Roughening instability of broken extremals

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Abstract

We derive a new general jump condition on a broken Weierstrass-Erdmann extremal of a vectorial variational problem. Such extremals, containing surfaces of gradient discontinuity, are ubiquitous in shape optimization and in the theory of elastic phase transformations. The new condition, which does not have a one dimensional analog, reflects the stationarity of the singular surface with respect to two-scale variations that are nontrivial generalizations of Weierstrass needles. The over-determinacy of the ensuing free boundary problem suggests that typical stable configurations must involve microstructures or chattering controls.

1 Introduction

Our general mathematical inquiry has its origin in the two related physical problems: optimal design of materials and equilibrium coexistence of elastic phases during martensitic transformations [43]. In the optimal design framework the question of whether classical smooth surfaces of discontinuity are compatible with optimality was addressed in [48, 58, 59, 40, 73] (see reviews [49, 62, 51, 8, 1]). In the phase transition theory, where broken extremals correspond to multiphase equilibria, the analogous problem concerning stability of classical smooth phase boundaries was raised in [14, 12, 39, 36, 32] (see reviews [34, 68, 63, 7]). The underlying mathematical problem is the minimization of an integral functional with non quasiconvex energy density.

Consider the energy functional

$$E(\boldsymbol{y}) = \int_{\Omega} W(\boldsymbol{x}, \boldsymbol{y}(\boldsymbol{x}), \nabla \boldsymbol{y}(\boldsymbol{x})) d\boldsymbol{x} \tag{1.1}$$

defined on Lipschitz maps $\boldsymbol{y} : \overline{\Omega} \to \mathbb{R}^m$ which satisfy given boundary conditions. Here Ω is an open and bounded domain in $\mathbb{R}^d$. The regularity of the boundary of Ω and specific form of the boundary conditions will be unimportant for our purposes. Let $\mathbb{M}$ denote the space of all $m \times d$ matrices. We assume that the energy density $W : \overline{\Omega} \times \mathbb{R}^m \times \mathbb{M} \to \mathbb{R}$ is continuous and bounded from below. In addition we assume that W is of class C^2 on an open neighborhood of the range of a given map $\boldsymbol{x} \mapsto (\boldsymbol{x}, \boldsymbol{y}(\boldsymbol{x}), \nabla \boldsymbol{y}(\boldsymbol{x}))$. We call $\boldsymbol{y}(\boldsymbol{x})$ a strong local minimizer if

$E(\boldsymbol{y}+\boldsymbol{\phi}_n) \geq E(\boldsymbol{y})$ for all n large enough and for all admissible strong variations $\boldsymbol{\phi}_n$. Here by admissible strong variations we mean sequences $\{\boldsymbol{\phi}_n\}$ of Lipschitz functions, such $\boldsymbol{\phi}_n \to \boldsymbol{0}$ uniformly as $n \to \infty$ and $\boldsymbol{y}+\boldsymbol{\phi}_n$ satisfies the imposed boundary conditions. In what follows we identify stable phase equilibria with strong local minimizers in the above sense.

Assume that the Lipschitz continuous strong local minimizer $\boldsymbol{y} : \Omega \to \mathbb{R}^m$ is such that $\boldsymbol{F}(\boldsymbol{x}) = \nabla \boldsymbol{y}(\boldsymbol{x})$ has a jump discontinuity across a smooth surface $\Sigma \subset \Omega$ and suppose $\boldsymbol{x}_0 \in \Sigma$. By definition of a jump discontinuity, there exist matrices $\{\boldsymbol{F}_+, \boldsymbol{F}_-\} \subset \mathbb{M}$, such that for any $\boldsymbol{z} \in \mathbb{R}^d \setminus \{\boldsymbol{0}\}$

$$\lim_{\epsilon \to 0} \boldsymbol{F}(\boldsymbol{x}_0 + \epsilon \boldsymbol{z}) = \overline{\boldsymbol{F}}(\boldsymbol{z}) = \begin{cases} \boldsymbol{F}_+, & \text{if } \boldsymbol{z} \cdot \boldsymbol{n} > 0, \\ \boldsymbol{F}_-, & \text{if } \boldsymbol{z} \cdot \boldsymbol{n} < 0. \end{cases} \tag{1.2}$$

In this paper we address the question: what are the equalities that the pair of $m \times d$ matrices $\boldsymbol{F}_\pm$ must satisfy in order to be associated with a strong local minimizer via (1.2)?

Classical necessary identities on the jump are known as the Weierstrass-Erdmann conditions. The Lipschitz continuity of $\boldsymbol{y}(\boldsymbol{x})$ implies that there exists $\boldsymbol{a} \in \mathbb{R}^m$ such that

$$[\![\boldsymbol{F}]\!] = \boldsymbol{a} \otimes \boldsymbol{n}. \tag{1.3}$$

Here $[\![A]\!] = A_+ - A_-$ is the jump across the interface and $\boldsymbol{n}$ is the unit normal to the singular surface pointing from the "$-$" side into the "$+$" side. The first Weierstrass-Erdmann condition [11] reads

$$[\![W_{\boldsymbol{F}}]\!]\boldsymbol{n} = \boldsymbol{0}, \tag{1.4}$$

where $W_{\boldsymbol{F}}$ denotes the matrix of partial derivatives $\partial W / \partial F_{i\alpha}$. The second Weierstrass-Erdmann condition [11] reads

$$[\![W]\!] - (\{\!\!\{ W_{\boldsymbol{F}} \}\!\!\}, [\![\boldsymbol{F}]\!]) = 0, \tag{1.5}$$

where $\{\!\!\{ A \}\!\!\} = \dfrac{1}{2}(A_+ + A_-)$ and we use the inner product notation $(\cdot,\cdot)$ to denote the dot product of two vectors or a Frobenius inner product of two matrices. In optimization context the general vectorial condition (1.5) was derived in [49] (see also [37]). In the phase transition literature (1.5) is known as the elastic Maxwell condition. Maxwell dealt with the case of fluids [56] when (1.5) reduces to the equality of the chemical potentials in coexisting phases. Condition (1.5) was generalized to solid-liquid equilibria by Gibbs [28] and to solid-solid equilibria by Eshelby [14]; later it was independently rediscovered several times (see e.g. [64, 41, 33, 39]).

The three conditions (1.3)–(1.5) constitute a set of relations which have been routinely used in the modeling of phase coexistence in nonlinear elasticity, for example [17, 20, 24, 42, 66]), and in optimal design problems, for example [49, 61, 8, 1]. In this paper we derive a set of additional general jump conditions

$$[\![W_{\boldsymbol{F}}]\!]^T [\![\boldsymbol{F}]\!]\boldsymbol{n} = \boldsymbol{0}. \tag{1.6}$$

Among these d equalities $d-1$ are independent.

The necessity of additional equalities on smooth broken extremals was first realized by Lurie [48] in the context of optimal design of resistivity of the working medium in a magnetic-hydrodynamic generator (see more recent exposition and extensions in [49, 51, 8]). In an application to a scalar phase equilibrium problem a special form of the condition (1.6) was found by Gurtin [36]. Gurtin's condition was later used by Silling [71] in a complete characterization of classical and generalized solutions for anti-plane shear boundary value problem for a two-phase material. In the case of 2D isotropic non-linear materials a condition equivalent to (1.6) was implicitly obtained by Šilhavý [70] (see also [69]). Various special forms of (1.6) appeared earlier in physical and optimization literature where the functional was minimized with respect to the orientation of the layered microstructure, see [65, 53, 51, 67, 45]. A need for an additional equality on the equilibrium phase boundary was also realized in the series of papers on ellipsoidal inclusions of a new phase appearing in an elastic matrix (see e.g. [44, 18]). However, to the knowledge of the authors, the general form of the condition (1.6) and its link to a particular mode of instability of an interface has not been previously reported in the literature.

In this paper we derive the condition (1.6) in three different ways. First, we exhibit an explicit two-scale Weierstrass needle-like variation on the surface of discontinuity leading to the new condition. The new variation can be viewed as the combination of a *platelet* and an *antiplatelet* attached to the smooth interface, with the effect of a strong variation of its normal (see Fig. 1). The implied mode of surface instability requires local perturbation of the surface *orientation* and can be associated with roughening. While this variation has a lot in common with the plate-like variation of Weierstrass, it leads to a necessary condition in the form of *equality* rather than an inequality.

The Weierstrass plate-like variation for vectorial variational problems have been employed in [9, 31] to derive what is now called rank-one convexity inequality in Calculus of Variations. In the context of optimal design such variations, first used in [46, 47], became an essential tool in deriving optimality conditions, eventually evolving into the concept of a topological gradient (see e.g. [60, 72, 13, 26, 1]). The first application of the Weierstrass positivity condition to phase transitions is due to Ericksen [12] and to general non-linear elasticity to Ball [5], where it was understood that a stronger quasiconvexity condition is the appropriate generalization of the Weierstrass condition in Calculus of Variations.

The mechanism of emergence of the equality (1.6) from the rank one convexity inequality is noteworthy. Recall that both the quasiconvexity and the rank one convexity conditions lead to inequalities because the variational functional is not differentiable with respect to strong variations. Our explicit construction of the platelet-antiplatelet variation shows that the presence of equilibrium surfaces of gradient discontinuity creates "directions" in the space of strong variations along which the functional becomes differentiable, which leads to necessary conditions in the form of equalities.

Our second derivation of the new condition is based on the application of rank one convexity inequality simultaneously to two coexisting states. The idea to combine rank one convexity with Weierstrass-Erdmann jump conditions belongs to Lurie [48]; in the phase transition framework the interaction of the two types of conditions was first exhibited in

[36]. We go further and show that the combination of rank one convexity with Weierstrass-Erdmann jump conditions can be interpreted as a minimality condition of a certain function of the interface normal. The vanishing of the first derivative leads to the new condition (1.6), while the positive semidefiniteness of the Hessian results in a new inequality. The latter can be regarded as a condition of non-negativity of second variation corresponding to our two-scale platelet-antiplatelet variation.

Our third derivation of the new condition is based on the study of geometry of the Maxwell set, first introduced in [21, 22] (see also [19, 23]). The Maxwell set contains all rank one connected matrices $\boldsymbol{F}_{\pm}$ satisfying the classical Weierstrass-Erdmann conditions (1.4), (1.5). We show that the interior of the Maxwell set violates the rank one convexity condition, meaning that stable configurations must correspond to points on the boundary of the Maxwell set and are, therefore, singled out by a set of $d-1$ additional relations. These relations are provided by (1.6), which is satisfied on the boundary of the Maxwell set. The necessity of failure of the Legendre-Hadamard condition at some points of the Maxwell set was first shown in [42].

An analysis of the free boundary problem for the broken extremal with a smooth surface of gradient discontinuity shows that adding the new condition (1.6) to the classical set of Weierstrass-Erdmann conditions (1.3)–(1.5) leads to an over-determined problem. This over-determinacy suggests that typically a smooth surface of jump discontinuity is unstable. It is natural to associate this instability with roughening of the surface and the formation of an extended zone where the fields are represented by Young measures [48, 58]; such singular behavior is known in the general control theory as "chattering controls" [15, 25]. This interpretation is also compatible with an idea that solutions of non rank one convex problems may contain infinitely fine microstructures (see e.g. [6]). In the context of elastic phase transitions the numerical studies of the microstructures were initiated in [71] and more recently the numerical reproduction of the roughening instability of solid-solid interfaces has attracted a lot of attention in the physics literature (see, for instance, [3, 2]). In the present paper we illustrate (1.6) by providing a proof of the instability of the non-hydrostatically stressed solid in equilibrium contact with its melt [28, 4, 32]. A brief announcement of the main results of this paper can be found in [30].

2 Classical conditions

For a point $\boldsymbol{x}_0 \in \Sigma$ to be in (mechanical) equilibrium, it is necessary that the energy is stationary with respect to smooth inner and outer variations which we can present as a variation of the graph $\Gamma_{\boldsymbol{y}} = \{(\boldsymbol{x}, \boldsymbol{y}(\boldsymbol{x})) : \boldsymbol{x} \in \Omega\} \subset \mathbb{R}^d \times \mathbb{R}^m$ of $\boldsymbol{y}(\boldsymbol{x})$ (see [29]). The perturbed graph is

$$\Gamma_{\boldsymbol{y}_\epsilon} = \{(\boldsymbol{x} + \epsilon\boldsymbol{\theta}(\boldsymbol{x}), \boldsymbol{y}(\boldsymbol{x}) + \epsilon\boldsymbol{\phi}(\boldsymbol{x})) : \boldsymbol{x} \in \Omega\}. \tag{2.1}$$

where $\boldsymbol{\phi} \in C_0^1(\overline{\Omega}; \mathbb{R}^m)$ and $\boldsymbol{\theta} \in C_0^1(\overline{\Omega}; \mathbb{R}^d)$. When ϵ is sufficiently small the set $\Gamma_{\boldsymbol{y}_\epsilon}$ is a graph of a function $\boldsymbol{y}_\epsilon(\boldsymbol{x})$. It is not hard to see [27, 68] that if a Lipschitz map $\boldsymbol{y}(\boldsymbol{x})$ is an equilibrium configuration it must satisfy (in the sense of distributions) the Euler-Lagrange equation

$$\nabla \cdot \boldsymbol{P} = W_{\boldsymbol{y}} \tag{2.2}$$

and the Eshelby equation

$$\nabla \cdot \boldsymbol{P}^* = W_{\boldsymbol{x}}, \tag{2.3}$$

where

$$\boldsymbol{P}(\boldsymbol{x}) = W_{\boldsymbol{F}}(\boldsymbol{x}, \boldsymbol{y}(\boldsymbol{x}), \nabla \boldsymbol{y}), \qquad \boldsymbol{P}^*(\boldsymbol{x}) = W(\boldsymbol{x}, \boldsymbol{y}(\boldsymbol{x}), \nabla \boldsymbol{y})\boldsymbol{I} - (\nabla \boldsymbol{y})^T \boldsymbol{P}(\boldsymbol{x})$$

are the Piola-Kirchhoff and the the Eshelby stress tensors, respectively. These equilibrium equations imply the continuity of tractions

$$[\![\boldsymbol{P}]\!]\boldsymbol{n} = \boldsymbol{0}, \tag{2.4}$$

and the Maxwell relation

$$p^* = [\![W]\!] - (\{\!\!\{\boldsymbol{P}\}\!\!\}, [\![\boldsymbol{F}]\!]) = 0. \tag{2.5}$$

The last two equalities arise as conditions of equilibrium with respect to smooth perturbations (2.1) of the graph of $\boldsymbol{y}(\boldsymbol{x})$. As such, they can be regarded as necessary conditions for *weak local minima*, where the notions of weak local minima and weak variations are understood in the sense of graphs: in this way weak variations become compatible with non-smooth (Lipschitz) extremals and variable domains.

In the classical theory of *strong local minima* the necessary conditions for weak local minima are supplemented by the Weierstrass condition ensuring stability with respect to needle-type variations. In vectorial variational problems the analogous result is the quasiconvexity inequality at points of continuity of the deformation gradient [57, 5]. To obtain this generalization of the Weierstrass condition we need to consider variations of the form [5]

$$\boldsymbol{y}(\boldsymbol{x}) \mapsto \boldsymbol{y}_\epsilon = \boldsymbol{y}(\boldsymbol{x}) + \epsilon \boldsymbol{\phi}\left(\frac{\boldsymbol{x} - \boldsymbol{x}_0}{\epsilon}\right), \tag{2.6}$$

where $\boldsymbol{\phi} \in C_0^1(B(\boldsymbol{0}, 1); \mathbb{R}^m)$. If $\boldsymbol{x}_0$ is the point of continuity of $\boldsymbol{F}(\boldsymbol{x}_0)$, we obtain the quasiconvexity condition

$$\lim_{\epsilon \to 0} \frac{E(\boldsymbol{y}_\epsilon) - E(\boldsymbol{y})}{\epsilon^d} = \delta E(\boldsymbol{\phi}) = \int_{B(\boldsymbol{0},1)} \{W_0(\boldsymbol{F}(\boldsymbol{x}_0) + \nabla \boldsymbol{\phi}) - W_0(\boldsymbol{F}(\boldsymbol{x}_0))\} d\boldsymbol{z} \geq 0, \tag{2.7}$$

where $W_0(\boldsymbol{F}) = W(\boldsymbol{x}_0, \boldsymbol{y}(\boldsymbol{x}_0), \boldsymbol{F})$. From now on $W(\boldsymbol{F})$ will denote $W_0(\boldsymbol{F})$.

Remark 2.1. *In (2.7) we obtained the inequality, because the functional $\delta E(\boldsymbol{\phi})$ is not linear in $\boldsymbol{\phi}$, which is the consequence of the lack of differentiability of the functional $E(\boldsymbol{y})$ with respect to variations (2.6).*

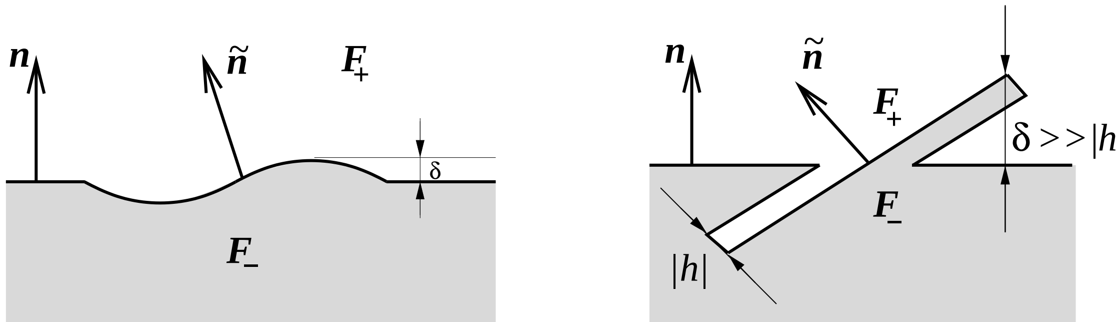

Figure 1: Sketch of the classical inner variation (left) and the Weierstrass type inner variation (right) of the interface in the reference space.

3 Two-scale surface variations

In this section we construct a special needle variation localized at $\boldsymbol{x}_0 \in \Sigma$ with respect to which the energy functional becomes differentiable. In Fig. 1 we show two ways of how the surface can be perturbed locally in the reference configuration. The figure on the left shows the classical smooth variation (2.1) corresponding to the displacement of the interface in the direction of its normal. The figure on the right shows how the local orientation of the surface, but not its location, can be perturbed. In the left figure, the normal of the perturbed surface is uniformly close to the normal of the original surface. By contrast, the right figure shows a strong variation of the normal which is akin to the classical "Weierstrass needle" applied to the orientation of the surface.

As we show below the desired variation has the form (2.6), where $\boldsymbol{x}_0 \in \Sigma$ and $\boldsymbol{\phi}(\boldsymbol{z})$ depends on two small parameters h and δ (see Fig. 1). The new variation is constructed from the infinite strip of thickness $2|h|$

$$\boldsymbol{\phi}_{h,\delta}(\boldsymbol{z}) = \begin{cases} (\boldsymbol{n}+\delta\boldsymbol{\eta}, \boldsymbol{z})\boldsymbol{a}, & \text{if } |(\boldsymbol{n}+\delta\boldsymbol{\eta}, \boldsymbol{z}/h))| < 1, \\ h\boldsymbol{a}, & \text{if } (\boldsymbol{n}+\delta\boldsymbol{\eta}, \boldsymbol{z}/h) \geq 1, \\ -h\boldsymbol{a}, & \text{if } (\boldsymbol{n}+\delta\boldsymbol{\eta}, \boldsymbol{z}/h) \leq -1. \end{cases}$$

Here $\boldsymbol{n}$ and $\boldsymbol{a}$ are as in (1.3) and the vector $\boldsymbol{\eta} \in \mathbb{R}^d$ is arbitrary. The variation of the normal is achieved by splitting the double-strip $\boldsymbol{\phi}_{h,\delta}$ into single strips

$$\boldsymbol{\phi}_{h,\delta}(\boldsymbol{z}) = \boldsymbol{\phi}^+_{h,\delta}(\boldsymbol{z}) + \boldsymbol{\phi}^-_{h,\delta}(\boldsymbol{z}),$$

where

$$\boldsymbol{\phi}^+_{h,\delta}(\boldsymbol{z}) = \begin{cases} (\boldsymbol{n}+\delta\boldsymbol{\eta}, \boldsymbol{z})\boldsymbol{a}, & \text{if } 0 < (\boldsymbol{n}+\delta\boldsymbol{\eta}, \boldsymbol{z}/h)) < 1, \\ \boldsymbol{0}, & \text{if } (\boldsymbol{n}+\delta\boldsymbol{\eta}, \boldsymbol{z}/h) \leq 0, \\ h\boldsymbol{a}, & \text{if } (\boldsymbol{n}+\delta\boldsymbol{\eta}, \boldsymbol{z}/h) \geq 1 \end{cases}$$

and

$$\boldsymbol{\phi}^-_{h,\delta}(\boldsymbol{z}) = -\boldsymbol{\phi}^+_{h,\delta}(-\boldsymbol{z}) = \begin{cases} (\boldsymbol{n}+\delta\boldsymbol{\eta}, \boldsymbol{z})\boldsymbol{a}, & \text{if } -1 < (\boldsymbol{n}+\delta\boldsymbol{\eta}, \boldsymbol{z}/h)) < 0, \\ \boldsymbol{0}, & \text{if } (\boldsymbol{n}+\delta\boldsymbol{\eta}, \boldsymbol{z}/h) \geq 0, \\ -h\boldsymbol{a}, & \text{if } (\boldsymbol{n}+\delta\boldsymbol{\eta}, \boldsymbol{z}/h) \leq -1. \end{cases}$$

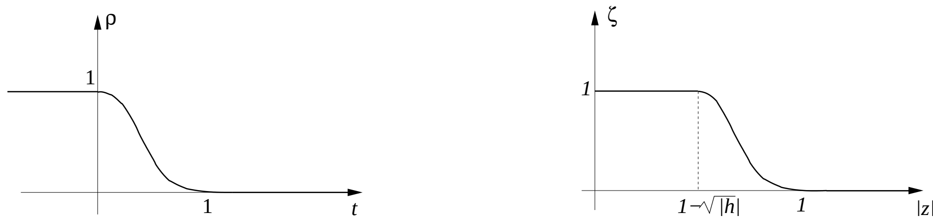

Figure 2: Cut-off functions $\rho(t)$ and $\zeta(|\boldsymbol{z}|)$.

The strip variations $\boldsymbol{\phi}^{\pm}_{h,\delta}$ are not supported on the unit ball, as required in (2.6). This can be dealt with by means of cut-off functions. Let $\rho(t) \in C^\infty(\mathbb{R})$ be such that $\rho(t) = 1$, when $t \le 0$ and $\rho(t) = 0$, when $t \ge 1$, while $0 < \rho(t) < 1$, when $t \in (0,1)$. Let $\zeta_h(s) \in C^\infty([0,\infty))$ be such that $\zeta_h(s) = 1$, when $0 \le s \le 1 - \sqrt{|h|}$ and $\zeta_h(s) = 0$, when $s \ge 1$. In addition $0 \le \zeta_h(s) < 1$ and $|\zeta_h'(s)| \le C/\sqrt{|h|}$ for some $C > 0$ and all $s \ge 0$. See Fig. 2. We define the platelet variation

$$\boldsymbol{\Phi}^+_h(\boldsymbol{z}) = \boldsymbol{\phi}^+_{h,\delta(h)}(\boldsymbol{z})\rho\left(\frac{(\boldsymbol{z},\boldsymbol{n})}{\sqrt{|h|}}\right)\zeta_h(|\boldsymbol{z}|),$$

and the antiplatelet variation

$$\boldsymbol{\Phi}^-_h(\boldsymbol{z}) = -\boldsymbol{\phi}^-_{h,\delta(h)}(\boldsymbol{z})\rho\left(-\frac{(\boldsymbol{z},\boldsymbol{n})}{\sqrt{|h|}}\right)\zeta_h(|\boldsymbol{z}|) = \boldsymbol{\Phi}^+_h(-\boldsymbol{z}).$$

We also define the total platelet-antiplatelet variation

$$\boldsymbol{\Phi}_h(\boldsymbol{z}) = \boldsymbol{\Phi}^+_h(\boldsymbol{z}) + \boldsymbol{\Phi}^-_h(\boldsymbol{z}). \tag{3.1}$$

The first important feature of the new class of variations is its two-scale structure. Our particular construction requires that $\delta(h) \sim |h|^\alpha$, with $0 < \alpha < 1/2$, to ensure that the variation $\delta E(\boldsymbol{\phi}_{h,\delta})$, defined in (2.7), depends on the parameter $\boldsymbol{\eta}$ linearly (i.e. exhibiting differentiability of $E(\boldsymbol{y})$ with respect to the variations (3.1)). The second important aspect of the variation (3.1) is that the perturbation of the local surface orientation is strong despite the smallness of the parameter δ. In fact, the limiting orientation of the normal is multivalued at the point $\boldsymbol{x}_0$, as $\epsilon \to 0$, $h \to 0$ and $\delta(h) \to 0$.

Figure 3 shows regions of different behavior of $\nabla\boldsymbol{\Phi}^+_h(\boldsymbol{z})$. The key technical step in our analysis is the observation that when $\boldsymbol{x}_0 \in \Sigma$

$$\delta E(\boldsymbol{\Phi}_h) = \int_{B(\boldsymbol{0},1)} W^\circ(\overline{\boldsymbol{F}}(\boldsymbol{z}), \nabla\boldsymbol{\Phi}_h(\boldsymbol{z}))d\boldsymbol{z}, \tag{3.2}$$

where $\overline{\boldsymbol{F}}(\boldsymbol{z})$ is given by (1.2) and

$$W^\circ(\boldsymbol{F},\boldsymbol{H}) = W(\boldsymbol{F}+\boldsymbol{H}) - (W_{\boldsymbol{F}}(\boldsymbol{F}),\boldsymbol{H}) - W(\boldsymbol{F})$$

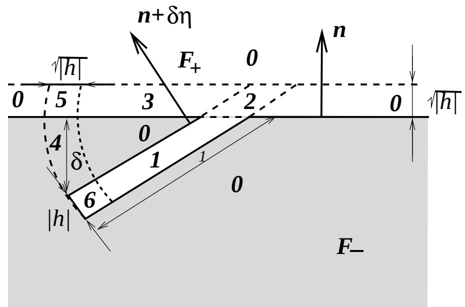

Figure 3: Weierstrass needle variation of the phase boundary.

is a version of the Weierstrass excess function. Indeed, the same calculation that led to (2.7) for points $\boldsymbol{x}_0$ of continuity of $\boldsymbol{F}(\boldsymbol{x})$ leads to the inequality

$$\delta E(\boldsymbol{\Phi}_h) = \int_{B(\boldsymbol{0},1)} \{W(\overline{\boldsymbol{F}}(\boldsymbol{z}) + \nabla\boldsymbol{\Phi}_h) - W(\overline{\boldsymbol{F}}(\boldsymbol{z}))\}d\boldsymbol{z} \geq 0, \tag{3.3}$$

when $\boldsymbol{x}_0 \in \Sigma$. It remains to observe that due to (2.4)

$$\int_{B(\boldsymbol{0},1)} (W_{\boldsymbol{F}}(\overline{\boldsymbol{F}}(\boldsymbol{z})), \nabla\boldsymbol{\Phi}_h)d\boldsymbol{z} = \int_{T_{\boldsymbol{x}_0}\Sigma\cap B(\boldsymbol{0},1)} ([\![\boldsymbol{P}]\!]\boldsymbol{n}, \boldsymbol{\Phi}_h)dS = 0,$$

where $T_{\boldsymbol{x}_0}\Sigma$ is the tangent space to Σ at $\boldsymbol{x}_0$. The formula (3.2) is established.

Now, we are ready to estimate $\delta E(\boldsymbol{\Phi}_h)$, using a simple observation that $|W^\circ(\boldsymbol{F}, \boldsymbol{H})| \leq C|\boldsymbol{H}|^2$, when $\boldsymbol{F}$ and $\boldsymbol{H}$ are uniformly bounded. Observe that the supports of $\nabla\boldsymbol{\Phi}_h^+(\boldsymbol{z})$ and $\nabla\boldsymbol{\Phi}_h^-(\boldsymbol{z})$ are disjoint. Therefore, for each $\boldsymbol{z}$ the value of the total platelet-antiplatelet variation gradient $\nabla\boldsymbol{\Phi}_h(\boldsymbol{z})$ is equal either to $\nabla\boldsymbol{\Phi}_h^+(\boldsymbol{z})$ or to $\nabla\boldsymbol{\Phi}_h^-(\boldsymbol{z})$. Therefore,

$$\int_{B(\boldsymbol{0},1)} W^\circ(\overline{\boldsymbol{F}}(\boldsymbol{z}), \nabla\boldsymbol{\Phi}_h)d\boldsymbol{z} = \int_{B(\boldsymbol{0},1)} W^\circ(\overline{\boldsymbol{F}}(\boldsymbol{z}), \nabla\boldsymbol{\Phi}_h^+)d\boldsymbol{z} + \int_{B(\boldsymbol{0},1)} W^\circ(\overline{\boldsymbol{F}}(\boldsymbol{z}), \nabla\boldsymbol{\Phi}_h^-)d\boldsymbol{z}.$$

It is sufficient to examine only the first term on the right-hand side of the above equality.

Region 1. Here $\rho = 1$, $\zeta_h = 1$ and $\boldsymbol{\phi}_{h,\delta}^+(\boldsymbol{z}) = (\boldsymbol{n} + \delta\boldsymbol{\eta}, \boldsymbol{z})\boldsymbol{a}$. Therefore, $\nabla\boldsymbol{\Phi}_h^+(\boldsymbol{z}) = \boldsymbol{a} \otimes (\boldsymbol{n} + \delta(h)\boldsymbol{\eta})$. Volume $V_1(h)$ of Region 1 is of order h:

$$\lim_{h\to 0} \frac{V_1(h)}{|h|} = V_1^\circ > 0.$$

Also $\overline{\boldsymbol{F}}(\boldsymbol{z}) = \boldsymbol{F}_-$ in Region 1. Therefore, by (1.3)

$$W^\circ(\overline{\boldsymbol{F}}(\boldsymbol{z}), \nabla\boldsymbol{\Phi}_h^+(\boldsymbol{z})) = W(\boldsymbol{F}_+ + \delta(h)\boldsymbol{a}\otimes\boldsymbol{\eta}) - (\boldsymbol{P}_-, [\![\boldsymbol{F}]\!] + \delta(h)\boldsymbol{a}\otimes\boldsymbol{\eta}) - W(\boldsymbol{F}_-).$$

Expanding in powers of $\delta(h)$ we get, using (2.4),

$$W^\circ(\overline{\boldsymbol{F}}(\boldsymbol{z}), \nabla\boldsymbol{\Phi}_h^+(\boldsymbol{z})) = p^* + \delta(h)([\![\boldsymbol{P}]\!], \boldsymbol{a}\otimes\boldsymbol{\eta}) + O(\delta(h)^2).$$

Thus,

$$\int_{\text{Region 1}} W^\circ(\overline{\boldsymbol{F}}(\boldsymbol{z}), \nabla\boldsymbol{\Phi}_h^+(\boldsymbol{z}))d\boldsymbol{z} = |h|V_1^\circ p^* + |h|\delta(h)V_1^\circ([\![\boldsymbol{P}]\!], \boldsymbol{a}\otimes\boldsymbol{\eta}) + o(h\delta(h)).$$

Region 2. Here $\zeta_h(\boldsymbol{z}) = 1$ and $\boldsymbol{\phi}_{h,\delta}^+(\boldsymbol{z}) = (\boldsymbol{n}+\delta\boldsymbol{\eta}, \boldsymbol{z})\boldsymbol{a}$. Therefore,

$$\nabla\boldsymbol{\Phi}_h^+(\boldsymbol{z}) = \boldsymbol{a}\otimes(\boldsymbol{n}+\delta(h)\boldsymbol{\eta})\rho\left(\frac{(\boldsymbol{z},\boldsymbol{n})}{\sqrt{|h|}}\right) + \rho'\left(\frac{(\boldsymbol{z},\boldsymbol{n})}{\sqrt{|h|}}\right)\frac{(\boldsymbol{n}+\delta(h)\boldsymbol{\eta},\boldsymbol{z})}{\sqrt{|h|}}\boldsymbol{a}\otimes\boldsymbol{n}.$$

In Region 2 $|(\boldsymbol{n}+\delta(h)\boldsymbol{\eta},\boldsymbol{z})| \le |h|$, therefore $\nabla\boldsymbol{\Phi}_h^+(\boldsymbol{z})$ is uniformly bounded. The volume $V_2(h)$ of Region 2 is of order $h\sqrt{|h|}$. Thus,

$$\int_{\text{Region 2}} W^\circ(\overline{\boldsymbol{F}}(\boldsymbol{z}), \nabla\boldsymbol{\Phi}_h^+(\boldsymbol{z}))d\boldsymbol{z} = O(h\sqrt{|h|}) = o(h\delta(h)).$$

Region 3. Here $\zeta_h(\boldsymbol{z}) = 1$ and $\boldsymbol{\phi}_{h,\delta}^+(\boldsymbol{z}) = h\boldsymbol{a}$. Therefore,

$$\nabla\boldsymbol{\Phi}_h^+(\boldsymbol{z}) = \sqrt{|h|}\rho'\left(\frac{(\boldsymbol{z},\boldsymbol{n})}{\sqrt{|h|}}\right)\boldsymbol{a}\otimes\boldsymbol{n} = O(\sqrt{|h|}).$$

So, $W^\circ(\overline{\boldsymbol{F}}(\boldsymbol{z}), \nabla\boldsymbol{\Phi}_h^+(\boldsymbol{z})) = O(h)$. The volume $V_3(h)$ of Region 3 is of order $\sqrt{|h|}$. Therefore,

$$\int_{\text{Region 3}} W^\circ(\overline{\boldsymbol{F}}(\boldsymbol{z}), \nabla\boldsymbol{\Phi}_h^+(\boldsymbol{z}))d\boldsymbol{z} = O(h\sqrt{|h|}) = o(h\delta(h)).$$

Region 4. Here $\rho = 1$ and $\boldsymbol{\phi}_{h,\delta}^+(\boldsymbol{z}) = h\boldsymbol{a}$. Therefore, $\nabla\boldsymbol{\Phi}_h^+(\boldsymbol{z}) = h\zeta_h'\boldsymbol{a}\otimes\widehat{\boldsymbol{z}} = O(\sqrt{|h|})$, where $\widehat{\boldsymbol{z}} = \boldsymbol{z}/|\boldsymbol{z}|$. So, $W^\circ(\overline{\boldsymbol{F}}(\boldsymbol{z}), \nabla\boldsymbol{\Phi}_h^+(\boldsymbol{z})) = O(h)$. The volume $V_4(h)$ of Region 4 is of order $\delta(h)\sqrt{|h|}$. Therefore,

$$\int_{\text{Region 4}} W^\circ(\overline{\boldsymbol{F}}(\boldsymbol{z}), \nabla\boldsymbol{\Phi}_h^+(\boldsymbol{z}))d\boldsymbol{z} = O(h\delta(h)\sqrt{|h|}) = o(h\delta(h)).$$

Region 5. Here $\boldsymbol{\phi}_{h,\delta}^+(\boldsymbol{z}) = h\boldsymbol{a}$. Therefore,

$$\nabla\boldsymbol{\Phi}_h^+(\boldsymbol{z}) = h\zeta_h'(|\boldsymbol{z}|)\rho\left(\frac{(\boldsymbol{z},\boldsymbol{n})}{\sqrt{|h|}}\right)\boldsymbol{a}\otimes\widehat{\boldsymbol{z}} + \sqrt{|h|}\zeta_h(|\boldsymbol{z}|)\rho'\left(\frac{(\boldsymbol{z},\boldsymbol{n})}{\sqrt{|h|}}\right)\boldsymbol{a}\otimes\boldsymbol{n} = O(\sqrt{|h|}).$$

So, $W^\circ(\overline{\boldsymbol{F}}(\boldsymbol{z}), \nabla\boldsymbol{\Phi}_h^+(\boldsymbol{z})) = O(h)$. The volume $V_5(h)$ of Region 5 is of order h. Therefore,

$$\int_{\text{Region 5}} W^\circ(\overline{\boldsymbol{F}}(\boldsymbol{z}), \nabla\boldsymbol{\Phi}_h^+(\boldsymbol{z}))d\boldsymbol{z} = O(h^2) = o(h\delta(h)).$$

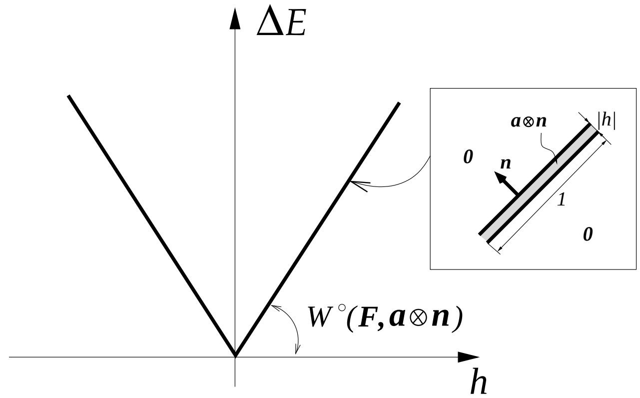

Figure 4: Non-differentiability of the energy with respect to the platelet variation at the point of continuity of the deformation gradient.

Region 6. Here $\rho = 1$ and $\boldsymbol{\phi}^+_{h,\delta}(\boldsymbol{z}) = (\boldsymbol{n} + \delta\boldsymbol{\eta}, \boldsymbol{z})\boldsymbol{a}$. Therefore,

$$\nabla\boldsymbol{\Phi}^+_h(\boldsymbol{z}) = \zeta_h(|\boldsymbol{z}|)\boldsymbol{a} \otimes (\boldsymbol{n} + \delta(h)\boldsymbol{\eta}) + \zeta'_h(|\boldsymbol{z}|)(\boldsymbol{n} + \delta(h)\boldsymbol{\eta}, \boldsymbol{z})\boldsymbol{a} \otimes \widehat{\boldsymbol{z}}.$$

In Region 6 $|(\boldsymbol{n} + \delta(h)\boldsymbol{\eta}, \boldsymbol{z})| \le |h|$, therefore $\nabla\boldsymbol{\Phi}^+_h(\boldsymbol{z})$ is uniformly bounded. The volume $V_6(h)$ of Region 6 is of order $h\sqrt{|h|}$. Thus,

$$\int_{\text{Region 6}} W^\circ(\overline{\boldsymbol{F}}(\boldsymbol{z}), \nabla\boldsymbol{\Phi}^+_h(\boldsymbol{z}))d\boldsymbol{z} = O(h\sqrt{|h|}) = o(h\delta(h)).$$

We have shown that

$$\delta E(\boldsymbol{\Phi}^+_h) = |h|V^\circ_1 p^* + |h|\delta(h)([\![\boldsymbol{P}]\!]^T\boldsymbol{a}, \boldsymbol{\eta})V^\circ_1 + o(h\delta(h)).$$

Similarly,

$$\delta E(\boldsymbol{\Phi}^-_h) = -|h|V^\circ_1 p^* + |h|\delta(h)([\![\boldsymbol{P}]\!]^T\boldsymbol{a}, \boldsymbol{\eta})V^\circ_1 + o(h\delta(h)).$$

Therefore,

$$\delta E(\boldsymbol{\Phi}_h) = 2|h|\delta(h)([\![\boldsymbol{P}]\!]^T\boldsymbol{a}, \boldsymbol{\eta})V^\circ_1 + o(h\delta(h)).$$

Now, the inequality (3.3) implies that $([\![\boldsymbol{P}]\!]^T\boldsymbol{a}, \boldsymbol{\eta}) \ge 0$ for an arbitrary vector $\boldsymbol{\eta} \in \mathbb{R}^d$. We conclude that in order for the interface to be stable the equality

$$[\![\boldsymbol{P}]\!]^T\boldsymbol{a} = \boldsymbol{0}. \tag{3.4}$$

has to be satisfied. Due to continuity of the fields (1.3), the condition (3.4) is equivalent to (1.6).

4 Rank one convexity

The heterogeneity introduced by the phase boundary Σ is responsible for the multiscale nature of the variation (3.1), while the equilibrium condition (2.4) is responsible for the

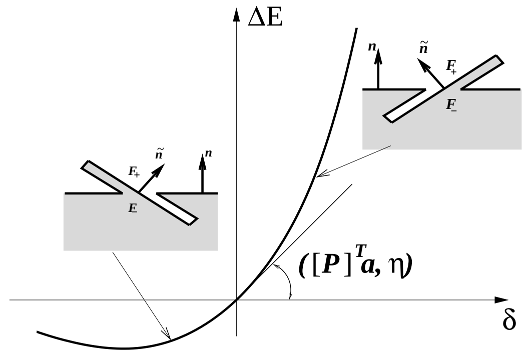

Figure 5: Differentiability of the energy functional with respect to variation of the interface normal.

differentiability of the energy functional $E(\boldsymbol{y})$ with respect to the variations (3.1). We recall that a very similar single scale variation

$$\boldsymbol{\phi}_h(\boldsymbol{z}) = \begin{cases} (\boldsymbol{n}, \boldsymbol{z})\boldsymbol{a}, & \text{if } -1 < (\boldsymbol{n}, \boldsymbol{z}/h) < 0, \\ \boldsymbol{0}, & \text{if } (\boldsymbol{n}, \boldsymbol{z}/h) \geq 0, \\ -h\boldsymbol{a}, & \text{if } (\boldsymbol{n}, \boldsymbol{z}/h) \leq -1 \end{cases} \tag{4.1}$$

produces the rank one convexity inequality

$$W^\circ(\boldsymbol{F}(\boldsymbol{x}_0), \boldsymbol{a} \otimes \boldsymbol{n}) \geq 0, \tag{4.2}$$

which can also be obtained directly from the quasiconvexity inequality (2.7), see [9, 31, 57, 5]. Here $\boldsymbol{a}$ and $\boldsymbol{n}$ are arbitrary vectors in $\mathbb{R}^m$ and $\mathbb{R}^d$, respectively, while $\boldsymbol{x}_0$ is a point of continuity of $\boldsymbol{F}(\boldsymbol{x})$. The cut-off function is $\zeta_h(|\boldsymbol{z}|)$ and analysis is similar (but much simpler) to the one in Section 3, except the result is not the equality (3.4) but the inequality (4.2), since the energy functional is not differentiable in h, see Fig. 4. We now see that the slope $W^\circ(\boldsymbol{F}, \boldsymbol{a} \otimes \boldsymbol{n})$ in Fig. 4 becomes zero, when $\boldsymbol{F} = \boldsymbol{F}_-$ and $\boldsymbol{a} \otimes \boldsymbol{n} = [\![\boldsymbol{F}]\!]$, due to the phase boundary equilibrium condition (2.4) and the Maxwell relation (2.5). Hence, the energy becomes differentiable with respect to the variation (3.1), see Fig. 5. In fact, the platelet-antiplatelet structure of the new variation makes the energy differentiable when only the traction continuity condition (2.4) holds.

Let us now show that both the Maxwell relation (2.5) and the new phase boundary equilibrium condition (3.4) can be obtained as consequences of the rank one convexity inequality (4.2) applied simultaneously to both fields coexisting at the jump discontinuity, provided that kinematic compatibility condition (1.3) and the continuity of tractions (2.4) hold. In the case of the Maxwell identity this has already been done in [49].

THEOREM **4.1.** *Assume that $W(\boldsymbol{F})$ is of class C^2 on the neighborhoods of $\boldsymbol{F}_+$ and $\boldsymbol{F}_-$. Assume that the jump conditions (1.3) and (1.4) hold. Assume also that the rank one convexity inequalities hold at $\boldsymbol{F}_\pm$:*

$$W(\boldsymbol{F}_\pm + \boldsymbol{u} \otimes \boldsymbol{v}) \geq W(\boldsymbol{F}_\pm) + (\boldsymbol{P}_\pm \boldsymbol{v}, \boldsymbol{u}). \tag{4.3}$$

for all $\boldsymbol{u} \in \mathbb{R}^m$ and $\boldsymbol{v} \in \mathbb{R}^d$. Then both (2.5) and (3.4) hold.

Proof. Let $\boldsymbol{u} = \mp\boldsymbol{a}$ in (4.3). We obtain

$$\omega_\pm(\boldsymbol{v}) = W(\boldsymbol{F}_\pm \mp \boldsymbol{a}\otimes\boldsymbol{v}) - W(\boldsymbol{F}_\pm) \pm (\boldsymbol{P}_\pm\boldsymbol{v}, \boldsymbol{a}) \geq 0 \tag{4.4}$$

for all $\boldsymbol{v} \in \mathbb{R}^d$. Observe that (1.3) and (2.4) imply that $\omega_\pm(\boldsymbol{n}) = \pm p^*$. The inequalities (4.4) then imply $p^* = 0$. Therefore, the non-negative functions $\omega_\pm(\boldsymbol{v})$ achieve their global minima equal to zero at $\boldsymbol{v} = \boldsymbol{n}$ and, hence,

$$\boldsymbol{0} = \nabla\omega_\pm(\boldsymbol{n}) = \mp[\![\boldsymbol{P}]\!]^T\boldsymbol{a}.$$

□

We can translate the arguments in the proof above into the language of variations. Replacing $\boldsymbol{F}(\boldsymbol{x}_0)$ in (4.2) with $\boldsymbol{F}_\pm$ and differentiating $\omega_\pm(\boldsymbol{v})$ at $\boldsymbol{v} = \boldsymbol{n}$ can be interpreted as the variation of the interface normal by means of combined platelet-antiplatelet variation.

Remark 4.2. *The differentiability of the energy functional with respect to the variations shown in Fig. 1 allows the computation of the second variation, whose non-negativity is a necessary condition for the interface stability. The derivation and applications of the new inequality will be presented elsewhere while here we only state the result. Let*

$$(\boldsymbol{A}'_\pm(\boldsymbol{u})\boldsymbol{v}, \boldsymbol{v}) = (\boldsymbol{A}_\pm(\boldsymbol{v})\boldsymbol{u}, \boldsymbol{u}) = (W_{\boldsymbol{FF}}(\boldsymbol{F}_\pm)(\boldsymbol{u}\otimes\boldsymbol{v}), \boldsymbol{u}\otimes\boldsymbol{v})$$

and

$$(\boldsymbol{B}_\pm(\boldsymbol{u}, \boldsymbol{v})\boldsymbol{\eta}, \boldsymbol{\xi}) = (W_{\boldsymbol{FF}}(\boldsymbol{F}_\pm)(\boldsymbol{u}\otimes\boldsymbol{\eta}), \boldsymbol{\xi}\otimes\boldsymbol{v}).$$

Assume that the acoustic tensors $\boldsymbol{A}_\pm(\boldsymbol{n})$ are positive definite in the sense of quadratic forms. Then the $d \times d$ matrices

$$\mathbb{B}_\pm(\boldsymbol{a}, \boldsymbol{n}) = \boldsymbol{A}'_\pm(\boldsymbol{a}) - (\boldsymbol{B}_\pm(\boldsymbol{a}, \boldsymbol{n}) + [\![\boldsymbol{P}]\!])^T\boldsymbol{A}_\pm^{-1}(\boldsymbol{n})(\boldsymbol{B}_\pm(\boldsymbol{a}, \boldsymbol{n}) + [\![\boldsymbol{P}]\!]) \tag{4.5}$$

must be non-negative definite on $(\mathbb{R}\boldsymbol{n})^\perp$.

5 The Maxwell set

Definition 5.1. *The Maxwell set $\mathfrak{M}$ is the set of all matrices $\boldsymbol{F} \in \mathbb{M}$ for which there exist a vector $\boldsymbol{a} \in \mathbb{R}^m \setminus \{\boldsymbol{0}\}$ and a unit vector $\boldsymbol{n} \in \mathbb{R}^d$ such that $\boldsymbol{F}_- = \boldsymbol{F}$ and $\boldsymbol{F}_+ = \boldsymbol{F} + \boldsymbol{a}\otimes\boldsymbol{n}$ satisfy (2.4) and (2.5).*

Following [21, 22] we observe that the system of md kinematic conditions (1.3), m mechanical equilibrium conditions (2.4) and one Maxwell condition (2.5) constitute the set of $md + m + 1$ equalities constraining $2md + m + d - 1$ unknown fields $\boldsymbol{F}_+$, $\boldsymbol{F}_-$, $\boldsymbol{a}$ and $\boldsymbol{n}$ at any equilibrium phase boundary. One can conclude that the solution set forms an $md + d - 2$ parameter family. This means that the value of say $\boldsymbol{F}_-$ can be chosen from a set of full dimension in $\mathbb{M}$, while the corresponding deformation gradient $\boldsymbol{F}_+$ will belong to a $d-2$-dimensional parametric family of $m \times d$ matrices. Hence, generically, $\mathfrak{M}$ has a non-empty interior.

We claim, however, that the entire interior of the Maxwell set violates the rank one convexity condition. This can be conveniently stated in terms of the instability set

$$\mathfrak{S} = \{\boldsymbol{F} \in \mathbb{M} : RW(\boldsymbol{F}) < W(\boldsymbol{F})\}, \tag{5.1}$$

where $RW(\boldsymbol{F})$ is the rank one convex envelope of $W(\boldsymbol{F})$, [10, 43]. This set is an example of the "forbidden region" introduced in [49, 8]. Below we show that $\boldsymbol{F} \in \mathfrak{S}$ for all matrices $\boldsymbol{F}$ in the interior of the Maxwell set.

THEOREM **5.2.** *Suppose that the pair $\boldsymbol{F}_+$, $\boldsymbol{F}_-$ satisfies (1.3), (2.4) and (2.5). Suppose that $(\boldsymbol{A}_-(\boldsymbol{n})\boldsymbol{a}, \boldsymbol{a}) > 0$. Let $\boldsymbol{F}_t = t\boldsymbol{F}_+ + (1-t)\boldsymbol{F}_-$. Then $\boldsymbol{F}_t \in \mathfrak{S}$ when $t > 0$ is small enough.*

Proof. We have

$$RW(\boldsymbol{F}_t) \le tRW(\boldsymbol{F}_+) + (1-t)RW(\boldsymbol{F}_-) \le tW(\boldsymbol{F}_+) + (1-t)W(\boldsymbol{F}_-),$$

since $\boldsymbol{F}_+$ and $\boldsymbol{F}_-$ are rank one related, according (1.3). Then

$$RW(\boldsymbol{F}_t) - W(\boldsymbol{F}_t) \le tW(\boldsymbol{F}_+) + (1-t)W(\boldsymbol{F}_-) - W(\boldsymbol{F}_t).$$

Let

$$\Psi(t) = tW(\boldsymbol{F}_+) + (1-t)W(\boldsymbol{F}_-) - W(\boldsymbol{F}_t).$$

We observe that

$$\Psi(0) = 0, \quad \Psi'(0) = p^* = 0.$$

We also compute

$$\Psi''(0) = -(W_{\boldsymbol{FF}}(\boldsymbol{F}_-)[\![\boldsymbol{F}]\!], [\![\boldsymbol{F}]\!]) = -(\boldsymbol{A}_-(\boldsymbol{n})\boldsymbol{a}, \boldsymbol{a}) < 0,$$

by assumption. Therefore, $RW(\boldsymbol{F}_t) - W(\boldsymbol{F}_t) \le \Psi(t) < 0$, when $t > 0$ is sufficiently small. $\square$

We conclude that stable values $\boldsymbol{F}_-$ must belong to the $md-1$-dimensional boundary of $\mathfrak{M}$. This shows that exactly $d-1$ relations are missing from the classical set of jump conditions (1.3), (2.4) and (2.5).

Let us now consider $\boldsymbol{F}_0 \in \mathfrak{M}$, and apply the implicit function theorem to the system of equations (1.3), (2.4), (2.5) to determine when $\boldsymbol{F}_0$ lies in the interior of $\mathfrak{M}$.

THEOREM **5.3.** *Let $\boldsymbol{F}_0 \in \mathfrak{M}$. Let $\boldsymbol{a}_0$ and $\boldsymbol{n}_0$ be the vectors from Definition 5.1 of $\mathfrak{M}$, corresponding to $\boldsymbol{F}_0$. Assume that $[\![\boldsymbol{P}]\!]^T\boldsymbol{a}_0 \neq \boldsymbol{0}$ and the acoustic tensor $\boldsymbol{A}(\boldsymbol{n}_0)$ is non-singular. Then $\boldsymbol{F}_0$ is in the interior of $\mathfrak{M}$.*

Proof. Our assumption of invertibility of the matrix $\boldsymbol{A}(\boldsymbol{n}_0)$ implies, via the implicit function theorem, that the system of equations (2.4), $W_{\boldsymbol{F}}(\boldsymbol{F}+\boldsymbol{a}\otimes\boldsymbol{n})\boldsymbol{n}-W_{\boldsymbol{F}}(\boldsymbol{F})\boldsymbol{n}=\boldsymbol{0}$, can be solved for $\boldsymbol{a}$ in the neighborhood of $\boldsymbol{a}_0$ for all $\boldsymbol{F}$ and $\boldsymbol{n}$ sufficiently close to $\boldsymbol{F}_0$ and $\boldsymbol{n}_0$. Hence, we may regard $\boldsymbol{a}$ as a function of $\boldsymbol{F}$ and $\boldsymbol{n}$ defined on the neighborhood of $\boldsymbol{F}_0$ and $\boldsymbol{n}_0$, respectively. Let

$$p^*(\boldsymbol{n};\boldsymbol{F})=W(\boldsymbol{F}+\boldsymbol{a}(\boldsymbol{F},\boldsymbol{n})\otimes\boldsymbol{n})-W(\boldsymbol{F})-(W_{\boldsymbol{F}}(\boldsymbol{F})\boldsymbol{a}(\boldsymbol{F},\boldsymbol{n}),\boldsymbol{n})$$

which we regard as a function on the unit sphere $\mathbb{S}^{d-1}$ depending on md parameters $\boldsymbol{F}$. Observe that $p^*(\boldsymbol{n}_0;\boldsymbol{F}_0)=p^*=0$. The implicit function theorem states that the equation $p^*(\boldsymbol{n};\boldsymbol{F})=0$ has a solution $\boldsymbol{n}\in\mathbb{S}^{d-1}$, near $\boldsymbol{n}_0$ for all $\boldsymbol{F}$ sufficiently close to $\boldsymbol{F}_0$, if the differential $dp^*(\boldsymbol{n}_0,\boldsymbol{F}_0):T_{\boldsymbol{n}_0}\mathbb{S}^{d-1}\to\mathbb{R}$ is non-zero. Differentiating, we obtain, using (2.4),

$$dp^*(\boldsymbol{n}_0,\boldsymbol{F}_0)\dot{\boldsymbol{n}}=([\![\boldsymbol{P}]\!]^T\boldsymbol{a}_0,\dot{\boldsymbol{n}})+([\![\boldsymbol{P}]\!]\boldsymbol{n}_0,d\boldsymbol{a}\dot{\boldsymbol{n}})=([\![\boldsymbol{P}]\!]^T\boldsymbol{a}_0,\dot{\boldsymbol{n}}),$$

where $\dot{\boldsymbol{n}}$ is an arbitrary vector in $T_{\boldsymbol{n}_0}\mathbb{S}^{d-1}$. We conclude that, due to (2.4), $dp^*\neq 0$ if and only if $[\![\boldsymbol{P}]\!]^T\boldsymbol{a}_0\neq\boldsymbol{0}$. The theorem is proved. □

To summarize, the new interface condition (3.4) is necessary for stability, because, if it fails (and $\boldsymbol{A}_-(\boldsymbol{n})$ is positive definite), then $\boldsymbol{F}_-$ must belong to the interior of $\mathfrak{M}$, in which case the rank one convexity condition $\boldsymbol{F}_-\not\in\mathfrak{S}$ is violated.

The vector equation (3.4) comprises d scalar equations. However, one linear combination of these equations

$$([\![\boldsymbol{P}]\!]^T\boldsymbol{a},\boldsymbol{n})=0 \tag{5.2}$$

is a consequence of (2.4). Equation (5.2) is the Hill's orthogonality relation [38]. The remaining $d-1$ equations, if added to the system of classical jump conditions (1.3), (2.4), (2.5), will now constrain $\boldsymbol{F}_\pm$ to lie on a co-dimension 1 surface in $\mathbb{M}$ called the *jump set*.

Definition 5.4. *The jump set $\mathfrak{J}$ is the set of matrices $\boldsymbol{F}\in\mathfrak{M}$ such that there exist vectors $\boldsymbol{a}\in\mathbb{R}^m\setminus\{\boldsymbol{0}\}$ and $\boldsymbol{n}\in\mathbb{R}^d$, $|\boldsymbol{n}|=1$ such that $\boldsymbol{F}_+=\boldsymbol{F}+\boldsymbol{a}\otimes\boldsymbol{n}$ and $\boldsymbol{F}_-=\boldsymbol{F}$ satisfy (1.3), (2.4), (2.5) and (3.4).*

Remark 5.5. *Theorem 5.3 implies that $\partial\mathfrak{M}\cap\mathfrak{M}\subset\mathfrak{J}$, while Theorem 5.2 implies that those points of $\mathfrak{J}$ that are in the interior of $\mathfrak{M}$ are unstable.*

The requirement that the deformation gradients on the stable interface must belong to the jump set is rather strong. For example in the case of anti-plane shear Silling has shown [71] that equilibrium configurations satisfying both classical and the new equilibrium condition are very special and are generated by a single complex potential which is analytic in the whole domain (rather than two potentials analytic on each phase separately). Generic Weierstrass-Erdmann solutions would be incompatible with such restrictions (roughening instability) and the corresponding smooth phase discontinuities would be replaced by the generalized surfaces in the sense of Young [74].

6 Solid-melt instability

As an example of the ability of (1.6) to indicate instability, consider an elastic solid in equilibrium with its melt. This problem was first addressed by Gibbs [28] who concluded that a non-hydrostatically stressed solid in equilibrium with a hydrostatically stressed fluid is always unstable. His argument was that a stressed element of solid surface can always dissolve into fluid and then recrystallize inside the fluid under hydrostatic conditions. This instability was later studied more systematically by Asaro and Tiller [4] in linear framework and by Grinfeld [32, 35] in the geometrically and physically nonlinear setting. In the work of Grinfeld the classical second variation was used and the unconditional instability was found. Here we show that the instability of a stressed solid-melt phase boundary can also be detected by checking our new jump condition (3.4). However, the implied mode of instability is closer to the one envisaged by Gibbs than to the one studied by Grinfeld.

To match our general setting we assume that the liquid is described as a hyperelastic solid with the energy density $W(\boldsymbol{F})$ that depends only on $\det \boldsymbol{F}$. The liquid does not have a preferred reference state, therefore, the representation $v = \det \nabla \boldsymbol{y}(\boldsymbol{x})$ is only formal. Indeed, if $\boldsymbol{y}'(\boldsymbol{x}')$ defined on the domain $\Omega' \subset \mathbb{R}^d$ is such that $\boldsymbol{y}'(\Omega') = \boldsymbol{y}(\Omega) = \Omega^*$ and $\det \nabla \boldsymbol{y}'((\boldsymbol{y}')^{-1}(\boldsymbol{z})) = \det \nabla \boldsymbol{y}(\boldsymbol{y}^{-1}(\boldsymbol{z}))$ for all $\boldsymbol{z} \in \Omega^*$ then the two states $\boldsymbol{y}(\boldsymbol{x})$ and $\boldsymbol{y}'(\boldsymbol{x}')$ are equivalent. We therefore assume that any statement about the liquid must hold for all equivalent deformation fields compatible with the prescribed function $v(\boldsymbol{z}) = \det \nabla \boldsymbol{y}(\boldsymbol{y}^{-1}(\boldsymbol{z}))$.

Let $w(v)$ be such that $W(\boldsymbol{F}) = w(\det \boldsymbol{F})$. Then the equations of equilibrium say $\nabla p = \boldsymbol{0}$, where $p(\boldsymbol{x}) = -w'(\det \nabla \boldsymbol{y}(\boldsymbol{x}))$. Hence, $p(\boldsymbol{x}) = \mathit{const}$. In the absence of liquid-liquid phase transitions $v(\boldsymbol{x}) = \det \boldsymbol{F}(\boldsymbol{x})$ must also be constant. Now, assume that there is a smooth surface Σ separating the solid and the liquid phase, that is capable of changing its position in Lagrangian coordinates. In other words, we assume that the solid and liquid phases can transform into one another.

If at the point $\boldsymbol{x}_0 \in \Sigma$ the values of the deformation gradients are $\boldsymbol{F}_s$ and $\boldsymbol{F}_l$ for the solid and the liquid, respectively, then the interface condition (1.3) states that $\boldsymbol{F}_l = \boldsymbol{F}_s + \boldsymbol{a} \otimes \boldsymbol{n}$ at the point $\boldsymbol{y}(\boldsymbol{x}_0)$ in Eulerian coordinates. Then

$$v_l = \det \boldsymbol{F}_l = \det \boldsymbol{F}_s + (\mathrm{cof} \boldsymbol{F}_s \boldsymbol{n}, \boldsymbol{a}) = v_s + (\boldsymbol{n}^*, \boldsymbol{a}) |\mathrm{cof} \boldsymbol{F}_s \boldsymbol{n}|,$$

where $\boldsymbol{n}^*$ is the unit normal to the solid-liquid interface in Eulerian coordinates. We conclude that replacing $\boldsymbol{a}$ with $\boldsymbol{a}'$ such that $(\boldsymbol{a}, \boldsymbol{n}^*) = (\boldsymbol{a}', \boldsymbol{n}^*)$ produces an equivalent state of the system, where Ω is the half-space $\mathbb{H}_{\boldsymbol{n}} = \{\boldsymbol{x} \in \mathbb{R}^d : (\boldsymbol{n}, \boldsymbol{x}) > 0\}$. Obviously,

$$(\boldsymbol{F}_s + \boldsymbol{a} \otimes \boldsymbol{n})\mathbb{H}_{\boldsymbol{n}} = (\boldsymbol{F}_s + \boldsymbol{a}' \otimes \boldsymbol{n})\mathbb{H}_{\boldsymbol{n}} = \{\boldsymbol{z} \in \mathbb{R}^d : (\boldsymbol{z}, \boldsymbol{n}^*) > 0\},$$

provided, $(\boldsymbol{a}, \boldsymbol{n}^*) = (\boldsymbol{a}', \boldsymbol{n}^*)$.

Let $p = -w'(v_l)$ be the pressure in the liquid and $\boldsymbol{\sigma} = \boldsymbol{P}_s \boldsymbol{F}_s^T / \det \boldsymbol{F}_s$ the Cauchy stress tensor of the solid. The continuity of tractions (2.4) can be written as

$$\boldsymbol{\sigma} \boldsymbol{n}^* = -p \boldsymbol{n}^*.$$

For a liquid phase we have

$$\boldsymbol{P}_l^T \boldsymbol{a} = -p\mathrm{cof}(\boldsymbol{F}_s + \boldsymbol{a} \otimes \boldsymbol{n})^T \boldsymbol{a} = -p(\mathrm{cof}\boldsymbol{F}_s)^T \boldsymbol{a} = -p(\det \boldsymbol{F}_s)\boldsymbol{F}_s^{-1}\boldsymbol{a}.$$

The new condition (3.4) then becomes

$$\boldsymbol{P}_s^T \boldsymbol{a} = -p \det \boldsymbol{F}_s \boldsymbol{F}_s^{-1} \boldsymbol{a}.$$

Equivalently, in terms of the Cauchy stress tensor, $\boldsymbol{\sigma}^T \boldsymbol{a} = -p\boldsymbol{a}$. Using the symmetry of $\boldsymbol{\sigma}$ we obtain

$$\boldsymbol{\sigma}\boldsymbol{a} = -p\boldsymbol{a}.$$

According to our assumption about equivalent states, we must also have $\boldsymbol{\sigma}\boldsymbol{a}' = -p\boldsymbol{a}'$ for all $\boldsymbol{a}'$, such that $(\boldsymbol{a}', \boldsymbol{n}^*) = (\boldsymbol{a}, \boldsymbol{n})$, which means $\boldsymbol{\sigma} = -p\boldsymbol{I}$. In other words, the solid which is in stable equilibrium with a fluid must be hydrostatically stressed.

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