Normal Modes Analysis of Subsonic Phase Boundaries in Elastic Materials

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1 Introduction

1.1 Equations and Assumptions

Consider the equations of nonthermal elasticity with no external forces,

$$\begin{aligned} U_t - \nabla_x V &= 0, \\ V_t - \operatorname{div}_x \sigma(U) &= 0, \end{aligned} \tag{1}$$

where $(x,t) \in \mathbb{R}^d \times [0,+\infty)$, $d \geq 2$, $U \in \mathbb{R}_+^{d\times d}$ is the local deformation gradient, and $V \in \mathbb{R}^d$ is the local velocity. Equation (1) is subject to the constraints

$$\operatorname{curl}_x U = 0. \tag{2}$$

In (1), $\sigma = \sigma(U)$ denotes the first Piola–Kirchhoff stress and is supposed to derive from a stored-energy density function $W : \mathbb{R}_+^{d\times d} \to \mathbb{R}$ as $\sigma(U) = \partial W/\partial U$. System (1) is hyperbolic at U if W is rank-one convex at U [Ci88], i.e., if the acoustic tensor $\mathcal{N}(U,\xi) := D^2W(U)(\xi,\xi)$ is positive definite for all $\xi \in \mathbb{R}^d$. We are interested in the stability of subsonic phase boundaries, which are weak solutions to (1) of form

$$(U,V)(x,t) = \begin{cases} (U^-,V^-), & x\cdot N < st, \\ (U^+,V^+), & x \cdot N > st, \end{cases} \tag{3}$$

with direction of propagation $N \in S^{d-1}$, and speed s satisfying the subsonicity condition

$$0 \leq s^2 < \min\,\{\text{eigenvalues of}\,(\mathcal{N}(U^\pm, N))\}. \tag{4}$$

Note that $s = 0$ is included in definition (4). Configurations (3) are subject to the classical Rankine–Hugoniot jump conditions

$$\begin{aligned} -s[U] - [V] \otimes N &= 0, \\ -s[V] - [\sigma(U)]N &= 0, \end{aligned} \tag{5}$$

expressing conservation across the front. In addition, solutions (3) are required to satisfy an additional jump condition or *kinetic rule*

$$g((U^-, V^-), (U^+, V^+), s, N) = 0, \tag{6}$$

where g is real-valued and continuously differentiable. We can assemble both the Rankine–Hugoniot and the kinetic jump conditions into one vector relation $h((U^-, V^-), (U^+, V^+), s, N) = 0$, where h takes values in $\mathbb{R}^{d^2+d+1}$.

Due to its importance for applications, we pay special attention to the static configuration

$$(U, V)(x, t) = \begin{cases} (U^A, 0), & x \cdot N^* < 0, \\ (U^B, 0), & x \cdot N^* > 0, \end{cases} \tag{7}$$

again with $N^* \in S^{d-1}$, and where $U^A \neq U^B \in \mathbb{R}_+^{d\times d}$ corresponds to martensitic wells, local minima of W, and, by physical considerations [Mu99], rank one connected: rank $(U^A - U^B) = 1$.

For applicability of the existing stability theory for subsonic undercompressive shocks [Me90, Co03] we assume also the constant-multiplicity condition of Métivier [Me00], namely, that the eigenvalues of $\mathcal{N}(U, \xi)$ are all semi-simple and their multiplicities are independent of U and ξ, locally; and the nondegeneracy of the jump relations, introduced by Coulombel [Co03], requiring the matrix $(d_{(U^+,V^+)}h,\, d_{(U^-,V^-)}h)$ to have full rank.

1.2 The Lopatinski Determinant

Thanks to the fundamental work of Majda and Métivier [Ma83, Me90, Me01], the nonlinear stability of shock fronts like (3) is determined by the Lopatinski conditions of linear hyperbolic problems [K71]. The Majda–Métivier theory has been extended to general undercompressive shocks [F98, Co03], and subsonic phase boundaries like (3) fit into this setting. The starting point of these analyses is the Fourier decomposition in normal modes of the constant coefficients linearized problem at the end states, leading to the analysis of the so-called *Lopatinski determinant.* If $A_\xi^\pm = \sum A_j^\pm \xi_j$ denotes the linearization of system (1) in direction $\xi \in \mathbb{R}^d$ at $(U^\pm, V^\pm)$, one may verify (see [F98]) that for subsonic phase boundaries (3) with $s \neq 0$, the Lopatinski (or stability) function [Ma83] takes the form of the $(d^2+d+1) \times (d^2+d+1)$ determinant

$$\varDelta(\lambda, \xi) = \det \begin{pmatrix} R_-^s & Q & R_+^u \\ -(d_{u^-}g)(A_N^- - sI)^{-1}R_-^s & q & (d_{u^+}g)(A_N^+ - sI)^{-1}R_+^u \end{pmatrix}, \tag{8}$$

where $(\lambda, \xi) \in \varGamma_N := \{\operatorname{Re}\lambda \geq 0, \xi \cdot N = 0, |\lambda|^2 + |\xi|^2 = 1\}$; Q and q are the "jump vector" fields associated to conditions (5) and (6), respectively (see [FP05]); $R_\pm^{s,u}(\lambda, \xi)$ denotes the right invariant stable/unstable subspaces of $\mathcal{A}_\pm(\lambda, \xi) = (\lambda I + i \sum \xi_j A_j^\pm)(A_N^\pm - s)^{-1}$. In [FP05] we establish the following,

Theorem 1. *For* $((U^+,V^+),(U^-,V^-),s,N)$*,* g *and* W *satisfying hyperbolicity, constant-multiplicity, and subsonicity assumptions, together with jump conditions* (5) *and* (6)*, the stability behavior of* (3) *is determined by the stability function*

$$\hat{\Delta}(U^-,U^+) = \det\begin{pmatrix} \hat{R}^s_{s,N}(U^-) & \hat{Q} & \hat{R}^u_{s,N}(U^+)) \\ \hat{p}^- & \hat{q} & \hat{p}^+ \end{pmatrix} : \Gamma_N \to \mathbb{C}, \tag{9}$$

in which
$$\begin{aligned} \hat{Q}(\lambda,\xi) &:= \begin{pmatrix} [U]N \\ -(\lambda s[U]N + i[\sigma(U)]\xi) \end{pmatrix}, \\ \hat{q}(\lambda,\xi) &:= -\lambda(d_s g) + i(\xi\cdot d_N)g, \\ \hat{p}^-(\lambda,\xi) &:= -(d_{(U^-,V^-)}g)\mathcal{K}_{s,N}(U^-)\hat{R}^s_{s,N}(U^-), \\ \hat{p}^+(\lambda,\xi) &:= (d_{(U^+,V^+)}g)\mathcal{K}_{s,N}(U^+)\hat{R}^u_{s,N}(U^+), \end{aligned}$$

in the sense that if $\hat{\Delta}$ *has no zero on* Γ_N*, then* (3) *is nonlinearly stable; if* $\hat{\Delta}$ *vanishes for some* $(\lambda,\xi)\in\Gamma_N$ *with* $\mathrm{Re}\,\lambda > 0$*, then* (3) *is strongly unstable; and, if* $\hat{\Delta}$ *does not vanish on* $\Gamma_N \cap \{\mathrm{Re}\,\lambda > 0\}$ *then* (3) *is weakly stable.* $\hat{\Delta}$ *is a* $(2d+1)\times(2d+1)$ *determinant, in which* $\hat{R}^s$ *and* $\hat{R}^u$ *represent the right stable and unstable spaces of a matrix field* $\mathbb{M}_{s,N}(U) : \Gamma_N \to \mathbb{C}^{2d\times 2d}$*, and* $\mathcal{K}_{s,N}$ *denotes a continuous mapping* $\mathcal{K}_{s,N} : \Gamma_N \to \mathbb{C}^{(d^2+d)\times 2d}$*.* $\mathbb{M}$ *and* $\mathcal{K}$ *are given by explicit formulae in terms of the first and second derivatives of* W*. Moreover,* $\mathbb{M}, \hat{R}^s, \hat{R}^u$ *and* $\mathcal{K}$ *depend continuously on* (U,s,N) *in their domains of definition, which is given by*

$$s^2 < \min\{\text{eigenvalues of } \mathcal{N}(U,N)\}$$

(including $s = 0$*).*

Corollary 1. *If* W*,* g*,* U^A*, and* U^B *satisfy the hypotheses of Theorem 1 for the equilibrium configuration with* $s=0$*, then the dynamic stability of the phase boundary* (7) *is uniformly controlled by the static-case Lopatinski function*

$$\hat{\Delta}(U^A,U^B) : \Gamma_{N^*} \to \mathbb{C},$$

in the sense detailed in Theorem 1.

Remark 1. Theorem 1 states that it suffices to perform the normal modes analysis on a sub-bundle $\mathbb{G}$ of amplitudes. This simplifies the analysis greatly. In particular, $\mathbb{G}$ is also regular in the characteristic limit $s = 0$, including static configurations into the analysis. This last feature is highlighted in Corollary 1 because of its importance. The theorem and the corollary offer a contribution to the problem of modeling phase-boundary dynamics in real materials, in the sense that any kinetic rule which does not satisfy such a multidimensional stability condition can hardly be accepted as a mathematical description of stably moving boundaries.

2 The Normal Modes Analysis

Let us specify the notation used in [FP05]. U_j will denote the jth column of U, and, accordingly, the stress tensor has columns $\sigma(U)_j = W_{U_j}$. $\{e_j\}$ denotes the canonical basis of $\mathbb{R}^d$. We gather the second derivatives of W into the following $\mathbb{R}^{d\times d}$ matrices $B_i^j(U) := \partial\sigma_j/\partial U_i$, whose (l,k)-component is $\partial^2 W/\partial U_{lj}\partial U_{ki}$. Clearly, B_i^i is symmetric, and $(B_j^i)^\top = B_i^j$. Then, the fluxes and Jacobians of system (1) are expressed as,

$$f_j(U,V) := -\begin{pmatrix} 0 \\ \vdots \\ V \\ \vdots \\ 0 \\ \sigma(U)_j \end{pmatrix}, \qquad A_j(U) = Df_j(U) = -\begin{pmatrix} & & & 0 \\ & & & \vdots \\ & 0 & & I \\ & & & \vdots \\ & & & 0 \\ B_1^j(U) & \cdots & B_d^j(U) & 0 \end{pmatrix}.$$

Notice the high multiplicity characteristic zero mode. Under hyperbolicity and symmetrizability with constant multiplicity, for any $N \in \mathbb{R}^d \setminus \{0\}$, the characteristic speeds of $\sum A_j(U)N_j$ are: $a_0(N,U) = 0$ with constant algebraic multiplicity $\alpha_0 = d^2 - d$, and $a_j^\pm(N,U) = \pm\sqrt{\kappa_j(N,U)}$, $j = 1,\ldots,m$, where κ_j are the m distinct semi-simple eigenvalues of $\mathcal{N}$, $m \le d$, with constant multiplicities α_j, satisfying $\sum \alpha_j = d$. Hence, the planar front corresponds to an undercompressive shock with degree of undercompressivity $l = 1$ (see [F95]).

2.1 The Space $\mathbb{G}$

Without loss of generality assume $N = e_1$. Suppose W is hyperbolic at U, s subsonic with respect to (e_1, U). The squares of the characteristic speeds are therefore the positive eigenvalues of $B_1^1(U)$. The set of time–space frequencies is thus $\Gamma = \{(\lambda,\tilde\xi) \in \mathbb{C}\times\mathbb{R}^{d-1} : \operatorname{Re}\lambda \ge 0, |\lambda|^2 + |\tilde\xi|^2 = 1\}$. We are interested in the matrix field

$$\mathcal{A}(U,s,\lambda,\tilde\xi) = C(s)^{-1}(\lambda I + i\sum_{j\neq 1}\xi_j A_j(U))(A_1(U) - sI)^{-1}C(s),$$

where

$$C(s) := \begin{pmatrix} I_d & & \\ & sI_{d^2-d} & \\ & & I_d \end{pmatrix}.$$

Denote $\hat B(s) := (s^2 - B_1^1)^{-1}$ (its invertibility is guaranteed by subsonicity, and it is regular at $s = 0$). It is easy to verify that the matrix fields $C(s)^{-1}(A_1 - sI)$ and $(A_1 - sI)^{-1}C(s)$ are analytic for all subsonic s, including $s = 0$ [FP05]. Define on Γ the $2d$-dimensional bundle

$$\mathbb{G}(\lambda,\tilde\xi) := \Big\{(\lambda Y, i\xi_2 Y, \ldots, i\xi_d Y, Z)^\top \;:\; Y, Z \in \mathbb{C}^d\Big\}. \tag{10}$$

Lemma 1 ([FP05]). *For $(\lambda, \tilde{\xi}) \in \Gamma$ and s subsonic, $\mathbb{G}$ is an invariant subspace for $\mathcal{A}$, and the $2d \times 2d$ matrix field $\mathbb{M}(U, s, \lambda, \tilde{\xi}) = \left(\begin{smallmatrix} M_1^1 & M_1^2 \\ M_2^1 & M_2^2 \end{smallmatrix}\right)$ that expresses the action of $\mathcal{A}$ on $\mathbb{G}$ has the $d \times d$-block components*

$$M_1^1 := -\hat{B}(\lambda s I + i \sum_{j \neq 1} \xi_j B_j^1), \qquad M_1^2 := \hat{B},$$

$$M_2^1 := (\lambda s I + i \sum_{j \neq 1} \xi_j B_1^j) \hat{B} (\lambda s I + i \sum_{j \neq 1} \xi_j B_j^1) - \lambda^2 I - \sum_{i,j \neq 1} \xi_i \xi_j B_j^i,$$

$$M_2^2 := -(\lambda s I + i \sum_{j \neq 1} \xi_j B_1^j) \hat{B},$$

being $\mathbb{M}$ well defined and smooth for all subsonic s including 0. Moreover, the eigenvalues $-i\mu$ of $\mathbb{M}(U, s, \lambda, \tilde{\xi})$ satisfy $\det(\mathcal{N}(U, \mu, \tilde{\xi}) + (i\mu s - \lambda)^2 I) = 0$, with the property that for $\operatorname{Re} \lambda > 0$, d of these eigenvalues (counting multiplicities) have $\operatorname{Im} \mu > 0$, while the remaining d have $\operatorname{Im} \mu < 0$. Finally, $(Y, Z)^\top \in \mathbb{C}^{2d}$ is an eigenvector of $\mathbb{M}$ if and only if

$$Y \in \ker(\mathcal{N}(U, \mu, \tilde{\xi}) + (i\mu s - \lambda)^2 I), \ Y \neq 0 \text{ and}$$
$$Z = \Big(s(\lambda - i\mu s) I + i\mu B_1^1(U) + i \sum_{j \neq 1} \xi_j B_j^1(U)\Big) Y.$$

Remark 2. The restriction $\mathbb{M} = \mathcal{A}_{|\mathbb{G}}$ has a unique analytic extension to $s = 0$, even though $\mathcal{A}$ is not defined there. As a result, we only investigate the modes of $\mathcal{A}(U, s, \cdot, \cdot)$ whose amplitudes lie in $\mathbb{G}$. Another feature of $\mathbb{M}$ is the following.

Lemma 2 ([FP05]). *The matrix $\mathbb{M}$ satisfies the block structure assumption of Majda [Ma83].*

Remark 3. The last lemma follows from adapting the results of Métivier [Me00] to our setting. In [Cor93], Corli showed that $\mathcal{A}$ satisfies the block structure condition for noncharacteristic speeds s, i. e. excluding $s = 0$. (This is also a direct consequence of a later general theorem in [Me00].) Note that $\mathcal{A}$ has a singular eigenvalue $\beta_* = -\lambda/s$, and that the corresponding mode is exactly what is avoided by our restriction to $\mathbb{G}$.

The significance of Lemma 2 is that the restriction $\mathcal{A}_{|\mathbb{G}}$ satisfies the block structure also in the characteristic limit $s = 0$, allowing the construction of Kreiss' symmetrizers [K71, Me90, Co03] for the static case.

Therefore, the stable/unstable bundles of $\mathbb{M}$, namely $\hat{R}^{s,u}(\lambda, \xi)$, have dimension $2d$ each, and have continuous representations in all Γ (including $\operatorname{Re} \lambda = 0$), and for all subsonic $s \geq 0$, as required in Theorem 1. The key point regarding the case $s = 0$ now is the fact that thanks to the curl-free constraint (2), the Fourier analysis can be performed on the $2d$-dimensional bundle $\mathbb{G}$.

Indeed, if $(U, V)(x, t) = (\hat{U}(x_1 - st), \hat{V}(x_1 - st)) \exp(i\tilde{\xi} \cdot \tilde{x} + \lambda t)$ are normal modes solutions to (1) and (2) (where $x = (x_1, \tilde{x})$, $\tilde{x} \in \mathbb{R}^{d-1}$ and $(\lambda, \tilde{\xi}) \in \Gamma$), then necessarily, $C(s)^{-1}(A_1 - sI)(\hat{U}(\cdot), \hat{V}(\cdot))^\top \in \mathbb{G}$ (see [FP05]). One checks that (9) represents (8) in the restriction to $\mathbb{G}$. Then Theorem 1 and Corollary 1 follow from existing nonlinear theory [Co03, Me90, Ma83]. See [FP05] for details.

3 An Example: Martensite Twins

As an illustration, consider a crystal in two dimensions which is described by an energy function of form

$$W(U) = \tfrac{1}{8}(\beta_1 - (1+\delta^2))^2 + (\beta_2 - 1)^2 + \gamma(\beta_3^2 - \delta^2)^2, \tag{11}$$

with $\beta_1 := |U_1|^2$, $\beta_2 := |U_2|^2$, $\beta_3 := U_1^\top U_2$, with $\gamma > 0$, $\delta \neq 0$. W is rank-one convex at the two rank-one connected ("martensitic") wells

$$U^A = I - \delta e_2 \otimes e_1, \quad U^B = I + \delta e_2 \otimes e_1.$$

(Family (11) is also used to model orthorhombic to monoclinic phase transformations [Lu96]. The interest here is in martensite–martensite phase boundaries, however.) Each such W satisfies all previous hypotheses, plus "material frame-indifference". In particular (11) has constant multiplicity near U^A and U^B in an open nonempty set of the parameters (γ, δ) (see [FP06]). The choice of the kinetic relation is crucial. Motivated by the classical Hugoniot rule of fluid dynamics (see for example [W49] and, for use in connection with phase boundaries [B98, B99]), we consider a *generalized Hugoniot rule*

$$g = [W(U)] - N^\top [U]^\top \langle \sigma(U) \rangle N.$$

This rule expresses conservation of energy across the front. Here $\langle \sigma \rangle = \frac{1}{2}(\sigma^+ + \sigma^-)$. Also, we are interested in perturbations of the form $g \to g + \tilde{g}$, where $\tilde{g} \in C^1$ satisfies, (a) $\tilde{g} = 0$ for $s = 0$; (b) $\tilde{g} > 0$ for $s < 0$, $\tilde{g} < 0$ for $s > 0$; and (c) $d_s \tilde{g} < 0$. The family of perturbations is thus compatible with energy considerations. As a paradigmatic (though artificial) example, we reckon $\tilde{g} = -\epsilon s$ with $\epsilon > 0$, as artificial energy dissipation at rate ϵ.

Using Lemma 1 to represent the stable/unstable bundles associated to the static phase boundary, one can numerically compute the Lopatinski determinant. As a first step in the stability analysis, we look at the mapping $\lambda \mapsto \hat{\Delta}(\lambda, \pm 1)$ for an appropriately normalized version of $\hat{\Delta}$ of Corollary 1, and λ along the imaginary axis. Figure 1 shows the computed values of $\hat{\Delta}$ for $(\gamma, \delta) = (1, 1)$ and $\lambda = i\tau$, $\tau \in [-2, 2]$. The graph on the right shows the values of $\hat{\Delta}(i\tau, +1)$, with dots for $\tau > 0$, and with circles for $\tau < 0$. It corresponds to conservation of energy as kinetic rule, depicting two zeroes along the imaginary axis (weak stability). The graph on the right corresponds to a perturbation of conservation of energy under $\tilde{g} = -\epsilon s$ with $\epsilon = 0.75$, and the zeroes are left out of the contour, suggesting strong stability. These observations (and the concurrent treatment in [FP06]) seem to indicate that in

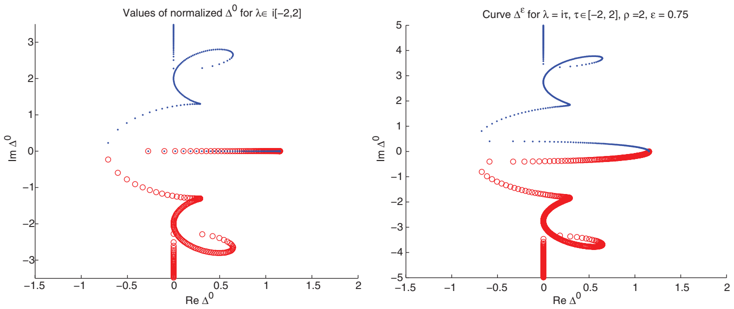

Fig. 1. Computed values of a normalized $\hat{\Delta}(i\tau, +1)$ for $\tau \in [-2, 2]$ under generalized Hugoniot kinetics or conservation of energy (*left*), and corresponding values of $\hat{\Delta}$ under small perturbations of the kinetic rule (*right*)

the case of the generalized Hugoniot rule, the static boundary is dynamically weakly stable, while it is strongly stable in the case of the above-mentioned perturbations of the generalized Hugoniot rule. This is similar to the picture for two-phase fluids [B98, B99]. Details will be provided in [FP06].

References

[B98] Benzoni-Gavage, S.: Stability of multi-dimensional phase transitions in a van der Waals fluid. Nonlinear Anal. **31**, no. 1-2, 243–263 (1998)

[B99] Benzoni-Gavage, S.: Stability of subsonic planar phase boundaries in a van der Waals fluid. Arch. Rational Mech. Anal. **150**, 23–55 (1999)

[Ci88] Ciarlet, P.G.: Mathematical elasticity. Vol. I: Three-dimensional elasticity. Vol. 20 of Studies in Mathematics and its Applications, North-Holland Publishing Co., Amsterdam (1988)

[Cor93] Corli, A.: Weak shock waves for second-order multi-dimensional systems. Boll. Un. Mat. Ital. B (7) **7**, no. 3, 493–510 (1993)

[Co03] Coulombel, J.-F.: Stability of multidimensional undercompressive shock waves. Interfaces Free Bound. **5**, no. 4, 360–390 (2003)

[F95] Freistühler, H.: A short note on the persistence of ideal shock waves. Arch. Math. (Basel) **64**, no. 4, 344–352 (1995)

[F98] Freistühler, H.: Some results on the stability of non-classical shock waves. J. Partial Diff. Eqs. **11**, no. 1, 25–38 (1998)

[FP05] Freistühler, H., Plaza, R.G.: Normal modes and nonlinear stability behaviour of dynamic phase boundaries in elastic materials. Arch. Rational Mech. Anal., to appear.

[FP06] Freistühler, H., Plaza, R.G.: In preparation.

[K71] Kreiss, H.O.: Initial boundary value problems for hyperbolic systems. Comm. Pure Appl. Math. **23**, 277–298 (1970)

[Lu96] Luskin, M.: On the computation of crystalline microstructure. In: Acta numerica, 1996, vol. 5 of Acta Numer., Cambridge Univ. Press, Cambridge (1996)

[Ma83] Majda, A.: The stability of multi-dimensional shock fronts. Mem. Amer. Math. Soc. **41**, no. 275 (1983)

[Me90] Métivier, G.: Stability of multidimensional weak shocks. Comm. Partial Differential Equations **15**, no. 7, 983–1028 (1990)

[Me00] Métivier, G.: The block structure condition for symmetric hyperbolic systems. Bull. London Math. Soc. **32**, no. 6, 689–702 (2000)

[Me01] Métivier, G.: Stability of multidimensional shocks. In Freistühler, H. and Szepessy, A. (eds.) Advances in the Theory of Shock Waves, vol. 47 of Progress in Nonlinear Differential Equations and Their Applications, Birkhäuser, Boston (2001)

[Mu99] Müller, S.: Variational models for microstructure and phase transitions. In Calculus of variations and geometric evolution problems (Cetraro, 1996), vol. 1713 of Lecture Notes in Math., Springer, Berlin (1999)

[W49] Weyl, H.: Shock waves in arbitrary fluids. Comm. Pure Appl. Math. **2**, 103–122 (1949)