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Maxwell's relation for isotropic bodies *

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Abstract. The paper determines the forms of equations of equilibrium of force and Maxwell's relations for stable coherent phase interfaces in isotropic two–dimensional solids. The interfaces fall within three distinct types; the forms of equilibrium equations depend on them. The first type is when the stresses of the two phases are hydrostatic; then the equilibrium of forces reduces to the equilibrium of pressures and Maxwell's relation reduces to the equality of Gibbs functions. The second, generic, case is when the principal stretches are different, the stress of at least one of the two phases is not hydrostatic and certain nondegeneracy condition holds. The force equilibrium is formulated in terms of a pair of scalar force-type quantities. These forces depend on whether the two principal stretches both increase (decrease) when crossing the interface or whether one of the stretches increases and the other decreases. Maxwell's relation involves these forces and reduces to the equality of generalized Gibbs-type potentials. The third case is when nondegeneracy condition is violated. The force equilibrium reduces to one scalar equation; Maxwell's relation reflects this fact.

Contents

1 Introduction

The conditions for phase equilibrium on stable coherent phase interfaces between phases A, B in a general nonlinear elastic material consist of

(a) the geometrical compatibility condition (Hadamard's condition)

$$\boldsymbol{B} - \boldsymbol{A} = \boldsymbol{a} \otimes \boldsymbol{n},$$

where $\boldsymbol{A}, \boldsymbol{B}$ are the deformation gradients of the two phases, $\boldsymbol{n}$ is the referential normal to the interface, and $\boldsymbol{a}$ is a vector called the amplitude of the interface,

(b) the balance of forces (mechanical equilibrium)

$$\boldsymbol{S}_A\, \boldsymbol{n} = \boldsymbol{S}_B\, \boldsymbol{n} \tag{1.1}$$

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where $\boldsymbol{S}_A$, $\boldsymbol{S}_B$ are the Piola–Kirchhoff stress of the phases A, B;

(c) Maxwell's relation (thermodynamical equilibrium):

$$f_B = f_A + \boldsymbol{S}_A \cdot (\boldsymbol{B} - \boldsymbol{A}), \tag{1.2}$$

where f_A , f_B are the values of free energy functions at the phases A, B,

(d) moreover, the stability considerations imply that the energy is rank 1 convex at the two phases (see Section 5).

The quantities in (1.1)–(1.2) are vectors and tensors. However, for fluids (to which the above general requirements apply as well), thanks to the fact that the symmetry group of the material is extremely large, it is possible to rewrite the conditions (b), (c) in a form involving only scalar quantites (Gibbsian thermostatics of fluids): the equality of pressures

$$p_A = p_B \tag{1.3}$$

and the equality of the Gibbs functions

$$g_A = g_B \tag{1.4}$$

where $g = f + pv$ is the Gibbs function and $v = \det \boldsymbol{F}$ the specific volume.

The goal of this note is to examine the analogues of (1.3) and (1.4) for two–dimensional isotropic solids. Thus the question is (α) whether the equality of the nomal components of forces (1.1) (which makes two scalar equations) can be formulated in terms of two predefined scalar quantities universal for this class, and (β) whether Maxwell's relation can be written in terms of some analog of Gibbs function. It turns out that the answer to both (α) and (β) is positive provided one divides all possible interfaces into three distinct types (A), (B), (C), and defines the universal forces and generalized Gibbs potentials for each class of interfaces separately. This allows one to pass from the tensorial equations to scalar equations involving the principal stretches only (see below).

To formulate the results, recall that the principal stretches $\alpha_1 \geq \alpha_2$ of a deformation gradient $\boldsymbol{A}$ are, by definition, the eigenvalues of $\sqrt{\boldsymbol{A}\boldsymbol{A}^{\mathrm{T}}}$; we write $\alpha = (\alpha_1, \alpha_2)$ for the ordered pair of singular values. If the body is isotropic then its stored energy $f : \mathbb{M}_+^{2\times 2} \to \mathbb{R}$, defined on the set $\mathbb{M}_+^{2\times 2}$ of 2×2 matrices with positive determinant, can be expressed also in terms if the principal stretches:

$$f(\boldsymbol{A}) = \tilde{f}(\alpha) \tag{1.5}$$

for every $\boldsymbol{A} \in \mathbb{M}_+^{2\times 2}$ where α are the principal stretches of $\boldsymbol{A}$ and $\tilde{f} : (0, \infty) \times (0, \infty) \to \mathbb{R}$ is a symmetric function (i.e., satisfies $\tilde{f}(\alpha_1, \alpha_2) = \tilde{f}(\alpha_2, \alpha_1)$). The function f is continuously differentiable on $\mathbb{M}_+^{2\times 2}$ if and only if $\tilde{f}$ is continuously differentiable on its domain ([3]), and if this is the case, we define the principal forces s_1, s_2 to be the functions on $(0, \infty) \times (0, \infty)$ given by

$$s_i(\alpha) = \frac{\partial \tilde{f}(\alpha)}{\partial \alpha_i}, \tag{1.6}$$

The Piola–Kirchhoff stress $\boldsymbol{S} = \boldsymbol{S}(\boldsymbol{A})$

$$\boldsymbol{S}(\boldsymbol{A}) = \frac{\partial f(\boldsymbol{A})}{\partial \boldsymbol{A}} \tag{1.7}$$

is diagonal of the form $\boldsymbol{S} = \mathrm{diag}(s_1, s_2)$ if $\boldsymbol{A}$ is diagonal: $\boldsymbol{A} = \mathrm{diag}(\alpha_1, \alpha_2)$.

Consider a stable interface with the deformation gradients $\boldsymbol{A}, \boldsymbol{B}$ whose principal stretches are $\alpha = (\alpha_1, \alpha_2), \beta = (\beta_1, \beta_2)$. The cases mentioned above are as follows. Case (A) is when the stresses of the two phases are hydrostatic:

$$\boldsymbol{S}_{\boldsymbol{A}} = -p_{\boldsymbol{A}}(\det \boldsymbol{A})\boldsymbol{A}^{-\mathrm{T}}, \quad \boldsymbol{S}_{\boldsymbol{B}} = -p_{\boldsymbol{B}}(\det \boldsymbol{B})\boldsymbol{B}^{-\mathrm{T}};$$

then the conditions of mechanical equilibrium and Maxwell's relation reduce to (1.3) and (1.4), respectively. Note that the stresses is certainly hydrostatic if $\alpha_1 = \alpha_2$; however, in nonelliptic solids exhibitting phase transitions the stress can be hydrostatic even if $\alpha_1 \neq \alpha_2$. In particular, it will be shown that (A) includes twinning: the case when $\alpha = \beta$.

Case (B) is when at least one of the stresses $\boldsymbol{S}_{\boldsymbol{A}}, \boldsymbol{S}_{\boldsymbol{B}}$ is not hydrostatic and $(\alpha_1 - \beta_2)(\beta_1 - \alpha_2) \neq 0$. Then, if $(\alpha_1 - \alpha_2)(\beta_1 - \beta_2) \geq 0$, the condition of mechanical equilibrium and Maxwell's relation read

$$k_+(\alpha) = k_+(\beta), \quad c_+(\alpha) = c_+(\beta), \quad g_+(\alpha) = g_+(\beta)$$

where

$$k_+ := \frac{\alpha_1 s_1 - \alpha_2 s_2}{\alpha_1 - \alpha_2}, \quad c_+ := -\frac{s_1 - s_2}{\alpha_1 - \alpha_2}, \tag{1.8}$$

$$g_+ = f - k_+(\alpha_1 + \alpha_2) - c_+ \alpha_1 \alpha_2 = f - \frac{\alpha_1^2 s_1 - \alpha_2^2 s_2}{\alpha_1 - \alpha_2}. \tag{1.9}$$

The quantities k_+, c_+ are the force type quantities in terms of which the equation of mechanical equilibrium is formulated. They are combinations of of the principal stresses. Similarly, g_+ is the analog of the Gibbs function appropriate to this case. If $(\alpha_1 - \alpha_2)(\beta_1 - \beta_2) \leq 0$, the condition of mechanical equilibrium and Maxwell's relation read

$$k_-(\alpha) = k_-(\beta), \quad c_-(\alpha) = c_-(\beta), \quad g_-(\alpha) = g_-(\beta),$$

provided where

$$k_- := \frac{\alpha_1 s_1 - \alpha_2 s_2}{\alpha_1 + \alpha_2}, \quad c_- := \frac{s_1 + s_2}{\alpha_1 + \alpha_2}, \tag{1.10}$$

$$g_- = f - k_-(\alpha_1 - \alpha_2) - c_- \alpha_1 \alpha_2 = f - \frac{\alpha_1^2 s_1 + \alpha_2^2 s_2}{\alpha_1 + \alpha_2}. \tag{1.11}$$

Case (C) is when at least one of the stresses $\boldsymbol{S}_{\boldsymbol{A}}, \boldsymbol{S}_{\boldsymbol{B}}$ is not hydrostatic and $(\alpha_1 - \beta_2)(\beta_1 - \alpha_2) = 0$. It follows that either $\beta_2 = \alpha_1$ or $\alpha_2 = \beta_1$ (or both) and then

$$s_1(\beta) = s_2(\alpha), \tag{1.12}$$

$$f_{\boldsymbol{A}} - s_2(\alpha)\alpha_2 = f_{\boldsymbol{B}} - s_1(\beta)\beta_1 \tag{1.13}$$

and

$$s_1(\alpha) = s_2(\beta), \tag{1.14}$$

$$f_{\boldsymbol{A}} - s_1(\alpha)\alpha_1 = f_{\boldsymbol{B}} - s_2(\beta)\beta_2, \tag{1.15}$$

respectively.

The quantities occurring in (1.3), (1.8), (1.10), (1.12), and (1.14) are the scalar force–type quantities which express the equations of mechanical equilibrium and the quantities (1.4), (1.9), (1.11), (1.13) abnd (1.15) are the Gibbs functions or their analogues which express the thermodynamical equilibrium.

$$2\frac{\alpha_1 \alpha_2 (\alpha_1 s_1 - \alpha_2 s_2)}{\alpha_1^2 - \alpha_2^2}$$

2 Stable coherent interfaces

We consider a two–dimensional isotropic body. We label the material points by their position $\boldsymbol{x}$ in a reference configuration $\Omega \subset \mathbb{R}^2$; a deformation is a function $\boldsymbol{u} : \Omega \to \mathbb{R}^2$ which gives the present position $\boldsymbol{y} = \boldsymbol{u}(\boldsymbol{x})$ in terms of $\boldsymbol{x} \in \Omega$; it is also assumed that the density of the body in the reference configuration is = 1. Assume that the body has a continuously differentiable stored energy function $f : \mathbb{M}^{2\times 2} \to \mathbb{R}$ and denote by $\boldsymbol{S} : \mathbb{M}^{2\times 2} \to \mathbb{M}^{2\times 2}$ the Piola–Kirchhoff stress as in (1.7). Throughout the paper, f is considered as given.

Deformations with coherent interfaces are adequately described by continuous and piecewise continuously differentiable deformation functions $\boldsymbol{u} : \Omega \to \mathbb{R}^2$. Thus Ω is divided into two open parts Ω_A, Ω_B, separated by a smooth surface $\mathscr{S} \subset \Omega$, such that the deformation gradient

$$\boldsymbol{F} := \frac{\partial \boldsymbol{u}(\boldsymbol{x})}{\partial \boldsymbol{x}}$$

is well-defined in Ω_A, Ω_B and has limits $\boldsymbol{A} = \boldsymbol{A}(\boldsymbol{x}), \boldsymbol{B} = \boldsymbol{B}(\boldsymbol{x})$ at every point $\boldsymbol{x} \in \mathscr{S}$ as $\boldsymbol{y}$ approaches $\boldsymbol{x}$ from Ω_A, Ω_B. The surface $\mathscr{S}$ then represents the interface in the reference configuratrion. If $\boldsymbol{n} = \boldsymbol{n}(\boldsymbol{x}), \boldsymbol{x} \in \mathscr{S}$ is the unit normal to $\mathscr{S}$ then by Hadamard's lemma, which follows from the continuity of $\boldsymbol{u}$, there exists a function $\boldsymbol{a} : \mathscr{S} \to \mathbb{R}^2$, called the amplitude of the jump, such that

$$\boldsymbol{B} = \boldsymbol{A} + \boldsymbol{a} \otimes \boldsymbol{n} \tag{2.1}$$

at every $\boldsymbol{x} \in \mathscr{S}$. Thus the geometrical compatibility on the interface assets that the jump $\boldsymbol{B} - \boldsymbol{A}$ in the deformation gradient is a rank 1 tensor: $\det(\boldsymbol{B} - \boldsymbol{A}) = 0$.

In the absence of external forces the total energy of the body in $\boldsymbol{u}$ is given by

$$I(\boldsymbol{u}) = \int_\Omega f(\boldsymbol{F})\, d\boldsymbol{x}.$$

We deal with deformations $\boldsymbol{u}$ which are stable in the sense that

$$I(\boldsymbol{u}) \le I(\boldsymbol{v}) \tag{2.2}$$

for each continuous and piecewise continuously differentiable deformation $\boldsymbol{v} : \Omega \to \mathbb{R}^2$ such that $\boldsymbol{u} = \boldsymbol{v}$ on the boundary $\partial\Omega$. It turns out that the minimum energy principle is a restriction on both the deformation and the energy function f; in particular, it implies that f must be rank 1 convex along the minimizer $\boldsymbol{u}$. The energy f is said to be rank 1 convex at $\boldsymbol{A} \in \mathbb{M}^{2\times 2}_+$ if

$$f(\boldsymbol{B}) \ge f(\boldsymbol{A}) + \boldsymbol{S}(\boldsymbol{A}) \cdot (\boldsymbol{B} - \boldsymbol{A}) \tag{2.3}$$

for every $\boldsymbol{B} \in \mathbb{M}^{2\times 2}_+$ that is rank 1 connected to $\boldsymbol{A}$,, i.e., $\det(\boldsymbol{B} - \boldsymbol{A}) = 0$. The minimum energy principle (2.2) implies that f is rank 1 convex at every $\boldsymbol{F}(\boldsymbol{x}), \boldsymbol{x} \in \Omega_A \cup \Omega_B$ and at the limiting values $\boldsymbol{A}(\boldsymbol{x}), \boldsymbol{B}(\boldsymbol{x})$ of $\boldsymbol{F}$ at $\boldsymbol{x} \in \mathscr{S}$. In addition, we have Maxwell's relation

$$f_B = f_A + \boldsymbol{S}_A \cdot (\boldsymbol{B} - \boldsymbol{A}) \tag{2.4}$$

where we write $f_A := f(\boldsymbol{A}), \boldsymbol{S}_A := \boldsymbol{S}(\boldsymbol{A})$ and similarly for $\boldsymbol{B}$.

For the considerations that follow we shall need just the above consequences of the minimum energy principle (2.2). We fix the point $\boldsymbol{x}$ on $\mathscr{S}$ and write $\boldsymbol{A}, \boldsymbol{B}$ for $\boldsymbol{A}(\boldsymbol{x}), \boldsymbol{B}(\boldsymbol{x})$. We say that $\boldsymbol{A}, \boldsymbol{B}, \boldsymbol{A} \ne \boldsymbol{B}$, form a stable interface if

(i) $\boldsymbol{A}, \boldsymbol{B}$ are rank 1 connected, i.e., (2.1) holds for some $\boldsymbol{a}, \boldsymbol{n} \in \mathbb{R}^2$;
(ii) both $\boldsymbol{A}, \boldsymbol{B}$ are points of rank 1 convexity of f;
(iii) Maxwell's relation (2.4) holds.

The equation of equilibrium of forces

$$\boldsymbol{S}_A \boldsymbol{n} = \boldsymbol{S}_B \boldsymbol{n} \tag{2.5}$$

is a consequence of (i)–(iii) together with the "conjugate" equation

$$\boldsymbol{S}_A^{\mathrm{T}} \boldsymbol{a} = \boldsymbol{S}_B^{\mathrm{T}} \boldsymbol{a}. \tag{2.6}$$

Indeed, since f is rank 1 convex at $\boldsymbol{A}$ we have

$$f(\boldsymbol{A} + \boldsymbol{b} \otimes \boldsymbol{n}) - f(\boldsymbol{A}) - \boldsymbol{S}_A \cdot (\boldsymbol{b} \otimes \boldsymbol{n}) \geq 0 \tag{2.7}$$

for each vector $\boldsymbol{b}$; in addition, Maxwell's relation says that the equality holds for $\boldsymbol{b} = \boldsymbol{a}$. Thus $\boldsymbol{b} = \boldsymbol{a}$ is a point of minimum of the function in the left–hand side of (2.7) and the differentiation with respect to $\boldsymbol{b}$ at $\boldsymbol{b} = \boldsymbol{a}$ gives (2.5). Similarly, we have

$$f(\boldsymbol{A} + \boldsymbol{a} \otimes \boldsymbol{m}) - f(\boldsymbol{A}) - \boldsymbol{S}_A \cdot (\boldsymbol{a} \otimes \boldsymbol{m}) \geq 0$$

for each $\boldsymbol{m} \in \mathbb{R}^2$ with the equality at $\boldsymbol{m} = \boldsymbol{n}$; the differentiation provides (2.6).

Let $\tilde{f} : (0,\infty) \times (0,\infty)$ be the symmetric function representing f as in (1.5) and let the principal forces be defined as in (1.6). We note that the symmetry of $\tilde{f}$ implies that for any $x \in (0,\infty) \times (0,\infty)$ we have $s_1(x_1, x_2) = s_2(x_2, x_1)$ and hence in particular

$$s_1(\gamma, \gamma) = s_2(\gamma, \gamma) \tag{2.8}$$

for any $\gamma > 0$, i.e., the principal forces coincide whenever the principal stretches coincide. If $\boldsymbol{A} \in \mathbb{M}_+^{2\times 2}$ has the singular values $\alpha = (\alpha_1, \alpha_2)$ then the singular–value decomposition theorem says that there exist proper orthogonal matrices $\boldsymbol{Q}, \boldsymbol{R} \in SO(2)$ such that

$$\boldsymbol{A} = \boldsymbol{Q} \operatorname{diag}(\alpha) \boldsymbol{R}; \tag{2.9}$$

the isotropy of the material then implies that

$$\boldsymbol{S}_A = \boldsymbol{Q} \operatorname{diag}(s) \boldsymbol{R} \tag{2.10}$$

where $s = s(\alpha)$ is the pair of principal forces. Note that the Cauchy stress $\boldsymbol{T}$ is related to $\boldsymbol{S}$ by $\boldsymbol{S} = \boldsymbol{T} \operatorname{cof} \boldsymbol{A}$ where $\operatorname{cof} \boldsymbol{A} = (\det \boldsymbol{A}) \boldsymbol{A}^{-\mathrm{T}}$ is the matrix of cofactors of $\boldsymbol{A}$.

A point $\boldsymbol{A}$ is said to be a point of liquefaction if

$$\boldsymbol{S}_A = -p \operatorname{cof} \boldsymbol{A} \tag{2.11}$$

for some $p \in \mathbb{R}$, called the pressure of $\boldsymbol{A}$. A necessary and sufficient condition for $\boldsymbol{A}$ to be a liquefaction point is that the corresponding principal forces $s = s(\alpha)$ satisfy

$$s_1 \alpha_1 = s_2 \alpha_2. \tag{2.12}$$

Indeed, if $\boldsymbol{A}$ is a liquefaction point and $\boldsymbol{Q}, \boldsymbol{R}$ are as in (2.9) then $\operatorname{cof} \boldsymbol{A} = \boldsymbol{A}(\operatorname{diag}(\alpha))^{-1} \boldsymbol{R}$ and the comparison of (2.10) with (2.11) produces $-p\alpha_i^{-1} = s_i$, $i = 1, 2$; thus (2.12). Conversely, (2.12) implies (2.11) with $p = -s_1\alpha_1 = -s_2\alpha_2$.

3 Maxwell's relation

For any $\alpha \in \mathbb{H}^2$ and any $\varepsilon \in \{1, -1\}$ we define the quantities

$$\hat{\alpha}_\varepsilon = \alpha_1 + \varepsilon\alpha_2;$$

we furthermore set

$$k_\varepsilon(\alpha) = \frac{\alpha_1 s_1 - \alpha_2 s_2}{\alpha_1 - \varepsilon\alpha_2}, \quad c_\varepsilon(\alpha) = -\varepsilon\frac{s_1 - \varepsilon s_2}{\alpha_1 - \varepsilon\alpha_2} \tag{3.1}$$

whenever the denominators are nonzero. We also abbreviate $\hat{\alpha}_\pm := \hat{\alpha}_{\pm1}, k_\pm(\alpha) := k_{\pm1}(\alpha), c_\pm(\alpha) := c_{\pm1}(\alpha)$ and notice that $k_\pm, c_\pm$ coincide with the quantities defined in Introduction. If $\alpha, \beta \in \mathbb{H}^2$, we further define

$$\varepsilon(\alpha, \beta) = \operatorname{sgn}\left((\beta_1 - \alpha_1)(\beta_2 - \alpha_2)\right).$$

For any $i \in \{1, 2\}$ we denote by $\bar{\imath} \in \{1, 2\}$ the complementary index, i.e., the unique $j \in \{1, 2\}$ such that $i \neq j$. The following theorem determines the forms of condition of mechanical and thermodynamical equilibrium:

3.1 Theorem. *Let $\boldsymbol{A}, \boldsymbol{B} \in \mathbb{M}^{2\times 2}_+$, with singular values α, β, respectively, form a stable interface. We have the following assertions:*
(i) *if $\alpha = \beta$ then $\boldsymbol{A}, \boldsymbol{B}$ are points of liquefaction of equal pressures:*

$$\boldsymbol{S_A} = -p_{\boldsymbol{A}} \operatorname{cof} \boldsymbol{A}, \quad \boldsymbol{S_B} = -p_{\boldsymbol{B}} \operatorname{cof} \boldsymbol{B} \tag{3.2}$$

with

$$p_{\boldsymbol{A}} = p_{\boldsymbol{B}}; \tag{3.3}$$

Maxwell's relation is a consequence of (3.3)*;*
(ii) *if $\alpha_i \neq \beta_j$ for all $i,j \in \{1, 2\}$* (*and hence $\alpha \neq \beta$*) *then setting $\varepsilon =: \varepsilon(\alpha, \beta)$ we have $\varepsilon \neq 0$, the quantities $k_\varepsilon(\alpha), k_\varepsilon(\beta), c_\varepsilon(\alpha), c_\varepsilon(\beta)$ are well-defined* (*see* (3.1)) *and*

$$k_\varepsilon(\alpha) = k_\varepsilon(\beta), \quad c_\varepsilon(\alpha) = c_\varepsilon(\beta) \tag{3.4}$$

and

$$\tilde{f}(\alpha) - k_\varepsilon(\alpha)\hat{\alpha}_\varepsilon - c_\varepsilon(\alpha)\alpha_1\alpha_2 = \tilde{f}(\beta) - k_\varepsilon(\beta)\hat{\beta}_\varepsilon - c_\varepsilon(\beta)\beta_1\beta_2; \tag{3.5}$$

(iii) *if $\alpha \neq \beta$ and $\alpha_i = \beta_j$ for some $i,j \in \{1, 2\}$ then*

$$s_{\bar{\imath}}(\alpha) = s_{\bar{\jmath}}(\beta), \tag{3.6}$$

$$\tilde{f}(\alpha) - s_{\bar{\imath}}(\alpha)\alpha_{\bar{\imath}} = \tilde{f}(\beta) - s_{\bar{\jmath}}(\beta)\beta_{\bar{\jmath}}. \tag{3.7}$$

It is noted that the Items (i)–(iii) are exhaustive and mutually exclusive.

Proof Let $\boldsymbol{B} = \boldsymbol{A} + \boldsymbol{a} \otimes \boldsymbol{n}$ and assume without any loss of generality that $\boldsymbol{A} = \operatorname{diag}(\alpha)$.
(i): Since $\alpha = \beta$, we have $\tilde{f}(\alpha) = \tilde{f}(\beta)$, and Maxwell's relation implies

$$\boldsymbol{S_A}\boldsymbol{n} \cdot \boldsymbol{a} = 0; \tag{3.8}$$

moreover, if we normalize to $|\boldsymbol{n}| = 1$ then $\boldsymbol{a}$ is given by (4.2). Since $\boldsymbol{A}$ is diagonal, we have $\boldsymbol{S} = \boldsymbol{S_A} = \operatorname{diag}(s)$ where $s := s(\alpha)$. The combination of (3.8) with (4.2) leads to

$$\boldsymbol{S}\boldsymbol{A}^{-1}\boldsymbol{n} \cdot \boldsymbol{n} = |\boldsymbol{A}^{-1}\boldsymbol{n}|^2 \boldsymbol{S}\boldsymbol{A}\boldsymbol{n} \cdot \boldsymbol{n}. \tag{3.9}$$

If we denote by n_1, n_2 the components of $\boldsymbol{n}$ then a rearrangement of (3.9) and the use of $|\boldsymbol{n}| = 1$ give

$$\frac{n_1^2(n_1^2-1)(\alpha_1^2-\alpha_2^2)(s_1\alpha_1-s_2\alpha_2)}{\alpha_1^2\alpha_2^2} = 0.$$

Note that $n_1 \neq 0, n_2 \neq 0$. Indeed, otherwise $\boldsymbol{n}$ is an eigenvector of $\boldsymbol{A}$ and (4.2) implies $\boldsymbol{a} = 0$, which contradicts $\boldsymbol{A} \neq \boldsymbol{B}$. Thus we have

$$(\alpha_1^2-\alpha_2^2)(s_1\alpha_1-s_2\alpha_2) = 0. \tag{3.10}$$

If $\alpha_1^2 = \alpha_2^2$, i.e., $\alpha_1 = \alpha_2$ then $s_1 = s_2$ by (2.8); so $s_1\alpha_1 - s_2\alpha_2 = 0$, i.e., $\boldsymbol{A}$ is a liquefaction point. If $\alpha_1^2 \neq \alpha_2^2$, then $s_1\alpha_1 - s_2\alpha_2 = 0$ by (3.10) and thus $\boldsymbol{A}$ is a liquefaction point again. By symmetry also $\boldsymbol{B}$ is a liquefaction point. Thus (3.2) holds for some $p_{\boldsymbol{A}}, p_{\boldsymbol{B}} \in \mathbb{R}$; comparing (2.5) with $\operatorname{cof} \boldsymbol{An} = \operatorname{cof} \boldsymbol{Bn}$ (which follows from (2.1), see [4]) we obtain (3.3). To show that Maxwell's relation (2.4) holds automatically, note that with $(3.3)_1$ and (2.1), Maxwell's relation takes the form

$$\tilde{f}(\beta) = \tilde{f}(\alpha) - p_{\boldsymbol{A}}(\det \boldsymbol{A})\boldsymbol{A}^{-\mathrm{T}}\boldsymbol{n}\cdot\boldsymbol{a}. \tag{3.11}$$

From $\alpha = \beta$ we deduce $\det \boldsymbol{A} = \det \boldsymbol{B}$; a combination with $\det \boldsymbol{B} = \det(\boldsymbol{A} + \boldsymbol{a}\otimes\boldsymbol{n}) \equiv \det \boldsymbol{A}(1 + \boldsymbol{A}^{-\mathrm{T}}\boldsymbol{n}\cdot\boldsymbol{a})$ leads to $\boldsymbol{A}^{-\mathrm{T}}\boldsymbol{n}\cdot\boldsymbol{a} = 0$. Hence (3.11) reduces to $\tilde{f}(\alpha) = \tilde{f}(\beta)$ which is certainly true since $\alpha = \beta$.

To proceed to the proofs of the cases (ii)–(iii), we note that since f is rank 1 convex at $\boldsymbol{A}$, Theorem 4.5, Proposition 4.6(i) and Maxwell's relation imply that

$$\begin{aligned}\tilde{f}(\beta) &\geq \tilde{f}(\alpha) + H(\alpha,\beta)\\ &\geq \tilde{f}(\alpha) + \boldsymbol{S}(\boldsymbol{A})\cdot(\boldsymbol{B}-\boldsymbol{A})\\ &= \tilde{f}(\beta).\end{aligned}$$

Thus we have the equality signs throughout; in particular

$$\tilde{f}(\beta) = \tilde{f}(\alpha) + H(\alpha,\beta). \tag{3.12}$$

(ii): The condition $\alpha_i \neq \beta_j$ for all $i,j \in \{1,2\}$ implies $(\beta_1-\alpha_1)(beta_2-\alpha_2) \neq 0$ and

$$(\alpha_1-\beta_2)(\beta_1-\alpha_2) \neq 0; \tag{3.13}$$

thus $\varepsilon \neq 0$ and equation (3.12) takes the form

$$\tilde{f}(\beta) = \tilde{f}(\alpha) + k_\varepsilon(\alpha)(\hat{\beta}_\varepsilon - \hat{\alpha}_\varepsilon) + c_\varepsilon(\alpha)(\beta_1\beta_2 - \alpha_1\alpha_2); \tag{3.14}$$

by symmetry also

$$\tilde{f}(\alpha) = \tilde{f}(\beta) + k_\varepsilon(\beta)(\hat{\alpha}_\varepsilon - \hat{\beta}_\varepsilon) + c_\varepsilon(\beta)(\alpha_1\alpha_2 - \beta_1\beta_2).$$

Consider the case $\varepsilon = 1$. By Remark 4.2 we have either $\alpha_1 > \alpha_2$ or $\beta_1 > \beta_2$; assume the latter and note that

$$(\beta_1-\alpha_1)(\beta_2-\alpha_2) > 0, \quad (\alpha_1-\beta_2)(\beta_1-\alpha_2) > 0, \quad \beta_1 > \beta_2 > 0. \tag{3.15}$$

Indeed, the first inequality is $\varepsilon = 1$. The second inequality is a combination of (3.13) with (4.1). The third inequality is our assumption. By (3.15) then

$$(\gamma_1-\alpha_1)(\gamma_2-\alpha_2) > 0, \quad (\alpha_1-\gamma_2)(\gamma_1-\alpha_2) > 0, \quad \gamma_1 > \gamma_2 > 0$$

for all $\gamma \in \mathbb{R}^2$ sufficiently close to β. Thus, since f is rank 1 convex at $\boldsymbol{A}$, an appeal to Theorem 4.5 shows that

$$\tilde{f}(\gamma) \geq \tilde{f}(\alpha) + k_+(\alpha)(\hat{\gamma}_+ - \hat{\alpha}_+) + c_+(\alpha)(\gamma_1\gamma_2 - \alpha_1\alpha_2)$$

for all γ sufficiently close to β; moreover, for $\gamma = \beta$ we have the equality sign by (3.14). Thus the differentiation with respect to γ at $\gamma = \beta$ provides

$$s_1(\beta) = k_+(\alpha) + c_+(\alpha)\beta_2, \quad s_2(\beta) = k_+(\alpha) + c_+(\alpha)\beta_1;$$

consequently

$$s_1(\beta)\beta_1 - s_2(\beta)\beta_2 = k_+(\alpha)(\beta_1 - \beta_2), \quad s_1(\beta) - s_2(\beta) = c_+(\alpha)(\beta_2 - \beta_1). \tag{3.16}$$

Since $\beta_1 > \beta_2$, we see that $k_+(\beta), c_+(\beta)$ are defined and equations (3.16) imply (3.4) with $\varepsilon = 1$. With (3.4), equation (3.14) implies (3.5) with $\varepsilon = 1$. Let $\varepsilon = -1$; noting that again either $\alpha_1 > \alpha_2$ or $\beta_1 > \beta_2$ we assume the latter and observe that

$$(\beta_1 - \alpha_1)(\beta_2 - \alpha_2) < 0, \quad (\alpha_1 - \beta_2)(\beta_1 - \alpha_2) > 0, \quad \beta_1 > \beta_2 > 0.$$

Here the first inequality is a restatement of $\varepsilon = -1$, the second follows from (3.13), (4.1) as above and the third inequality is our assumption. Then we have

$$(\gamma_1 - \alpha_1)(\gamma_2 - \alpha_2) < 0, \quad (\alpha_1 - \gamma_2)(\gamma_1 - \alpha_2) > 0, \quad \gamma_1 > \gamma_2 > 0$$

for all γ sufficiently close to β. Thus, since f is rank 1 convex at $\boldsymbol{A}$, an appeal to Theorem 4.5 shows that

$$\tilde{f}(\gamma) \geq \tilde{f}(\alpha) + k_-(\alpha)(\hat{\gamma}_- - \hat{\alpha}_-) + c_-(\alpha)(\gamma_1\gamma_2 - \alpha_1\alpha_2)$$

with the equality holding at $\gamma = \beta$. Thus the differentiation provides

$$s_1(\beta) = k_-(\alpha) + c_-(\alpha)\beta_2, \quad s_2(\beta) = -k_-(\alpha) + c_-(\alpha)\beta_1;$$

these relations immediately imply (3.4) with $\varepsilon = -1$. With (3.4), equation (3.14) implies (3.5) with $\varepsilon = -1$.

(iii): Consider first the case $i = j = 1$ so that $\bar{i} = \bar{j} = 2$ and $\beta_1 = \alpha_1$. Using that either $\alpha_1 > \alpha_2$ or $\beta_1 > \beta_2$ we assume without any loss of generality the latter. If φ is the function defined in Remark 4.7 then the inequality (4.6) holds for each $\tau > 0$; moreover, for $\tau = \beta_2$ the equality holds in (4.6) by (3.12). The differentiation provides $\varphi'(\beta_2) = s_2(\alpha)$. The definition of φ and the use of $\beta_2 < \beta_1 = \alpha_1$ gives that $\varphi'(\beta_2) = \tilde{f}_2(\alpha_1, \beta_2) = \tilde{f}_2(\beta) = s_2(\beta)$. Thus we have (3.6) and with that equation the equality (4.6) at $\tau = \beta_2$ gives (3.7). The case $i = j = 2$ is similar. Next consider the case $i = 1, j = 2$ so that $\bar{i} = 2, \bar{j} = 1$ and $\beta_1 = \alpha_2$. Let ψ be the function defined in Remark 4.7. Then we have the inequality (4.6) for each $\tau > 0$ and for $\tau = \beta_2$ the equality holds by (3.12). Thus the differentiation provides $\psi'(\beta_2) = s_1(\alpha)$. The definition of ψ gives that $\psi'(\beta_2) = \tilde{f}_2(\alpha_2, \beta_2) = \tilde{f}_2(\beta_1, \beta_2) = s_2(\beta)$. Thus we have (3.6) and with that equation the equality (4.6) at $\tau = \beta_2$ gives (3.7). The case $i = 2, j = 1$ is similar. □

The following assertion shows that in the cases (C), (D) the deformation gradient of the phase B is essentially uniquely determined by the deformation of the phase A : and the singular values of $\boldsymbol{B}$, and the form of the dependence is independent of the material in question. and

$$\tilde{f}(\alpha) + p_A v_A = \tilde{f}(\beta) + p_B v_B$$

where $v_A = \det \boldsymbol{A}, v_B = \det \boldsymbol{B}$;

3.2 Theorem. *Let* $\boldsymbol{A}, \boldsymbol{B} \in \mathbb{M}_{+}^{2\times 2}$ *form a stable interface where* $\boldsymbol{A} = \operatorname{diag}(\alpha)$, $\alpha \in \mathbb{H}^2$, *and* $\boldsymbol{B}$ *has the singular values* β. *If* $\boldsymbol{A}$ *is not a liquefaction point then* $\boldsymbol{B} = \boldsymbol{A} + \boldsymbol{a} \otimes \boldsymbol{n}$, *where* $\boldsymbol{a}, \boldsymbol{n}$, *with* $|\boldsymbol{n}| = 1$, *satisfy*

$$\left.\begin{aligned} n_1^2 &= \frac{\alpha_1 - \sigma\beta_2}{\alpha_1 - \sigma\alpha_2}\left|\frac{\beta_1 - \alpha_1}{\hat{\beta}_\sigma - \hat{\alpha}_\sigma}\right|, \quad n_2^2 = \frac{\beta_1 - \sigma\alpha_2}{\alpha_1 - \sigma\alpha_2}\left|\frac{\beta_2 - \alpha_2}{\hat{\beta}_\sigma - \hat{\alpha}_\sigma}\right|, \\ a_1 &= (\hat{\beta}_\sigma - \hat{\alpha}_\sigma)n_1, \quad a_2 = \sigma(\hat{\beta}_\sigma - \hat{\alpha}_\sigma)n_2 \end{aligned}\right\} \tag{3.17}$$

where

$$\sigma = \begin{cases} \varepsilon(\alpha,\beta) & \text{if} \quad \varepsilon(\alpha,\beta) \neq 0, \\ 1 & \text{if} \quad \varepsilon(\alpha,\beta) = 0. \end{cases} \tag{3.18}$$

4 Rank 1 perturbations and invariant rank 1 convex functions

This appendix reviews be background of notions and results employed in the preceding text. We first address the question of the possible singular values of rank 1 perturbations.

4.1 Proposition ([1]). *If* $\boldsymbol{A} \in \mathbb{M}_{+}^{2\times 2}$ *has the singular values* α *then* $\beta \in \mathbb{H}^2$ *are singular values of some rank 1 perturbation of* $\boldsymbol{A}$ *if and only if*

$$(\alpha_1 - \beta_2)(\beta_1 - \alpha_2) \geq 0; \tag{4.1}$$

equivalently, if and only if

$$\alpha_1 \geq \beta_2, \quad \beta_1 \geq \alpha_2.$$

The above Proposition has the following useful corollary:

4.2 Remark. *If* $\boldsymbol{A}, \boldsymbol{B} \in \mathbb{M}_{+}^{2\times 2}$ *are two rank 1 connected matrices whose singular values satisfy* $\alpha \neq \beta$ *then either* $\alpha_1 > \alpha_2$ *or* $\beta_1 > \beta_2$.

Two matrices $\boldsymbol{A}, \boldsymbol{B} \in \mathbb{M}_{+}^{2\times 2}$ are said to be twins if (i) they are rank 1 connected (i.e., $\det(\boldsymbol{A} - \boldsymbol{B}) = 0$) and (ii) have the same singular values.

4.3 Proposition. *If* $\boldsymbol{A}, \boldsymbol{B} \in \mathbb{M}_{+}^{2\times 2}$ *are twins then there exists an* $\boldsymbol{n} \in \mathbb{R}^2$, $|\boldsymbol{n}| = 1$, *such that* $\boldsymbol{B} = \boldsymbol{A} + \boldsymbol{a} \otimes \boldsymbol{n}$ *where*

$$\boldsymbol{a} = 2\left(\frac{\boldsymbol{A}^{-1}\boldsymbol{n}}{|\boldsymbol{A}^{-1}\boldsymbol{n}|^2} - \boldsymbol{A}\boldsymbol{n}\right). \tag{4.2}$$

4.4 Proposition ([5]). *If* $\alpha, \beta \in \mathbb{H}^2$, $\alpha \neq \beta$, *satisfy* (4.1) *and if* $\boldsymbol{a}, \boldsymbol{n} \in \mathbb{R}^2$ *are given by* (3.17), *then* $\boldsymbol{B} := \operatorname{diag}(\alpha) + \boldsymbol{a} \otimes \boldsymbol{n}$ *has the singular values* β. *Moreover, if* σ *is given by* (3.18) *then with* $\boldsymbol{J}_\sigma := \operatorname{diag}(1, \sigma)$ *we have*

$$\operatorname{tr}\big(\boldsymbol{J}_\sigma(\boldsymbol{B} - \boldsymbol{A})\big) = \hat{\beta}_\sigma - \hat{\alpha}_\sigma.$$

The following result is a characterization of rank 1 convexity of rotationally invariant rank 1 convex functions, [2, 5].

4.5 Theorem. *The function f is rank 1 convex at* $\operatorname{diag}(\alpha)$, $\alpha \in \mathbb{H}^2$, *if and only if the following two conditions hold simultaneously with* $s = s(\alpha)$*:*
(i) $s_1\alpha_1 - s_2\alpha_2 \geq 0$;
(ii) *if* $\beta \in \mathbb{H}^2$ *satisfies* (4.1) *and if we write* $\varepsilon := \varepsilon(\alpha, \beta)$ *then*

$$\tilde{f}(\beta) \geq \tilde{f}(\alpha) + H(\alpha, \beta) \tag{4.3}$$

where

$$H(\alpha,\beta) = \begin{cases} k_\varepsilon(\alpha)(\hat{\beta}_\varepsilon - \hat{\alpha}_\varepsilon) + c_\varepsilon(\alpha)(\beta_1\beta_2 - \alpha_1\alpha_2) & \text{if} \quad \varepsilon \neq 0, \\ s(\alpha)\cdot(\beta - \alpha) & \text{if} \quad \varepsilon = 0. \end{cases}$$

It is noted that the function $H(\alpha, \beta)$ pays the role of the Weierstrass excess function in the convexity theory. Here H is nonlinear in the increments of the arguments. The following result shows that $H(\alpha, \beta)$ is the maximum of the right hand side of inequality (2.3) subject to fixed singular values of $\boldsymbol{A}$, $\boldsymbol{B}$ and establishes the status of maximizers for the special rank 1 perturbations occurring in Proposition 4.4.

4.6 Proposition. *Let f be rank 1 convex at* $\boldsymbol{A} = \operatorname{diag}(\alpha)$, $\alpha \in \mathbb{H}^2$ *and let* $\boldsymbol{B} \in \mathbb{M}^{2\times 2}_+$, *with singular values β, be rank 1 connected to $\boldsymbol{A}$. Then:*
(i)

$$H(\alpha,\beta) \geq \boldsymbol{S}(\boldsymbol{A})\cdot(\boldsymbol{B} - \boldsymbol{A})$$

(ii) *if* $\boldsymbol{B} = \boldsymbol{A} + \boldsymbol{a} \otimes \boldsymbol{n}$ *where* $\boldsymbol{a}, \boldsymbol{n}$ *are as in* (3.17) *then*

$$H(\alpha,\beta) = \boldsymbol{S}(\boldsymbol{A})\cdot(\boldsymbol{B} - \boldsymbol{A}); \tag{4.4}$$

(iii) *if for* $s := s(\alpha)$ *we have* $s_1\alpha_1 - s_2\alpha_2 > 0$ *then* (4.4) *holds only if* $\boldsymbol{B} = \boldsymbol{A} + \boldsymbol{a} \otimes \boldsymbol{n}$ *where* $\boldsymbol{a}, \boldsymbol{n}$ *are as in* (3.17).

Proof Items (i), (ii) follow from the considerations underlying the proof of Theorem 4.5 in [5]. Thus it suffices to prove (iii). Let $\boldsymbol{B}$ be a rank 1 perturbation with singular values β and let σ be given by (3.18). We seek to prove that $\boldsymbol{B}$ is of the asserted special form. We have $\boldsymbol{S} := \boldsymbol{S}(\boldsymbol{A}) = \operatorname{diag}(s)$ and the inequality $s_1\alpha_1 - s_2\alpha_2 > 0$ implies that $\alpha_1 > \alpha_2$ (for otherwise we would have $s_1 = s_2$). Thus $k_\sigma := k_\sigma(\alpha), c_\sigma := c_\sigma(\alpha)$ are well defined and using this fact, it is easy to establish the following formula for $\boldsymbol{S}$:

$$\boldsymbol{S} = k_\sigma \boldsymbol{J}_\sigma + c_\sigma \operatorname{cof} \boldsymbol{A}$$

where $\boldsymbol{J}_\sigma := \operatorname{diag}(1, \sigma)$. Using this expression and

$$\beta_1\beta_2 - \alpha_1\alpha_2 = \det \boldsymbol{B} - \det \boldsymbol{A} = \operatorname{cof} \boldsymbol{A} \cdot (\boldsymbol{B} - \boldsymbol{A}),$$

which is valid for any rank 1 perturbation of $\boldsymbol{A}$, we obtain that

$$\boldsymbol{S}\cdot(\boldsymbol{B} - \boldsymbol{A}) = k_\sigma \operatorname{tr}(\boldsymbol{J}_\sigma(\boldsymbol{B} - \boldsymbol{A})) + c_\sigma(\beta_1\beta_2 - \alpha_1\alpha_2).$$

Comparing this expression with the definition of $H(\alpha, \beta)$ and using $k_\sigma > 0$, which follows from $s_1\alpha_1 - s_2\alpha_2 > 0$, we obtain

$$\operatorname{tr}(\boldsymbol{J}_\sigma(\boldsymbol{B} - \boldsymbol{A})) = \hat{\beta}_\sigma - \hat{\alpha}_\sigma.$$

Using $\boldsymbol{A} = \operatorname{diag}(\alpha)$ this finally reduces to

$$\operatorname{tr}(\boldsymbol{J}_\sigma \boldsymbol{B}) = \hat{\beta}.$$

The differentiation implies that $\boldsymbol{J}_\sigma \boldsymbol{B}$ is symmetric. The eigenvalues of $\boldsymbol{B}$ are $\mu_1\beta_1, \mu_2 = \beta_2, \mu_1\mu_2 = 1$. This implies that the eigenvalues are β. Thus $\boldsymbol{B}$ is a symmetric rank 1 perturbation of the symmetric matrix and thus of my form. □

The following remark is the well–known separate convexity of rank 1 convex functions (cf..). The result also follows from Theorem 4.5.

4.7 Remark. *Let f be rank 1 convex at* $\operatorname{diag}(\alpha)$, $\alpha \in \mathbb{H}^2$, *let* $i \in \{1, 2\}$ *and define* $\varphi : (0, \infty) \to \mathbb{R}$ *by*

$$\varphi(\tau) = \tilde{f}(\alpha_i, \tau), \tag{4.5}$$

$\tau \in (0, \infty)$. *Then*

$$\varphi(\tau) \geq \varphi(\alpha_{\bar{i}}) + s_{\bar{i}}(\alpha)(\tau - \alpha_{\bar{i}}) \tag{4.6}$$

for all $\tau > 0$.

5 Complements

A function $g : D \to \mathbb{R} \cup \{\infty\}, D \subset \mathbb{H}^2$, is said to be BE–monotonic at an $\alpha \in D$ if

$$g(\alpha) \leq g(\beta)$$

for each $\beta \in D$ satisfying

$$\alpha_1 \leq \beta_1, \quad \alpha_1\alpha_2 = \beta_1\beta_2.$$

The function $g : D \to \mathbb{R} \cup \{\infty\}$ is said to be BE–monotonic if it is BE–monotonic at every $\alpha \in D$.

5.1 Proposition. *A tensor $\boldsymbol{A}$ is a linear combination of twins of singular values β if and only if its singular values α satisfy*

$$\alpha_1 \leq \beta_1, \quad \alpha_1\alpha_2 = \beta_1\beta_2.$$

Proof Let $\boldsymbol{A} = \operatorname{diag}(\alpha)$,

$$\boldsymbol{B}_\pm = \begin{bmatrix} \alpha_1 & \pm t \\ 0 & \alpha_2 \end{bmatrix}, \quad t = \sqrt{\beta_1^2 + \beta_2^2 - (\alpha_1^2 + \alpha_2^2)}.$$

Then the signed singular values of $\boldsymbol{B}_\pm$ are β and

$$\boldsymbol{A} = \tfrac{1}{2}(\boldsymbol{B}_+ + \boldsymbol{B}_-).$$

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