the  $v^2, v_*^2, h$ -space. Typical cross sections of this region in the  $v^2, h$  and  $v_*^2, h$ -planes are shown at the end of next section in Figures 3.5 and 3.6.

### 3.4 Driving traction, kinetic relation and nucleation criterion.

As pointed out in Section 3.3.2, the solution involving two phase boundaries is not unique. The postulation of a kinetic relation at each phase boundary settles the uniqueness issue. In order to introduce the kinetic relation, the explicit form of the driving traction acting on each phase boundary is given below.



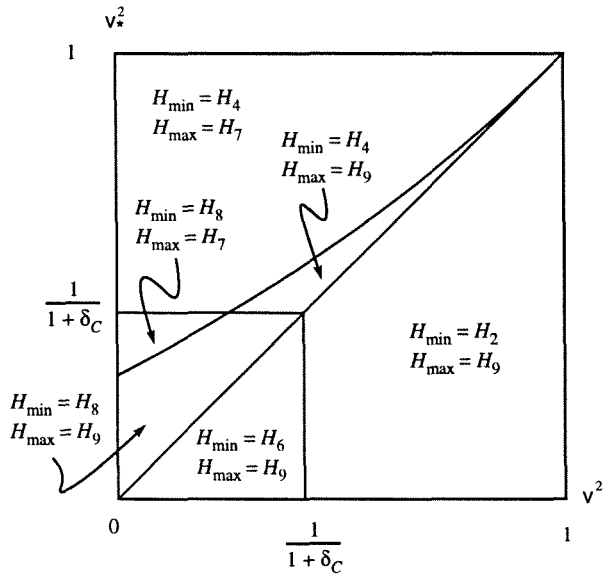


Figure 3.3: Lower and upper limits for  $h$  on the  $v^2, v_*^2$ -plane.

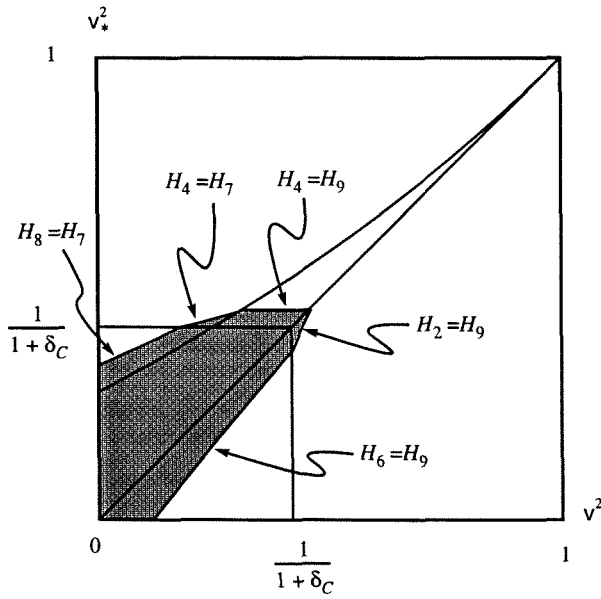


Figure 3.4: Projection of the admissible region on the  $v^2, v_*^2$ -plane.

### 3.4.1 Driving traction for phase boundaries.

For the thermoelastic material undergoing an adiabatic process, equation (2.33) at the phase boundary which has the high strain phase on its *right* becomes, with  $\alpha = 0$ ,

$$f = -\rho c \langle \theta \rangle \left\{ \log \frac{\theta^+}{\theta^-} - \frac{\lambda_T}{c\theta_T} \right\} . \quad (3.26)$$

If the high strain phase is on the *left* of the phase boundary, then (2.33) becomes

$$f = \rho c \langle \theta \rangle \left\{ \log \frac{\theta^-}{\theta^+} - \frac{\lambda_T}{c\theta_T} \right\} . \quad (3.27)$$

Consider a dimensionless driving traction defined as

$$\mathbf{f} \equiv \frac{f}{\mu \gamma_T^2} . \quad (3.28)$$

From (2.53), (3.26), (3.27), (3.15) and (3.16), the driving traction at the phase boundary  $x/at = \mathbf{v}$  is

$$\mathbf{f} = -F [T_L, r(\mathbf{v}, \mathbf{v}_*)] , \quad (3.29)$$

and the driving traction at the phase boundary  $x/at = \mathbf{v}_*$  is

$$\mathbf{f}_* = F [T_R, r_*(\mathbf{v}, \mathbf{v}_*)] , \quad (3.30)$$

where

$$F(T, r) = \left( T + \frac{r}{2} \right) \left\{ \log \left( 1 + \frac{r}{T} \right) - \frac{l_T}{T} \right\} , \quad (3.31)$$

and  $r, r_*$  are given by (3.17)-(3.18). In the purely mechanical case, ABEYARATNE & KNOWLES [2] showed that, under certain assumptions, the corresponding Riemann problem was symmetric in the sense that  $\mathbf{v} = -\mathbf{v}_*$  and  $\mathbf{f} = -\mathbf{f}_*$  so that the problem reduces to a one-parameter family of solutions. The adiabatic Riemann problem does

not exhibit such symmetry. One has to consider, separately, a kinetic relation for each propagating phase boundary. Nevertheless, one can easily check that the solution is symmetric when  $T_L = T_R$ .

### 3.4.2 Kinetic relations.

From (2.27), (2.29), (2.30) and (2.31), the dimensionless rate of entropy production for a segment of the bar containing a phase boundary during some time interval can be expressed by

$$\bar{\Gamma} \equiv \frac{1}{\rho ac} \Gamma = \frac{\mathbf{fv}}{\langle T \rangle} . \quad (3.32)$$

If, following [1] and [3], the quantity  $\mathbf{f}/\langle T \rangle$  is identified as an *affinity* and  $\mathbf{v}$  as the corresponding *flux*, then the kinetic relation relates the affinity to the flux and, in this case, to the temperature on one side of the phase boundary. The temperature is not considered as an affinity (it describes the state of the material). Therefore, the relation between the affinity and the flux is of the form

$$\frac{\mathbf{f}}{\langle T \rangle} = \varphi_{ij}(T, \mathbf{v}) ,$$

where the subscripts refer to the low and high strain phases  $P_1$  and  $P_3$ . Thus,

$$\frac{\mathbf{f}}{T_L + r/2} = \varphi_{13}(T_L, \mathbf{v}) , \quad (3.33)$$

$$\frac{\mathbf{f}_*}{T_R + r_*/2} = \varphi_{31}(T_R, \mathbf{v}_*) . \quad (3.34)$$

Clearly, it is required that

$$\varphi_{13}(\cdot, \mathbf{v}) = -\varphi_{31}(\cdot, -\mathbf{v}) . \quad (3.35)$$

The kinetic relation has to satisfy some restrictions that arise upon enforcement of the entropy inequality. Since  $\bar{\Gamma}$  is non-negative, then  $\varphi_{ij}$  must be such that

$$\varphi_{ij}(T, \mathbf{v})\mathbf{v} \geq 0 .$$

This implies that if  $\varphi_{ij}$  is differentiable with respect to  $\mathbf{v}$ , then

$$\varphi_{ij}(T, 0) = 0 , \quad \frac{\partial \varphi_{ij}}{\partial \mathbf{v}}(T, 0) \geq 0 . \quad (3.36)$$

Furthermore, *assume* that  $\varphi_{ij}$  is strictly monotonically increasing with  $\mathbf{v}$ .

Returning to the special case where  $l_T = 0$ , from (3.33), (3.34), (3.35), (3.29), (3.30) and (3.31), one has

$$\log \left( 1 + \frac{r}{T_L} \right) = \varphi_{31}(T_L, -\mathbf{v}) , \quad \log \left( 1 + \frac{r_*}{T_R} \right) = \varphi_{31}(T_R, \mathbf{v}_*) ;$$

therefore,

$$r = T_L (e^{\varphi_{31}(T_L, -\mathbf{v})} - 1) , \quad r_* = T_R (e^{\varphi_{31}(T_R, \mathbf{v}_*)} - 1) .$$

Using (3.17) and (3.18) with  $l_T = 0$  provides

$$h + \frac{1}{2} \left( \frac{\mathbf{v}}{1 - \mathbf{v}^2} - \frac{\mathbf{v}_*}{1 + \mathbf{v}_*} \right) = T_L (e^{\varphi_{31}(T_L, -\mathbf{v})} - 1) , \quad (3.37)$$

$$h + \frac{1}{2} \left( -\frac{\mathbf{v}_*}{1 - \mathbf{v}_*^2} + \frac{\mathbf{v}}{1 - \mathbf{v}} \right) = T_R (e^{\varphi_{31}(T_R, \mathbf{v}_*)} - 1) . \quad (3.38)$$

Consider the restriction of the function  $\varphi_{31}(T, \cdot)$  to non-negative values of its argument. Define

$$\tilde{\varphi}_{31}(T, \mathbf{v}^2) \equiv \varphi_{31}(T, \mathbf{v}) \quad \text{for } \mathbf{v} \geq 0 . \quad (3.39)$$

Recall that the phase velocities are  $-\mathbf{v} > 0$  and  $\mathbf{v}_* > 0$ , hence, subtracting (3.38)

from (3.37) and using (3.39) gives

$$\frac{v_*^2}{1-v_*^2} + 2T_R \left( e^{\tilde{\varphi}_{31}(T_R, v_*^2)} - 1 \right) = \frac{v^2}{1-v^2} + 2T_L \left( e^{\tilde{\varphi}_{31}(T_L, v^2)} - 1 \right). \quad (3.40)$$

From the properties of the kinetic relation  $\varphi_{31}$ , the function  $\tilde{\varphi}_{31}$  increases monotonically with  $v^2$ . As a function of  $v^2$ , (resp.  $v_*^2$ ), the left-hand side (right-hand side) of (3.40) is strictly monotonically increasing from 0 at  $v^2 = 0$  ( $v_*^2 = 0$ ) to  $+\infty$  at  $v^2 = 1$  ( $v_*^2 = 1$ ). Thus, there is a unique  $v_*^2 \in [0, 1)$  for a given  $v^2 \in [0, 1)$ . Therefore, it is possible to define a functional relation between  $v_*^2$  and  $v^2$ , say

$$v^2 = \Phi(v_*^2, T_L, T_R). \quad (3.41)$$

Notice that, since  $v < 0$ , then

$$v = -\sqrt{\Phi(v_*^2, T_L, T_R)}.$$

Henceforth, let

$$\begin{aligned} V &= \sqrt{\Phi(v_*^2, T_L, T_R)}, \\ \varphi_L &= \tilde{\varphi}_{31}(T_L, v^2) = \tilde{\varphi}_{31}(T_L, \Phi(v_*^2, T_L, T_R)), \\ \varphi_R &= \tilde{\varphi}_{31}(T_R, v_*^2). \end{aligned}$$

Adding (3.37) and (3.38) and using (3.39), (3.41) and the above notation, one has

$$\begin{aligned} h &= \Psi(v_*^2, T_L, T_R) \\ &= \frac{T_L}{2} (e^{\varphi_L} - 1) + \frac{T_R}{2} (e^{\varphi_R} - 1) + \frac{1}{2} \left\{ \frac{2v_* - v_*^2}{1-v_*^2} + \frac{2V - V^2}{1-V^2} \right\}. \end{aligned} \quad (3.42)$$

The function  $\Psi$  is strictly monotonically increasing in  $v_*^2$  from 0 at  $v_*^2 = 0$  to  $+\infty$  at  $v_*^2 = 1$ . Therefore, for a given  $h$  in the admissible range, (3.42) singles out a unique  $v_*^2$  which, by (3.41), provides a unique  $v^2$ . This fully determines a unique solution of

the form (3.12).

The fact that a solution exists can be seen by the following analysis. The lower bounds  $H_6$  and  $H_8$  of the admissible region can be expressed as

$$\begin{aligned}\tilde{H}_6(v_*^2, T_L, T_R) &= H_6(\Phi(v_*^2, T_L, T_R), v_*^2) \\ &= \frac{1}{2} \left\{ \frac{1 + V - V^2}{1 - V^2} - \frac{1}{1 + v_*} \right\}, \\ \tilde{H}_8(v_*^2, T_L, T_R) &= H_8(\Phi(v_*^2, T_L, T_R), v_*^2) \\ &= \frac{1}{2} \left\{ \frac{1 + v_* - v_*^2}{1 - v_*^2} - \frac{1}{1 + V} \right\}.\end{aligned}$$

Notice that  $\Psi(v_*, T_L, T_R) \geq \max_{v_*^2} [\tilde{H}_6(v_*^2, T_L, T_R), \tilde{H}_8(v_*^2, T_L, T_R)]$ . Moreover, the upper bound  $H_9$  is such that  $H_9 = (T_C - T_R)$  for  $v_* = v = 0$ . Hence, by continuity, there exists a range of values of  $h$  in the admissible region for which  $\max[H_6, H_8] \leq h = \Psi < H_9$ , thus the *existence* of a solution of the form (3.12) is guaranteed. A complete analysis of solvability requires further knowledge of a specific kinetic relation.

### 3.4.3 Nucleation criterion.

As shown in Sections 3.3.1 and 3.3.2, there are two different kinds of solutions for the adiabatic Riemann problem. One can interpret the no-phase boundary solution as the limit of the two-phase boundary solution when  $v \rightarrow 0^-$  and  $v_* \rightarrow 0^+$ . Now, if the initial datum satisfies (3.11), it is possible to have a solution with no phase boundaries of the form (3.8). Assuming that  $T_R > T_L$  and using (3.21)<sub>1</sub>, then (3.10) becomes

$$-1 < h \leq \frac{1}{2} - M(T_C - T_L). \quad (3.43)$$

On the other hand, the lower bound for  $h$  corresponding to the solution with two phase boundaries at  $v^2 = v_*^2 = 0$  is  $H_{\min}(0, 0) = 0$  and the upper bound is  $H_{\max}(0, 0) =$

$(T_C - T_R)$ . Moreover, the curve defined by (3.42) passes through the origin, hence, if

$$\frac{1}{2} - \mathbf{M}(T_C - T_L) < (T_C - T_R)$$

then there exists an overlapping range for the initial datum  $h$  for which it is possible to have either kind of solution:

$$\text{if } \begin{cases} -1 < h \leq 0 \\ 0 < h \leq \frac{1}{2} - \mathbf{M}(T_C - T_L) \end{cases} \text{ then } \begin{cases} \text{No phase change solution.} \\ \text{Both types of solutions.} \end{cases} \quad (3.44)$$

To select the appropriate solution, a nucleation criterion is required. Following [2], assume there is a critical value  $f_{\text{cr}}(T)$  of the driving traction at which a transformation from low to high strain phase occurs. In this case, the critical value depends on the temperature of the corresponding low strain phase temperature. From (3.17), (3.18), (3.29), (3.30) and (3.31), nucleation occurs when

$$|f| = F(T_L, r(h, \mathbf{v}, \mathbf{v}_*)) = f_{\text{cr}}(T_L) \quad (3.45)$$

for the leftward moving phase boundary and

$$f_* = F(T_R, r_*(h, \mathbf{v}, \mathbf{v}_*)) = f_{\text{cr}}(T_R) \quad (3.46)$$

for the rightward moving phase boundary. Although  $h$  is considered as fixed (initial conditions), the explicit dependence of  $r$  and  $r_*$  on  $h$  is shown for clarity. Equations (3.45) and (3.46) define two surfaces on the  $\mathbf{v}^2, \mathbf{v}_*^2, h$ -space. The intersection of the region where  $f \geq f_{\text{cr}}(T_L)$  and  $|f_*| \geq f_{\text{cr}}(T_R)$  corresponds to the region where nucleation occurs. Typical cross sections of this region are shown by the shaded area in Figures 3.5 and 3.6.

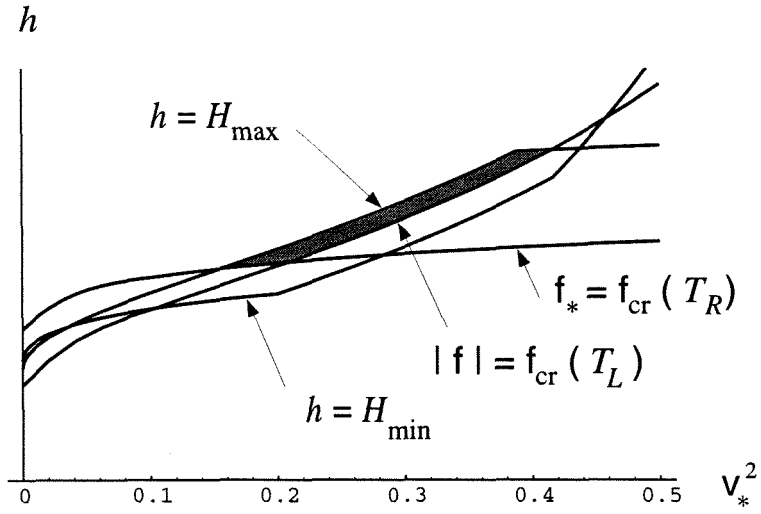


Figure 3.5: Admissible values of  $h$  on the plane  $v_*^2 = 0.2$ .

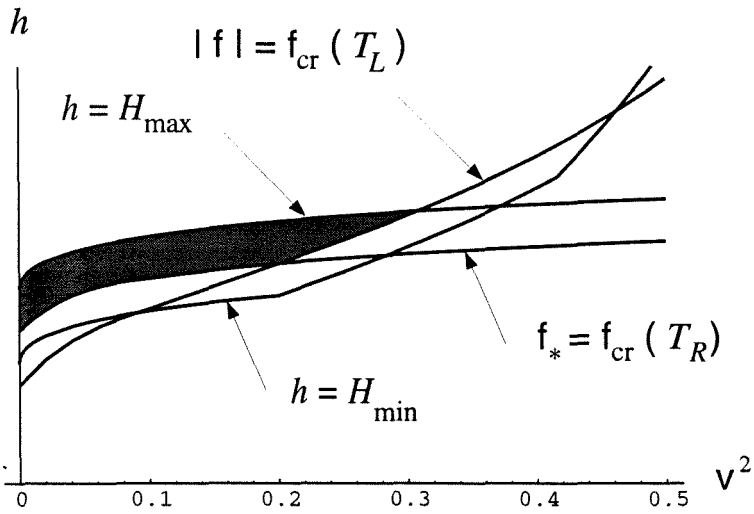


Figure 3.6: Admissible values of  $h$  on the plane  $v_*^2 = 0.2$ .



### 3.5 Nucleation: nontrivial solution for uniform data.

The importance of the Riemann problem with uniform initial data is related to its connection with the nucleation criterion. Since the bar is initially in the same phase and there are no discontinuities, the existence of a *nontrivial* solution (where two phase boundaries nucleate from an arbitrary point) could, in principle, provide a restriction on the critical value of the driving traction  $f_{cr}$ . Suppose that the initial data of the Riemann problem of Section 3.3.2 is such that  $\delta_L = \delta_R = \delta_*$  and  $T_L = T_R = T_*$ . Since the system of equations (3.1)-(3.3) and the jump conditions (3.4)-(3.6) are homogeneous, then the problem admits a trivial solution  $\delta(x, t) = \delta_*$  and  $T(x, t) = T_* \forall x, t$ . Nevertheless, there is also a nontrivial solution. Since  $T_L = T_R$  and in view of the properties of the kinetic relation  $\varphi_{ij}$ , equation (3.40) implies that

$$v^2 = v_*^2 \quad \Rightarrow \quad v = -v_* .$$

From (3.13)-(3.18), there exists a one-parameter family of nontrivial solutions for the Riemann problem with uniform initial data of the following form (parametrized by  $v_*$ ):

$$\delta(x, t) = \begin{cases} \delta_* & -\infty < x < -at , \\ \delta_0 & -at < x < -av_*t , \\ \delta_1 & -av_*t < x < av_*t , \\ \delta_0 & av_*t < x < at , \\ \delta_* & at < x < \infty , \end{cases} \quad (3.47)$$

and

$$T(x, t) = \begin{cases} T_* & -\infty < x < -av_*t , \\ T' & -av_*t < x < av_*t , \\ T_* & av_*t < x < \infty , \end{cases} \quad (3.48)$$

where

$$\begin{aligned}\delta_0 &= \delta_* - \left( \frac{v_*}{1 - v_*^2} \right), \\ \delta_1 &= \delta_* + \left( \frac{1}{1 + v_*} \right), \\ T' &= \delta_* - \frac{1}{2} \left( \frac{2v_* - v_*^2}{1 - v_*^2} \right) + T_*.\end{aligned}$$

Notice that, in view of the analysis of Section 3.4.2, a solution of the form (3.47), (3.48) exists. Using the notation of Section 3.4.2, it follows that  $V = v_*$  and  $\varphi_L = \varphi_R = \varphi_* = \tilde{\varphi}(T_*, v_*^2)$ . Equation (3.42), together with (3.9), becomes

$$h = \delta_* = T_* (e^{\varphi_*} - 1) + \left\{ \frac{2v_* - v_*^2}{1 - v_*^2} \right\}.$$

The nucleation criterion was introduced in terms of the driving traction which, in this case, can be written as

$$f(T_*, r(\delta_*, v_*)) = \left( T_* + \frac{r(\delta_*, v_*)}{2} \right) \left[ \log \left( 1 + \frac{r(\delta_*, v_*)}{T_*} \right) \right],$$

where

$$r(\delta_*, v_*) = \delta_* - \frac{1}{2} \left[ \frac{2v_* - v_*^2}{1 - v_*^2} \right].$$

In order to have an admissible solution, the phase segregation conditions and entropy inequality requirements have to be enforced. From Section 3.3.3, the lower bound for the value of  $h$  is given by

$$H_{\min} = \begin{cases} \tilde{H}_6 = \tilde{H}_8 = \frac{1}{2} \left( \frac{2v_* - v_*^2}{1 - v_*^2} \right) & 0 < v_*^2 < c_1^2, \\ \tilde{H}_2 = \tilde{H}_4 = \frac{v_*}{1 - v_*^2} - 1 & c_1^2 < v_*^2 < 1. \end{cases}$$

Recall that the functions  $\tilde{H}_6$  and  $\tilde{H}_8$  are related to the entropy inequality (3.5)<sub>4</sub> and (3.6)<sub>4</sub>, whereas the functions  $\tilde{H}_2$  and  $\tilde{H}_4$  represent the restriction  $T' = T'' < T_C$ . The

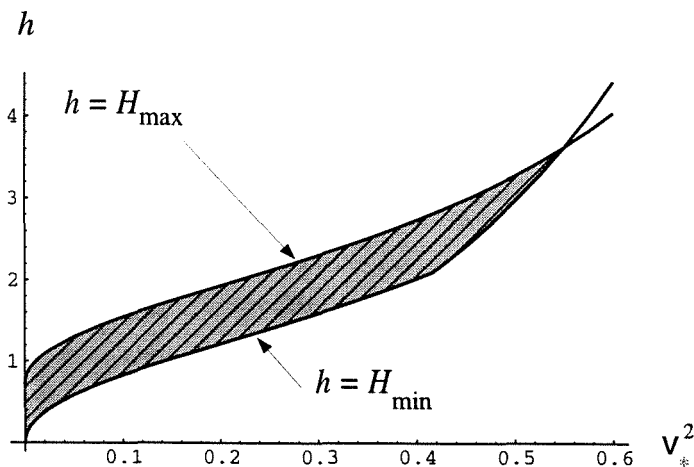


Figure 3.7: Admissible region for uniform data problem.

upper bound for the admissible region is given by

$$H_{\max} = H_7 = H_9 = \frac{1}{2} \left( \frac{2v_* - v_*^2}{1 - v_*^2} \right).$$

The admissible region is shown in Figure 3.7. From this, one can see that there is a minimum value for  $\delta_*$  below which no nucleation occurs (in this case,  $\delta_* = 0$  at  $v_*^2 = 0$ ). Observe that this lower bound is given by the entropy inequality (it corresponds to  $f = 0$ ). This analysis confirms the fact that nucleation occurs at a critical value such that  $f_{\text{cr}} v_* \geq 0$  (as required by the entropy inequality) but *fails* to restrict the nucleation criterion in any other way.

# Chapter 4 Augmented theory and structured traveling wave

## 4.1 Introduction.

Although the classical thermoelastic theory of phase transitions has room (and, in fact, requires) a kinetic relation, such a piece of constitutive information is introduced in the theory, in a sense, as a supplement. Some other theories have built-in features from which the equivalent of a kinetic relation can be *derived*. In fact, FRIED & GURTIN [18] argue that a kinetic relation is not part of the constitutive theory but follows as a consequence of new balance principles. Here, nevertheless, a viewpoint consistent with ABEYARATNE & KNOWLES [1] is taken. An augmented theory that includes viscosity, strain gradient and heat conduction is introduced. From an admissibility criterion for a special class of solutions, namely traveling waves, a special kinetic relation in the thermomechanical case is derived. This procedure follows well established techniques used in fluid and solid mechanics in a purely mechanical context (see ABEYARATNE & KNOWLES [6], HATTORI [21], ROSAKIS [27], SLEMROD [29], TRUSKINOVSKY [31]).

In the augmented theory, the phase boundary acquires a *structure*, as opposed to the classical theory where the phase boundary corresponds to a sharp interface. By “structure” it is meant that there is a region where the field quantities vary rapidly but continuously from one solid phase to another.

By using the classical form of the balance principles and enforcing the second law of thermodynamics for all admissible processes, GURTIN [20], generalizing a result established by COLEMAN & NOLL [13], proved that the Helmholtz potential cannot depend on higher order derivatives of the strain. In order to obtain a thermodynamically consistent theory that includes strain gradient and viscosity effects, DUNN &

SERRIN [15] proposed a modification of the energy balance to take into account long range interactions by introducing the concept of *interstitial working*. An alternative approach is used by TRUSKINOVSKY [31].

In this chapter, DUNN & SERRIN's model is specialized for the one-dimensional case and some general features of a structured traveling wave are analyzed.

## 4.2 Basic equations.

In the regularized theory, one introduces from the onset a new fundamental quantity: the *interstitial working*  $p$ . Hence, neglecting body forces and radiation terms, the fundamental quantities are: the deformation  $y$ , the absolute temperature  $\theta$ , the specific internal energy  $\epsilon$ , the entropy  $\eta$ , the stress  $\sigma$ , the heat flux  $q$  and the interstitial working  $p$ . All quantities are defined at a particle  $x$  at time  $t$ . Let  $u(x, t) = y(x, t) - x$  be the displacement. The strain  $\gamma$  and the velocity  $v$  are given as usual by  $\gamma = u_x$  and  $v = u_t$ . As in the classical theory of Chapter 2, the momentum equation is given by (2.1), but by introducing the interstitial working  $p$  and considering heat conduction, the energy equation is

$$[\sigma v + p + q]_{x_1}^{x_2} = \frac{d}{dt} \int_{x_1}^{x_2} \rho \left( \epsilon + \frac{1}{2} v^2 \right) dx . \quad (4.1)$$

The Clausius-Duhem inequality has the same form as in the classical theory with heat conduction, i.e.,

$$\Gamma(t) = \frac{d}{dt} \int_{x_1}^{x_2} \rho \eta dx - \left[ \frac{q}{\theta} \right]_{x_1}^{x_2} \geq 0 . \quad (4.2)$$

At points where the field quantities have enough differentiability, the local form of the balance of linear momentum, the energy equation and the Clausius-Duhem inequality

(dissipation inequality) are

$$\sigma_x = \rho v_t , \quad (4.3)$$

$$(\sigma v + q + p)_x = \rho \left( \epsilon + \frac{1}{2} v^2 \right)_t , \quad (4.4)$$

$$\left( \frac{q}{\theta} \right)_x \leq \rho \eta_t , \quad (4.5)$$

and the compatibility equation is

$$v_x = \gamma_t . \quad (4.6)$$

Although in the regularized theory it is common to assume enough differentiability, for the specific thermoelastic material introduced in Section 2.5 it is necessary to consider that at some points some of the field quantities are discontinuous. Hence, to complement the local form of the balance principles, one has to consider the corresponding jump conditions across a point of discontinuity  $x = s(t)$ , i.e.,

$$\left. \begin{aligned} [v] + \dot{s}[\gamma] &= 0 , \\ [\sigma] - \rho \dot{s}^2 [\gamma] &= 0 , \\ [q + p] + \dot{s} \{ \rho [\epsilon] - \langle \sigma \rangle [\gamma] \} &= 0 , \\ \left[ \frac{q}{\theta} \right] + \rho \dot{s} [\eta] &\leq 0 . \end{aligned} \right\} \quad (4.7)$$

Moreover, assuming that  $\gamma$  and  $\theta$  are continuous, the jump conditions (4.7) become

$$\left. \begin{aligned} [v] &= 0 , \\ [\sigma] &= 0 , \\ [q + p] + \rho \dot{s} [\epsilon] &= 0 , \\ [q] + \rho \dot{s} \theta [\eta] &\leq 0 . \end{aligned} \right\} \quad (4.8)$$

Using equation (4.3) in equation (4.4) provides

$$\sigma v_x + q_x + p_x = \rho \epsilon_t . \quad (4.9)$$

Furthermore, expanding the dissipation inequality (4.5) and using the expression of  $q_x$  provided by the energy equation (4.9) yields

$$\rho (\epsilon_t - \theta \eta_t) - \sigma v_x - p_x - \frac{q \theta_x}{\theta} \leq 0 .$$

In terms of the free energy potential  $\psi$ , the dissipation inequality now becomes

$$\rho (\psi_t + \theta_t \eta) - \sigma v_x - p_x - \frac{q \theta_x}{\theta} \leq 0 . \quad (4.10)$$

In order to introduce higher gradient effects into the theory, the following constitutive assumptions are made:

$$\left. \begin{aligned} \psi &= \hat{\psi}(\gamma, \theta, \gamma_x, \gamma_{xx}, \theta_x, \gamma_t) , \\ p &= \hat{p}(\gamma, \theta, \gamma_x, \gamma_{xx}, \theta_x, \gamma_t) , \\ \eta &= \hat{\eta}(\gamma, \theta, \gamma_x, \gamma_{xx}, \theta_x, \gamma_t) , \\ \sigma &= \hat{\sigma}(\gamma, \theta, \gamma_x, \gamma_{xx}, \theta_x, \gamma_t) , \\ q &= \hat{q}(\gamma, \theta, \gamma_x, \gamma_{xx}, \theta_x, \gamma_t) . \end{aligned} \right\} \quad (4.11)$$

Notice that all functionals depend on the same set of variables since there is no *a priori* reason to discard any of them. (This is known as the principle of equipresence.) Nevertheless, some restrictions arise in connection with the second law of thermodynamics.

### 4.3 Thermodynamic restrictions.

The constitutive assumption (4.11) is compatible with thermodynamics if every admissible thermodynamic process satisfies the dissipation inequality (4.10). This re-

quirement restricts the functional form of (4.11). Equations (4.10), (4.11)<sub>1,2</sub> and (4.6) provide

$$\begin{aligned} & \rho \left[ \hat{\psi}_\gamma \gamma_t + (\hat{\psi}_\theta + \hat{\eta}) \theta_t + \hat{\psi}_{\gamma_x} \gamma_{xt} + \hat{\psi}_{\gamma_{xx}} \gamma_{xxt} + \hat{\psi}_{\theta_x} \theta_{xt} + \hat{\psi}_{\gamma_t} \gamma_{tt} \right] - \hat{\sigma} \gamma_t \\ & - (\hat{p}_\gamma \gamma_x + \hat{p}_\theta \theta_x + \hat{p}_{\gamma_x} \gamma_{xx} + \hat{p}_{\gamma_{xx}} \gamma_{xxx} + \hat{p}_{\theta_x} \theta_{xx} + \hat{p}_{\gamma_t} \gamma_{xt}) - \frac{\hat{q} \theta_x}{\theta} \leq 0 . \end{aligned}$$

This inequality has to be satisfied for all deformations and all temperatures at any point  $(x, t)$ .

It is possible to find a deformation and a temperature field for which, at a given point  $(x, t)$ , the quantities  $\theta_t, \gamma_{xt}, \gamma_{xxt}, \theta_{xt}, \gamma_{tt}, \gamma_{xxx}$  and  $\theta_{xx}$  are independent of the values of  $\gamma, \theta, \gamma_x, \gamma_{xx}, \theta_x$  and  $\gamma_t$  at the same point. Therefore, in order to satisfy the dissipation inequality, the following terms must vanish:

$$\hat{\psi}_\theta + \hat{\eta} = 0 , \quad (4.12)$$

$$\rho \hat{\psi}_{\gamma_x} - \hat{p}_{\gamma_t} = 0 , \quad (4.13)$$

and

$$\hat{\psi}_{\gamma_{xx}} = 0 , \quad \hat{\psi}_{\theta_x} = 0 , \quad \hat{\psi}_{\gamma_t} = 0 , \quad (4.14)$$

$$\hat{p}_{\gamma_{xx}} = 0 , \quad \hat{p}_{\theta_x} = 0 . \quad (4.15)$$

The formal role of the interstitial working and the connection between the viscosity and the strain gradient can be observed from equation (4.13). Without the interstitial working term or without a dependence of the interstitial working on  $\gamma_t$ , then the Helmholtz potential would not be a function of  $\gamma_x$ .

The dissipation inequality reduces to

$$\rho \hat{\psi}_\gamma \gamma_t - \hat{\sigma} \gamma_t - (\hat{p}_\gamma \gamma_x + \hat{p}_\theta \theta_x + \hat{p}_{\gamma_x} \gamma_{xx}) - \frac{\hat{q} \theta_x}{\theta} \leq 0 . \quad (4.16)$$



Equation (4.14) implies that the free energy cannot depend on these variables, hence

$$\psi = \hat{\psi}(\gamma, \theta, \gamma_x) . \quad (4.17)$$

Similarly, equation (4.15) implies

$$p = \hat{p}(\gamma, \theta, \gamma_x, \gamma_t) . \quad (4.18)$$

Notice that equation (4.12) corresponds to the same relation between entropy and free energy as in the classical theory. Since  $\hat{\psi}$  does not depend on  $\gamma_t$ , then (4.13) can be integrated, i.e.,

$$\hat{p}(\gamma, \theta, \gamma_x, \gamma_t) = \rho \hat{\psi}_{\gamma_x}(\gamma, \theta, \gamma_x) \gamma_t + p^0(\gamma, \theta, \gamma_x) , \quad (4.19)$$

where  $p^0$  is the equilibrium part of the interstitial work. Using this expression for the interstitial working in the dissipation inequality (4.16) gives

$$\left\{ \rho \left[ \hat{\psi}_{\gamma} - \left( \hat{\psi}_{\gamma_x} \right)_x \right] - \hat{\sigma} \right\} \gamma_t - \left( p_{\theta}^0 + \frac{\hat{q}}{\theta} \right) \theta_x - (p_{\gamma}^0 \gamma_x + p_{\gamma_x}^0 \gamma_{xx}) \leq 0 . \quad (4.20)$$

The third term in this inequality is independent of  $\theta_x$  and  $\gamma_t$ ; therefore, it should satisfy

$$p_{\gamma}^0(\gamma, \theta, \gamma_x) \gamma_x + p_{\gamma_x}^0(\gamma, \theta, \gamma_x) \gamma_{xx} \geq 0 ,$$

for all  $\gamma, \theta, \gamma_x, \gamma_{xx}$ . Since  $\gamma_{xx}$  can be specified independently of  $\gamma, \theta, \gamma_x$  then, necessarily,

$$p_{\gamma_x}^0 = 0 ,$$

but then  $p^0$  is independent of  $\gamma_x$  and the same inequality implies

$$p_{\gamma}^0 = 0 .$$

Therefore,  $p^0$  can only be a function of  $\theta$  and the dissipation inequality (4.20) becomes

$$\left\{ \rho \left[ \hat{\psi}_\gamma - \left( \hat{\psi}_{\gamma_x} \right)_x \right] - \hat{\sigma} \right\} \gamma_t - \left( p_\theta^0 + \frac{\hat{q}}{\theta} \right) \theta_x \leq 0 . \quad (4.21)$$

The equilibrium values of  $\sigma$  and  $q$  can be obtained by replacing  $\theta_x$  and  $\gamma_t$  by  $h\theta_x$  and  $h\gamma_t$  respectively and taking the limit  $h \rightarrow 0$  in the dissipation inequality (4.21), i.e.,

$$\left\{ \rho \left[ \hat{\psi}_\gamma - \left( \hat{\psi}_{\gamma_x} \right)_x \right] - \sigma_{\text{eq}} \right\} \gamma_t - \left( p_\theta^0 + \frac{q_{\text{eq}}}{\theta} \right) \theta_x \leq 0 , \quad (4.22)$$

where

$$\sigma_{\text{eq}} = \hat{\sigma}(\gamma, \theta, \gamma_x, 0, 0) , \quad (4.23)$$

$$q_{\text{eq}} = \hat{q}(\gamma, \theta, \gamma_x, 0, 0) . \quad (4.24)$$

Since the first term in (4.22) is linear in  $\gamma_t$  and the second is linear in  $\theta_x$ , then the equilibrium stress is given by

$$\sigma_{\text{eq}} = \rho \left[ \hat{\psi}_\gamma - \left( \hat{\psi}_{\gamma_x} \right)_x \right] , \quad (4.25)$$

and the equilibrium heat is

$$q_{\text{eq}} = -p_\theta^0 \theta . \quad (4.26)$$

For *elastic* materials where  $\hat{\psi}$  and  $\hat{q}$  are *independent* of  $\gamma_t$ , the first term of the dissipation inequality (4.21) is linear in  $\gamma_t$ , hence the elastic part of the stress is completely determined by the free energy as

$$\sigma_{\text{el}} = \rho \left[ \hat{\psi}_\gamma - \left( \hat{\psi}_{\gamma_x} \right)_x \right] . \quad (4.27)$$

Notice that the elastic stress is equal to the equilibrium stress (when  $\theta_x = 0$ ).

Define the *viscous* stress as

$$\sigma_v = \hat{\sigma} - \sigma_{\text{el}} ,$$

and the “non-equilibrium” heat flux as

$$q_{\text{ne}} = \hat{q} - q_{\text{eq}} .$$

In the general case, the elastic stress can be obtained from the Helmholtz free energy, but for the viscous stress an additional constitutive assumption is required.

Returning to the general case, using the expression (4.27) for the elastic stress and the definitions of the viscous stress and the non-equilibrium heat flux, the dissipation inequality (4.21) can be expressed as

$$\sigma_v \gamma_t + \frac{q_{\text{ne}} \theta_x}{\theta} \geq 0 .$$

Moreover, the balance of linear momentum (4.3) now takes the form

$$\rho \left[ \hat{\psi}_\gamma - \left( \hat{\psi}_{\gamma_x} \right)_x \right] + (\sigma_v)_x - \rho v_t = 0 . \quad (4.28)$$

The energy equation (4.9), with the use of (2.15) and (4.12) becomes

$$\hat{\sigma} \gamma_t + \hat{p}_x + \hat{q}_x = \rho \hat{\psi}_t - \rho \hat{\psi}_\theta \theta_t + \rho \theta \hat{\eta}_t .$$

Furthermore, from the expression (4.19) for the interstitial work, the above equation yields

$$\hat{\sigma} \gamma_t + \rho \left( \hat{\psi}_{\gamma_x} \right)_x \gamma_t + p_\theta^0 \theta_x + \hat{q}_x = \rho \hat{\psi}_\gamma \gamma_t + \rho \theta \hat{\eta}_t .$$

From the decomposition of the stress into its elastic and viscous parts and the heat flux into its equilibrium and non-equilibrium parts, the energy equation now becomes

$$\sigma_v \gamma_t - \left( p_\theta^0 \right)_x \theta + (q_{\text{ne}})_x = \rho \theta \hat{\eta}_t . \quad (4.29)$$

This is the classical energy equation with two additional terms: the work done by

the viscous stress  $(\sigma_\nu \gamma_t)$  and the interstitial working term  $(p_\theta^0)_x \theta$ . Moreover, only the non-equilibrium part of the heat flux is present.

## 4.4 Specific constitutive assumptions.

Introduce the following constitutive assumptions: Assume that the Helmholtz potential is of the form

$$\hat{\psi}(\gamma, \theta, \gamma_x) = \bar{\psi}(\gamma, \theta) + \frac{1}{2} \lambda \gamma_x^2, \quad (4.30)$$

where  $\lambda$  is the strain gradient coefficient. This coefficient is formally analogous to the concept of capillarity in fluid mechanics. Moreover, assume that the viscous stress is given by

$$\sigma_\nu = \rho \nu \gamma_t, \quad (4.31)$$

where  $\nu$  is the viscosity, and, finally, assume that the equilibrium heat flux is zero and the non-equilibrium heat flux is only a linear function of  $\theta_x$  (i.e., Fourier's law<sup>1</sup>)

$$\hat{q}(\theta_x) = q_{ne}(\theta_x) = k \theta_x, \quad (4.32)$$

where  $k$  is the thermal conductivity. Alternatively, it is convenient to define the thermal diffusivity  $\kappa$  (in the reference configuration) as

$$\kappa = \bar{\kappa}(\gamma, \theta) = \frac{k}{\rho \bar{c}(\gamma, \theta)}. \quad (4.33)$$

For simplicity, the strain gradient coefficient, viscosity and thermal conductivity are assumed constant for all phases. Notice that the viscous stress is assumed as a function of  $\gamma_t$  only and the non-equilibrium heat flux as a function of  $\theta_x$  only. These assumptions are consistent with the thermodynamical restrictions. The internal en-

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<sup>1</sup>Recall that in the linear theory (linearized about a reference temperature), the heat flux can only depend linearly on the temperature gradient (see, e.g., CARLSON [10]).

ergy of the regularized theory is

$$\epsilon = \hat{\epsilon}(\gamma, \theta, \gamma_x) = \hat{\psi}(\gamma, \theta, \gamma_x) - \theta \hat{\psi}_\theta(\gamma, \theta, \gamma_x) ,$$

which, by (4.30), can be expressed as

$$\epsilon = \hat{\epsilon}(\gamma, \theta, \gamma_x) = \bar{\epsilon}(\gamma, \theta) + \frac{1}{2} \lambda \gamma_x^2 , \quad (4.34)$$

where

$$\bar{\epsilon}(\gamma, \theta) = \bar{\psi}(\gamma, \theta) - \theta \bar{\psi}_\theta(\gamma, \theta) . \quad (4.35)$$

Moreover, since the equilibrium heat flux is zero, then, from (4.26), it follows that the equilibrium part of the interstitial work,  $p^0$ , can at most be a constant. Since the energy equation and the dissipation inequality only involve derivatives of  $p^0$ , then without loss of generality for a material that follows Fourier's law, one can take  $p^0 = 0$ . With assumptions (4.30), (4.31) and (4.32) enforced, the stress becomes

$$\hat{\sigma}(\gamma, \theta, \gamma_{xx}, \gamma_t) = \rho [\bar{\psi}_\gamma(\gamma, \theta) - \lambda \gamma_{xx} + \nu \gamma_t] , \quad (4.36)$$

the balance of linear momentum (4.28) takes the form

$$(\bar{\psi}_\gamma)_x - \lambda \gamma_{xxx} + \nu \gamma_{xt} - v_t = 0 , \quad (4.37)$$

and the energy equation (4.29) reduces to

$$\nu \gamma_t^2 + \frac{k}{\rho} \theta_{xx} + \theta (\bar{\psi}_\theta)_t = 0 . \quad (4.38)$$

Recall that the strain and particle velocity are related through (4.6). The dissipation inequality (4.21) can be expressed as

$$\rho \nu \gamma_t^2 + \frac{k}{\theta} \theta_x^2 \geq 0 , \quad (4.39)$$

which is satisfied if

$$\nu \geq 0, \quad k \geq 0.$$

By setting  $\nu = \lambda = 0$  in equations (4.37) and (4.38), one recovers the corresponding equations for a classical thermoelastic material with heat conduction.

With the constitutive assumptions (4.30)-(4.32) enforced, the jump conditions (4.8) can be written as

$$\begin{aligned} [[v]] &= 0, \\ [[\bar{\psi}_\gamma(\gamma, \theta)]] - \lambda[[\gamma_{xx}]] + \nu[[\gamma_t]] &= 0, \\ \frac{k}{\rho}[[\theta_x]] + \lambda[[\gamma_x \gamma_t]] + \dot{s}[[\bar{\epsilon}(\gamma, \theta) + \frac{1}{2}\lambda\gamma_x^2]] &= 0, \\ \frac{k}{\rho}[[\theta_x]] - \dot{s}\theta[[\bar{\psi}_\theta(\gamma, \theta)]] &\leq 0. \end{aligned}$$

Now, assume that  $\bar{\psi}_\gamma$ ,  $\bar{\psi}_\theta$  and  $\bar{\epsilon}$  are continuous functions of  $\gamma$  and  $\theta$ , then it follows that

$$\left. \begin{aligned} \lambda[[\gamma_{xx}]] - \nu[[\gamma_t]] &= 0, \\ \frac{k}{\rho}[[\theta_x]] + \lambda[[\gamma_x \gamma_t]] + \frac{1}{2}\dot{s}[[\gamma_x^2]] &= 0, \\ \frac{k}{\rho}[[\theta_x]] &\leq 0. \end{aligned} \right\} \quad (4.40)$$

In the case where  $\nu = \lambda = 0$ , the jump conditions (4.40) are equivalent to  $[[\theta_x]] = 0$ .

## 4.5 Traveling wave: Generalities.

A steady, structured traveling wave corresponds to the case when all fields satisfy (4.3)-(4.6) and depend only on the variable

$$\xi = x - st, \quad (4.41)$$

where  $\dot{s}$ , the wave speed, is a constant. A moving discontinuity (either a shock wave or a phase boundary) can be viewed, within the context of the adiabatic, sharp interface theory, as the limit of a structured wave within the framework of the regularized theory. The limit is achieved when the viscosity, strain gradient coefficient and heat conductivity tend to zero in an appropriate sense. Hence, in an infinitely long bar, the conditions at  $\pm\infty$  for a structured wave should correspond to the front and back states of a moving discontinuity.

The precise statement of the traveling wave problem will be given in Chapters 5 and 6. In this chapter, some general characteristics of the traveling wave are recorded for future use. Notice that although in the classical theory of Chapter 2 the function  $\bar{\psi}$  corresponds to the Helmholtz free energy, in the regularized theory, the free energy is given by  $\hat{\psi}$ .

Assume there exists a structured, steady traveling wave for  $\xi \in \mathbb{R}$ . From (4.3), (4.4) and (4.6) it follows that

$$\sigma' + \rho\dot{s}v' = 0 , \quad (4.42)$$

$$v' + \dot{s}\gamma' = 0 , \quad (4.43)$$

$$(\sigma v)' + q' + p' + \rho\dot{s} \left( \epsilon + \frac{1}{2}v^2 \right)' = 0 , \quad (4.44)$$

where  $(\cdot)'$  denotes differentiation with respect to  $\xi$ . Assuming the existence of a solution, integrate to get

$$\sigma + \rho\dot{s}v = H_1 , \quad (4.45)$$

$$v + \dot{s}\gamma = H_2 , \quad (4.46)$$

$$\sigma v + q + p + \rho\dot{s} \left( \epsilon + \frac{1}{2}v^2 \right) = H_3 , \quad (4.47)$$

where the  $H$ 's are integration constants. Let the conditions at  $\xi \rightarrow \pm\infty$  be given by

$$\gamma(-\infty) = \gamma^-, \quad \gamma(+\infty) = \gamma^+, \quad (4.48)$$

$$v(-\infty) = v^-, \quad v(+\infty) = v^+, \quad (4.49)$$

$$\theta(-\infty) = \theta^-, \quad \theta(+\infty) = \theta^+, \quad (4.50)$$

and all derivatives of these quantities vanish when  $\xi \rightarrow \pm\infty$ . Hence, the integration constants must satisfy

$$H_1 = \sigma^+ + \rho \dot{s} v^+ = \sigma^- + \rho \dot{s} v^-, \quad (4.51)$$

$$H_2 = v^+ + \dot{s} \gamma^+ = v^- + \dot{s} \gamma^-, \quad (4.52)$$

$$H_3 = \sigma^+ v^+ + \rho \dot{s} \left( \epsilon^+ + \frac{1}{2} (v^+)^2 \right) = \sigma^- v^- + \rho \dot{s} \left( \epsilon^- + \frac{1}{2} (v^-)^2 \right), \quad (4.53)$$

where

$$\sigma^\pm = \hat{\sigma}(\gamma^\pm, \theta^\pm, 0, 0),$$

$$\epsilon^\pm = \hat{\psi}(\gamma^\pm, \theta^\pm, 0) - \theta^\pm \hat{\psi}_\theta(\gamma^\pm, \theta^\pm, 0).$$

With the foregoing constitutive assumptions (4.30), (4.31) and (4.32), the stress  $\sigma^\pm$  (given by equation (4.36)) is

$$\sigma^\pm = \rho \bar{\psi}_\gamma(\gamma^\pm, \theta^\pm) \quad (4.54)$$

and the internal energy  $\epsilon^\pm$  becomes

$$\epsilon^\pm = \bar{\psi}(\gamma^\pm, \theta^\pm) - \theta^\pm \bar{\psi}_\theta(\gamma^\pm, \theta^\pm). \quad (4.55)$$

Therefore, from equations (4.51)-(4.53), the values given in (4.48)-(4.50) must satisfy the adiabatic jump conditions (2.9)-(2.11).



For a traveling wave, the jump conditions (4.40) reduce to

$$\left. \begin{aligned} \lambda[\gamma''] + \dot{s}\nu[\gamma'] &= 0, \\ \frac{k}{\rho}[\theta'] - \frac{1}{2}\dot{s}\lambda[\gamma'^2] &= 0, \\ \frac{k}{\rho}[\theta'] &\leq 0. \end{aligned} \right\} \quad (4.56)$$

In the case where  $\nu = \lambda = 0$ , these are equivalent to

$$[\theta'] = 0. \quad (4.57)$$

These jump conditions apply *within* the structured wave and should not be confused with restrictions on the values  $(\gamma^\pm, \theta^\pm)$  at  $\xi \rightarrow \pm\infty$ . Whenever it is clear by the context, the symbol  $[\cdot]$  is also used in this section as the difference between the values at  $\xi \rightarrow \pm\infty$ .

## 4.6 Driving traction.

If a traveling wave solution exists then, from equation (4.29), it necessarily satisfies

$$-\rho\dot{s}\eta' = \rho\dot{s}^2\nu\frac{\gamma'^2}{\theta} + k\frac{\theta''}{\theta}.$$

Integrate from  $\xi \rightarrow -\infty$  to  $\xi \rightarrow \infty$  to get

$$-\rho\dot{s}[\eta] = \int_{-\infty}^{\infty} \left\{ \rho\dot{s}^2\nu\frac{\gamma'^2}{\theta} + k\frac{\theta''}{\theta} \right\} d\xi,$$

where  $[\eta] = \eta^+ - \eta^- = -\bar{\psi}_\theta(\gamma^+, \theta^+) + \bar{\psi}_\theta(\gamma^-, \theta^-)$ . Integrating by parts the second term in the integral and using the conditions at  $\pm\infty$  provides

$$-\rho\dot{s}[\eta] = \int_{-\infty}^{\infty} \left\{ \rho\dot{s}^2\nu\frac{\gamma'^2}{\theta} + k\left(\frac{\theta'}{\theta}\right)^2 \right\} d\xi \geq 0.$$

This inequality remains true even in the case when there is only heat conduction (i.e., when  $\nu = 0$ ). To make the connection with the classical adiabatic theory, consider the driving traction  $f$  given by (2.31), i.e.,

$$\frac{f\dot{s}}{\langle\theta\rangle} = -\rho\dot{s}[\eta] .$$

Thus, the values in (4.48)-(4.50) must also satisfy

$$f\dot{s} \geq 0 ,$$

which corresponds to the entropy jump inequality (2.34). The previous analysis shows that the field values at  $\xi \rightarrow \pm\infty$  for the traveling wave problem must satisfy all the corresponding jump conditions of the classical adiabatic problem. Moreover, the condition for the existence of a traveling wave solution for the regularized theory should provide an additional relation for the phase boundary velocity  $\dot{s}$  in terms of the driving traction  $f$ .

## 4.7 Basic equations.

Evaluate the constants  $H_i$  in equations (4.45), (4.46) and (4.47) using the conditions at an *arbitrary* point  $\xi = \xi_0$  (one could choose either  $\xi \rightarrow \pm\infty$  but, in view of the regularity of the trilinear material introduced in Section 2.5, it will be more convenient to develop the equations for any point  $\xi_0$ ). These equations can be written as follows:

$$\sigma - \sigma_0 + \rho\dot{s}(v - v_0) = 0 , \quad (4.58)$$

$$(v - v_0) + \dot{s}(\gamma - \gamma_0) = 0 , \quad (4.59)$$

$$(\sigma v - \sigma_0 v_0) + q - q_0 + p - p_0 + \rho\dot{s} \left( \epsilon - \epsilon_0 + \frac{1}{2}(v^2 - v_0^2) \right) = 0 , \quad (4.60)$$

where  $\sigma_0 = \hat{\sigma}(\gamma_0, \theta_0, \gamma_0'', -\dot{s}\gamma_0')$ , etc., and  $\gamma_0 = \gamma(\xi_0)$ , etc. The velocity  $v$  can be eliminated from equations (4.58) and (4.60) by use of equation (4.59). The momentum

equation (4.58) becomes

$$\sigma - \rho \dot{s}^2 \gamma = \sigma_0 - \rho \dot{s}^2 \gamma_0 , \quad (4.61)$$

and the energy equation (4.60) can be expressed as

$$q - q_0 + p - p_0 = -\dot{s} \left[ \rho(\epsilon - \epsilon_0) - \left( \frac{\sigma + \sigma_0}{2} \right) (\gamma - \gamma_0) \right] . \quad (4.62)$$

Alternatively, using the expression for  $\sigma$  given by (4.61), the previous equation can be written as

$$q - q_0 + p - p_0 + \rho \dot{s} \left[ (\epsilon - \epsilon_0) - \frac{\dot{s}^2}{2} (\gamma - \gamma_0)^2 - \frac{\sigma_0}{\rho} (\gamma - \gamma_0) \right] = 0 . \quad (4.63)$$

Equation (4.63) is therefore a combination of the compatibility, momentum and energy equations. Notice that equations (4.61) and (4.62) (or (4.63)) are general in the sense that they do not depend upon any constitutive assumption. Moreover, it is clear that by choosing the conditions *behind* (resp. *ahead*) a right-traveling wave in equations (4.51), (4.52) and (4.53), i.e., the “−” side (resp. the “+” side), equations (4.61) and (4.63) are also valid with the subscript 0 replaced by “−” (resp. by “+”) and with  $q^- = p^- = 0$  (resp.  $q^+ = p^+ = 0$ ).

Notice also that equation (4.61) is similar to the equation that defines the Rayleigh set in the classical adiabatic theory (see Section 2.4), except that in this case the stress  $\sigma$  might depend on  $\gamma'$  and  $\gamma''$ , hence it is no longer an algebraic relation but rather a differential equation. Similarly, the quantity in brackets on the right-hand side of equation (4.62) is related to the Hugoniot set but it is not an algebraic expression if the stress  $\sigma$  and the internal energy  $\epsilon$  depend on  $\gamma'$  and  $\gamma''$ .

With the foregoing constitutive assumptions (4.30), (4.31) and (4.32), the heat

flux  $q$  and the interstitial work  $p$  are, for the traveling wave problem,

$$\left. \begin{aligned} q &= k\theta' , \\ p &= -\rho\dot{s}\lambda\gamma'^2 . \end{aligned} \right\} \quad (4.64)$$

The stress given by equation (4.36) is

$$\sigma = \rho [\bar{\psi}_\gamma(\gamma, \theta) - \lambda\gamma'' - \nu\dot{s}\gamma'] \quad (4.65)$$

and, from equation (4.34), the internal energy is

$$\epsilon = \bar{\epsilon}(\gamma, \theta) + \frac{1}{2}\lambda\gamma'^2 , \quad (4.66)$$

where  $\bar{\epsilon}$  is given by (4.35).

# Chapter 5   Structured wave: Heat conduction only

## 5.1 Introduction.

There are several possibilities for connecting the regularized theory to the sharp interface one. The three structuring mechanisms are related to viscous, strain gradient and heat conduction effects. The approach taken here is as follows: first, the heat conductivity is assumed to be positive but the viscosity  $\nu$  and strain gradient coefficient  $\lambda$  are taken as zero. This *reduced* problem, analyzed in this chapter, corresponds to the basic solution of the singularly perturbed system. Secondly, the case when the viscosity and strain gradient coefficient are assumed small (in a sense to be specified) is analyzed in the next chapter, where it is shown that a kinetic relation can be inherited when  $\lambda, \nu, k \rightarrow 0$  and that the augmented theory reduces to the sharp interface theory.

The problem for a shock wave is analyzed in Section 5.3 and for a phase boundary in Sections 5.4-5.8. It is found that only propagating phase boundaries that satisfy a restricted version of the subsonic-supersonic condition are possible. Some special cases are analyzed in the last section.

## 5.2 Basic equations.

There are two possible situations regarding the conditions at  $\xi \rightarrow \pm\infty$ , viz., either  $(\gamma^\pm, \theta^\pm)$  are in the same phase (shock wave) or in different phases (phase boundary).

Consider first the case when the viscosity and strain gradient coefficient are removed (i.e., take  $\lambda = \nu = 0$ ). Using equations (4.64), (4.65) and (4.66) in the

governing equations (4.61) and (4.62) gives

$$\begin{aligned} & [\bar{\psi}_\gamma(\gamma, \theta) - \bar{\psi}_\gamma(\gamma_0, \theta_0)] - \dot{s}^2(\gamma - \gamma_0) = 0 , \\ \theta' - \theta'_0 = & -\frac{\rho\dot{s}}{k} \left\{ \bar{\epsilon}(\gamma, \theta) - \bar{\epsilon}(\gamma_0, \theta_0) - \frac{1}{2} [\bar{\psi}_\gamma(\gamma, \theta) + \bar{\psi}_\gamma(\gamma_0, \theta_0)] (\gamma - \gamma_0) \right\} . \end{aligned} \quad (5.1)$$

Equation (5.1)<sub>1</sub> is a purely algebraic relation that corresponds to the Rayleigh set (i.e., *all* points in the traveling wave are necessarily in the Rayleigh set). This equation can be expressed as

$$R(\gamma, \theta) = 0 ,$$

where the Rayleigh function  $R$  is defined by (2.36) and generated by  $(\gamma_0, \theta_0)$  and  $\dot{s}$ . For a point of the Rayleigh set where  $R_\gamma \neq 0$ , equations (5.1) can be written as

$$\begin{aligned} \gamma &= \gamma^R(\theta) , \\ \theta' - \theta'_0 &= -\frac{\rho\dot{s}}{k} H(\gamma^R(\theta), \theta) , \end{aligned} \quad (5.2)$$

where  $H$  is the Hugoniot function defined by (2.35) and  $\gamma^R$  corresponds to the Rayleigh set as introduced in Section 2.4. To analyze the autonomous differential equation (5.2)<sub>2</sub>, consider the following derivative of the Hugoniot function along the Rayleigh set (parametrized by  $\theta$ ):

$$\frac{dH}{d\theta}(\gamma^R(\theta), \theta) = H_\gamma(\gamma^R(\theta), \theta)\gamma_\theta^R(\theta) + H_\theta(\gamma^R(\theta), \theta) .$$

Using the expression (2.35) and dropping momentarily the arguments, this derivative becomes

$$\frac{dH}{d\theta} = \left\{ \bar{\epsilon}_\gamma - \frac{1}{2} [\bar{\psi}_\gamma + \bar{\psi}_\gamma^0 + \bar{\psi}_{\gamma\gamma}(\gamma - \gamma_0)] \right\} \gamma_\theta^R + \bar{\epsilon}_\theta - \frac{1}{2} \bar{\psi}_{\gamma\theta}(\gamma - \gamma_0) .$$

Since  $\bar{\epsilon}_\gamma = \bar{\psi}_\gamma - \theta\bar{\psi}_{\gamma\theta}$  and  $\bar{\epsilon}_\theta = -\theta\bar{\psi}_{\theta\theta}$ , then, rearranging terms,

$$\frac{dH}{d\theta} = -\theta(\bar{\psi}_{\gamma\theta}\gamma_\theta^R + \bar{\psi}_{\theta\theta}) + \frac{1}{2} [\bar{\psi}_\gamma - \bar{\psi}_\gamma^0 - \bar{\psi}_{\gamma\gamma}(\gamma - \gamma_0)] \gamma_\theta^R - \frac{1}{2} \bar{\psi}_{\gamma\theta}(\gamma - \gamma_0) .$$

In view of the expression for  $\gamma_\theta^R$  given by (2.37) and using equation (5.1)<sub>1</sub>, it follows that

$$\frac{dH}{d\theta} = -\theta \bar{\psi}_{\theta\theta} \left[ \frac{(\bar{\psi}_{\theta\theta})^{-1} (\bar{\psi}_{\gamma\gamma} \bar{\psi}_{\theta\theta} - \bar{\psi}_{\gamma\theta}^2) - \dot{s}^2}{\bar{\psi}_{\gamma\gamma} - \dot{s}^2} \right]. \quad (5.3)$$

For clarity, it is useful to express (5.3) using the parameters defined by (2.18)<sub>1,2</sub>, (2.22) and (2.24) as follows:

$$\frac{dH}{d\theta} = c \left( \frac{a_e^2 - \dot{s}^2}{a^2 - \dot{s}^2} \right),$$

where  $c$ ,  $a_e^2$  and  $a^2$  are evaluated at  $(\gamma^R(\theta), \theta)$ . Notice that the isothermal and isentropic sound speed are complex in the unstable region.

As shown above, in the case where the only structuring mechanism is heat conduction, all points of a traveling wave belong to the Rayleigh set. The relevant portion of  $\mathcal{R}$  depends on the given traveling wave problem since the end points  $(\gamma^-, \theta^-)$  and  $(\gamma^+, \theta^+)$  correspond to the conditions at  $\xi \rightarrow \pm\infty$ .

For a phase boundary propagation problem,  $\mathcal{R}$  is parametrized by  $\xi = x - \dot{s}t$  as  $\{(\theta(\xi), \gamma(\xi))\}$ . In that case, the parameter  $\xi$  varies (for fixed  $x$  or fixed  $t$ ) from  $-\infty$  to  $+\infty$  or vice-versa *depending on the sign of  $\dot{s}$* . This has important physical consequences.

Notice also that the continuity of  $\gamma(\xi)$ ,  $\theta(\xi)$  and  $\theta'(\xi)$ ,  $\gamma'(\xi)$  with respect to  $\xi$  is *not necessarily* equivalent to the continuity of  $\gamma^R$  and  $\gamma_\theta^R$  with respect to the parameter  $\theta$  or the continuity of  $\theta^R$  and  $\theta_\gamma^R$  with respect to  $\gamma$ .

The Helmholtz free energy  $\hat{\psi}(\gamma, \theta, \gamma_x)$  was specified in Section 4.4 up to the function  $\bar{\psi}(\gamma, \theta)$ . Now, to fully characterize the material, consider the function  $\bar{\psi}$  introduced in Section 2.5. In view of (2.40), the stress is given by equation (4.65) with  $\lambda = \nu = 0$ , i.e.,

$$\sigma = \mu\gamma - \alpha\mu\theta + H_4, \quad (5.4)$$

where

$$H_4 = \begin{cases} \alpha\mu\theta_T & \text{low strain phase,} \\ \alpha\mu\theta_T - \mu\gamma_T & \text{high strain phase.} \end{cases} \quad (5.5)$$

Similarly, by (4.66) and (2.40), the internal energy  $\epsilon$  is given (with  $\lambda = 0$ ) by

$$\epsilon = \bar{\epsilon}(\gamma, \theta) = \frac{\mu}{2\rho}\gamma^2 + c\theta + \frac{H_4}{\rho}\gamma + H_5, \quad (5.6)$$

where

$$H_5 = \begin{cases} 0 & \text{low strain phase,} \\ \frac{\mu\gamma_T}{2\rho} - \frac{\alpha\mu\gamma_T\theta_T}{\rho} - \lambda_T & \text{high strain phase.} \end{cases} \quad (5.7)$$

### 5.3 Traveling shock wave.

Suppose that *all* points in an infinite bar (parametrized by  $\xi = x - st$ ) are in the *same* phase (either low or high strain phase). This assumption, referred to as the *phase segregation* condition, can be stated as

$$\forall \xi \in \mathbb{R} \quad 0 < \theta(\xi) \leq \theta_C \quad \text{and} \quad -1 \leq \gamma(\xi) \leq \gamma_M(\theta(\xi)) \quad (5.8)$$

for the low strain phase or

$$\forall \xi \in \mathbb{R} \quad 0 < \theta(\xi) \leq \theta_C \quad \text{and} \quad \gamma(\xi) \geq \gamma_m(\theta(\xi)) \quad (5.9)$$

for the high strain phase. The traveling shock wave problem is stated as follows:

**Shock wave problem:** *given one end state, say  $(\gamma^+, \theta^+)$ , find continuous functions  $\gamma(\xi)$  and  $\theta(\xi)$ ,  $\xi \in \mathbb{R}$ , that satisfy equations (5.1) and the corresponding phase segre-*



gation condition (i.e., (5.8) or (5.9)).

Alternatively, the state  $(\gamma^-, \theta^-)$  could be prescribed, although, physically, the previous alternative is preferred. The state  $(\gamma^-, \theta^-)$  at  $\xi \rightarrow -\infty$  and the shock wave speed  $\dot{s}$  are unknown. From (5.4) and (5.6) and for a given state  $(\gamma^+, \theta^+)$ ,

$$\bar{\psi}_\gamma(\gamma, \theta) - \bar{\psi}_\gamma(\gamma^+, \theta^+) = a^2(\gamma - \gamma^+) - \alpha a^2(\theta - \theta^+) ,$$

and

$$\bar{\epsilon}(\gamma, \theta) - \epsilon^+ = \frac{a^2}{2}(\gamma^2 - \gamma^{+2}) + c(\theta - \theta^+) + \frac{H_4}{\rho}(\gamma - \gamma^+) .$$

Since

$$\frac{1}{2} [\bar{\psi}_\gamma(\gamma, \theta) + \bar{\psi}_\gamma(\gamma^+, \theta^+)] = \frac{a^2}{2}(\gamma + \gamma^+) - \frac{\alpha a^2}{2}(\theta + \theta^+) + \frac{H_4}{\rho} ,$$

then (5.1) becomes, assuming  $R_\gamma = a^2 - \dot{s}^2 \neq 0$ ,

$$\left\{ \begin{array}{l} \gamma = \frac{\alpha a^2}{a^2 - \dot{s}^2}(\theta - \theta^+) + \gamma^+ , \\ \theta' = -\frac{\rho \dot{s}}{k} \left\{ c(\theta - \theta^+) + \frac{\alpha a^2}{2}(\theta + \theta^+)(\gamma - \gamma^+) \right\} . \end{array} \right.$$

The case  $\dot{s}^2 = a^2$  is analyzed at the end of this section. The first equation corresponds to the Rayleigh set given as  $\gamma = \gamma^R(\theta)$ . Substitution of  $\gamma$  by  $\gamma^R(\theta)$  in the second equation gives

$$\left\{ \begin{array}{l} \gamma = \frac{\alpha a^2}{a^2 - \dot{s}^2}(\theta - \theta^+) + \gamma^+ , \\ \theta' = r_1(\dot{s})(\theta - \theta^+)^2 + r_2(\dot{s}, \theta^+)(\theta - \theta^+) , \end{array} \right. \quad (5.10)$$

where

$$\begin{cases} r_1(\dot{s}) = -\frac{\rho\dot{s}}{k} \left( \frac{\alpha^2 a^4}{2(a^2 - \dot{s}^2)} \right), \\ r_2(\dot{s}, \theta^+) = -\frac{\rho\dot{s}}{k} \left( c + \frac{\alpha^2 a^4 \theta^+}{a^2 - \dot{s}^2} \right). \end{cases}$$

These functions can be written as

$$\begin{cases} r_1(\dot{s}) = -\frac{\rho c}{k} \dot{s} \left( \frac{G}{2} \right) \gamma_\theta^R, \\ r_2(\dot{s}, \theta^+) = -\frac{\rho c}{k} \dot{s} \left( \frac{(a_e^+)^2 - \dot{s}^2}{a^2 - \dot{s}^2} \right). \end{cases} \quad (5.11)$$

Notice that these functions are essentially the same as  $r_1$  and  $r_2$  defined by (2.60).

**Stability of equilibrium points:** Equation (5.10)<sub>2</sub> has two equilibrium points, i.e.,

$$\theta_1 = \theta^+, \quad \theta_2 = -\frac{r_2(\dot{s}, \theta^+)}{r_1(\dot{s})} + \theta^+.$$

Observe that for  $\theta_2$  to be positive, then, in view of (5.11),

$$\theta_2 = -\frac{2c(a^2 - \dot{s}^2)}{\alpha^2 a^4} - \theta^+ > 0,$$

which implies that

$$\dot{s}^2 > \dot{s}_{\min}^2 > a^2,$$

where

$$\dot{s}_{\min}^2 = (a_e^+)^2 - \frac{\alpha^2 a^4 \theta^+}{2c}.$$

Linearizing (5.10)<sub>2</sub> about  $\theta_{1,2}$  gives

$$\theta' = r_2(\dot{s}, \theta^+)(\theta - \theta^+) \quad \text{at } \theta = \theta_1,$$

$$\theta' = -r_2(\dot{s}, \theta^+)(\theta - \theta^+) \quad \text{at } \theta = \theta_2.$$

Therefore, if  $r_2(\dot{s}, \theta^+) > 0$ , then  $\theta_1$  is a source and  $\theta_2$  is a sink. If  $r_2(\dot{s}, \theta^+) < 0$ , the situation is reversed.

**Explicit solution:** Equation (5.10)<sub>2</sub> is a Riccati equation that can be solved, assuming  $r_1(\dot{s}) \neq 0$ , using the transformation

$$\theta(\xi) = -\frac{1}{r_1} \frac{d}{d\xi} \log w(\xi)$$

and solving the corresponding linear equation for the function  $w$ . The case  $r_2(\dot{s}, \theta^+) = 0$  corresponds to  $\dot{s}^2 = (a_e^+)^2$ . From (5.10)<sub>2</sub>, the corresponding solution is such that  $\theta(-\infty) = \theta(+\infty) = \theta^+$  and has a singularity at  $\xi = -1/[(\theta^+ - \theta_0)r_1(\dot{s})]$ , where  $\theta_0 = \theta(0)$ . Therefore, this is not an admissible structured wave. Hence, assuming  $r_2(\dot{s}, \theta^+) \neq 0$ , the temperature is given by

$$\theta(\xi) = \left\{ K_0 e^{-r_2 \xi} - \frac{r_1}{r_2} \right\}^{-1} + \theta^+ ,$$

where  $K_0$  is an integration constant and  $r_1 = r_1(\dot{s})$ ,  $r_2 = r_2(\dot{s}, \theta^+)$ . The constant  $K_0$  corresponds only to a translation of  $\xi$  (i.e., change of origin), which is irrelevant for a steady wave. The case  $K_0 \rightarrow \infty$  corresponds to the trivial solution  $\theta(\xi) = \theta^+$ . For the nontrivial solution, there are two cases to consider, viz.,

**Case 1:** Suppose  $r_2 > 0$ . Therefore,

$$\lim_{\xi \rightarrow -\infty} \theta(\xi) = \theta^+ .$$

Hence (4.50)<sub>1</sub> cannot be satisfied except for the trivial case  $\theta^- = \theta^+$ .

**Case 2:** Suppose  $r_2 < 0$ . Therefore,

$$\lim_{\xi \rightarrow +\infty} \theta(\xi) = \theta^+ ,$$

which corresponds to (4.50)<sub>2</sub>. On the other hand,

$$\lim_{\xi \rightarrow -\infty} \theta(\xi) = -\frac{r_2}{r_1} + \theta^+ = -\frac{2c(a^2 - \dot{s}^2)}{\alpha^2 a^4} - \theta^+ .$$

To satisfy (4.50)<sub>1</sub> then, necessarily,  $|\dot{s}|$  must be the same as the shock wave speed of the adiabatic theory as given by (2.46). Moreover, from (2.46) and (5.11)<sub>1</sub>,

$$r_2 = \frac{\rho c \dot{s}}{k} \left( \frac{\theta^+ - \theta^-}{\theta^+ + \theta^-} \right) .$$

Hence, since the sign of  $r_2$  depends on the signs of  $\dot{s}$  and  $\theta^+ - \theta^-$ , it follows that  $r_2 < 0$  is equivalent to the entropy jump condition of the adiabatic theory as given by (2.48) (except for the trivial case).

**Singularities:** Observe that the temperature, as a function of  $\xi$ , has a singularity if  $K_0$  and  $r_1/r_2$  have the same sign. Let  $\theta_0$  be the (unknown) temperature at  $\xi = 0$ . Therefore, in terms of  $\theta_0$ , the constant  $K_0$  can be expressed as

$$K_0 = \frac{1}{\theta_0 - \theta^+} + \frac{r_1}{r_2} .$$

Moreover, for a solution with no singularities, it is required that

$$\frac{r_2}{r_1} K_0 = \frac{r_2}{r_1(\theta_0 - \theta^+)} + 1 < 0 .$$

From (5.11), the above inequality becomes

$$\left( \frac{2c}{\alpha^2 a^4} \right) \frac{(a_e^+)^2 - \dot{s}^2}{\theta_0 - \theta^+} + 1 < 0 .$$

Now, suppose first that  $\dot{s} > 0$ . By the regularity of the Rayleigh set and in view of the entropy inequality (2.48), it follows that

$$\forall |\xi| < \infty \quad \theta^+ < \theta(\xi) < \theta^- .$$

Hence,  $\theta_0 - \theta^+ > 0$  and, therefore,

$$(a_e^+)^2 - \dot{s}^2 + \frac{\alpha^2 a^4}{2c} (\theta_0 - \theta^+) < 0 ,$$

or

$$a^2 \left( 1 + \frac{\alpha^2 a^2}{2c} (\theta_0 + \theta^+) \right) - \dot{s}^2 < 0 .$$

In view of (2.46) and since  $\theta_0 < \theta^-$ , the above inequality is satisfied and the solution does not have a singularity. The case  $\dot{s} < 0$  is similar.

Expressing  $\tau_1$  in terms of  $\theta^+$  and  $\theta^-$ , the temperature can be written as

$$\theta(\xi) = \llbracket \theta \rrbracket \left\{ \llbracket \theta \rrbracket K_0 \exp \left[ -\frac{2\dot{s}\llbracket \theta \rrbracket}{\kappa\langle \theta \rangle} \xi \right] - 1 \right\}^{-1} + \theta^+ ,$$

where  $\kappa$  is the thermal diffusivity as defined in (4.33),  $\dot{s}$  is related to  $\theta^\pm$  through (2.50) and the symbols  $\llbracket \cdot \rrbracket$ ,  $\langle \cdot \rangle$  are used here as notation for the difference and the average of the values at  $\xi \rightarrow \pm\infty$ . Therefore, the values  $(\gamma^\pm, \theta^\pm)$  satisfy all the jump conditions of the adiabatic theory as given in (2.46), (2.47). The corresponding strain is, from (5.10)<sub>1</sub>,

$$\gamma(\xi) = -\frac{1}{G} \frac{\llbracket \theta \rrbracket}{\langle \theta \rangle} \left\{ \llbracket \theta \rrbracket K_0 \exp \left[ -\frac{2\dot{s}\llbracket \theta \rrbracket}{\kappa\langle \theta \rangle} \xi \right] - 1 \right\}^{-1} + \gamma^+ .$$

**A one-parameter family of solutions:** Apart from the constant  $K_0$ , the solution to the traveling shock wave problem remains undetermined up to one unknown in the following sense: if  $(\gamma^+, \theta^+)$  are given, then one can *choose* a shock wave speed such that  $\dot{s}^2 > (a_e^+)^2$  for  $\dot{s} > 0$  or  $\dot{s}^2 < (a_e^+)^2$  for  $\dot{s} < 0$ . Using the momentum and energy jump conditions (2.46) and (2.47)<sub>2</sub>, it is possible to obtain the (back) state  $(\gamma^-, \theta^-)$  (as long as it is in the same phase). Therefore, the temperature and strain, as functions of  $\xi$ , remain undetermined up to  $\dot{s}$ . This shows that there exists a one-parameter family of steady, structured, compressive shock waves that satisfy the shock wave problem for a trilinear material.

In the limit, as the heat conduction is removed, the structured wave tends to the solution for the traveling wave problem within the framework of the classical adiabatic theory, i.e.,

$$\gamma(\xi) = \begin{cases} \gamma^- & \text{for } \xi < 0, \\ \gamma^+ & \text{for } \xi > 0, \end{cases}$$

and

$$\theta(\xi) = \begin{cases} \theta^- & \text{for } \xi < 0, \\ \theta^+ & \text{for } \xi > 0. \end{cases}$$

Also, the jump conditions (2.47) are satisfied and  $\dot{s}^2$  is given by (2.46).

It is useful to write this solution in dimensionless form using the parameters defined in Section 2.7. Introduce a nondimensional coordinate  $z$ ,

$$z = \frac{a}{\kappa} \xi,$$

hence, the temperature can be written as

$$T(z) = -[[T]] \left\{ \exp \left[ -2\nu \frac{[[T]]}{\langle T \rangle} z \right] + 1 \right\}^{-1} + T^+,$$

where the solution was normalized by taking  $\theta(0) = \langle \theta \rangle$  which implies  $K_0 = -[[\theta]]^{-1}$ .

Similarly, the strain can be written as

$$\delta(z) = \frac{1}{G} \frac{[[T]]}{\langle T \rangle} \left\{ \exp \left[ -2\nu \frac{[[T]]}{\langle T \rangle} z \right] + 1 \right\}^{-1} + \delta^+.$$

**Special case of zero thermal expansion:** It was assumed that  $R_\gamma = a^2 - \dot{s}^2 \neq 0$ . Suppose now that  $\dot{s}^2 = a^2$ . From (5.1)<sub>1</sub> and (5.4), this implies that, for a shock wave,  $\alpha a^2(\theta(\xi) - \theta^+) = 0$ . Except for the isothermal case  $\theta(\xi) = \theta^+$ , this equation is not satisfied unless  $\alpha = 0$  (the case  $a^2 = 0$  is physically irrelevant). Henceforth, as a special case, assume that the thermal expansion coefficient  $\alpha$  is zero. The speed of propagation of the shock wave  $\dot{s}^2 = a^2$  is consistent with (2.46) with  $\alpha = 0$ . This is a degenerate case in the sense that the momentum equation (5.1)<sub>1</sub> is satisfied by *any*

pair  $(\gamma, \theta)$ , i.e., the Rayleigh set is the whole  $\gamma$ - $\theta$  plane. Equation (5.1)<sub>2</sub> reduces to

$$\theta' = -\frac{\dot{s}}{\kappa}(\theta - \theta^+) , \quad (5.12)$$

hence

$$\theta(\xi) = \theta_0 \exp \left[ -\frac{\dot{s}}{\kappa} \xi \right] + \theta^+ .$$

If  $\dot{s} > 0$  then the condition (4.50)<sub>1</sub> cannot be satisfied and if  $\dot{s} < 0$  then the condition (4.50)<sub>2</sub> cannot be satisfied. Hence, it is *not* possible to have a structured shock wave when  $\alpha = 0$ .

## 5.4 Traveling phase boundary.

Suppose that the conditions at  $\xi \rightarrow +\infty$  correspond to the *high strain* phase and the conditions at  $\xi \rightarrow -\infty$  correspond to the *low strain* phase. Presumably, if the strain varies continuously, there is an interval, say  $(0, b)$ , where the points are in the *unstable* phase. In this case, since the special material under consideration is such that  $\bar{\psi}_{\gamma\gamma}$  is piecewise continuous (continuous in each phase), the phase boundary propagation problem is naturally divided into three sub-problems. From the above considerations and in view of the continuity requirements of the traveling wave, the solution must satisfy the following conditions:

$$\begin{aligned} \theta(0^-) &= \theta(0^+) = \theta_0 , \\ \gamma(0^-) &= \gamma(0^+) = \gamma_M(\theta_0) , \\ \theta(b^-) &= \theta(b^+) = \theta_b , \\ \gamma(b^-) &= \gamma(b^+) = \gamma_m(\theta_b) , \end{aligned}$$

where the functions  $\gamma_m$  and  $\gamma_M$  are given by (2.39). Observe that the strains  $\gamma_0$  and  $\gamma_b$  and the temperatures  $\theta_0$  and  $\theta_b$  are unknown. The phase segregation conditions must be satisfied, i.e., the solution must be such that the material is in its low strain phase

in  $(-\infty, 0)$ , unstable phase in  $(0, b)$  and high strain phase in  $(b, +\infty)$ . Moreover, the temperature has to be below the critical value  $\theta_C$ . These conditions can be expressed as

$$\left. \begin{aligned} -1 < \gamma(\xi) \leq \gamma_M(\theta(\xi)) & \text{ for } -\infty < \xi < 0, \\ \gamma_M(\theta(\xi)) \leq \gamma(\xi) \leq \gamma_m(\theta(\xi)) & \text{ for } 0 < \xi < b, \\ \gamma(\xi) \geq \gamma_m(\theta(\xi)) & \text{ for } b < \xi < +\infty, \\ \theta(\xi) \leq \theta_C & \text{ for } -\infty < \xi < +\infty. \end{aligned} \right\} \quad (5.13)$$

Additionally, at  $\xi = 0$  and  $\xi = b$ , the corresponding jump condition (4.57) (continuity of  $\theta'$ ) has to be satisfied. Formally, the conditions at  $\xi \rightarrow \pm\infty$  are given by (4.48) and (4.50), although only one of them is known a priori. The problem can now be stated as follows:

**Structured phase boundary traveling wave problem:** *Given one end state, say  $(\gamma^+, \theta^+)$  (or, alternatively,  $(\gamma^-, \theta^-)$ ) find continuous functions  $\gamma(\xi)$  and  $\theta(\xi)$ ,  $\xi \in \mathbb{R}$ , that satisfy the phase segregation conditions (5.13), the jump condition (4.57) at  $\xi = 0$  and  $\xi = b$  and the following three problems:*

**Problem 1:** Low strain phase. Suppose that for  $\xi \in (-\infty, 0)$  the material is in its low strain phase. Using the conditions at  $-\infty$  in (5.1) and the corresponding expressions of  $\bar{\psi}(\gamma, \theta)$ ,  $\bar{\epsilon}(\gamma, \theta)$ ,  $\epsilon^-$  and  $\sigma^-$  given by equations (2.42) and (2.44), the governing equations are

$$\begin{cases} \gamma = \frac{\alpha a^2}{a^2 - \dot{s}^2}(\theta - \theta^-) + \gamma^-, \\ \theta' = r_1(\dot{s})(\theta - \theta^-)^2 + r_2(\dot{s}, \theta^-)(\theta - \theta^-), \end{cases} \quad (5.14)$$

where the functions  $r_1$  and  $r_2$  are defined by (5.11) and the functions  $\gamma(\xi)$  and  $\theta(\xi)$



satisfy

$$\gamma(-\infty) = \gamma^-, \quad \theta(-\infty) = \theta^-, \quad (5.15)$$

$$\gamma(0^-) = \gamma_0 = \gamma_C + M(\theta_0 - \theta_C), \quad \text{where } \theta(0^-) = \theta_0. \quad (5.16)$$

The values of  $\gamma^-$ ,  $\theta^-$ ,  $\gamma_0$ ,  $\theta_0$  and  $\dot{s}$  are unknown.

**Problem 2:** Unstable phase. Suppose that for  $\xi \in (0, b)$  the material is in its unstable phase. In view of (5.2), the governing equations are

$$\begin{cases} \gamma = \gamma^{R,u}(\theta), \\ \theta' - \theta'_0 = -\frac{\rho\dot{s}}{k} H^u(\gamma^{R,u}(\theta), \theta), \end{cases} \quad (5.17)$$

where  $\gamma^{R,u}$  and  $H^u$  correspond to the Rayleigh set and the Hugoniot function for the *unstable* phase generated at  $(\gamma_0, \theta_0)$ <sup>1</sup> and the functions  $\gamma(\xi)$  and  $\theta(\xi)$  satisfy

$$\gamma(0^+) = \gamma_C + M(\theta_0 - \theta_C), \quad \text{where } \theta(0^+) = \theta_0, \quad (5.18)$$

$$\gamma(b^-) = \gamma_C + m(\theta_b - \theta_C), \quad \text{where } \theta(b^-) = \theta_b. \quad (5.19)$$

The temperature  $\theta_b$  is unknown.

**Problem 3:** High strain phase. Suppose that for  $\xi \in (b, +\infty)$  the material is in its high strain phase. The governing equations are

$$\begin{cases} \gamma = \frac{\alpha a^2}{a^2 - \dot{s}^2}(\theta - \theta^+) + \gamma^+, \\ \theta' = r_1(\dot{s})(\theta - \theta^+)^2 + r_2(\dot{s}, \theta^+)(\theta - \theta^+), \end{cases} \quad (5.20)$$

---

<sup>1</sup>Equivalently, one can use the point  $(\gamma_b, \theta_b)$ . The explicit expressions are not relevant here, although they will be given below for computational purposes.

and the functions  $\gamma(\xi)$  and  $\theta(\xi)$  satisfy

$$\gamma(b^+) = \gamma_C + m(\theta_b - \theta_C), \quad \text{where } \theta(b^+) = \theta_b, \quad (5.21)$$

$$\gamma(+\infty) = \gamma^+, \quad \theta(+\infty) = \theta^+. \quad (5.22)$$

The values of  $\gamma^+$  and  $\theta^+$  are given.

**Preliminary remarks:** The original problem has been divided into three *a priori* independent sub-problems. The connection between them is through the continuity of the temperature, the temperature gradient and the strain at  $\xi = 0$  and  $\xi = b$ . Additionally, since the original equations (4.45)-(4.47) were obtained by integration of (4.42)-(4.44), the values at  $\xi \rightarrow \pm\infty$  are related (formally) via the jump conditions (2.52). It is expected that the solution of the phase boundary propagation problem will deliver values  $(\gamma^\pm, \theta^\pm)$  that satisfy (2.52) in view of the following: the (integrated) momentum equation, applied successively between  $\xi = -\infty, 0, b$  and  $+\infty$ , gives

$$\sigma^- - \sigma_0^- = \rho \dot{s}^2 (\gamma^- - \gamma_0^-),$$

$$\sigma_0^+ - \sigma_b^- = \rho \dot{s}^2 (\gamma_0^+ - \gamma_b^-),$$

$$\sigma_b^+ - \sigma^+ = \rho \dot{s}^2 (\gamma_b^+ - \gamma^+),$$

where the symbols have obvious meaning. Enforcing the continuity of temperature and strain at  $\xi = 0$  and  $\xi = b$  guarantees that, since  $\bar{\sigma}$  is continuous in  $\gamma$  and  $\theta$ ,

$$\sigma^+ - \sigma^- = \rho \dot{s}^2 (\gamma^+ - \gamma^-),$$

which is (2.52)<sub>2</sub>. Similarly, from the energy equation, it is not hard to see that enforcing continuity of  $\theta$ ,  $\theta'$  and  $\gamma$  at  $\xi = 0$  and  $\xi = b$  results in the energy jump condition

$$\epsilon^+ - \epsilon^- = \frac{1}{2\rho} (\sigma^+ + \sigma^-) (\gamma^+ - \gamma^-),$$

which corresponds to (2.52)<sub>3</sub>.

Moreover, the jump condition (4.57) requires that  $\theta'$  be continuous at  $\xi = 0$  and  $\xi = b$ , hence, since at those points

$$[[\theta']] = [[\theta_\gamma^R \gamma']] = \langle \theta_\gamma^R \rangle [[\gamma']] + \langle \gamma' \rangle [[\theta_\gamma^R]] = 0$$

and, generally,  $[[\theta_\gamma^R]] \neq 0$ , then it is expected that  $\gamma'$  will be *discontinuous* at  $\xi = 0$  and  $\xi = b$ . The above remarks will be verified in the following analysis.  $\square$

The solution to the phase boundary propagation problem can be obtained explicitly for the metastable phases (problems 1 and 3) and implicitly for the unstable phase (problem 2).

## 5.5 The metastable phases.

Equations (5.14)<sub>2</sub> and (5.20)<sub>2</sub> are Riccati equations. This provides, assuming  $r_1(\dot{s}) \neq 0$ ,  $r_2(\dot{s}, \theta^-) \neq 0$  and  $r_2(\dot{s}, \theta^+) \neq 0$ ,

$$\theta(\xi) = \begin{cases} \left\{ \left\{ K_1 \exp[-r_2(\dot{s}, \theta^-)\xi] - \frac{r_1(\dot{s})}{r_2(\dot{s}, \theta^-)} \right\}^{-1} + \theta^- \right. & \text{for } \xi < 0, \\ \left. \left\{ \left\{ K_3 \exp[-r_2(\dot{s}, \theta^+)\xi] - \frac{r_1(\dot{s})}{r_2(\dot{s}, \theta^+)} \right\}^{-1} + \theta^+ \right. \right. & \text{for } \xi > b, \end{cases} \quad (5.23)$$

where  $K_1$  and  $K_3$  are unknown constants. The cases when either  $r_1 = 0$  or  $r_2 = 0$  are analyzed in Section 5.8. The cases  $K_1 \rightarrow \infty$  and  $K_3 \rightarrow \infty$  correspond to the trivial solutions  $\theta(\xi) = \theta^-$  for  $\xi < 0$  and  $\theta(\xi) = \theta^+$  for  $\xi > b$  respectively. The constants  $K_1$  and  $K_3$  can, alternatively, be expressed in terms of the (unknown) temperatures  $\theta_0$  and  $\theta_b$  and other parameters as

$$K_1 = K_1(\dot{s}, \theta_0, \theta^-) = \frac{1}{\theta_0 - \theta^-} + \frac{r_1(\dot{s})}{r_2(\dot{s}, \theta^-)}, \quad (5.24)$$

$$K_3 = K_3(\dot{s}, \theta_b, \theta^+, b) = e^{r_2(\dot{s}, \theta^+)b} \left[ \frac{1}{\theta_b - \theta^+} + \frac{r_1(\dot{s})}{r_2(\dot{s}, \theta^+)} \right]. \quad (5.25)$$

It is convenient to use (5.14) and (5.20) together with (5.16) and (5.21) to express  $\theta_0$  and  $\theta_b$  in terms of the conditions at  $\pm\infty$ . It follows that

$$\theta_0 = \left( \frac{\alpha a^2}{a^2 - \dot{s}^2} - M \right)^{-1} [\gamma_C - \gamma^- + M(\theta^- - \theta_C)] + \theta^- , \quad (5.26)$$

$$\theta_b = \left( \frac{\alpha a^2}{a^2 - \dot{s}^2} - m \right)^{-1} [\gamma_C - \gamma^+ + m(\theta^+ - \theta_C)] + \theta^+ . \quad (5.27)$$

Moreover, in view of (5.14)<sub>1</sub> and (5.20)<sub>1</sub>, the conditions for the strain at  $\xi \rightarrow \pm\infty$ , i.e., (5.15)<sub>1</sub> and (5.22)<sub>1</sub>, are satisfied as long as the conditions for the temperature, (5.15)<sub>2</sub> and (5.22)<sub>2</sub>, hold. At this point, from (5.23)-(5.27), the temperature and the strain in the metastable phases, as functions of  $\xi$ , are known in terms of  $(\dot{s}, \theta^-, \gamma^-)$  for  $\xi < 0$  and in terms of  $(\dot{s}, \theta^+, \gamma^+, b)$  for  $\xi > b$ .

For the low strain phase, if  $r_2(\dot{s}, \theta^-) < 0$  (or  $K_1 = 0$ ), then, from (5.23),

$$\lim_{\xi \rightarrow -\infty} \theta(\xi) = -\frac{r_2(\dot{s}, \theta^-)}{r_1(\dot{s})} + \theta^- .$$

hence the condition (5.15)<sub>2</sub> cannot be satisfied. Therefore, consider  $r_2(\dot{s}, \theta^-) > 0$ , which gives

$$\lim_{x \rightarrow -\infty} \theta(\xi) = \theta^- ,$$

as required by (5.15)<sub>2</sub>. Similarly, for the high strain phase, if  $r_2(\dot{s}, \theta^+) > 0$  (or  $K_3 = 0$ ), then,

$$\lim_{\xi \rightarrow +\infty} \theta(\xi) = -\frac{r_2(\dot{s}, \theta^+)}{r_1(\dot{s})} + \theta^+ ,$$

and the condition (5.22)<sub>2</sub> cannot be satisfied. If  $r_2(\dot{s}, \theta^+) < 0$ , then

$$\lim_{x \rightarrow +\infty} \theta(\xi) = \theta^+ ,$$

as required by (5.22)<sub>2</sub>. Hence, a necessary condition for the existence of a nontrivial

propagating phase boundary is

$$\begin{cases} r_2(\dot{s}, \theta^-) > 0, \\ r_2(\dot{s}, \theta^+) < 0. \end{cases}$$

The propagating phase boundary is nontrivial in the sense that both  $|K_1| < \infty$  and  $|K_3| < \infty$ . The case where one of these two constants tends to  $\infty$  will be analyzed in Section 5.8. An additional restriction is that the constants  $K_1$  and  $K_3$  have to be different from zero. There are two cases to consider, viz.,

**Case 1:** Suppose  $\dot{s} > 0$ ; from the expression for  $r_2$  given by (5.11)<sub>2</sub>, it follows that the above condition is equivalent to

$$\begin{cases} \frac{(a_e^-)^2 - \dot{s}^2}{a^2 - \dot{s}^2} < 0, \\ \frac{(a_e^+)^2 - \dot{s}^2}{a^2 - \dot{s}^2} > 0. \end{cases}$$

In the metastable phases, these inequalities can be satisfied simultaneously only if  $\dot{s}^2 > a^2$  and

$$(a_e^+)^2 < \dot{s}^2 < (a_e^-)^2.$$

Additionally, for this restriction to hold, it is required that

$$\theta^+ < \theta^-.$$

**Case 2:** Suppose  $\dot{s} < 0$ ; the necessary condition for the existence of a traveling phase boundary is equivalent to

$$\begin{cases} \frac{(a_e^-)^2 - \dot{s}^2}{a^2 - \dot{s}^2} > 0, \\ \frac{(a_e^+)^2 - \dot{s}^2}{a^2 - \dot{s}^2} < 0. \end{cases}$$

In the metastable phases, these inequalities can be satisfied simultaneously only if

$\dot{s}^2 > a^2$  and

$$(a_e^-)^2 < \dot{s}^2 < (a_e^+)^2 .$$

For this restriction to hold, it is required that

$$\theta^+ > \theta^- .$$

Now, the values at  $\xi \rightarrow \pm\infty$  for a steady traveling wave have to satisfy the same jump conditions that apply to a moving discontinuity in the adiabatic theory where the conditions ahead of and behind of the discontinuity correspond to the values at  $\pm\infty$ . If the conditions at  $+\infty$  correspond to the high strain phase and the conditions at  $-\infty$  to the low strain phase then, in particular, equation (2.52)<sub>2</sub> has to hold. This equation can be written as

$$(\dot{s}^2 - a^2)(\gamma^+ - \gamma^-) + \alpha a^2(\theta^+ - \theta^-) = -a^2 \gamma_T .$$

Assume henceforth that  $\gamma^+ > \gamma^-$ . This is a working assumption that has to be verified *a posteriori*. Therefore, the left-hand side of the above equation is positive for case 2 (in which  $\dot{s} < 0$  and  $\theta^+ > \theta^-$ ). Since the right-hand side is negative (recall that  $\gamma_T > 0$ ), then case 2 cannot correspond to a traveling phase boundary and hence  $\dot{s}$  cannot be negative. However, case 1 ( $\dot{s} > 0$ ) is not ruled out since  $\theta^+ < \theta^-$  and therefore the left-hand side could be negative. Consequently, only *compressive* waves are allowed if  $\gamma^+ > \gamma^-$ . The specific thermoelastic material used here is intended to model materials in tension. It is possible to introduce a similar thermoelastic material to model compressive waves more appropriately. See ABEYARATNE & KNOWLES [5]. Furthermore, after proving that there is a feasible solution in the metastable phases, it is important at this point to analyze the additional restrictions that arise from the fact that the solution (5.23) cannot have singularities.

**Movable singularities:** Suppose that the solution (5.23) for the metastable phases has a singularity at  $\xi = \xi_* < 0$  for the low strain phase and/or at  $\xi = \xi_{**} > b$  for the high strain phase. This occurs if the denominator vanishes, i.e., if one (or both) of

the following values exists:

$$\xi_* = \frac{1}{r_2(\dot{s}, \theta^-)} \log \left[ \frac{r_2(\dot{s}, \theta^-) + r_1(\dot{s})(\theta_0 - \theta^-)}{r_1(\dot{s})(\theta_0 - \theta^-)} \right] \quad \xi_* < 0 ,$$

$$\xi_{**} - b = \frac{1}{r_2(\dot{s}, \theta^+)} \log \left[ \frac{r_2(\dot{s}, \theta^+) + r_1(\dot{s})(\theta_b - \theta^+)}{r_1(\dot{s})(\theta_b - \theta^+)} \right] \quad \xi_{**} - b > 0 .$$

Now, for case 1, the slope of the Rayleigh curve in the  $\gamma, \theta$ -plane is negative for each metastable phase, hence  $\theta_0 - \theta^- < 0$  and  $\theta_b - \theta^+ > 0$ . Moreover, in case 1 one has  $r_1(\dot{s}) < 0$ ,  $r_2(\dot{s}, \theta^-) > 0$  and  $r_2(\dot{s}, \theta^+) < 0$ . From the above expressions for  $\xi_*$  and  $\xi_{**}$ , it follows that if any of the quantities in brackets (i.e., the arguments of the logarithmic function) is positive, then there is at least one singularity. Hence, to avoid the presence of a singularity (by “moving” it), it is necessary that

$$\begin{cases} r_2(\dot{s}, \theta^-) + r_1(\dot{s})(\theta_0 - \theta^-) > 0 , \\ r_2(\dot{s}, \theta^+) + r_1(\dot{s})(\theta_b - \theta^+) < 0 . \end{cases} \quad (5.28)$$

Define a “mean” isentropic sound speed (along the Rayleigh curve) for each metastable phase as

$$a_{e,ls}^2 = a^2 \left( 1 + G\alpha \frac{\theta_0 + \theta^-}{2} \right) , \quad a_{e,hs}^2 = a^2 \left( 1 + G\alpha \frac{\theta_b + \theta^+}{2} \right) .$$

Therefore, from the expressions for  $r_1$  and  $r_2$  given by (5.11), the restrictions (5.28) can also be expressed as  $a_{e,hs}^2 < \dot{s}^2 < a_{e,ls}^2$ . Since, in this case,  $\theta_0 < \theta^-$  and  $\theta_b > \theta^+$ , then this restriction is stronger than the subsonic-supersonic condition, i.e.,

$$(a_e^+)^2 < a_{e,hs}^2 < \dot{s}^2 < a_{e,ls}^2 < (a_e^-)^2 . \quad (5.29)$$

## 5.6 The unstable phase.

The Rayleigh set for the unstable phase generated at  $(\gamma_0, \theta_0)$  can be obtained from (2.40) and (5.1)<sub>1</sub>, although the explicit form of  $\gamma^{R,u}(\theta)$  is not required here. Henceforth, the analysis will be carried out only for case 1 of the previous section. Recall that the following assumptions and restrictions are enforced:

$$\begin{aligned} \gamma^+ &> \gamma^- , \quad \theta^+ < \theta^- , \quad \dot{s} > 0 , \\ a^2 &< (a_e^+)^2 < \dot{s}^2 < (a_e^-)^2 . \end{aligned}$$

Henceforth, assume the existence of an admissible Rayleigh set  $\gamma^{R,u}(\theta)$ . It is important to remark that since  $\gamma^{R,u}(\theta)$  is generated at  $(\gamma_0, \theta_0)$ , then the Rayleigh set is given in terms of  $(\dot{s}, \theta_0, \gamma_0)$ . In view of (5.16) and (5.26), it is possible to express the Rayleigh set in terms of  $(\dot{s}, \theta^-, \gamma^-)$ . Moreover, since  $\theta(0) = \theta_0$  and  $\gamma(0) = \gamma_0$  then, continuity of  $\gamma^R(\theta)$  at  $\theta = \theta_0$  and  $\theta = \theta_b$  is equivalent to continuity of  $\gamma(\xi)$  and  $\theta(\xi)$  at  $\xi = 0$  and  $\xi = b$ . By construction,  $\gamma^R(\theta)$  is continuous at  $\theta = \theta_0$ . It is a matter of algebra to prove that  $\gamma^R(\theta)$  is continuous at  $\theta_b$  as long as the values at  $\xi \rightarrow \pm\infty$  satisfy the restriction (2.52)<sub>2</sub>, which corresponds to the momentum jump condition of the sharp interface theory (see remark at the end of Section 5.4).

The next step is to prove the existence of a solution for equation (5.17)<sub>2</sub>. The derivative of the right-hand side of (5.17)<sub>2</sub> with respect to  $\theta$  is given by (5.3). It can be shown that  $\bar{\psi}_{\gamma\gamma} < 0$  for the unstable phase. Now, since

$$\bar{\psi}_{\theta\theta} = -\frac{c}{\theta} + \frac{a^2\gamma_T(\gamma - \gamma_C)^2}{\theta(M - m)(\theta - \theta_C)^3} ,$$

then  $\bar{\psi}_{\theta\theta} < 0$  in the unstable region (see end of Section 2.5). It was shown in Section 2.2 that

$$\tilde{\epsilon}_{\gamma\gamma}(\gamma, \bar{\eta}(\gamma, \theta)) = \frac{\bar{\psi}_{\gamma\gamma}\bar{\psi}_{\theta\theta} - \bar{\psi}_{\gamma\theta}^2}{\bar{\psi}_{\theta\theta}} ;$$

therefore, the sign of  $dH^u/d\theta$  depends on the sign of  $\tilde{\epsilon}_{\gamma\gamma}$ . From stability arguments,



the thermoelastic material is unstable if  $\tilde{\epsilon}_{\gamma\gamma} < 0$ , hence,

$$\frac{dH^u}{d\theta} \geq 0$$

throughout the unstable phase and it follows that  $H^u(\gamma^{R,u}(\theta), \theta)$  is a nondecreasing function of  $\theta$ . As mentioned before, the Rayleigh set can be viewed as given by  $(\dot{s}, \theta^-, \gamma^-)$  hence the Hugoniot function also depends on the same parameters. Notice that, by construction,

$$H^u(\gamma^{R,u}(\theta_0), \theta_0) = 0 .$$

It is important to remark that this Hugoniot *function* is generated at  $(\gamma_0, \theta_0)$  which does *not* belong to the Hugoniot *set* of the problem. The Hugoniot sets  $\mathcal{H}_\pm$  are given by the Hugoniot functions based at  $(\gamma^+, \theta^+)$  and  $(\gamma^-, \theta^-)$  respectively and they do not coincide in general with the set of points where  $H^u$  vanishes. Now, from (5.17)<sub>2</sub>,

$$-\int_{\theta}^{\theta_0} \left[ -\frac{\rho\dot{s}}{k} H^u(\gamma^{R,u}(\check{\theta}), \check{\theta}) + \theta'_0 \right]^{-1} d\check{\theta} = \xi \quad \text{for } 0 < \xi < b, \quad (5.30)$$

where  $\theta'_0$  can be obtained from the expression of the temperature in the high strain phase ( $\xi < 0$ ) and by enforcing the jump condition (4.57) at  $\xi = 0$ , i.e.,

$$\theta'_0 = \left. \frac{d\theta}{d\xi} \right|_{\xi=0^-} = \left. \frac{d\theta}{d\xi} \right|_{\xi=0^+} .$$

From (5.23) and (5.24), this derivative can be viewed as given in terms of  $(\dot{s}, \theta^-, \gamma^-)$ , i.e.,

$$\theta'_0 = [r_1(\dot{s})(\theta_0 - \theta^-) + r_2(\dot{s}, \theta^-)] (\theta_0 - \theta^-) . \quad (5.31)$$

Enforcing condition (5.28)<sub>1</sub> guarantees that  $\theta'_0 < 0$ . Since the Hugoniot function  $H^u$  is positive throughout the unstable phase—it vanishes only at  $(\gamma^{R,u}(\theta_0), \theta_0)$ —and since in this case  $\dot{s} > 0$ , the integrand in (5.30) is a nondecreasing function of  $\check{\theta}$ , hence this relation defines implicitly  $\theta(\xi)$  in the unstable region. More precisely,  $\theta(\xi)$  decreases

from  $\theta_0$  at  $\xi = 0$  to  $\theta_b$  at  $\xi = b$  and the integrand increases from  $1/\theta'_0$  at  $\check{\theta} = \theta_b$  to  $1/\theta'_b$  at  $\check{\theta} = \theta_0$ . Moreover, as shown below, the restriction (5.28)<sub>2</sub> guarantees that  $\theta'_b < 0$ . From the foregoing analysis,  $\theta(\xi)$  depends on  $(\dot{s}, \theta^-, \gamma^-)$ . The continuity of  $\theta'(\xi)$  at  $\xi = 0$  is thus guaranteed by construction. From (5.30), the width of the unstable region can be expressed as

$$b = - \int_{\theta_b}^{\theta_0} \left[ -\frac{\rho \dot{s}}{k} H^u(\gamma^{R,u}(\check{\theta}), \check{\theta}) + \theta'_0 \right]^{-1} d\check{\theta} . \quad (5.32)$$

Therefore and in view of (5.27), equation (5.32) can be thought of as a relation of the type

$$b = b(\dot{s}, \gamma^-, \theta^-, \gamma^+, \theta^+) .$$

At this point, the only remaining condition to be fulfilled is the jump condition (4.57) at  $\xi = b$ , i.e.,

$$\left. \frac{d\theta}{d\xi} \right|_{\xi=b^-} = \left. \frac{d\theta}{d\xi} \right|_{\xi=b^+} . \quad (5.33)$$

Now, from (5.23) and (5.25), the right-hand side of (5.33) is given by

$$\left. \frac{d\theta}{d\xi} \right|_{\xi=b^+} = [r_1(\dot{s})(\theta_b - \theta^+) + r_2(\dot{s}, \theta^+)] (\theta_b - \theta^+) .$$

From (5.17) and (5.31), the left hand-side of (5.33) can be expressed as

$$\left. \frac{d\theta}{d\xi} \right|_{\xi=b^-} = -\frac{\rho \dot{s}}{k} H^u(\gamma_b, \theta_b) + [r_1(\dot{s})(\theta_0 - \theta^-) + r_2(\dot{s}, \theta^-)] (\theta_0 - \theta^-) .$$

Now, by definition, the Hugoniot function generated at  $(\gamma_0, \theta_0)$  and evaluated at  $(\gamma_b, \theta_b)$  is, from (2.35),

$$\epsilon(\gamma_b, \theta_b) - \epsilon(\gamma_0, \theta_0) - \frac{1}{2\rho} (\sigma(\gamma_b, \theta_b) + \sigma(\gamma_0, \theta_0)) (\gamma_b - \gamma_0) .$$

Since continuity of  $\gamma$  and  $\theta$  has been enforced at  $\xi = 0$  and  $\xi = b$  and since  $\epsilon$  and  $\sigma$  are continuous functions of strain and temperature, then it is possible to use the

expressions of these functions in the low and high strain phases respectively. From this point, it is just a matter of algebra to check that, as mentioned in Section 5.4, the continuity of  $\theta'(\xi)$  at  $\xi = b$  is equivalent to the energy jump condition (2.59).

## 5.7 A one-parameter family of solutions.

It is shown in this section that admissible solutions to the phase boundary propagation problem are known up to the phase boundary velocity  $\dot{s}$ . This velocity can be viewed as a parameter that defines a family of solutions. Hence, the presence of heat conduction only regularizes the moving discontinuity, but fails to deliver an additional restriction on the values  $(\gamma^\pm, \theta^\pm)$  and the phase boundary velocity  $\dot{s}$ . In view of the above, it is useful to recapitulate the steps to construct a solution, presented here in nondimensional form.

**Dimensionless solution:** Define a dimensionless coordinate  $z$  by

$$z = \frac{\rho c a}{k} \xi .$$

This is the same dimensionless coordinate as in the shock wave problem. Now, for given conditions  $(\delta^+, T^+)$  in the high strain phase, *choose a supersonic* phase boundary velocity  $v$  in a given interval  $v_{\min}^2 < v^2 < v_{\max}^2$  shown below. Obtain the temperature  $T^-$  by solving (2.59). Obtain the corresponding strain  $\delta^-$  from (2.58)<sub>1</sub>. The temperature  $T_0$  at  $z = 0$  is related to the values at  $-\infty$  by

$$T_0 = \left( \frac{G}{1 - v^2} - M \right)^{-1} [\delta_C - \delta^- + M(T^- - T_C)] + T^- ,$$

and the corresponding strain is

$$\delta_0 = \delta_C + M(T_0 - T_C) .$$

The temperature at  $z = b$  is given by

$$T_b = \left( \frac{G}{1 - v^2} - m \right)^{-1} [\delta_C - \delta^+ + m(T^+ - T_C)] + T^+ .$$

Define the function

$$K(v, T_*, T) = \frac{r_2(v, T)}{r_1(v)} \left( \frac{1}{T_* - T} \right) + 1 ,$$

where the functions  $r_1$  and  $r_2$  are given by (2.60). The explicit form of the temperature in the metastable phases is

$$T(z) = \begin{cases} \frac{r_2(v, T^-)}{r_1(v)} \{K_1 \exp[-r_2(v, T^-)z] - 1\}^{-1} + T^- & z < 0 , \\ \frac{r_2(v, T^+)}{r_1(v)} \{K_3 \exp[-r_2(v, T^+)(z - b)] - 1\}^{-1} + T^+ & z > b , \end{cases}$$

where  $K_1 = K(v, T_0, T^-)$ ,  $K_3 = K(v, T_b, T^+)$ . The width  $b$  of the unstable region is given below. The temperature gradient at  $z = 0$  is given by

$$T'_0 = \left. \frac{dT}{dz} \right|_{z=0} = [r_1(v)(T_0 - T^-) + r_2(v, T^-)] (T_0 - T^-) .$$

The temperature inside the unstable region can be obtained by solving the following equation:

$$- \int_{T_0}^T \{ -vH^u(\delta^{R,u}(\check{T}), \check{T}) + T'_0 \}^{-1} d\check{T} = z , \quad (5.34)$$

where the Rayleigh set is given by

$$\delta^{R,u}(T) = \frac{\delta_0 - \delta_C - M(T - T_C) + G(m - M)(T - T_C)(T - T_0)}{(1 - v^2)(m - M)(T - T_C) - 1} + \delta_0 ,$$

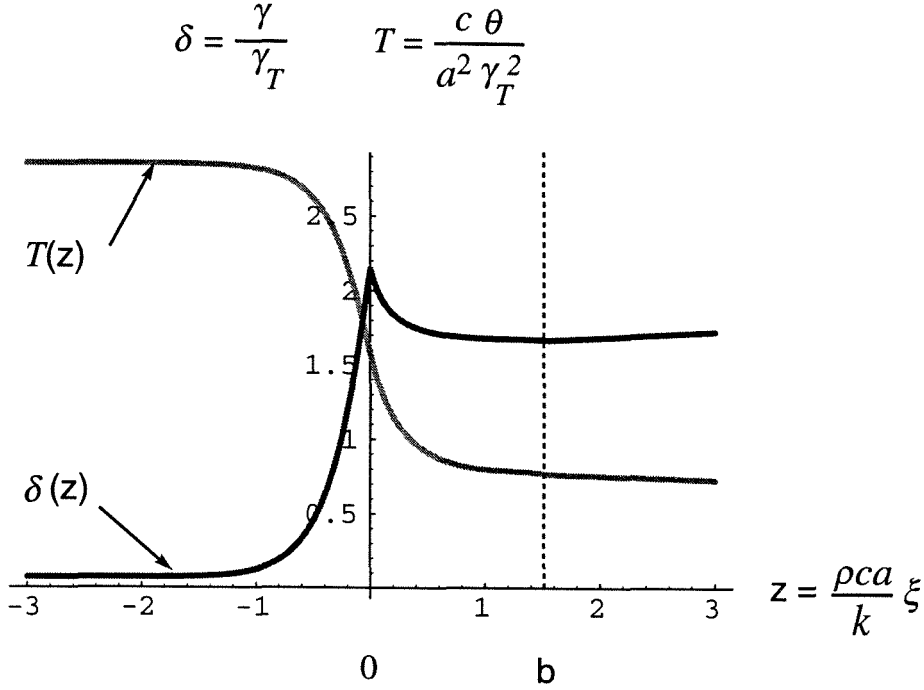


Figure 5.1: Structured traveling phase boundary (temperature and strain).

and the Hugoniot function is expressed as

$$H^u(\delta, T) = \frac{1}{2(m-M)} \left\{ \frac{(\delta - \delta_C) [T_C(\delta_0 - \delta_C) - T(\delta + \delta_0 - 2\delta_C)]}{(T - T_C)^2} + M(\delta + \delta_0 - 2\delta_C) + M^2 T_C \right\} + \frac{G}{2}(T + T_0)(\delta - \delta_0) + T - T_0 .$$

The width  $b$  is obtained by setting  $z = b$  in equation (5.34) with  $T = T_b$  in the upper limit of the integral. A typical solution is shown in Figures 5.1 (temperature and strain) and 5.2 (stress and entropy). The corresponding Rayleigh curve in the  $\delta, T$ -plane is the same as shown in Figure 2.2. The bar is in the (front) state  $(\delta^+, T^+)$  for  $t \rightarrow -\infty$  and ends up in the (back) state  $(\delta^-, T^-)$  as  $t \rightarrow +\infty$ .

**Family of solutions (restrictions on  $v^2$ ):** from the restriction (5.29) (in nondimensional form) it follows that the phase boundary speed has to satisfy

$$G^2(T_b + T^+) < 2(v^2 - 1) < G^2(T_0 + T^-) .$$

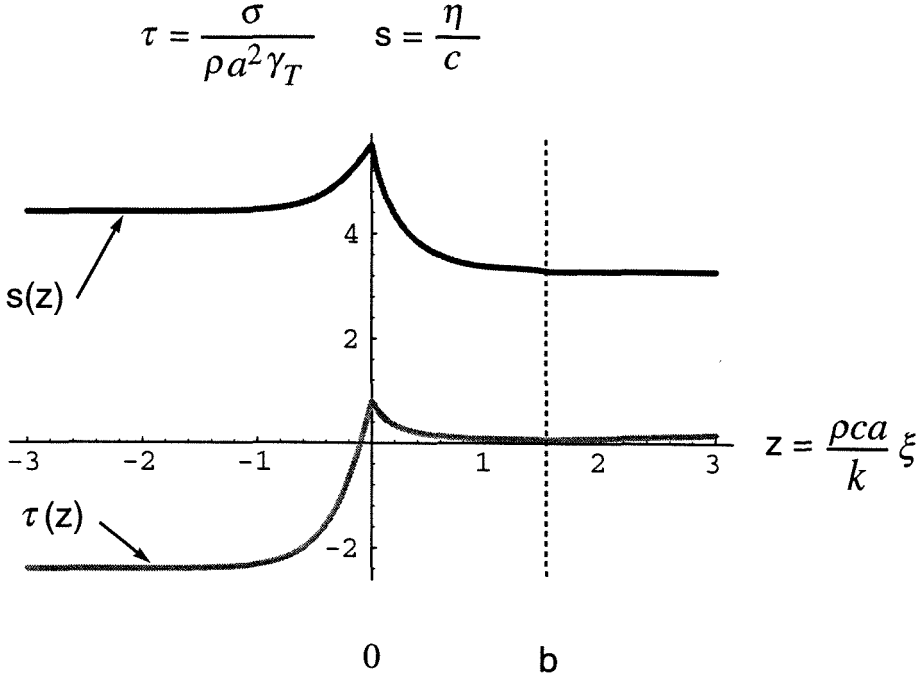


Figure 5.2: Structured traveling phase boundary (stress and entropy).

Using equations (5.26) and (5.27) to eliminate the temperatures  $T_b$  and  $T_0$  in the above relation gives

$$\begin{cases} G^2 \left( \frac{1 - v^2}{G - M(1 - v^2)} \right) [\delta_C - \delta^- + M(T^- - T_C)] + 2(1 - v^2) + 2G^2 T^- > 0, \\ G^2 \left( \frac{1 - v^2}{G - m(1 - v^2)} \right) [\delta_C - \delta^+ + m(T^+ - T_C)] + 2(1 - v^2) + 2G^2 T^+ < 0. \end{cases}$$

Furthermore, assume that  $m > 0$  and, since in this case  $1 - v^2 < 0$ , then the above inequalities can be expressed as (recall that  $M > 0$ )

$$\begin{cases} w^2 + h_1(\delta^-, T^-, M)w + h_2(T^-, M) < 0, \\ w^2 + h_1(\delta^+, T^+, m)w + h_2(T^+, m) > 0, \end{cases}$$

where

$$w = 1 - v^2$$

and

$$\begin{cases} h_1(\delta, T, n) = -\frac{G^2}{2n} \left[ \frac{2}{G} + \delta_C - \delta - n(T + T_C) \right] , \\ h_2(T, n) = -\frac{G^3 T}{n} . \end{cases}$$

Let  $h_1^+ = h_1(\delta^+, T^+, m)$ ,  $h_1^- = h_1(\delta^-, T^-, M)$  and similarly for  $h_2$ . If  $m > 0$ , then  $h_2^\pm < 0$  and it follows that the roots of the equations  $w^2 + h_1^\pm w + h_2^\pm = 0$  are real and have opposite signs. Denote by  $w_\pm^-$  and  $w_\pm^+$  the corresponding roots of these equations, where the subscript of  $w$  refers to its sign. Hence, the above restrictions can be expressed as

$$1 - w_-^+ < v^2 < 1 - w_-^- \quad \text{if } w_-^+ > w_-^- . \quad (5.35)$$

If  $w_-^+ < w_-^-$  then there are no solutions. Expanding  $w_\pm^\pm$  in powers of  $G$  gives

$$w_\pm^\pm = -G^2 T^\pm + O(G^3) ,$$

hence, for small  $G$  and up to  $O(G^3)$ ,  $w_-^+ > w_-^-$ . Any value of  $v^2$  that satisfies (5.35) determines an admissible solution for the phase boundary propagation problem. Nevertheless, notice that the conditions in the phase boundary propagation problem are given for one side only (either at  $z \rightarrow +\infty$  or  $z \rightarrow -\infty$ ) and the conditions on the other side depend on  $v^2$ . Hence, one bound is well defined but the other is not. It is possible to obtain the unknown bound numerically as follows: suppose that the state  $(\delta^+, T^+)$  is known and fixed. From (2.59) and (2.58)<sub>1</sub> one has

$$\begin{aligned} \delta^- &= \delta^-(v^2, \delta^+, T^+) , \\ T^- &= T^-(v^2, \delta^+, T^+) . \end{aligned}$$

It follows that

$$w_-^- = w_-^-(v^2, \delta^+, T^+) .$$

Although it is not proved here, there is numerical evidence that the inequality

$$v^2 < 1 - w_-(v^2, \delta^+, T^+)$$

corresponds to

$$v^2 < v_{\max}^2,$$

where  $v_{\max}^2$  depends on  $(\delta^+, T^+)$  only. Let  $v_{\min}^2 = 1 - w_+(\delta^+, T^+)$ , hence there is an interval

$$v_{\min}^2 < v^2 < v_{\max}^2$$

whose limits depend only on  $(\delta^+, T^+)$  and in which any value  $v^2$  provides an admissible solution as shown above.

## 5.8 Special cases.

### 5.8.1 Phase boundary traveling at the isentropic sound speed.

In the previous section it was assumed that  $r_2(\dot{s}, \theta^\pm) \neq 0$ . Suppose now that  $r_2(\dot{s}, \theta^-) = 0$ , which corresponds to  $\dot{s}^2 = (a_e^-)^2$  (the case  $r_2(\dot{s}, \theta^+) = 0$  which corresponds to  $\dot{s}^2 = (a_e^+)^2$  is similar). Solving equation (5.14)<sub>2</sub> with  $r_2(\dot{s}, \theta^-) = 0$ , gives the temperature in the high strain phase, i.e.,

$$\theta(\xi) = -\frac{\theta_0 - \theta^-}{r_1(\dot{s})(\theta_0 - \theta^-)\xi - 1} + \theta^- \quad \text{for } \xi < 0,$$

where  $\theta_0 = \theta(0)$ . Regardless of the sign of  $\dot{s}$  and the value of  $\theta_0$ , the condition (5.15)<sub>2</sub> is satisfied. For the low strain phase (i.e., for  $\xi \geq b$ ), following a similar analysis as in the previous section, a necessary condition for the existence of a solution is  $r_2(\dot{s}, \theta^+) < 0$ . There are two cases to consider, viz.,



**Case 1:** Suppose  $\dot{s} > 0$ ; then, necessarily,

$$\dot{s}^2 = (a_e^+)^2 < (a_e^-)^2 ,$$

hence  $\theta^+ < \theta^-$ .

**Case 2:** Suppose  $\dot{s} < 0$ ; then, necessarily,

$$\dot{s}^2 = (a_e^+)^2 > (a_e^-)^2 ,$$

hence  $\theta^+ > \theta^-$ .

As in the previous section, the second case can be discarded by virtue of the momentum jump condition if  $\gamma^+ > \gamma^-$ . From the first case, it follows that

$$r_1(\dot{s}) > 0 .$$

Moreover, since the slope of the Rayleigh set in the  $\gamma, \theta$ -plane is negative, then  $\theta_0 < \theta^-$ , and it follows that there is a point  $\xi_* < 0$  where

$$r_1(\dot{s})(\theta_0 - \theta^-)\xi_* - 1 = 0 .$$

This means that the temperature, as given above, is unbounded at  $\xi = \xi_*$ , hence this is not an admissible structured traveling wave. The case  $r_2(\dot{s}, \theta^+) = 0$  is similar in the sense that the solution for  $\xi > b$  has a singularity.

### 5.8.2 Semi-structured wave.

It is possible to take the solution for one phase as the trivial solution. For definiteness, assume that the solution for the low strain phase (i.e.,  $\xi < 0$ ) is  $\theta(\xi) = \theta^-$ ,  $\forall \xi < 0$  (the case  $\theta(\xi) = \theta^+$ ,  $\forall \xi > b$  is similar). For a nontrivial solution in the high strain phase, it is necessary that  $r_2(\dot{s}, \theta^+) < 0$ . In that case, from (5.23), the temperature

in the stable phases is

$$\theta(\xi) = \begin{cases} \theta^- & \text{for } \xi < 0, \\ \left\{ K_3 \exp[-r_2(\dot{s}, \theta^+) \xi] - \frac{r_1(\dot{s})}{r_2(\dot{s}, \theta^+)} \right\}^{-1} + \theta^+ & \text{for } \xi > b. \end{cases}$$

Now, since  $\forall \xi < 0$ ,  $\theta'(\xi) = 0$ , then, from (5.17) and the jump condition (4.57), the temperature is given in the unstable phase by

$$\int_{\theta_0}^{\theta} \left[ -\frac{\rho \dot{s}}{k} H^u(\gamma^{R,u}(\check{\theta}), \check{\theta}) \right]^{-1} d\check{\theta} = \xi \quad \text{for } 0 < \xi < b.$$

The Hugoniot function  $H^{R,u}$  based at  $(\gamma_0, \theta_0)$  for the unstable phase satisfies

$$H^{R,u}(\gamma_0, \theta_0) = 0.$$

Therefore, the above integral diverges and it is not possible to find a solution in the unstable phase. Hence, the semi-structured phase boundary is not admissible.

### 5.8.3 Zero thermal expansion.

In the previous section, it was assumed that  $r_1(\dot{s}) \neq 0$ . Consider the case when  $r_1(\dot{s}) = 0$ , which occurs if  $\alpha = 0$ . The phase boundary propagation problem, as given by (5.14)-(5.22), can be formulated for  $\alpha = 0$  as follows:

**Problem 1:** Low strain phase. Equation (5.14) becomes

$$\begin{cases} \gamma = \gamma^-, \\ \theta' = -\frac{\dot{s}}{\kappa}(\theta - \theta^-). \end{cases}$$

The condition (5.15)<sub>1</sub> is automatically satisfied and the remaining condition for the strain, (5.16)<sub>1</sub>, is fulfilled if the corresponding temperature  $\theta_0$  is given by

$$\theta_0 = \theta_C - \frac{\gamma_C - \gamma^-}{M}.$$

The condition (5.15)<sub>2</sub> remains unchanged.

**Problem 2:** Unstable phase. Similarly, from equation (5.17), one has, in  $(0, b)$ ,

$$\begin{cases} \gamma = \gamma^{R,u}(\theta) , \\ \theta' - \theta'_0 = -\frac{\rho\dot{s}}{k} H^u(\gamma^{R,u}(\theta), \theta) . \end{cases}$$

The conditions (5.18) and (5.19) become in this case  $\gamma(0^+) = \gamma^+$ ,  $\gamma(b^-) = \gamma^-$ ,  $\theta(0^+) = \theta_0$  and  $\theta(b^-) = \theta_b$ , where the requirement of continuity at  $\xi = 0$  and  $\xi = b$  was enforced (see also problem 3 below).

**Problem 3:** High strain phase. From equation (5.20), in  $(b, +\infty)$  the problem can be expressed as

$$\begin{cases} \gamma = \gamma^+ , \\ \theta' = -\frac{\dot{s}}{\kappa}(\theta - \theta^+) . \end{cases}$$

The condition (5.22)<sub>1</sub> is automatically satisfied and the requirement (5.21)<sub>1</sub> is satisfied if the temperature  $\theta_b$  is given by

$$\theta_b = \theta_C - \frac{\gamma_C - \gamma^+}{m} .$$

The condition (5.22)<sub>2</sub> remains unchanged.

The temperature in the metastable phases is given by

$$\theta(\xi) = \begin{cases} K_1 \exp\left[-\frac{\dot{s}}{\kappa}\xi\right] + \theta^- & \text{for } \xi < 0 , \\ K_3 \exp\left[-\frac{\dot{s}}{\kappa}\xi\right] + \theta^+ & \text{for } \xi > b , \end{cases}$$

where  $K_1$  and  $K_3$  are constants. Notice that, since  $\kappa > 0$ , then if  $\dot{s} > 0$ ,  $\lim_{\xi \rightarrow +\infty} \theta(\xi) = \theta^+$  but the temperature grows unboundedly as  $\xi \rightarrow -\infty$ . Conversely, if  $\dot{s} < 0$ , then  $\lim_{\xi \rightarrow -\infty} \theta(\xi) = \theta^-$  but the temperature grows unboundedly as  $\xi \rightarrow +\infty$ . Hence, in

order to have a nontrivial solution, one of the constants  $K$  must be taken as zero. Suppose first that  $\dot{s} > 0$  and take  $K_1 = 0$ . Therefore, the temperature is given by

$$\theta(\xi) = \begin{cases} \theta^- & \text{for } \xi < 0, \\ K_3 \exp\left[-\frac{\dot{s}}{\kappa}\xi\right] + \theta^+ & \text{for } \xi > b, \end{cases}$$

hence

$$\theta'_0 = 0.$$

For the unstable phase, the temperature is given implicitly by

$$\xi = - \int_{\theta_0}^{\theta} \left\{ -\frac{\rho\dot{s}}{k} H^u(\gamma^{R,u}(\check{\theta}), \check{\theta}) \right\}^{-1} d\check{\theta},$$

but, by construction,  $H^u(\gamma_0, \theta_0) = 0$ . Based on the Hugoniot function, it is not hard to see that the singularity at  $\theta = \theta_0$  is stronger than  $1/\sqrt{\theta}$ , hence the above integral diverges and it is not possible to find a temperature profile in the unstable region. One can interpret this result as having an infinite unstable phase (i.e.,  $b \rightarrow +\infty$ ) since  $(\gamma^-, \theta^-)$  has to lie in the boundary between the low strain phase and the unstable phase. The case  $\dot{s} < 0$  is similar.

# Chapter 6 Structured wave: Viscosity, strain gradient and heat conduction

## 6.1 Introduction.

The traveling wave problem is analyzed here within the context of the augmented theory including viscosity, strain gradient and heat conduction. Section 6.2 deals with the basic equations and a linear stability analysis. Classical techniques of singular perturbation theory are then used to identify the region where the viscosity and strain gradient play an important role (i.e., the “inner” solution) and the region where heat conduction is the relevant structuring mechanism (i.e., the “outer” solution). A uniformly valid approximation is then obtained from the asymptotic matching of the inner and outer solutions and a kinetic relation is derived for a subsonically traveling phase boundary.

It is important to remark that the presence of heat conduction induces some structure to the phase boundary but, more significantly, it permits specification of different temperatures at  $+\infty$  and  $-\infty$ . This in turn allows an appropriate connection with the *adiabatic* limit case.

## 6.2 Basic equations.

Using equations (4.64), (4.65) and (4.66) in the governing equations (4.61) and (4.63) gives

$$\lambda(\gamma'' - \gamma_0'') + \nu \dot{s}(\gamma' - \gamma_0') - [\bar{\psi}_\gamma(\gamma, \theta) - \bar{\psi}_\gamma(\gamma_0, \theta_0)] + \dot{s}^2(\gamma - \gamma_0) = 0 , \quad (6.1)$$

$$\frac{k}{\rho}(\theta' - \theta'_0) + \dot{s} \left\{ \bar{\epsilon}(\gamma, \theta) - \bar{\epsilon}(\gamma_0, \theta_0) - \frac{1}{2}\lambda(\gamma'^2 - \gamma_0'^2) - \frac{1}{2}\dot{s}^2(\gamma - \gamma_0)^2 - [\bar{\psi}_\gamma(\gamma_0, \theta_0) - \lambda\gamma_0'' - \nu\dot{s}\gamma_0'](\gamma - \gamma_0) \right\} = 0. \quad (6.2)$$

The following stability analysis, with some modifications, follows from [25]. Introduce a new function  $w = \gamma'$ . Equations (6.1) and (6.2) can be expressed as a system of first order ordinary differential equations:

$$\left\{ \begin{array}{l} \gamma' = w \\ w' - w'_0 = -\frac{1}{\lambda} \{ \nu\dot{s}(w - w_0) - [\bar{\psi}_\gamma(\gamma, \theta) - \bar{\psi}_\gamma(\gamma_0, \theta_0)] + \dot{s}^2(\gamma - \gamma_0) \} \\ \theta' - \theta'_0 = -\frac{\rho\dot{s}}{k} \left\{ \bar{\epsilon}(\gamma, \theta) - \bar{\epsilon}(\gamma_0, \theta_0) - \frac{\lambda}{2}(w^2 - w_0^2) - \frac{\dot{s}^2}{2}(\gamma - \gamma_0)^2 - [\bar{\psi}_\gamma(\gamma_0, \theta_0) - \lambda w'_0 - \nu\dot{s}w_0](\gamma - \gamma_0) \right\} \end{array} \right. \quad (6.3)$$

Let  $(\gamma_*, w_*, \theta_*)$  be an equilibrium point of this dynamical system. Therefore, from (6.3) and assuming  $\dot{s} \neq 0$ , these points satisfy

$$\left\{ \begin{array}{l} w_* = 0 \\ \bar{\psi}_\gamma(\gamma_*, \theta_*) - \frac{\sigma^+}{\rho} = \dot{s}^2(\gamma_* - \gamma^+) \\ \bar{\epsilon}(\gamma_*, \theta_*) - \epsilon^+ = \frac{1}{2} \left( \bar{\psi}_\gamma(\gamma_*, \theta_*) + \frac{\sigma^+}{\rho} \right) (\gamma_* - \gamma^+) \end{array} \right. \quad (6.4)$$

Hence, the equilibrium points of the regularized traveling wave problem satisfy the jump conditions of the classical adiabatic theory for a given  $\gamma$  state  $(\gamma^+, \theta^+)$ ; see relations (2.13) and (2.14). The states at  $\xi \rightarrow \pm\infty$  given by (4.48)-(4.50) are equilibrium points.

To analyze the nature of the equilibria, consider the linearized system around an

equilibrium point:

$$W' = AW ,$$

where  $W = (\gamma, w, \theta)$  and

$$A = \begin{bmatrix} 0 & 1 & 0 \\ -\frac{1}{\lambda} [\dot{s}^2 - \psi_{\gamma\gamma}^*] & -\frac{\nu\dot{s}}{\lambda} & \frac{\psi_{\gamma\theta}^*}{\lambda} \\ \frac{\rho\dot{s}}{k} \theta_* \psi_{\gamma\theta}^* & 0 & \frac{\rho\dot{s}}{k} \theta_* \psi_{\theta\theta}^* \end{bmatrix} , \quad (6.5)$$

where  $\psi_{\gamma\gamma}^* = \bar{\psi}_{\gamma\gamma}(\gamma_*, \theta_*)$ ,  $\psi_{\gamma\theta}^* = \bar{\psi}_{\gamma\theta}(\gamma_*, \theta_*)$ ,  $\psi_{\theta\theta}^* = \bar{\psi}_{\theta\theta}(\gamma_*, \theta_*)$ . Notice that to obtain the term  $A_{31}$ , the relation  $\bar{\epsilon}_\gamma = \bar{\psi}_\gamma - \theta \bar{\psi}_{\gamma\theta}$  and (6.4)<sub>2</sub> were used. The term  $A_{33}$  was obtained using  $\bar{\epsilon}_\theta = -\theta \bar{\psi}_{\theta\theta}$ . Let  $\beta = \beta_i$ ,  $i = 1, 2, 3$ , be the eigenvalues of  $A$ . The characteristic polynomial of  $A$  is  $\beta^3 - I_1\beta^2 + I_2\beta - I_3 = 0$ , where  $I_i$ ,  $i = 1, 2, 3$ , are the principal invariants of  $A$ . A direct calculation gives

$$\text{tr } A = -\dot{s} \left( \frac{\nu}{\lambda} + \frac{\rho c_*}{k} \right) , \quad (6.6)$$

$$\frac{1}{2} [(\text{tr } A)^2 - \text{tr } A^2] = -\frac{1}{\lambda} \left[ \frac{\mu_*}{\rho} - \dot{s}^2 \left( \nu \left( \frac{\rho c_*}{k} \right) + 1 \right) \right] , \quad (6.7)$$

$$\det A = \frac{\dot{s}}{\lambda} \left( \frac{\rho c_*}{k} \right) \left[ \frac{\mu_{e*}}{\rho} - \dot{s}^2 \right] , \quad (6.8)$$

where, using the material parameters introduced in Section 2.2,

$$\begin{aligned} c_* &= -\theta_* \psi_{\theta\theta}^* , \\ \mu_* &= \rho \psi_{\gamma\gamma}^* , \\ \mu_{e*} &= \rho \left( \frac{\psi_{\gamma\gamma}^* \psi_{\theta\theta}^* - \psi_{\gamma\theta}^{*2}}{\psi_{\theta\theta}^*} \right) . \end{aligned}$$

Let  $a_*$  and  $a_{e*}$  be the values of the isothermal and isentropic sound speeds and  $\kappa_*$ , the value of the thermal diffusivity at an equilibrium point  $(\gamma_*, \theta_*)$ . The principal

invariants can then be written as

$$I_1 = -\dot{s} \left( \frac{\nu}{\lambda} + \frac{1}{\kappa_*} \right) , \quad (6.9)$$

$$I_2 = -\frac{1}{\lambda} \left[ a_*^2 - \dot{s}^2 \left( \frac{\nu}{\kappa_*} + 1 \right) \right] , \quad (6.10)$$

$$I_3 = \frac{\dot{s}}{\lambda \kappa_*} \left[ a_{e*}^2 - \dot{s}^2 \right] . \quad (6.11)$$

Define

$$\begin{aligned} \iota_1 &= I_3 + \frac{I_1 I_2}{3} - \frac{2}{27} I_1^3 , \\ \iota_2 &= \frac{I_2}{3} - \frac{I_1^2}{9} , \\ \iota_3 &= \iota_1^2 + 4\iota_2^3 , \end{aligned} \quad (6.12)$$

then, when  $\iota_3 < 0$ , all three eigenvalues are real and different; when  $\iota_3 = 0$ , all eigenvalues are real and two of them are equal and when  $\iota_3 > 0$  one solution is real and the two other are complex. The eigenvalues  $\beta_i$  satisfy

$$\begin{aligned} \beta_1 + \beta_2 + \beta_3 &= I_1 , \\ \beta_1 \beta_2 \beta_3 &= I_3 , \end{aligned}$$

hence if the three eigenvalues are real, and since  $I_1 < 0$  when  $\dot{s} > 0$ , then the three eigenvalues cannot be all positive. Therefore, if  $I_3 > 0$ , the equilibrium saddle point has a two-dimensional *stable* manifold and a one-dimensional *unstable* manifold. If  $\dot{s} < 0$ , then the equilibrium point has a two-dimensional *unstable* manifold and a one-dimensional *stable* manifold. If  $I_3 < 0$  then the situation is reversed.

Consider the thermoelastic material characterized by the Helmholtz potential (2.40). In this case, the stress given by equation (4.65) becomes

$$\sigma = \mu\gamma - \alpha\mu\theta - \rho\lambda\gamma'' - \rho\nu\dot{s}\gamma' + H_4 , \quad (6.13)$$



where

$$H_4 = \begin{cases} \alpha\mu\theta_T & \text{low strain phase,} \\ \alpha\mu\theta_T - \mu\gamma_T & \text{high strain phase.} \end{cases}$$

Similarly, by (4.34), (4.35) and (2.40), the internal energy  $\epsilon$  is given by

$$\begin{aligned} \epsilon &= \bar{\epsilon}(\gamma, \theta) + \frac{1}{2}\lambda\gamma'^2 \\ &= \frac{\mu}{2\rho}\gamma^2 + c\theta + \frac{H_4}{\rho}\gamma + H_5 + \frac{1}{2}\lambda\gamma'^2, \end{aligned} \quad (6.14)$$

where

$$H_5 = \begin{cases} 0 & \text{low strain phase,} \\ \frac{\mu\gamma_T}{2\rho} - \frac{\alpha\mu\gamma_T^2\theta_T}{\rho} - \lambda_T & \text{high strain phase.} \end{cases}$$

### 6.3 Traveling shock wave.

Suppose that for a given  $\xi$ , all the points in  $[\xi, +\infty)$  are in the *low strain* phase so that, from (6.13) and (6.14),

$$\bar{\psi}_\gamma(\gamma, \theta) - \frac{\sigma^+}{\rho} = a^2(\gamma - \gamma^+) - \alpha a^2(\theta - \theta^+),$$

and

$$\bar{\epsilon}(\gamma, \theta) - \epsilon^+ = \frac{a^2}{2}(\gamma^2 - \gamma^{+2}) + c(\theta - \theta^+) + \frac{H_4}{\rho}(\gamma - \gamma^+).$$

Since

$$\frac{\sigma^+}{\rho} = a^2\gamma^+ - \alpha a^2\theta^+ + \frac{H_4}{\rho},$$

the system (6.3) becomes

$$\left\{ \begin{array}{l} \gamma' = w \\ w' = -\frac{1}{\lambda} \{ \nu \dot{s} w - (a^2 - \dot{s}^2)(\gamma - \gamma^+) + \alpha a^2(\theta - \theta^+) \} \\ \theta' = -\frac{\rho \dot{s}}{k} \left\{ \frac{1}{2} (a^2 - \dot{s}^2) (\gamma - \gamma^+)^2 + \alpha a^2 \theta^+ (\gamma - \gamma^+) \right. \\ \left. + c(\theta - \theta^+) - \frac{\lambda w^2}{2} \right\}. \end{array} \right. \quad (6.15)$$

**Special case: zero thermal expansion:** Henceforth, as a special case, assume that the thermal expansion coefficient  $\alpha$  is zero. In this case the problem is very simple since the system is uncoupled. The corresponding equation for the strain is, from (6.15)<sub>1,2</sub> with  $\alpha = 0$ , given by

$$\lambda \gamma'' + \nu \dot{s} \gamma' = 0, \quad (6.16)$$

hence

$$\gamma(\xi) = c_1 \exp \left[ -\frac{\dot{s} \nu \xi}{\lambda} \right] + c_2,$$

where  $c_1, c_2$  are constants. Now, the conditions at  $\xi \rightarrow \pm$  are  $\gamma(+\infty) = \gamma^+$  and  $\gamma(-\infty) = \gamma^-$  which cannot be satisfied simultaneously.

Even though the idea in the regularized theory is to obtain a solution where  $\gamma \in C^3(\mathbb{R})$  and  $\theta \in C^2(\mathbb{R})$ , it is possible to relax the regularity requirements. Divide the real axis into two intervals, namely  $(-\infty, 0)$  and  $(0, +\infty)$ , and consider functions  $\gamma \in C^0(\mathbb{R}) \cup C^3(\mathbb{R} - \{0\})$  and  $\theta \in C^0(\mathbb{R}) \cup C^2(\mathbb{R} - \{0\})$  (i.e., continuous functions whose derivatives might be discontinuous at  $\xi = 0$ ). For definiteness, assume that  $\dot{s} > 0$  (the case  $\dot{s} < 0$  is similar). Enforcing the conditions at  $\xi \rightarrow \pm\infty$  and requiring

that  $\gamma$  be continuous at  $\xi = 0$  provides the following solution for (6.16):

$$\gamma(\xi) = \begin{cases} \gamma^- & \text{for } \xi \in (-\infty, 0) , \\ (\gamma^- - \gamma^+) \exp \left[ -\frac{\dot{s}\nu\xi}{\lambda} \right] + \gamma^+ & \text{for } \xi \in [0, +\infty) . \end{cases} \quad (6.17)$$

Now, since there is a jump in  $\gamma'$  and  $\gamma''$  at  $\xi = 0$ , the appropriate jump conditions have to be satisfied. In the regularized theory, the momentum jump condition is  $[[\hat{\sigma}]] - \rho\dot{s}^2[[\gamma]] = 0$ . If  $\gamma$  is continuous at  $\xi = 0$ , then, from (6.13) and since  $[[\bar{\sigma}]] = 0$ , one has

$$\lambda[[\gamma'']] + \nu\dot{s}[[\gamma']] = 0 ,$$

which, from (6.17), implies that

$$\gamma^+ = \gamma^- ,$$

and hence there is no nontrivial solution to the problem.

## 6.4 Traveling phase boundary.

In this case, since the fields under consideration are piecewise differentiable, the traveling phase boundary problem has to be divided into three sub-problems. Suppose that the conditions at  $\xi \rightarrow +\infty$  correspond to the *low strain* phase and the conditions at  $\xi \rightarrow -\infty$  correspond to the *high strain* phase. Presumably there is an interval, say  $(0, b)$ , where the points are in the unstable phase. From the above considerations and in view of the smoothness requirements of the traveling wave, the solution must satisfy conditions (4.48), (4.50) and the following:

$$\begin{aligned} \theta(0^-) &= \theta(0^+) = \theta_0 , \\ \gamma(0^-) &= \gamma(0^+) = \gamma_m(\theta_0) , \\ \theta(b^-) &= \theta(b^+) = \theta_b , \\ \gamma(b^-) &= \gamma(b^+) = \gamma_M(\theta_b) , \end{aligned}$$

where the functions  $\gamma_m$  and  $\gamma_M$  are given by (2.39) and the temperatures  $\theta_0$  and  $\theta_b$  are unknown. The jump conditions (4.56) also have to be satisfied at  $\xi = 0$  and  $\xi = b$ . Additionally, for the class of traveling waves considered here, the phase segregation conditions must be enforced, i.e., the solution must be such that the material is in its high strain phase in  $(-\infty, 0)$ , unstable phase in  $(0, b)$  and low strain phase in  $(b, +\infty)$ . Moreover, the temperature has to be below the critical value  $\theta_C$ . These conditions are formally the same as (5.13).

**Structured phase boundary traveling wave problem:** *Given one end state, say  $(\gamma^-, \theta^-)$  at  $\xi \rightarrow -\infty$ , (or, alternatively,  $(\gamma^+, \theta^+)$  at  $\xi \rightarrow +\infty$ ) find all admissible states  $(\gamma^+, \theta^+)$  at  $\xi \rightarrow +\infty$  in the high strain phase such that  $(\gamma^-, \theta^-)$  and  $(\gamma^+, \theta^+)$  can be connected via a traveling wave. A connection between the end states is achieved if there exist functions  $\gamma(\xi)$  and  $\theta(\xi)$ ,  $\xi \in \mathbb{R}$ , that satisfy the phase segregation conditions (5.13), the jump condition (4.56) at  $\xi = 0$  and  $\xi = b$  and the following three problems:*

**Problem 1:** Low strain phase. Suppose that for  $\xi \in (-\infty, 0)$  the material is in its low strain phase. Using the conditions at  $-\infty$  in system (6.3) and the corresponding expressions of  $\bar{\psi}(\gamma, \theta)$ ,  $\bar{\epsilon}(\gamma, \theta)$ ,  $\epsilon^-$  and  $\sigma^-$  given by equations (2.42) and (2.44), the governing equations are

$$\left\{ \begin{array}{l} \gamma' = w \\ w' = -\frac{1}{\lambda} \{ \nu \dot{s} w - (a^2 - \dot{s}^2)(\gamma - \gamma^-) + \alpha a^2 (\theta - \theta^-) \} \\ \theta' = -\frac{\rho \dot{s}}{k} \left\{ \frac{1}{2} (a^2 - \dot{s}^2) (\gamma - \gamma^-)^2 + \alpha a^2 \theta^- (\gamma - \gamma^-) \right. \\ \quad \left. + c(\theta - \theta^-) - \frac{\lambda}{2} w^2 \right\} \end{array} \right. \quad (6.18)$$

subject to the following boundary conditions:

$$\gamma(-\infty) = \gamma^-, \quad \theta(-\infty) = \theta^-, \quad (6.19)$$

$$\gamma(0^-) = \gamma_0 = \gamma_C + M(\theta_0 - \theta_C), \quad \text{where } \theta_0 = \theta(0^-). \quad (6.20)$$

The temperature  $\theta_0$  is not known a priori.

**Problem 2:** Unstable phase. Suppose that for  $\xi \in (0, b)$  the material is in its unstable phase. The governing equations are

$$\left\{ \begin{array}{l} \gamma' = w \\ w' = -\frac{1}{\lambda} \left\{ \nu \dot{s} w - (a^2 - \dot{s}^2)(\gamma - \gamma^-) + \alpha a^2 (\theta - \theta^-) \right. \\ \quad \left. + a^2 \frac{\gamma_T(\gamma - \gamma_M(\theta))}{\gamma_m(\theta) - \gamma_M(\theta)} \right\} \\ \theta' = -\frac{\rho \dot{s}}{k} \left\{ \frac{1}{2} (a^2 - \dot{s}^2) (\gamma - \gamma^-)^2 + \alpha a^2 \theta^- (\gamma - \gamma^-) + c(\theta - \theta^-) - \frac{\lambda}{2} w^2 \right. \\ \quad \left. + \frac{a^2 \gamma_T}{2(M - m)} \left[ \frac{(2\theta - \theta_C)(\gamma - \gamma_C)^2}{(\theta - \theta_C)^2} - M^2 \theta_C - 2M(\gamma - \gamma_C) \right] \right\}, \end{array} \right. \quad (6.21)$$

subject to the following initial conditions:

$$\gamma(0^+) = \gamma_0 = \gamma_C + M(\theta_0 - \theta_C) \quad \theta(0^+) = \theta_0, \quad (6.22)$$

$$\gamma'(0^+) = \gamma'(0^-). \quad (6.23)$$

**Problem 3:** High strain phase. Suppose that for  $\xi \in (b, +\infty)$  the material is in its

high strain phase. The governing equations are

$$\left\{ \begin{array}{l} \gamma' = w \\ w' = -\frac{1}{\lambda} \{ \nu \dot{s} w - (a^2 - \dot{s}^2)(\gamma - \gamma^+) + \alpha a^2 (\theta - \theta^+) \} \\ \theta' = -\frac{\rho \dot{s}}{k} \left\{ \frac{1}{2} (a^2 - \dot{s}^2) (\gamma - \gamma^+)^2 + \alpha a^2 \theta^+ (\gamma - \gamma^+) \right. \\ \quad \left. + c(\theta - \theta^+) - \frac{\lambda}{2} w^2 \right\} \end{array} \right. \quad (6.24)$$

subject to the following boundary conditions:

$$\gamma(b^+) = \gamma_b = \gamma_C + m(\theta_b - \theta_C), \quad \text{where } \theta_b = \theta(b^+), \quad (6.25)$$

$$\gamma(+\infty) = \gamma^+, \quad \theta(+\infty) = \theta^+. \quad (6.26)$$

The temperature  $\theta_b$  and the width of the unstable phase  $b$  are unknown a priori. Furthermore, there are three conditions that have to be enforced, i.e., the continuity of  $\gamma$ ,  $\theta$  and  $\gamma'$  at  $\xi = b$  (i.e.,  $\theta(b^+) = \theta(b^-)$ ,  $\gamma(b^+) = \gamma(b^-)$  and  $\gamma'(b^+) = \gamma'(b^-)$ ). The phase segregation conditions (5.13) also have to be satisfied. The continuity of  $\gamma'$  at  $\xi = 0$  and  $\xi = b$  guarantees the continuity of  $w' = \gamma''$  and  $\theta'$ , hence the jump conditions (4.56) are automatically satisfied.

## 6.5 Nondimensional parameters.

It is convenient to introduce a length parameter based on the viscosity and strain gradient coefficient and to use it to obtain nondimensional equations. Recall that the viscosity is given in terms of  $L^2 T^{-1}$ , where  $L$  is length and  $T$  is time, and the strain

gradient coefficient in terms of  $L^4T^{-2}$ . Let

$$z = \frac{\rho c a}{k} \xi ,$$

and

$$\omega = \frac{\nu}{\sqrt{\lambda}} , \quad \varpi = \frac{k}{\rho c \sqrt{\lambda}} .$$

Therefore, the system (6.18) can be expressed as

$$\left\{ \begin{array}{l} \delta' = w \\ w' = -\omega \varpi v w + \varpi^2 [(1 - v^2)(\delta - \delta^-) - G(T - T^-)] \\ T' = -v \left\{ \frac{1}{2} (1 - v^2) (\delta - \delta^-)^2 + G T^- (\delta - \delta^-) + (T - T^-) - \frac{1}{2 \varpi^2} w^2 \right\} \end{array} \right. \quad (6.27)$$

where

$$\delta' = \frac{d\delta}{dz} , \quad T' = \frac{dT}{dz} .$$

The boundary condition at  $z = 0$  is

$$\delta(0) = \delta_C + M(T(0) - T_C) . \quad (6.28)$$

The system (6.24) can be written as

$$\left\{ \begin{array}{l} \delta' = w \\ w' = -\omega \varpi v w + \varpi^2 [(1 - v^2)(\delta - \delta^+) - G(T - T^+)] \\ T' = -v \left\{ \frac{1}{2} (1 - v^2) (\delta - \delta^+)^2 + G T^+ (\delta - \delta^+) + (T - T^+) - \frac{1}{2 \varpi^2} w^2 \right\} \end{array} \right. \quad (6.29)$$

and the boundary condition at  $z = \mathbf{b}$  is

$$\delta(\mathbf{b}) = \delta_C + m(T(\mathbf{b}) - T_C) . \quad (6.30)$$

The dimensionless driving traction is defined as

$$\mathbf{f} = -[\mathbf{s}] \langle T \rangle = \frac{f}{\rho a^2 \gamma_T^2} ;$$

hence, if the conditions at  $+\infty$  correspond to the high strain phase, then, from (2.56),

$$\mathbf{f} = - \left[ \mathbf{G}([\delta] - 1) + \log \frac{T^+}{T^-} - \frac{l_T}{T_T} \right] \langle T \rangle . \quad (6.31)$$

For a given state  $(\delta^-, T^-)$  in the low strain phase, the state in the high strain phase for which the driving force vanishes corresponds, from equations (2.62) and (2.65), to

$$T^H(\delta) = T^I(\delta) , \quad \delta > \delta_m(T) . \quad (6.32)$$

Notice that  $\forall \delta, T^I(\delta) > 0$  and

$$\lim_{\delta \rightarrow +\infty} T^H(\delta) = -T^- + \frac{1}{\mathbf{G}} , \quad \lim_{\delta \rightarrow +\infty} T^I(\delta) = 0 ,$$

hence, since the functions  $T^H$  and  $T^I$  are monotonically decreasing in the high strain phase<sup>1</sup>, if  $T^- - 1/\mathbf{G} < 0$  then there is at least one real root for (6.32) if there exists a state (in the high strain phase) for which  $T^I(\delta) < T^H(\delta)$ . Likewise, if  $T^- - 1/\mathbf{G} > 0$ , then (6.32) has at least one real root if there is a state for which  $T^I(\delta) > T^H(\delta)$ . The values of  $\delta$  for which  $T^H(\delta) < 0$  are not admissible. Furthermore, only the smallest root of (6.32) is admissible.

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<sup>1</sup>Provided  $\delta > \delta^- - 2/\mathbf{G}$ .



The invariants of the linearized system can be expressed as

$$\begin{aligned} l_1 &= -v(1 + \omega\varpi) , \\ l_2 &= -\varpi^2 \left[ 1 - v^2 \left( \frac{\omega}{\varpi} + 1 \right) \right] , \\ l_3 &= v\varpi^2 (a_e^2 - v^2) . \end{aligned}$$

From (6.27)<sub>2</sub>, the temperature can be written in terms of the strain and its derivatives as

$$T(z) - T^- = \frac{1}{G} \left[ (1 - v^2)(\delta(z) - \delta^-) - \frac{1}{\varpi} \omega v \delta'(z) - \frac{1}{\varpi^2} \delta''(z) \right] , \quad (6.33)$$

hence, equation (6.27)<sub>3</sub> can be expressed as a single equation for the strain, i.e.,

$$\delta''' - l_1 \delta'' + l_2 \delta' - l_3 (\delta - \delta^-) + \frac{Gv}{2} \left[ (\delta')^2 - \varpi^2 (1 - v^2) (\delta - \delta^-)^2 \right] = 0 . \quad (6.34)$$

A similar equation can be obtained for the high strain phase.

## 6.6 Perturbation analysis.

To obtain an approximation of the solution in the metastable phases, consider a singular perturbation of the equations. Let

$$\varepsilon = \frac{1}{\varpi} ,$$

and consider the case where  $\lambda \ll 1$ ,  $\nu \ll 1$  but the ratio  $\omega$  remains *fixed*. Hence, assume that  $\varepsilon$  is a small parameter. For definiteness, the analysis is carried out for the low strain phase (it is formally the same for the high strain phase). As a general scheme of notation in this section, an overbar represents a quantity related to the inner expansion whereas no overbar usually represents a value related to the outer

expansion. A prime denotes differentiation with respect to the outer coordinate and a dot denotes differentiation with respect to the inner coordinate.

### 6.6.1 Outer solution

Assume that the asymptotic expansion for  $\delta$  corresponds to a power series in  $\varepsilon$  for fixed  $z \neq 0$ , i.e.,

$$\delta(z) - \delta^- \sim \phi_0(z) + \varepsilon\phi_1(z) + \varepsilon^2\phi_2(z) + \dots \quad \text{as } \varepsilon \rightarrow 0 .$$

This corresponds to the “outer” solution. Using this representation for  $\delta$  in equation (6.34) gives

$$\begin{aligned} & \varepsilon^2 (\phi_0''' + \varepsilon\phi_1''' + \varepsilon^2\phi_2''' + \dots) + \mathbf{v}(\varepsilon^2 + \omega\varepsilon) (\phi_0'' + \varepsilon\phi_1'' + \varepsilon^2\phi_2'' + \dots) \\ & + [\omega\mathbf{v}^2\varepsilon - (1 - \mathbf{v}^2)] (\phi_0' + \varepsilon\phi_1' + \varepsilon^2\phi_2' + \dots) - \mathbf{v} (\mathbf{a}_e^2 - \mathbf{v}^2) (\phi_0 + \varepsilon\phi_1 + \varepsilon^2\phi_2 + \dots) \\ & + \frac{\mathbf{G}\mathbf{v}}{2} \left[ \varepsilon^2 (\phi_0' + \varepsilon\phi_1' + \varepsilon^2\phi_2' + \dots)^2 - (1 - \mathbf{v}^2) (\phi_0 + \varepsilon\phi_1 + \varepsilon^2\phi_2 + \dots)^2 \right] = 0 . \end{aligned}$$

Collecting terms in powers of  $\varepsilon$  and setting each of the coefficients equal to zero gives, for the first term,

$$\phi_0' = r_2\phi_0 + r_0\phi_0^2 ,$$

where  $r_2$  is defined by (2.60) and

$$r_0(\mathbf{v}) = -\frac{\mathbf{G}\mathbf{v}}{2} . \quad (6.35)$$

The equation for the second term is

$$\phi_1' - (r_2 + 2r_0\phi_0)\phi_1 - r_4(\phi_0'' + \mathbf{v}\phi_0') = 0 ,$$

where

$$r_4(\mathbf{v}) = \frac{\omega\mathbf{v}}{1 - \mathbf{v}^2} . \quad (6.36)$$

There are two functions that satisfy the equation for  $\phi_0$  (one of them being the trivial solution).

**Nontrivial solution:** In this case the first term of the expansion is given by

$$\phi_0(z) = \frac{r_2}{r_0} \left\{ \frac{r_2}{r_0} c_0 \exp[-r_2 z] - 1 \right\}^{-1}, \quad (6.37)$$

where  $c_0$  is a constant. The second term can be expressed in terms of  $\phi_0$  as

$$\phi_1(z) = \phi_0'(z) \left\{ \frac{c_1}{r_2^3 c_0} - r_4 [(r_2 - v)z - 2 \log \phi_0(z)] \right\}, \quad (6.38)$$

where  $c_1$  is a constant. In order to enforce the condition that  $\phi_0(z) \rightarrow 0$  as  $z \rightarrow -\infty$ , it is required that  $r_2 = r_2(v, T^-) > 0$  in the low strain phase, but no further restriction is placed upon  $c_0$ . For the high strain phase the restriction is that  $r_2 = r_2(v, T^+) < 0$ . Observe that  $\forall n \in \mathbb{N}$ ,  $\phi_0^{(n)}(z) \rightarrow 0$  as  $z \rightarrow -\infty$  and similarly for  $\phi_1$ . The same occurs for  $z \rightarrow +\infty$ .

**Trivial solution:** In this case,  $\phi_0(z) = 0$ ; the second term is therefore given by

$$\phi_1(z) = c_1 e^{r_2 z}.$$

Since it is required that  $\phi_1(z) \rightarrow 0$  as  $z \rightarrow -\infty$ , then either  $r_2(v, T^-) > 0$  or  $c_1 = 0$ . For the high strain phase, since  $\phi_1(z) \rightarrow 0$  as  $z \rightarrow +\infty$ , then either  $r_2(v, T^+) < 0$  or  $c_1 = 0$ .

Formally, the strain gradient is given by

$$\delta'(z) \sim \phi_0'(z) + \varepsilon \phi_1'(z) + \dots,$$

and the temperature is given, from (6.33), by

$$T(z) - T^- \sim \frac{1 - v^2}{G} \phi_0(z) + \frac{\varepsilon}{G} [(1 - v^2)\phi_1(z) - \omega v \phi_0'(z)] + \dots ; \quad (6.39)$$

therefore, the boundary condition  $T(z) - T^- \rightarrow 0$  as  $z \rightarrow -\infty$  is satisfied.

### 6.6.2 Inner solution.

For the “inner” solution (close to  $z = 0$ ), consider a new coordinate defined as

$$x \equiv \frac{z}{\varepsilon} = \varpi z .$$

Assume the following asymptotic expansion for fixed  $x$ :

$$\delta(x) - \delta^- \sim \bar{\phi}_0(x) + \varepsilon \bar{\phi}_1(x) + \varepsilon^2 \bar{\phi}_2(x) + \dots .$$

Therefore, equation (6.34) can be expressed as

$$\begin{aligned} & \left( \ddot{\bar{\phi}}_0 + \varepsilon \ddot{\bar{\phi}}_1 + \varepsilon^2 \ddot{\bar{\phi}}_2 + \dots \right) + v(\varepsilon + \omega) \left( \ddot{\bar{\phi}}_0 + \varepsilon \ddot{\bar{\phi}}_1 + \varepsilon^2 \ddot{\bar{\phi}}_2 + \dots \right) \\ & + [\omega v^2 \varepsilon - (1 - v^2)] \left( \dot{\bar{\phi}}_0 + \varepsilon \dot{\bar{\phi}}_1 + \varepsilon^2 \dot{\bar{\phi}}_2 + \dots \right) - \varepsilon v (a_e^2 - v^2) (\bar{\phi}_0 + \varepsilon \bar{\phi}_1 + \varepsilon^2 \bar{\phi}_2 + \dots) \\ & + \varepsilon \frac{Gv}{2} \left[ \left( \dot{\bar{\phi}}_0 + \varepsilon \dot{\bar{\phi}}_1 + \varepsilon^2 \dot{\bar{\phi}}_2 + \dots \right)^2 - (1 - v^2) (\bar{\phi}_0 + \varepsilon \bar{\phi}_1 + \varepsilon^2 \bar{\phi}_2 + \dots)^2 \right] = 0 , \end{aligned}$$

where a dot denotes differentiation with respect to  $x$ . Proceeding as in the previous section, the equation to determine the first term of the expansion is

$$\ddot{\bar{\phi}}_0 + v\omega \ddot{\bar{\phi}}_0 - (1 - v^2) \dot{\bar{\phi}}_0 = 0 .$$

The solution  $\bar{\phi}_0$  is given by the sum of two exponentials plus a constant. The exponents are  $\beta_{\pm} x$ , where

$$\beta_{\pm} = \frac{1}{2} (-v\omega \pm \sqrt{v^2 \omega^2 + 4(1 - v^2)}) . \quad (6.40)$$

The exponents can be either real or complex. The different cases are as follows:

$$v > 1 \quad \left\{ \begin{array}{l} \omega \geq 2 \quad \beta^\pm < 0 \\ \omega < 2 \quad \left\{ \begin{array}{l} v^2 > 4/(4 - \omega^2) \quad \beta^\pm > 0 \\ 1 < v^2 < 4/(4 - \omega^2) \quad \beta^\pm \in \mathbb{C}, \Re(\beta^\pm) < 0 \end{array} \right. \end{array} \right.$$

$$0 < v < 1 \quad \beta^+ > 0, \beta^- < 0$$

$$-1 < v < 0 \quad \beta^\pm > 0$$

$$v < -1 \quad \left\{ \begin{array}{l} \omega \geq 2 \quad \beta^\pm > 0 \\ \omega < 2 \quad \left\{ \begin{array}{l} v^2 > 4/(4 - \omega^2) \quad \beta^\pm > 0 \\ 1 < v^2 < 4/(4 - \omega^2) \quad \beta^\pm \in \mathbb{C}, \Re(\beta^\pm) > 0 \end{array} \right. \end{array} \right.$$

In the low strain phase (where  $x < 0$ ), since the inner and outer solution must match in some region (as explained below), the exponential(s) with negative (or negative real part) exponent(s)—which would provide an unbounded term in the limit—should be discarded. For the high strain phase, the solution with positive (or positive real part) exponent(s) should be abandoned. If both exponents have the appropriate sign, then, in general,

$$\bar{\phi}_0(x) = \bar{c}_0 e^{\beta^+ x} + \bar{c}_1 e^{\beta^- x} + \bar{c}_2. \quad (6.41)$$

The equation for the next term is

$$\ddot{\phi}_1 + v\omega\ddot{\phi}_1 - (1 - v^2)\dot{\phi}_1 + v \left[ \ddot{\phi}_0 + v\omega\dot{\phi}_0 - (a_e^2 - v^2)\bar{\phi}_0 \right] + \frac{Gv}{2} \left[ \dot{\phi}_0^2 - (1 - v^2)\bar{\phi}_0^2 \right] = 0.$$

Using the general form for  $\bar{\phi}_0$  in the above equation and solving for  $\bar{\phi}_1$  gives

$$\bar{\phi}_1(\mathbf{x}) = (\bar{c}_3 + a_1\mathbf{x})e^{\beta^+\mathbf{x}} + a_2e^{2\beta^+\mathbf{x}} + (\bar{c}_4 + a_3\mathbf{x})e^{\beta^-\mathbf{x}} + a_4e^{2\beta^-\mathbf{x}} + a_5e^{(\beta^+ + \beta^-)\mathbf{x}} + a_6\mathbf{x} + \bar{c}_5, \quad (6.42)$$

where

$$\left. \begin{aligned} a_1 &= \frac{\bar{c}_0\mathbf{v}[(1 - \mathbf{a}_e^2) - \bar{c}_2\mathbf{G}(1 - \mathbf{v}^2)]}{(\beta^+ - \beta^-)\beta^+}, & a_2 &= \frac{\bar{c}_0^2\mathbf{G}\omega\mathbf{v}^2}{4\beta^+(2\beta^+ - \beta^-)}, \\ a_3 &= \frac{\bar{c}_1\mathbf{v}[(1 - \mathbf{a}_e^2) - \bar{c}_2\mathbf{G}(1 - \mathbf{v}^2)]}{(\beta^+ - \beta^-)\beta^-}, & a_4 &= \frac{\bar{c}_1^2\mathbf{G}\omega\mathbf{v}^2}{4\beta^-(2\beta^- - \beta^+)}, \\ a_5 &= \frac{2\bar{c}_0\bar{c}_1\mathbf{G}}{\omega}, & a_6 &= \bar{c}_2(\mathbf{r}_2 + \bar{c}_2\mathbf{r}_0). \end{aligned} \right\} \quad (6.43)$$

The constants  $\bar{c}_3, \bar{c}_4$  and  $\bar{c}_5$  are arbitrary. Observe that  $a_6 = 0$  corresponds to either

$$\bar{c}_2 = 0 \quad \text{or} \quad \bar{c}_2 = -\frac{\mathbf{r}_2}{\mathbf{r}_0}.$$

Notice that, from (6.12) in nondimensional form, the eigenvalues of the system linearized about the equilibrium point for the metastable phases are real and different if

$$-\frac{1}{27}(1 - \mathbf{v}^2)^2 [\mathbf{v}^2\omega^2 + 4(1 - \mathbf{v}^2)] + O(\varepsilon) < 0,$$

i.e., if  $\mathbf{v}^2\omega^2 + 4(1 - \mathbf{v}^2) > 0$  for small  $\varepsilon$ . Therefore, for small  $\varepsilon$ , the equilibrium points of the systems (6.27) (low strain phase) and (6.29) (high strain phase) have a two-dimensional stable manifold and a one-dimensional unstable manifold for  $0 < \mathbf{v} < 1$  and a one-dimensional stable manifold and a two-dimensional unstable manifold for  $-1 < \mathbf{v} < 0$ .

### 6.6.3 Unstable phase.

For the *unstable* phase, the system of equations (6.21) in nondimensional form and expressed in *inner* coordinates becomes

$$\left\{ \begin{array}{l} \dot{\delta} = \bar{w} \\ \dot{w} = -\omega v \bar{w} + \left[ (1 - v^2)(\delta - \delta^-) - G(T - T^-) + \frac{\delta - \delta_C - M(T - T_C)}{(M - m)(T - T_C)} \right] \\ \dot{T} = -\frac{v}{\varpi} \left\{ \frac{1}{2} (1 - v^2) (\delta - \delta^-)^2 + GT^-(\delta - \delta^-) + (T - T^-) - \bar{w}^2 \right. \\ \left. + \frac{1}{2(M - m)} \left[ \frac{(2T - T_C)(\delta - \delta_C)^2}{(T - T_C)^2} - M^2 T_C - 2M(\delta - \delta_C) \right] \right\} \end{array} \right. \quad (6.44)$$

Assuming that the strain, strain gradient and the temperature are bounded throughout the unstable phase, it is possible to conclude from (6.44)<sub>3</sub> that

$$T(x) - T_0 = O(\varepsilon) ,$$

where  $T_0$  is the (unknown) value of the temperature at  $x = 0$ . Therefore, assuming that

$$\delta(x) - \delta^- \sim \bar{\phi}_0(x) + \varepsilon \bar{\phi}_1(x) + \varepsilon^2 \bar{\phi}_2(x) + \dots ,$$

equations (6.44)<sub>1,2</sub> give, for the first term,

$$\ddot{\bar{\phi}}_0(x) + \omega v \dot{\bar{\phi}}_0(x) + k_1 \bar{\phi}_0(x) + k_2 = 0 ,$$

where

$$\left. \begin{array}{l} k_1 = - \left[ (1 - v^2) + \frac{1}{(M - m)(T_0 - T_C)} \right] , \\ k_2 = G(T_0 - T^-) - \frac{\delta^- - \delta_C - M(T_0 - T_C)}{(M - m)(T_0 - T_C)} . \end{array} \right\} \quad (6.45)$$

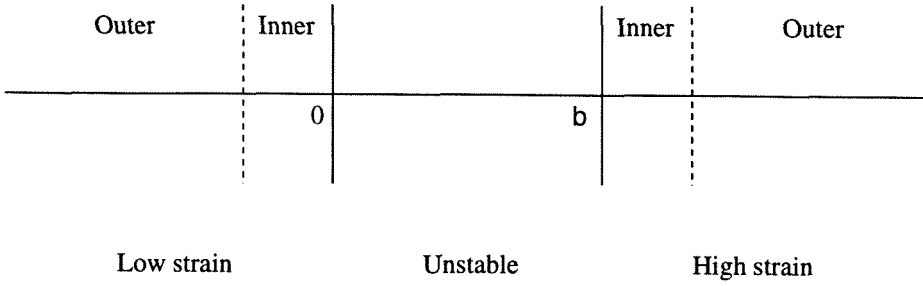


Figure 6.1: Outer and inner solutions for metastable phases.

Hence,

$$\bar{\phi}_0(x) = \bar{c}_1^+ e^{\beta_u^+ x} + \bar{c}_2^+ e^{\beta_u^- x} - \frac{k_2}{k_1}, \quad (6.46)$$

where

$$\beta_u^\pm = \frac{1}{2}(-v\omega \pm \sqrt{v^2\omega^2 - 4k_1}). \quad (6.47)$$

Notice that the exponents can be either real or complex. The following quantities will be useful in the foregoing analysis:

$$\left. \begin{aligned} P(v) &= \beta^+ - \beta^- = \sqrt{v^2\omega^2 + 4(1 - v^2)}, \\ Q(v, T_0) &= \beta_u^+ - \beta_u^- = \sqrt{v^2\omega^2 - 4k_1}. \end{aligned} \right\} \quad (6.48)$$

## 6.7 Subsonic case.

To obtain a uniformly valid approximation of the solution in the metastable phases, the inner and outer solutions must match. For the subsonic case (subsonic with respect to the isothermal sound speed) there are two cases to consider depending on the sign of the phase boundary velocity. The regions where the different approximations are valid are shown in Figure 6.1.



### 6.7.1 Positive velocity.

**Low strain phase:** Suppose that  $0 < v < 1$ . From (2.60)<sub>2</sub> it follows that  $r_2(v, T^\pm) < 0$ , hence the nontrivial outer solution for the low strain phase has to be abandoned in favor of the trivial solution. Furthermore, since  $\bar{\beta}^+ > 0$  and  $\bar{\beta}^- < 0$ , the inner solution for the low strain phase involves, up to  $O(\varepsilon^2)$ , only exponentials with exponents  $\bar{\beta}^+ x$  and  $2\bar{\beta}^+ x$ . From (6.41) and (6.42), the inner solution is given by

$$\delta(x) - \delta^- = \bar{\phi}_0(x) + \varepsilon \bar{\phi}_1(x) + O(\varepsilon^2), \quad (6.49)$$

where

$$\begin{aligned} \bar{\phi}_0(x) &= \bar{c}_0 e^{\bar{\beta}^+ x} + \bar{c}_2, \\ \bar{\phi}_1(x) &= (\bar{c}_3 + a_1 x) e^{\bar{\beta}^+ x} + a_2 e^{2\bar{\beta}^+ x} + a_6 x + \bar{c}_5. \end{aligned}$$

Before enforcing the boundary condition at  $x = 0$ , it is convenient first to analyze the restrictions imposed by the asymptotic matching of the inner and outer solutions. The inner expansion, rewritten in outer variables (i.e.,  $z$ ) and expanded for small  $\varepsilon$  and fixed  $z$  is given by

$$\bar{c}_2 + a_6 z + \varepsilon \bar{c}_5 + \dots$$

The two-term outer expansion of the two-term inner expansion rewritten in inner coordinates is

$$\bar{c}_2 + \varepsilon (a_6 x + \bar{c}_5).$$

For this expansion to match the (trivial) outer expansion, it is required that

$$\bar{c}_2 = a_6 = \bar{c}_5 = 0. \quad (6.50)$$

Notice that, as mentioned in the previous section,  $\bar{c}_2 = 0$  is consistent with  $a_6 = 0$ . The temperature can be expressed, from (6.33) in inner coordinates, as

$$T(x) - T^- = \frac{1}{G} \left[ (1 - v^2)(\delta(x) - \delta^-) - \omega v \dot{\delta}(x) - \ddot{\delta}(x) \right]. \quad (6.51)$$

The strain and the temperature at  $x = 0$  are related through the boundary condition (6.28). From (6.49), (6.50) and (6.51), the first term of the temperature's expansion at  $x = 0$  is

$$\frac{1}{G} \left[ (1 - \nu^2) \bar{\phi}_0(0) - \omega \nu \dot{\bar{\phi}}_0(0) - \ddot{\bar{\phi}}_0(0) \right] = \frac{1}{G} (1 - \nu^2) \bar{c}_2 = 0 ,$$

and the first term of the strain's expansion at  $x = 0$  is  $\bar{c}_0$ , hence, from (6.28) and matching coefficients of the same order gives, for the first term,

$$\bar{c}_0 = -\delta^- + \delta_C + M(T^- - T_C) . \quad (6.52)$$

From (6.51), the second term of the expansion in powers of  $\varepsilon$  at  $x = 0$  is

$$\frac{1}{G} \left[ (1 - \nu^2) \bar{\phi}_1(0) - \omega \nu \dot{\bar{\phi}}_1(0) - \ddot{\bar{\phi}}_1(0) \right] = -\frac{1}{G} \left[ (\beta^+ - \bar{\beta}) a_1 + \beta^+ (2\beta^+ - \bar{\beta}) a_2 \right] ,$$

and the second term of the strain's expansion is  $\bar{c}_3 + a_2$ ; hence, from (6.28), it follows that

$$\bar{c}_3 = -a_2 - \frac{M}{G} \left[ (\beta^+ - \bar{\beta}) a_1 + \beta^+ (2\beta^+ - \bar{\beta}) a_2 \right] . \quad (6.53)$$

Therefore, the strain, strain gradient and the temperature at  $z = 0$  are related to the conditions at  $z \rightarrow -\infty$  by

$$\left. \begin{aligned} \delta(0) - \delta^- &= \bar{c}_0 + \varepsilon(\bar{c}_3 + a_2) + O(\varepsilon^2) , \\ \dot{\delta}(0) &= \beta^+ \bar{c}_0 + \varepsilon(\bar{c}_3 \beta^+ + a_1 + 2\beta^+ a_2) + O(\varepsilon^2) , \\ T(0) - T^- &= \varepsilon \frac{1}{M} (\bar{c}_3 + a_2) + O(\varepsilon^2) , \end{aligned} \right\} \quad (6.54)$$

where, for given  $(\delta^-, T^-)$  and  $\nu$ ,  $\bar{c}_0$  is given by (6.52),  $\bar{c}_3$  by (6.53),  $a_{1,2}$  by (6.43) and  $\beta^\pm$  by (6.40). Observe that the strain gradient is given here with respect to the inner

coordinate. In view of the above, the composite expansion for the low strain phase is

$$\delta(\mathbf{z}) - \delta^- = (\bar{c}_0 + a_1 \mathbf{z}) e^{\bar{\beta} \mathbf{z} / \varepsilon} + \varepsilon \left[ \bar{c}_3 e^{\bar{\beta} \mathbf{z} / \varepsilon} + a_2 e^{2\bar{\beta} \mathbf{z} / \varepsilon} \right] + O(\varepsilon^2) \quad \text{for } \mathbf{z} < 0 .$$

Therefore, for given  $(\delta^-, T^-)$  and  $\mathbf{v}$ , the composite expansion for the low strain phase is completely determined up to  $O(\varepsilon^2)$ .

**High strain phase:** For the inner solution close to  $\mathbf{z} = \mathbf{b}$ , since  $\bar{\beta}^+ > 0$ , the exponential terms with exponents  $\bar{\beta}^+ \mathbf{x}$  and  $2\bar{\beta}^+ \mathbf{x}$  are discarded. Hence, the inner solution is

$$\delta(\mathbf{x}) - \delta^+ = \bar{\phi}_0(\mathbf{x}) + \varepsilon \bar{\phi}_1(\mathbf{x}) + O(\varepsilon^2) ,$$

where

$$\bar{\phi}_0(\mathbf{x}) = \bar{c}_1 e^{\bar{\beta}(\mathbf{x} - \bar{\mathbf{b}})} + \bar{c}_2 ,$$

$$\bar{\phi}_1(\mathbf{x}) = [\bar{c}_4 + a_3(\mathbf{x} - \bar{\mathbf{b}})] e^{\bar{\beta}(\mathbf{x} - \bar{\mathbf{b}})} + a_4 e^{2\bar{\beta}(\mathbf{x} - \bar{\mathbf{b}})} + a_6(\mathbf{x} - \bar{\mathbf{b}}) + \bar{c}_5 ,$$

and  $\bar{\mathbf{b}} = \mathbf{b} / \varepsilon$ . The boundary condition (6.30) at  $\mathbf{x} = \bar{\mathbf{b}}$  relates the strain and the temperature. From (6.51), expressed for the high strain phase, it follows that the lowest order term of the temperature's expansion at  $\mathbf{x} = \bar{\mathbf{b}}$  is

$$\frac{1}{\mathbf{G}} \left[ (1 - \mathbf{v}^2) \bar{\phi}_0(\bar{\mathbf{b}}) - \omega \mathbf{v} \dot{\bar{\phi}}_0(\bar{\mathbf{b}}) - \ddot{\bar{\phi}}_0(\bar{\mathbf{b}}) \right] = \frac{1}{\mathbf{G}} (1 - \mathbf{v}^2) \bar{c}_2 . \quad (6.55)$$

The first term of the strain's expansion at  $\mathbf{x} = \bar{\mathbf{b}}$  is  $\bar{c}_1 + \bar{c}_2$ , hence, using (6.55), the lowest order term in (6.30) gives

$$\bar{c}_1 + \bar{c}_2 - (\delta_C - \delta^+) = \mathbf{m} \left[ \frac{1}{\mathbf{G}} (1 - \mathbf{v}^2) \bar{c}_2 - (T_C - T^+) \right] . \quad (6.56)$$

Similarly, the next power of  $\varepsilon$  in (6.30) gives

$$\bar{c}_4 + \bar{c}_5 + a_4 = -\frac{\mathbf{m}}{\mathbf{G}} \left[ (\bar{\beta} - \bar{\beta}^+) a_3 + \bar{\beta} (2\bar{\beta} - \bar{\beta}^+) a_4 - (\bar{\beta} + \bar{\beta}^+) a_6 + \bar{\beta} \bar{\beta}^+ \bar{c}_5 \right] . \quad (6.57)$$

Therefore, the strain, strain gradient and the temperature at  $\mathbf{x} = \bar{\mathbf{b}}$  are related to the conditions at  $z \rightarrow +\infty$  by

$$\left. \begin{aligned} \delta(\bar{\mathbf{b}}) - \delta^+ &= \bar{c}_1 + \bar{c}_2 + \varepsilon(\bar{c}_4 + \bar{c}_5 + a_4) + O(\varepsilon^2) , \\ \dot{\delta}(\bar{\mathbf{b}}) &= \bar{\beta}\bar{c}_1 + \varepsilon(\bar{c}_4\bar{\beta} + a_3 + 2\bar{\beta}a_4 + a_6) + O(\varepsilon^2) , \\ T(\bar{\mathbf{b}}) - T^+ &= \frac{1}{G}(1 - \nu^2)\bar{c}_2 + \varepsilon\frac{1}{m}(\bar{c}_4 + \bar{c}_5 + a_4) + O(\varepsilon^2) . \end{aligned} \right\} \quad (6.58)$$

In this case, the outer solution is nontrivial and the first two terms are given by (6.37) and (6.38). For the high strain phase it is convenient to work with  $z - \mathbf{b}$  instead of  $z$ . The translation is absorbed by the integration constants  $c_0$  and  $c_1$ . The outer expansion, rewritten in inner variables and expanded for small  $\varepsilon$  (with  $\mathbf{x}$  fixed) gives

$$\frac{r_2}{r_2c_0 - r_0} + \varepsilon\frac{r_2^3}{(r_2c_0 - r_0)^2} \left[ c_0(\mathbf{x} - \bar{\mathbf{b}}) + c_1r_2^3 + 2c_0r_4 \log \frac{r_2}{r_2c_0 - r_0} \right] + \dots$$

where  $r_2 = r_2(\nu, T^+)$ . The inner expansion rewritten in outer coordinates, expanded for small  $\varepsilon$  (with  $z$  fixed) and rewritten in inner coordinates gives

$$\bar{c}_2 + \varepsilon [a_6(\mathbf{x} - \bar{\mathbf{b}}) + \bar{c}_5] + \dots ;$$

hence, for the inner and outer expansion to match asymptotically, it is necessary that

$$\left. \begin{aligned} \bar{c}_2 &= \frac{r_2}{r_2c_0 - r_0} , \\ \bar{c}_5 &= \frac{r_2^3}{(r_2c_0 - r_0)^2} \left[ c_1r_2^3 + 2c_0r_4 \log \frac{r_2}{r_2c_0 - r_0} \right] . \end{aligned} \right\} \quad (6.59)$$

Notice that it is also necessary that

$$a_6 = \frac{c_0r_2^3}{(r_2c_0 - r_0)^2} ,$$

but, in view of the expression for  $a_6$  given by (6.43), this is the same relation as (6.59)<sub>1</sub>. The two-term composite expansion is obtained by adding the two-term inner and outer expansions and subtracting the two-term outer expansion of the two-term

inner expansion, i.e.,

$$\begin{aligned} \delta(z) - \delta^+ &= \frac{r_2}{r_2 c_0 e^{-r_2(z-b)} - r_0} + [\bar{c}_1 + a_3(z-b)] e^{\bar{\beta}(z-b)/\varepsilon} \\ &+ \varepsilon \left[ \bar{c}_4 e^{\bar{\beta}(z-b)/\varepsilon} + a_4 e^{2\bar{\beta}(z-b)/\varepsilon} \right] \\ &+ \varepsilon \frac{r_2^3 c_0 e^{-r_2(z-b)}}{(r_2 c_0 e^{-r_2(z-b)} - r_0)^2} \left\{ \frac{c_1}{r_2^3 c_0} \right. \\ &\quad \left. - r_4 \left[ (r_2 - v)(z-b) - 2 \log \frac{r_2}{r_2 c_0 e^{-r_2(z-b)} - r_0} \right] \right\} \\ &+ O(\varepsilon^2) . \end{aligned}$$

The temperature in the high strain phase is, from (6.39), (6.51) and the above expression for the strain, given by

$$T(z) - T^+ = \frac{1}{G}(1 - v^2) \left[ \frac{r_2}{r_2 c_0 e^{-r_2(z-b)} - r_0} \right] + O(\varepsilon) .$$

Notice that the *inner* expansion of the temperature is, up to  $O(\varepsilon)$ , a *constant* given by  $(1/G)(1 - v^2)\bar{c}_2$ .

**Unstable phase:** Since  $T_0 = T(0^-) = T^- + O(\varepsilon)$ , then, from (6.46) and enforcing the continuity of the strain, strain gradient and temperature at  $x = 0$ , it follows that

$$\left. \begin{aligned} \bar{c}_1^u + \bar{c}_2^u - \frac{k_2}{k_1} &= \bar{c}_0 , \\ \bar{c}_1^u \beta_u^+ + \bar{c}_2^u \beta_u^- &= \beta \bar{c}_0 . \end{aligned} \right\}$$

Let

$$\delta_u = \delta^- - \frac{k_2}{k_1} . \quad (6.60)$$

Observe that the point  $(\delta_u, T^-)$  belongs to the Rayleigh set of the classical theory

with no strain gradient or viscosity as described in Section 2.8, i.e.,  $\delta_u = \delta^R(T^-)$ . Set

$$\begin{aligned}\delta_M &= \delta_M(T^-) = \delta_C + M(T^- - T_C) , \\ \delta_m &= \delta_m(T^-) = \delta_C + m(T^- - T_C) ;\end{aligned}$$

using the identities

$$\bar{c}_0 = \delta_M - \delta^- , \quad \frac{\delta_M - \delta_u}{\delta_M - \delta^-} = \frac{\beta^+ \beta^-}{\beta_u^+ \beta_u^-} ,$$

it follows that

$$\left. \begin{aligned}\bar{c}_1^u &= \frac{1}{Q} \left[ \frac{\bar{\beta}_u^+}{\bar{\beta}} (\beta_u^+ - \bar{\beta}) \right] (\delta_M - \delta_u) , \\ \bar{c}_2^u &= -\frac{1}{Q} \left[ \frac{\beta_u^+}{\bar{\beta}} (\bar{\beta}_u - \bar{\beta}) \right] (\delta_M - \delta_u) ,\end{aligned} \right\} \quad (6.61)$$

where  $Q = Q(\mathbf{v}, T^-)$  is given by (6.48),  $\bar{\beta}$  by (6.40),  $\delta_u$  by (6.60) and (6.45) and  $\bar{\beta}_u^\pm$  by (6.47). The phase segregation condition at  $x = \bar{\mathbf{b}}$  specifies that the material is on the interface between the unstable and the high strain phase. Since the temperature throughout the unstable phase is essentially constant (up to  $O(\varepsilon)$ ) then, from (6.46) and up to the leading term, this condition corresponds to

$$\bar{c}_1^u e^{\beta_u^+ \bar{\mathbf{b}}} + \bar{c}_2^u e^{\bar{\beta}_u \bar{\mathbf{b}}} = \delta_m - \delta_u . \quad (6.62)$$

Now, enforcing continuity of temperature at  $x = \bar{\mathbf{b}}$ , gives, from (6.58)<sub>3</sub>,

$$\bar{c}_2 = \frac{G}{1 - \nu^2} (T^- - T^+) .$$

Using the above expression in (6.56), the constant  $\bar{c}_1$  becomes

$$\bar{c}_1 = \delta_C - \delta^+ + m(T^- - T_C) - \frac{G}{1 - \nu^2} (T^- - T^+) .$$

Let

$$\delta_*^+ = \frac{1}{1 - \nu^2} + \delta^- . \quad (6.63)$$

This quantity can be thought of as the strain (in the high strain phase) corresponding to the front state  $(\delta_*^+, T^-)$  of an *isothermal* phase boundary for a given back state  $(\delta^-, T^-)$ . The state  $(\delta_*^+, T^-)$  can also be viewed as the back state of an *adiabatic* shock wave for a given front state  $(\delta^-, T^-)$ . It is important to notice that the strain gradient at  $(\delta_*^+, T^-)$  does not vanish, hence this state is not an equilibrium point of the system (6.29). Using (2.58)<sub>1</sub> and (6.63), the constants  $\bar{c}_{1,2}$  can be expressed as

$$\bar{c}_1 = \delta_m - \delta_*^+ , \quad \bar{c}_2 = \delta_*^+ - \delta^+ .$$

The boundary condition (6.30) was used to determine the asymptotic expansion in the high strain phase and (6.62) was obtained by enforcing the phase segregation condition for the asymptotic expansion in the unstable phase. Therefore, the continuity of the strain at  $x = \bar{b}$  is automatically satisfied from the continuity of the temperature. The only remaining condition that has not been enforced is the continuity of the strain gradient at  $x = \bar{b}$ . From the inner expansion for the strain in the high strain phase, it follows that

$$\dot{\delta}(\bar{b}^+) = \bar{\beta} \bar{c}_1 + O(\varepsilon) = \bar{\beta}(\delta_m - \delta_*^+) + O(\varepsilon) .$$

On the other hand, from the asymptotic expansion in the unstable phase, one has

$$\dot{\delta}(\bar{b}^-) = \beta_u^+ \bar{c}_1^u e^{\beta_u^+ \bar{b}} + \bar{\beta}_u \bar{c}_2^u e^{\bar{\beta}_u \bar{b}} + O(\varepsilon) ;$$

hence, up to the leading term, the closing condition for the construction of a traveling wave is

$$\beta_u^+ \bar{c}_1^u e^{\beta_u^+ \bar{b}} + \bar{\beta}_u \bar{c}_2^u e^{\bar{\beta}_u \bar{b}} = \bar{\beta}(\delta_m - \delta_*^+) . \quad (6.64)$$

It is possible to prove that

$$\frac{\delta_m - \delta_u}{\delta_m - \delta_*^+} = \frac{\beta^+ \beta^-}{\beta_u \beta_u}.$$

In view of the above relation and using (6.48) and (6.61), equations (6.62) and (6.64) can be expressed, after some simplifications, as

$$e^{Q\bar{b}} = \left( \frac{P - Q}{P + Q} \right)^2, \quad (6.65)$$

and

$$e^{-v\omega\bar{b}} = \left( \frac{-}{\beta} \right)^2 \left( \frac{\delta_m - \delta_u}{\delta_M - \delta_u} \right)^2. \quad (6.66)$$

Since  $v^2 < 1$ , then  $P > 0$ . Thus, if  $Q > 0$ , equation (6.65) has no solution since the left-hand side is always greater than the right-hand side for any  $\bar{b} > 0$ . Therefore, a necessary condition to obtain a solution is  $Q = i|Q|$ . Of all the possible roots of (6.65), only the smallest satisfies the phase segregation conditions, hence, choosing the argument of the complex number  $P + i|Q|$  to be in the interval  $(0, \pi/2)$ , then, from (6.65),

$$\bar{b} = \frac{1}{|Q|} [2\pi - 4 \arg(P + i|Q|)]. \quad (6.67)$$

The width of the unstable region is therefore determined as a function of the velocity and the temperature  $T^-$ .

Figure 6.2 shows a projection of the trajectory in the  $\delta$ - $T$  plane for a traveling wave such that  $T^+ > T^-$  (in this case  $v = 0.05$ ). The corresponding profiles are shown in Figures 6.3 (inner coordinates) and 6.4 (outer coordinates). These graphs were obtained using the following values:  $G = 0.8$ ,  $M = 1.4$ ,  $m = 1.2$ ,  $\delta_C = 3.1$ ,  $T_T = 1$ ,  $T_C = 3$ ,  $l_T = 0.5$ ,  $\omega = 1$  and  $\varepsilon = 1/\varpi = 10^{-5}$ . Similarly, Figures 6.5, 6.6 and 6.7 show a traveling wave such that  $T^+ < T^-$  (in this case  $v = 0.7$ ).



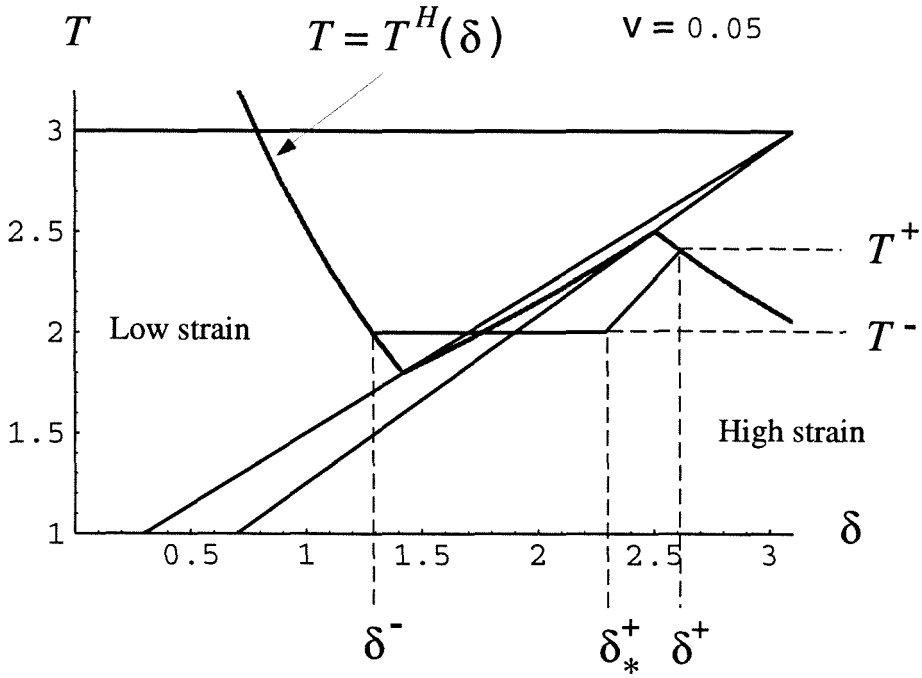


Figure 6.2: Projection of the traveling wave for  $T^+ > T^-$ .

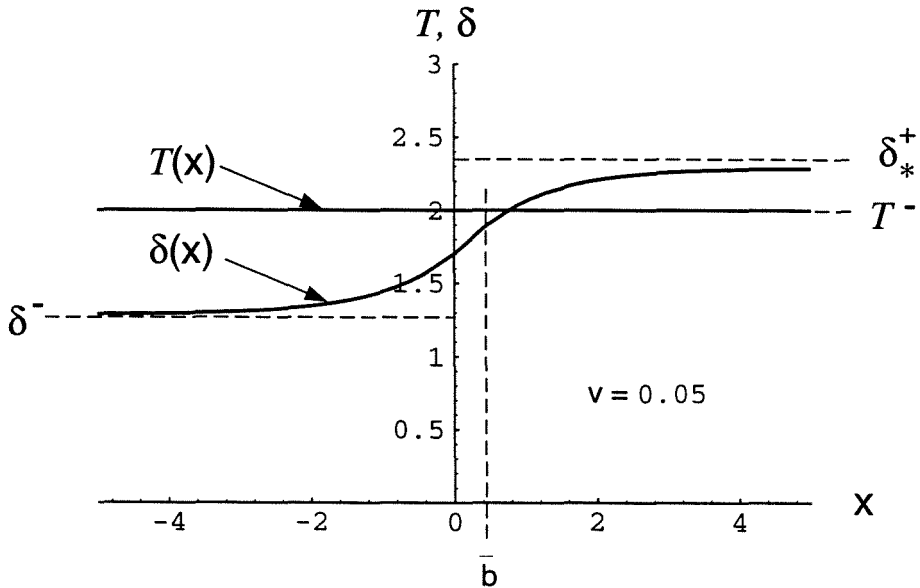


Figure 6.3: Wave profile in inner coordinates for  $v = 0.05$ .

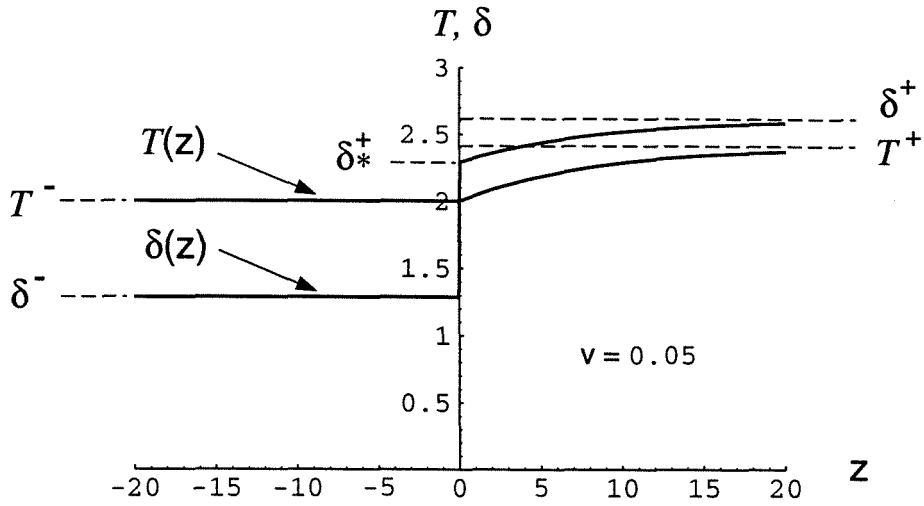


Figure 6.4: Wave profile in outer coordinates for  $v = 0.05$ .

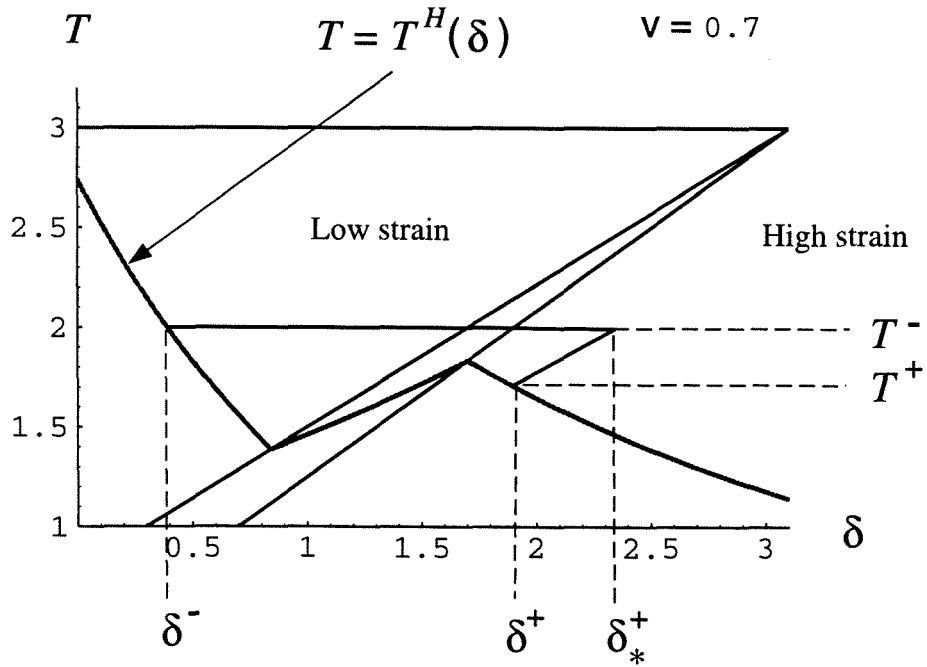


Figure 6.5: Projection of the traveling wave for  $T^+ < T^-$ .

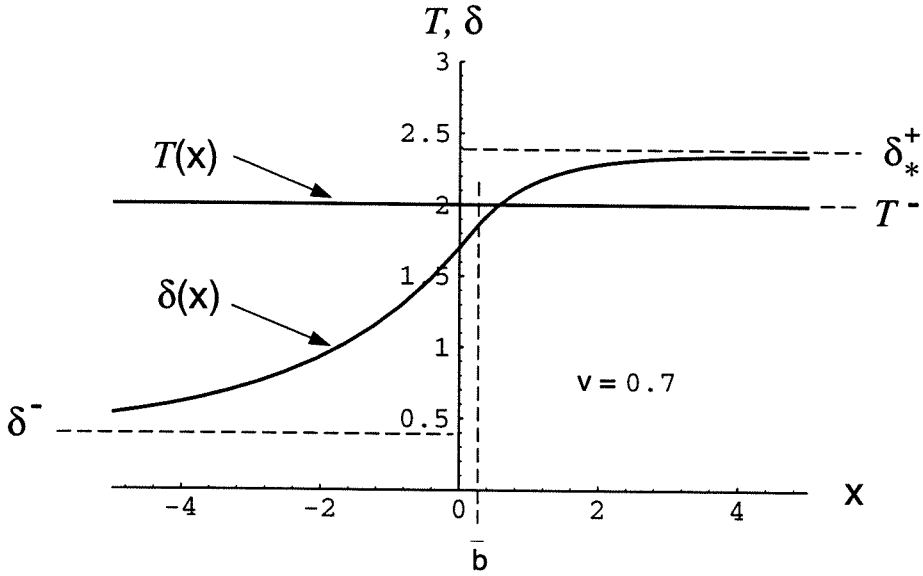


Figure 6.6: Wave profile in inner coordinates for  $v = 0.7$ .

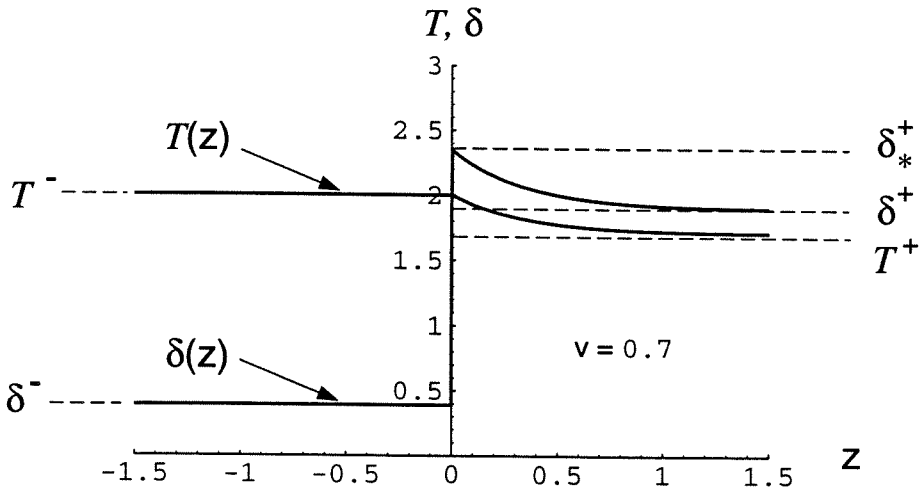


Figure 6.7: Wave profile in outer coordinates for  $v = 0.7$ .

**Kinetic relation:** As mentioned in Section 4.5, the values  $(\delta^\pm, T^\pm, \mathbf{v})$  are formally related via the jump conditions  $(2.58)_{1,2}$ . If equation (6.67) is used to compute  $\bar{\mathbf{b}}$ , then (6.66) can be viewed as an *additional restriction* on the values of  $(\delta^\pm, T^\pm, \mathbf{v})$ . Hence, for a given pair of values (e.g., back state  $(\delta^-, T^-)$  or front state  $(\delta^+, T^+)$  or other combinations), the system  $(2.58)_{1,2}$ , (6.67) provide the necessary restrictions to determine the other three values (e.g.,  $(\delta^+, T^+, \mathbf{v})$ , etc.). Notice that this relation only holds for  $0 < \mathbf{v} < 1$  and, from the entropy inequality, it is also required that the driving traction should be positive. The condition (6.66) can also be interpreted in terms of the driving traction. To this end, the strain  $\delta_u$  can be written, from (6.66), as

$$\delta_u = \delta_M + \frac{\delta_m - \delta_M}{1 - (\beta^+/\beta^-) \exp[-\mathbf{v}\omega\bar{\mathbf{b}}/2]} .$$

Therefore, from (6.45), (6.60) and (6.63), the strains  $\delta^-$  and  $\delta_*^+$  can be expressed as

$$\delta^- = \frac{1}{(1 - \mathbf{v}^2)} \left( \frac{\delta_u - \delta_M}{\delta_M - \delta_m} \right) + \delta_u ,$$

and

$$\delta_*^+ = \frac{1}{(1 - \mathbf{v}^2)} \left( \frac{\delta_u - \delta_m}{\delta_M - \delta_m} \right) + \delta_u .$$

Hence, formally, since  $\bar{\mathbf{b}}$  is a function of  $\mathbf{v}$  and  $T^-$  and  $\delta_m$  and  $\delta_M$  are functions of  $T^-$ , then  $\delta_u = \delta_u(\mathbf{v}, T^-)$  and  $\delta^- = \delta^-(\mathbf{v}, T^-)$ . Using this expression for  $\delta^-$  in (2.61), the temperature  $T^+$  can be obtained as a function of  $\mathbf{v}$  and  $T^-$ . The strain  $\delta^+$  in the high strain phase can be determined from  $(2.58)_1$ . Finally, from (6.31), it follows that

$$\mathbf{f} = \mathbf{f}(\mathbf{v}, T^-) .$$

It is also possible to use  $T^+$  as a reference temperature by solving for  $T^-$  and  $\delta^\pm$  for given  $T^+$  in which case

$$\mathbf{f} = \mathbf{f}(\mathbf{v}, T^+) .$$

Several kinetic curves, corresponding to different values of  $\omega$  and a common value of  $T^+ = 1.5$  are shown in Figure 6.8. The last point of each curve (for maximum  $\mathbf{v}$ ) cor-

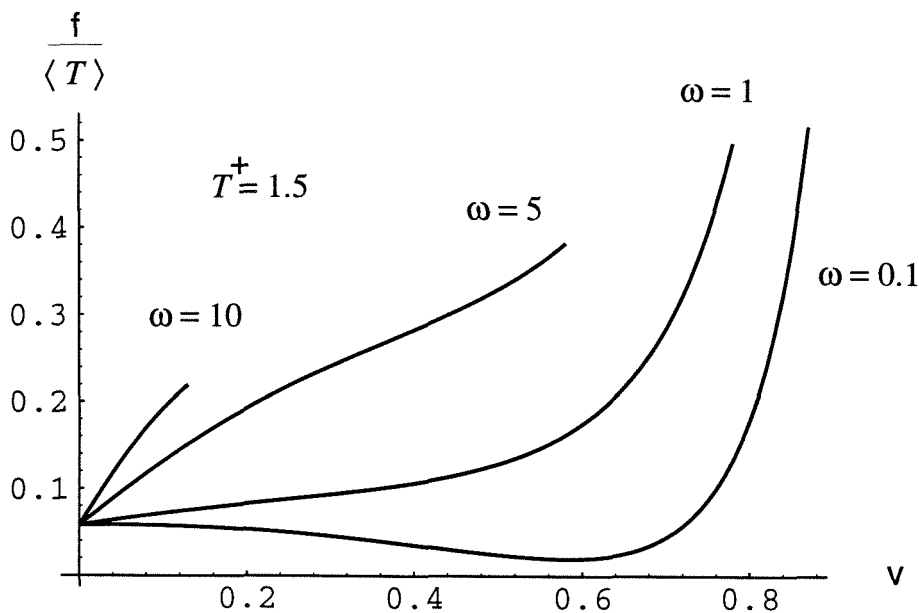


Figure 6.8: Kinetic curves for  $T^+ = 1.5$ .

responds to the limit  $\delta^+ = \delta_m$  as required by the phase segregation condition (5.13)<sub>3</sub>. All curves have a common value at  $v = 0$  (the parameter  $\omega$  is always multiplied by  $v$  in the equations). Observe that for values of  $\omega$  small enough, the corresponding kinetic curve is *non monotonic*. It is interesting to point out that setting  $v = 0$  in (6.27), (6.29) and (6.44) results in  $T(z)$  being constant, which is different from the limit  $v \rightarrow 0$  in the solution obtained by perturbation analysis. Moreover, the energy jump condition (2.58)<sub>2</sub> and the entropy inequality (2.58)<sub>3</sub> are trivially satisfied when  $v = 0$ . Figure 6.9 shows a set of kinetic relations for different values of  $T^+$  and a common value of  $\omega = 1$ . In this case, for a given velocity  $v$ , the driving traction decreases for increasing temperature  $T^+$  (the same behavior is observed when  $T^-$  is used as a reference temperature).

### 6.7.2 Negative velocity.

The negative velocity case is different than the positive one in the sense that  $\bar{\beta}^+$  and  $\bar{\beta}^-$  have the *same* sign. Even though it is possible to obtain a uniformly valid expansion for the low strain phase, there seems to be no simple way to construct such an

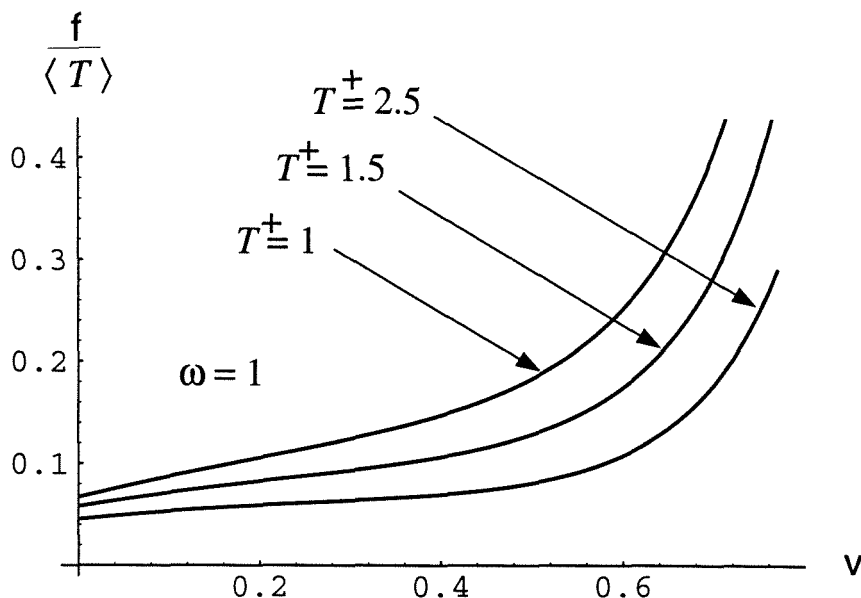


Figure 6.9: Kinetic curves for  $\omega = 1$ .

expansion for the high strain phase.

Since  $r_2(\mathbf{v}, T^+) > 0$ , the nontrivial outer solution for the high strain phase has to be abandoned in favor of the trivial solution. Furthermore, since  $\bar{\beta}^\pm > 0$ , the inner expansion for the low strain phase cannot match asymptotically the trivial outer expansion, unless  $\delta(\mathbf{b}) = \delta^+$  and  $T(\mathbf{b}) = T^+$  which corresponds to the degenerate case  $\bar{\mathbf{b}} \rightarrow \infty$ . Using asymptotic expansions of the form  $\delta(\mathbf{x}; \varepsilon) - \delta^+ \sim \sum_i \Delta_i(\varepsilon) \bar{\phi}_i(\mathbf{x})$ , where  $\Delta_i(\varepsilon)$  is an asymptotic sequence, did not yield the required expansion for different choices of asymptotic sequences and inner coordinates. Intermediate expansions or boundary layers at  $\mathbf{z} \rightarrow +\infty$  did not produce a uniformly valid expansion either<sup>2</sup>. In the case when  $\lambda = \nu = 0$  (see Chapter 5), it was found that  $\mathbf{v}$  could not be negative, but no equivalent proof was found in the case  $\lambda \neq 0, \nu \neq 0$ .

<sup>2</sup>For the general theory, see, e.g., KEVORKIAN & COLE [23], WHITHAM [32].

## Chapter 7 Concluding remarks

A Riemann problem with initial data in the same phase was analyzed and solved within the framework of the sharp interface theory. It was found that by enforcing a kinetic relation and a nucleation criterion, it is possible to single out a *unique* solution. This analysis shows that some concepts developed in the purely mechanical case carry over to the thermomechanical case. Furthermore, from the admissibility criterion for traveling wave solutions, a special kinetic relation for subsonically propagating phase boundaries was derived in the limit case when viscous, strain gradient and heat conduction effects are removed.

An interesting point that arises from the Riemann problem is that the temperature dependence in the kinetic relation and the nucleation criterion is somehow *arbitrary* in the sense that either the temperature in front of a phase boundary or the temperature in the back can be used as a reference temperature. This characteristic can also be observed in the kinetic relation obtained from the augmented theory proposed in Chapter 4.

Although it is possible to formally cast the admissibility criterion in terms of a kinetic relation of the type proposed in [4], there is no simple dependence on the temperature. This fact was also observed by NGAN & TRUSKINOVSKY [25] in their numerical simulations and suggests that the functional form of the kinetic relation in the thermoelastic case should be reconsidered. It is also interesting to point out that under certain conditions it is possible to derive a *nonmonotonic* kinetic relation. Relations of this kind have recently been considered by ROSAKIS & KNOWLES [28] in a purely mechanical context.

For the kinetic relation developed in Chapter 6, the case of negative velocity requires further analysis. The model delivers a kinetic relation for transformations from the high strain phase to the low strain phase, although one should expect, from a physical point of view, to obtain a kinetic relation for the inverse transformation.

If this is not possible, then the model should be modified to correct this flaw.

The special kinetic relation was derived using a limit where the nondimensional parameter  $\omega$  (as defined in Chapter 6) was maintained fixed and  $\varepsilon \ll 1$ . It is possible to analyze other limits although these are out of the scope of this work.



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