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Abstract. The paper gives a simple derivation of the relaxed energy W^{qc} for the quadratic double-well material with equal elastic moduli and analyzes W^{qc} in the transversely isotropic case. We observe that the energy W is a sum of a degenerate quadratic quasiconvex function and a function that depends on the strain only through a scalar variable. For such a W, the relaxation reduces to a one-dimensional convexification. W^{qc} depends on a constant g defined by a three-dimensional maximum problem. It is shown that in the transversely isotropic case the problem reduces to a maximization of a fraction of two quadratic polynomials over $[0, 1]$. The maximization reveals several regimes and explicit formulas are given in the case of a transversely isotropic, positive definite displacement of the wells.

1 Introduction

In the theory of phase transitions in crystalline solids, within the small deformation theory, one minimizes the energy functional

$$I(\mathbf{u}) = \int_{\Omega} W(\nabla^s \mathbf{u}), dx$$

where $\Omega \subset \mathbb{V}$ is an open bounded subset of an n-dimensional physical space $\mathbb{V}$, $\mathbf{u} : \Omega \to \mathbb{V}$ is a displacement with the symmetric gradient (the linear strain tensor) $\mathbf{E} = \nabla^s \mathbf{u} := \frac{1}{2}(\nabla \mathbf{u} + \nabla \mathbf{u}^T)$ and $W : \mathrm{Sym} \to \mathbb{R}$ is the stored energy defined on the set Sym of all symmetric second-order tensors (matrices).

The stored energy W has two or several relative minima corresponding to the phases of the material. In such situations, the effective energy of the crystal is given by the relaxation of I, i.e., by

$$\bar{I}(\mathbf{u}) = \int_{\Omega} W^{qc}(\nabla^s \mathbf{u})\, dx,$$

where W^{qc} is the quasiconvex hull of W, i.e., the largest quasiconvex function not exceeding W. See [1], [11], [8], [6], and [12]. Recall that a continuous function $W : \mathrm{Sym} \to \mathbb{R}$ is said to be quasiconvex [5] if

$$|E|W(\mathbf{E}) \le \int_E W(\mathbf{E} + \nabla^s \mathbf{v}(\mathbf{x}))\, d\mathbf{x}$$

for each $\mathbf{E} \in \mathrm{Sym}$, each open $E \subset \mathbb{V}$ and each $\mathbf{v} \in W_0^{1,\infty}(E)$; here $|E|$ is the Lebesgue measure of E. The idea behind relaxation is that the macroscopic deformation $\mathbf{E}$ may be a result of an averaging of a complicated microstructure consisting of different phases that may reduce the energy. Related to but simpler than W^{qc} is the rank 1 convex hull W^{rc} defined as the largest rank 1 convex function not exceeding W. Recall that W is said to be rank 1 convex if

$$W((1-t)\mathbf{F} + t\mathbf{G}) \le (1-t)W(\mathbf{F}) + tW(\mathbf{G}),$$

for each $\mathbf{F}, \mathbf{G} \in \mathrm{Sym}, t \in [0,1]$ such that

$$\mathbf{G} - \mathbf{F} = \mathbf{a} \odot \mathbf{n} \tag{1}$$

for some $\mathbf{a}, \mathbf{n} \in \mathbb{V}$, where $\mathbf{a} \odot \mathbf{n} := \frac{1}{2}(\mathbf{a} \otimes \mathbf{n} + \mathbf{n} \otimes \mathbf{a})$. It is well-known that the quasiconvexity implies rank 1 convexity; hence

$$W^{qc} \le W^{rc}. \tag{2}$$

Moreover, if one introduces W^{lo} by

$$W^{lo}(\mathbf{E}) := \inf\{(1-t)W(\mathbf{F}) + tW(\mathbf{G})\},$$

[3], where the infimum is taken over all $\mathbf{F}, \mathbf{G} \in \mathrm{Sym}, t \in [0,1]$ satisfying (1) and $\mathbf{E} = (1-t)\mathbf{F} + t\mathbf{G}$, then clearly

$$W^{rc} \le W^{lo}. \tag{3}$$

There are not so many examples where W^{qc} can be calculated explicitly. In Proposition 2.1, Section 2 we point out that W^{qc} is obtained elementarily if $W = F + G$ is a sum of a degenerate quasiconvex function F and a function G that depends on $\mathbf{E}$ only through a scalar variable $x = \mathbf{E} \cdot \mathbf{N}$ where $\mathbf{N}$ is a fixed direction in the space Sym. Namely,

$$W^{qc} = W^{rc} = W^{lo} = F + \tilde{G}$$

where $\tilde{G}$ is the convex hull of G. The hypothesis covers the quadratic double–well energy with equal elastic moduli by Lurie & Cherkaev [4], Kohn [2], and Pipkin [9]; the latter reference contains implicitly the result in the form $W^{qc} = F + \tilde{G}$.

The relaxed energy W^{qc} depends on a constant g defined by a three–dimensional auxiliary maximum problem introduced by Kohn and Pipkin which involves the tensor of elastic constants of the material and the displacement tensor $\mathbf{C}$ between the bottoms of the wells. The constant g is discussed in detail by Kohn for isotropic materials, with references. In the second part of the paper we examine g for a transversely isotropic material. To calculate g, one has to determine the inverse of the (isothermal) acoustic tensor $\mathbf{D}(\mathbf{n})$ (Section 3). Next we pass to the case when $\mathbf{C}$ has the transversal symmetry as well. It is shown that the problem reduces to a maximization of a fraction of two quadratic polynomials over $[0,1]$, and the problem of maximum is reduced to solving a quadratic equation. Surprisingly, and fortunately, the discriminant is a full square and thus the roots are given by rational expressions (no square roots) in the five elastic moduli $\alpha_1, \alpha_2, \alpha_3, \alpha_4, \alpha_5$, of the transversely isotropic material and the data of $\mathbf{C}$. The problem reduces to determining whether or not the root(s) fall in $[0,1]$. This leads to several regimes in which g is given by different expressions. We calculate g explicitly for the case of $\mathbf{C}$ transversely isotropic and positive semidefinite and specialize the results to the cases $\mathbf{C} = \mathbf{e} \otimes \mathbf{e}, \mathbf{C} = \mathbf{1} - \mathbf{e} \otimes \mathbf{e}, \mathbf{C} = \mathbf{1}$ where $\mathbf{e}$ is the preferred unit vector of transversal symmetry.

2 The quadratic double well energy with equal moduli

Let Lin be the space of all linear transformations (tensors) on $\mathbb{V}$, and write $\mathbf{A} \cdot \mathbf{B} = \operatorname{tr}(\mathbf{A}^T\mathbf{B}), |\mathbf{A}| = \sqrt{\mathbf{A} \cdot \mathbf{A}}$, $\mathbf{A}, \mathbf{B} \in$ Lin, for the inner product and norm on Lin, with $\mathbf{A}^T$ the transpose of $\mathbf{A}$ and tr the trace. For $\mathbf{a}, \mathbf{b} \in \mathbb{V}$, let $\mathbf{a} \otimes \mathbf{b}$ be the tensor defined by $(\mathbf{a} \otimes \mathbf{b})\mathbf{v} = (\mathbf{b} \cdot \mathbf{v})\mathbf{a}, \mathbf{v} \in \mathbb{V}$.

Proposition 2.1. *Let $W : \mathrm{Sym} \to \mathbb{R}$ be of the form*

$$W(\mathbf{E}) = F(\mathbf{E}) + G(x), \quad \mathbf{E} \in \mathrm{Sym}, \tag{4}$$

where $x := \mathbf{N} \cdot \mathbf{E}$, F is a quasiconvex function, $\mathbf{N} \in \mathrm{Sym}$ and $G : \mathbb{R} \to \mathbb{R}$. Assume that F is degenerate in the sense that there exist $\mathbf{b}, \mathbf{c} \in \mathbb{V}$ such that $\mathbf{N} \cdot (\mathbf{b} \odot \mathbf{c}) \neq 0$ and

$$F(\mathbf{E} + \lambda \mathbf{b} \odot \mathbf{c}) = F(\mathbf{E}) \tag{5}$$

for all $\mathbf{E} \in \mathrm{Sym}$, $\lambda \in \mathbb{R}$. Then $W^{lo} = W^{rc} = W^{qc}$ and

$$W^{qc}(\mathbf{E}) = F(\mathbf{E}) + \tilde{G}(x), \quad \mathbf{E} \in \mathrm{Sym}, \tag{6}$$

where $\tilde{G}$ is the convexification of G.

Proof. Let H denote the function on the right-hand side of (6). Since F is quasiconvex and $\mathbf{E} \mapsto \tilde{G}(\mathbf{N} \cdot \mathbf{E})$ convex, H is quasiconvex and since $H \le W$, we have $H \le W^{qc}$. By (2), (3), the proof will be complete if we show that $W^{lo} \le H$. Let $\mathbf{E} \in \mathrm{Sym}$ and $\epsilon > 0$. By the definition of $\tilde{G}$ there exist $y, z \in \mathbb{R}$ and $t \in (0,1)$ such that

$$x \equiv \mathbf{N} \cdot \mathbf{E} = (1-t)y + tz, \tag{7}$$

$$(1-t)G(y) + tG(z) < \tilde{G}(x) + \epsilon. \tag{8}$$

Let $\mathbf{b}, \mathbf{c}$ be as in the hypothesis and set $\mathbf{A} = \mathbf{b} \odot \mathbf{c}$. By $\mathrm{N} \cdot \mathbf{A} \neq 0$ and (7) there exists a $\lambda \in \mathbb{R}$ such that

$$y = x + (1-t)^{-1}\lambda \mathrm{N} \cdot \mathbf{A}, \quad z = x - t^{-1}\lambda \mathrm{N} \cdot \mathbf{A}.$$

Let

$$\mathbf{F} = \mathbf{E} + (1-t)^{-1}\lambda \mathbf{A}, \quad \mathbf{G} = \mathbf{E} - t^{-1}\lambda \mathbf{A},$$

so that $\mathbf{E} = (1-t)\mathbf{F} + t\mathbf{G}$ and hence $W^{lo}(\mathbf{E}) \leq (1-t)W(\mathbf{F}) + tW(\mathbf{G})$. By (5) we have $F(\mathbf{F}) = F(\mathbf{G}) = F(\mathbf{E})$ and hence

$$W(\mathbf{F}) = F(\mathbf{E}) + G(y), \quad W(\mathbf{G}) = F(\mathbf{E}) + G(z).$$

Consequently,

$$(1-t)W(\mathbf{F}) + tW(\mathbf{G}) = F(\mathbf{E}) + (1-t)G(y) + tG(z) \leq F(\mathbf{E}) + \tilde{G}(x) + \epsilon;$$

thus $W^{lo}(\mathbf{E}) \leq F(\mathbf{E}) + \tilde{G}(x) + \epsilon = H(\mathbf{E}) + \epsilon.$ □

The quadratic double well energy W with equal elastic moduli ([4], [2], [9]) is defined by

$$W(\mathbf{E}) = \min\{W_0(\mathbf{E}), W_1(\mathbf{E})\},$$

$$W_0(\mathbf{E}) = \tfrac{1}{2}\mathbb{C}\mathbf{E} \cdot \mathbf{E}, \quad W_1(\mathbf{E}) = \tfrac{1}{2}\mathbb{C}(\mathbf{E} - \mathbf{C}) \cdot (\mathbf{E} - \mathbf{C}) + d,$$

$\mathbf{E} \in \mathrm{Sym}$, where $\mathbb{C}, \mathbf{C}$, and d are as follows. $\mathbb{C}$ is a fourth-order tensor of elastic moduli, interpreted as linear transformation on Sym, and it is assumed that $\mathbb{C}$ is symmetric and positive definite, i.e.,

$$\mathbf{A} \cdot \mathbb{C}\mathbf{B} = \mathbf{B} \cdot \mathbb{C}\mathbf{A}, \quad \mathbf{A}, \mathbf{B} \in \mathrm{Sym},$$

and

$$\mathbf{E} \cdot \mathbb{C}\mathbf{E} > 0, \quad \mathbf{E} \in \mathrm{Sym}, \ \mathbf{E} \neq \mathbf{0}.$$

Furthermore, $\mathbf{C} \in \mathrm{Sym}$, $\mathbf{C} \neq \mathbf{0}$, is a constant tensor, the displacement between the relative minima of W, and $d \in \mathbb{R}$ the difference between the minima. We abbreviate

$$\mathrm{N} := \mathbb{C}\mathbf{C}, \quad C := \mathrm{N} \cdot \mathbf{C},$$

$$\mathsf{B}(\mathbf{a}, \mathbf{n}) := \mathbb{C}(\mathbf{a} \odot \mathbf{n}) \cdot (\mathbf{a} \odot \mathbf{n}), \quad \mathbf{a}, \mathbf{n} \in \mathbb{V},$$

and recall that the acoustic tensor $\mathbf{D} = \mathbf{D}(\mathbf{n}) \in \mathrm{Sym}$ corresponding to $\mathbf{n} \in \mathbb{S} := \{\mathbf{n} \in \mathbb{V} : |\mathbf{n}| = 1\}$ is defined by

$$\mathbf{D}(\mathbf{n})\mathbf{b} = \mathbb{C}(\mathbf{b} \odot \mathbf{n})\mathbf{n}, \quad \mathbf{b} \in \mathbb{V}. \tag{9}$$

The positive definiteness of $\mathbb{C}$ implies that $\mathbf{D}(\mathbf{n})$ is positive definite and hence invertible.

Theorem 2.2. [2] *We have* $W^{lo} = W^{rc} = W^{qc}$ *where*

$$W^{qc}(\mathbf{E}) = \begin{cases} \frac{1}{2}\mathbb{C}\mathbf{E}\cdot\mathbf{E} - (2g)^{-1}(\mathbf{N}\cdot\mathbf{E}-\xi)^2 & \text{if } \xi < \mathbf{N}\cdot\mathbf{E} < \xi + g, \\ W(\mathbf{E}) & \text{otherwise,} \end{cases}$$

$$g := \max\left\{(\mathbf{N}\mathbf{n}\cdot\mathbf{a})^2/\mathsf{B}(\mathbf{a},\mathbf{n}) : |\mathbf{a}| = |\mathbf{n}| = 1\right\}, \tag{10}$$

$$\xi := \tfrac{1}{2}C + d - \tfrac{1}{2}g. \tag{11}$$

The constant g has been introduced by Kohn [2], via (20) (below); we also refer to [2] for a detailed discussion of the behavior of W^{qc}.

Proof. We use Proposition 2.1. If $g > 0$ is arbitrary and F, G are defined by

$$F(\mathbf{E}) = \tfrac{1}{2}\mathbb{C}\mathbf{E}\cdot\mathbf{E} - (2g)^{-1}(\mathbf{N}\cdot\mathbf{E})^2,$$

$$G(x) = \min\{(2g)^{-1}x^2, (2g)^{-1}(x-g)^2 + \xi\}$$

where ξ is as in (11), then a calculation proves the structural formula (4). The second differential of F is

$$D^2F(\mathbf{E})(\mathbf{B},\mathbf{B}) = \mathbb{C}\mathbf{B}\cdot\mathbf{B} - g^{-1}(\mathbf{N}\cdot\mathbf{B})^2$$

for any $\mathbf{E}, \mathbf{B} \in \mathrm{Sym}$. We now want to choose g is such a way that all the remaining hypotheses of Proposition 2.1 are satisfied. Thus F must be quasiconvex, which for a quadratic function is equivalent to the Legendre–Hadamard condition $D^2F(\mathbf{E})(\mathbf{a}\odot\mathbf{n}, \mathbf{a}\odot\mathbf{n}) \geq 0$ for all $\mathbf{a}, \mathbf{n}, \mathbf{E}$, which is equivalent to

$$\mathsf{B}(\mathbf{a},\mathbf{n}) - g^{-1}(\mathbf{N}\mathbf{n}\cdot\mathbf{a})^2 \geq 0 \tag{12}$$

for all $\mathbf{a}, \mathbf{n}$. Furthermore, W must be degenerate in some rank 1 direction (5) which means here

$$\mathsf{B}(\mathbf{b},\mathbf{c}) - g^{-1}(\mathbf{N}\mathbf{c}\cdot\mathbf{b})^2 = 0 \tag{13}$$

for some nonvanishing $\mathbf{b}, \mathbf{c}$. The only possibility to satisfy (12) and (13) is to set (10). Indeed the definition gives immediately (12) and $\mathbf{b}, \mathbf{c}$ are realized as the maximizers in (10). Note that $\mathbf{C} \neq \mathbf{0}$ implies $g > 0$ and $\mathbf{N}\cdot(\mathbf{b}\odot\mathbf{c}) \neq 0$. Thus Proposition 2.1 requires us to calculate the convexification of G. Since

$$G(x) = \begin{cases} (2g)^{-1}x^2 & \text{if } x \leq \frac{1}{2}C + d \\ (2g)^{-1}(x-g)^2 + \xi & \text{if } x > \frac{1}{2}C + d, \end{cases}$$

the convexification of G is

$$\tilde{G}(x) = \begin{cases} (2g)^{-1}\xi(2x - \xi) & \text{if } \xi < x < \xi + g, \\ G(x) & \text{otherwise.} \end{cases}$$

This can be determined by the common tangent construction: G is replaced by the common tangent to the graph of G in the interval from $x := \xi$ to $y := \xi + g$, determined from

$$G'(y) = G'(x), \quad G(y) = G(x) + G'(x)(y - x).$$

The formula (6) now provides the result. □

The following three remarks deal with the properties and alternative definitions of g. We say that a $\mathbf{C} \in \mathrm{Sym}$ is compatible with $\mathbf{0}$ if $\mathbf{C} = \mathbf{b} \odot \mathbf{n}$ for some $\mathbf{b} \in \mathbb{V}, \mathbf{n} \in \mathbb{S}$.

Remark 2.3. *We have*

$$0 < g \leq C \tag{14}$$

and $g = C$ if and only if $\mathbf{C}$ is compatible with $\mathbf{0}$.

Proof. The inequality $g > 0$ is obvious. By Schwarz's inequality for the scalar product on Sym induced by $\mathbb{C}$,

$$(\mathbf{Nn} \cdot \mathbf{a})^2 = (\mathbb{C}\mathbf{C} \cdot (\mathbf{a} \odot \mathbf{n}))^2 \leq (\mathbf{N} \cdot \mathbf{C})\mathbb{C}(\mathbf{a} \odot \mathbf{n}) \cdot (\mathbf{a} \odot \mathbf{n}) = C\mathsf{B}(\mathbf{a}, \mathbf{n})$$

for any $\mathbf{a}, \mathbf{n} \in \mathbb{V}$, which by (10) implies $(14)_2$. Moreover, the equality holds if and only if $\mathbf{C}$ and $\mathbf{a} \odot \mathbf{n}$ are proportional. This shows that $g = C$ if and only if $\mathbf{C}$ is compatible with $\mathbf{0}$. □

Remark 2.4. *For each $\mathbf{n} \in \mathbb{S}$ let*

$$\hat{\mathbf{b}}(\mathbf{n}) = \mathbf{D}^{-1}(\mathbf{n})\mathbf{Nn}, \tag{15}$$

so that $\hat{\mathbf{b}}(\mathbf{n})$ is the unique solution of

$$\mathbb{C}(\hat{\mathbf{b}}(\mathbf{n}) \odot \mathbf{n})\mathbf{n} = \mathbf{Nn}; \tag{16}$$

the function $\hat{\mathbf{b}} : \mathbb{S} \to \mathbb{V}$ is infinitely differentiable and we have

$$g = \max\{h(\mathbf{n}) : \mathbf{n} \in \mathbb{S}\} \tag{17}$$

where

$$h(\mathbf{n}) = \mathbf{Nn} \cdot \hat{\mathbf{b}}(\mathbf{n}) = \mathsf{B}(\hat{\mathbf{b}}(\mathbf{n}), \mathbf{n}) = \mathbf{D}^{-1}(\mathbf{n}) \cdot (\mathbf{Nn} \otimes \mathbf{Nn}). \tag{18}$$

Proof. We recall that $\mathbf{D}(\mathbf{n})$ is positive definite and hence invertible. Thus the definition (15) is meaningful and simple considerations show that $\hat{\mathbf{b}}$ is infinitely differentiable. Alternatively, for each fixed $\mathbf{n}$, $\hat{\mathbf{b}}(\mathbf{n})$ is the unique point of minimum of the strictly convex function $r : \mathbb{V} \to \mathbb{R}$ defined by

$$r(\mathbf{a}) := \tfrac{1}{2}\mathsf{B}(\mathbf{a}, \mathbf{n}) - \mathbf{Nn} \cdot \mathbf{a}, \quad \mathbf{a} \in \mathbb{V}.$$

The equality of the three expressions in (18) is obvious and the existence of the maximum in (17) follows from the continuity of h. Let

$$s(\mathbf{a},\mathbf{n}) := (\mathbf{Nn}\cdot\mathbf{a})^2/\mathsf{B}(\mathbf{a},\mathbf{n})$$

for each $\mathbf{a} \neq \mathbf{0} \neq \mathbf{n}$. Using (16), we find that

$$s(\hat{\mathbf{b}}(\mathbf{n}),\mathbf{n}) = \mathsf{B}(\hat{\mathbf{b}}(\mathbf{n}),\mathbf{n})$$

and thus if we denote by $\bar{g}$ the maximum in (17), we have $g \geq \bar{g}$. To prove $g \leq \bar{g}$, it suffices to prove that

$$s(\mathbf{a},\mathbf{n}) \leq s(\hat{\mathbf{b}}(\mathbf{n}),\mathbf{n}) = \mathsf{B}(\hat{\mathbf{b}}(\mathbf{n}),\mathbf{n}) \tag{19}$$

for all $\mathbf{a} \neq \mathbf{0}, \mathbf{n} \in \mathbb{S}$. Let $\mathbf{n}$ be fixed. Since $\mathbf{b} := \hat{\mathbf{b}}(\mathbf{n})$ is a minimizer of r and $r(\mathbf{b}) = -\frac{1}{2}\mathbf{Nn}\cdot\mathbf{b}$ the inequality $r(\mathbf{a}) \geq -\frac{1}{2}\mathbf{Nn}\cdot\mathbf{b}$ gives

$$\tfrac{1}{2}\mathsf{B}(\mathbf{a},\mathbf{n}) - \mathbf{Nn}\cdot\mathbf{a} + \tfrac{1}{2}\mathbf{Nn}\cdot\mathbf{b} \geq 0.$$

Replacing $\mathbf{a}$ by $\lambda\mathbf{a}, \lambda \in \mathbb{R}$, we obtain

$$\tfrac{1}{2}\mathsf{B}(\mathbf{a},\mathbf{n})\lambda^2 - \mathbf{Nn}\cdot\mathbf{a}\lambda + \tfrac{1}{2}\mathbf{Nn}\cdot\mathbf{b} \geq 0.$$

Thus the discriminant of the quadratic form is nonpositive. This gives (19). □

Remark 2.5. *For each* $\mathbf{n} \in \mathbb{S}$ *let*

$$V(\mathbf{n}) = \{\mathbf{a}\odot\mathbf{n} \in \mathrm{Sym} : \mathbf{a} \in \mathbb{V}\}$$

and for each subspace $M \subset \mathrm{Sym}$ *let* $\mathsf{P}_M : \mathrm{Sym} \to \mathrm{Sym}$ *be the orthogonal projection onto* M. *Then*

$$g = \max\{|\mathsf{P}_{\mathbb{C}^{1/2}V(\mathbf{n})}\mathbb{C}^{1/2}\mathbf{C}|^2 : \mathbf{n} \in \mathbb{S}\}. \tag{20}$$

This is KOHN'S original definition of g.

Proof. Let $\mathbf{n} \in \mathbb{S}$, denote $\mathbf{P} := \mathsf{P}_{\mathbb{C}^{1/2}V(\mathbf{n})}\mathbb{C}^{1/2}\mathbf{C}$ and write $\mathbf{P} = \mathbb{C}^{1/2}(\mathbf{b}\odot\mathbf{n})$. One has

$$(\mathbf{P} - \mathbb{C}^{1/2}\mathbf{C})\cdot\mathbb{C}^{1/2}(\mathbf{a}\odot\mathbf{n}) = 0$$

for each $\mathbf{a} \in \mathbb{V}$, which gives $(\mathbb{C}^{1/2}\mathbf{P})\mathbf{n} = \mathbf{Nn}$ and hence

$$\mathbb{C}(\mathbf{b}\odot\mathbf{n})\mathbf{n} = \mathbf{Nn}.$$

In the notation of Remark 2.4 thus $\mathbf{b} = \hat{\mathbf{b}}(\mathbf{n})$. Furthermore,

$$|\mathsf{P}_{\mathbb{C}^{1/2}V(\mathbf{n})}\mathbb{C}^{1/2}\mathbf{C}|^2 = \mathbb{C}^{1/2}(\mathbf{b}\odot\mathbf{n})\cdot\mathbb{C}^{1/2}(\mathbf{b}\odot\mathbf{n}) = \mathsf{B}(\mathbf{b},\mathbf{n})$$

and a reference to Remark 2.4 completes the proof. □

3 Transversely isotropic elasticity tensor

Assume $n = 3$ henceforth. The elasticity tensor $\mathbb{C}$ is said to be transversely isotropic if there exists a unit vector $\mathbf{e} \in \mathbb{V}$ (the preferred direction of transverse isotropy) such that

$$\mathbb{C}(\mathbf{R}\mathbf{E}\mathbf{R}^T) = \mathbf{R}(\mathbb{C}\mathbf{E})\mathbf{R}^T$$

for all $\mathbf{E} \in \mathrm{Sym}$ and all orthogonal tensors satisfying $\mathbf{R}\mathbf{e} = \mathbf{e}$. To describe the form of the transversely isotropic elasticity tensor succinctly, for any $\mathbf{A}, \mathbf{B} \in \mathrm{Sym}$ we denote by $\mathbf{A} \otimes \mathbf{B}$ and $\mathbf{A} \boxtimes \mathbf{B}$ the linear transformations on Sym defined by

$$(\mathbf{A} \otimes \mathbf{B})\mathbf{H} = (\mathbf{B} \cdot \mathbf{H})\mathbf{A}, \quad (\mathbf{A} \boxtimes \mathbf{B})\mathbf{H} = \tfrac{1}{2}(\mathbf{A}\mathbf{H}\mathbf{B} + \mathbf{B}\mathbf{H}\mathbf{A}), \quad \mathbf{H} \in \mathrm{Sym}.$$

In [13] and [10] it has been proved that a linearly hyperelastic, transversely isotropic material is specified by only five elasticities as follows. Let $\mathbf{P} = \mathbf{e} \otimes \mathbf{e}$ be the orthogonal projection onto the line spanned by $\mathbf{e}$ and $\mathbf{Q} = \mathbf{1} - \mathbf{P}$ the projection onto the orthogonal complement of $\mathbf{e}$, and let $\mathbb{C}_1, \mathbb{C}_2, \mathbb{C}_3, \mathbb{C}_4, \mathbb{C}_5$ be the linear transformations on Sym defined by

$$\left.\begin{aligned} \mathbb{C}_1 &= \mathbf{P} \otimes \mathbf{P}, \\ \mathbb{C}_2 &= \mathbf{Q} \otimes \mathbf{Q}, \\ \mathbb{C}_3 &= \mathbf{P} \otimes \mathbf{Q} + \mathbf{Q} \otimes \mathbf{P}, \\ \mathbb{C}_4 &= 2\mathbf{P} \boxtimes \mathbf{Q}, \\ \mathbb{C}_5 &= 2\mathbf{Q} \boxtimes \mathbf{Q} - \mathbb{C}_2. \end{aligned}\right\} \tag{21}$$

A $\mathbb{C}$ is an elasticity tensor of a transversely isotropic material if and only if

$$\mathbb{C} = \alpha_1\mathbb{C}_1 + \alpha_2\mathbb{C}_2 + \alpha_3\mathbb{C}_3 + \alpha_4\mathbb{C}_4 + \alpha_5\mathbb{C}_5, \tag{22}$$

for some $\alpha_1, \alpha_2, \alpha_3, \alpha_4, \alpha_5 \in \mathbb{R}$. The tensor basis $\mathbb{C}_1, \mathbb{C}_2, \mathbb{C}_3, \mathbb{C}_4, \mathbb{C}_5$ used here coincides with the basis $\mathsf{P}_1, \mathsf{P}_2, \mathsf{P}_3, \mathsf{E}_1, \mathsf{E}_2$ in [10]. The tensor $\mathbb{C}$ is positive definite if and only if [13], [7]

$$\alpha_4 > 0, \quad \alpha_5 > 0, \quad \alpha_1 + 2\alpha_2 > 0, \quad \alpha_1\alpha_2 - \alpha_3^2 > 0, \tag{23}$$

which we assume throughout. We abbreviate

$$\alpha_6 := \alpha_2 + \alpha_5, \quad \alpha_7 := \alpha_3 + \alpha_4.$$

Note that (23) imply $\alpha_1 > 0, \alpha_2 > 0, \alpha_6 > 0$; thus only α_3 and α_7 can be negative. Furthermore, (23) specify an open convex subset of quintuples $(\alpha_1, \alpha_2, \alpha_3, \alpha_4, \alpha_5)$ in $\mathbb{R}^5$.

The explicit expression for $\hat{\mathbf{b}}$ can be obtained from (21). It is convenient to express $\mathbf{n}$ in cylindrical coordinates with the z-axis in the direction $\mathbf{e}$. That is, we write

$$\mathbf{n} = z\mathbf{e} + \boldsymbol{\rho}, \quad z = \mathbf{n} \cdot \mathbf{e}, \quad \boldsymbol{\rho} = \mathbf{Q}\mathbf{n}; \tag{24}$$

also denote $\rho = |\boldsymbol{\rho}|$. The acoustic tensor $\mathbf{D}(\mathbf{n})$ (see (9)) is

$$\mathbf{D}(\mathbf{n}) = (\alpha_1 z^2 + \alpha_4 \rho^2)\mathbf{P} + \alpha_2 \boldsymbol{\rho} \otimes \boldsymbol{\rho} + 2\alpha_7 z \mathbf{e} \odot \boldsymbol{\rho} + (\alpha_4 z^2 + \alpha_5 \rho^2)\mathbf{Q}. \quad (25)$$

To calculate $\mathbf{D}^{-1}(\mathbf{n})$, let us consider the case $\mathbf{Pn} \neq \mathbf{0}$ and $\boldsymbol{\rho} \neq \mathbf{0}$. Let $\mathbf{v}_1, \mathbf{v}_2, \mathbf{v}_3$ be the orthonormal basis

$$\mathbf{v}_1 = \mathbf{e}, \quad \mathbf{v}_2 = \boldsymbol{\rho}/\rho, \quad \mathbf{v}_3 = \mathbf{v}_1 \wedge \mathbf{v}_2.$$

We have

$$\mathbf{D}(\mathbf{n})\mathbf{v}_1 = \kappa_{11}\mathbf{v}_1 + \kappa_{12}\mathbf{v}_2, \quad \mathbf{D}(\mathbf{n})\mathbf{v}_2 = \kappa_{12}\mathbf{v}_1 + \kappa_{22}\mathbf{v}_2, \quad \mathbf{D}(\mathbf{n})\mathbf{v}_3 = \kappa_{33}\mathbf{v}_3,$$

where

$$\kappa_{11} = \alpha_1 z^2 + \alpha_4 \rho^2, \quad \kappa_{22} = \alpha_4 z^2 + \alpha_6 \rho^2,$$
$$\kappa_{12} = \alpha_7 z \rho, \quad \kappa_{33} = \alpha_4 z^2 + \alpha_5 \rho^2.$$

Due to the positive definiteness of $\mathbb{C}$ and the equality $z^2 + \rho^2 = 1$, the scalars κ_{33}, κ_{11} and κ_{22} are greater than zero whenever $|\mathbf{n}| = 1$ and

$$\mathbf{D}(\mathbf{n}) = \kappa_{11}\mathbf{v}_1 \otimes \mathbf{v}_1 + \kappa_{22}\mathbf{v}_2 \otimes \mathbf{v}_2 + 2\kappa_{12}\mathbf{v}_1 \odot \mathbf{v}_2 + \kappa_{33}\mathbf{v}_3 \otimes \mathbf{v}_3.$$

Hence

$$\mathbf{D}^{-1}(\mathbf{n}) = \omega^{-1}(\kappa_{22}\mathbf{v}_1 \otimes \mathbf{v}_1 + \kappa_{11}\mathbf{v}_2 \otimes \mathbf{v}_2 - 2\kappa_{12}\mathbf{v}_1 \odot \mathbf{v}_2) + \kappa_{33}^{-1}\mathbf{v}_3 \otimes \mathbf{v}_3, \quad (26)$$

where $\omega = \kappa_{11}\kappa_{22} - \kappa_{12}^2$, i.e.,

$$\omega = \alpha_4\alpha_6\rho^4 + \alpha_1\alpha_4 z^4 + (\alpha_1\alpha_6 - \alpha_3^2 - 2\alpha_3\alpha_4)\rho^2 z^2.$$

By (23), $\omega > 0$ for each $|\mathbf{n}| = 1$. Alternatively,

$$\mathbf{D}^{-1}(\mathbf{n}) = \frac{\kappa_{22}\kappa_{33}\mathbf{P} + \sigma\boldsymbol{\rho} \odot \boldsymbol{\rho} - 2\alpha_7 z \kappa_{33}\mathbf{e} \odot \boldsymbol{\rho} + \omega\mathbf{Q}}{\omega\kappa_{33}}$$

where

$$\sigma = (\alpha_7^2 - \alpha_1\alpha_2)z^2 - \alpha_2\alpha_4\rho^2$$

and it is noted that $\omega\kappa_{33} > 0$ for each $\mathbf{n} \neq \mathbf{0}$. Introducing $s_i = s_i(\mathbf{n}) = \mathbf{Nn} \cdot \mathbf{v}_i$, we find from (15) and (26) that

$$\hat{\mathbf{b}}(\mathbf{n}) = \omega^{-1}(\kappa_{22}s_1 - \kappa_{12}s_2)\mathbf{v}_1 + \omega^{-1}(\kappa_{11}s_2 - \kappa_{12}s_1)\mathbf{v}_2 + \kappa_{33}^{-1}s_3\mathbf{v}_3$$

and hence

$$h(\mathbf{n}) = \omega^{-1}(\kappa_{22}s_1^2 - 2\kappa_{12}s_1 s_2 + \kappa_{11}s_2^2) + \kappa_{33}^{-1}s_3^2. \quad (27)$$

From

$$\mathbf{N} = \alpha_1(\mathbf{P} \cdot \mathbf{C})\mathbf{P} + \alpha_2(\mathbf{Q} \cdot \mathbf{C})\mathbf{Q} + \alpha_3\big((\mathbf{Q} \cdot \mathbf{C})\mathbf{P} + (\mathbf{P} \cdot \mathbf{C})\mathbf{Q}\big)$$
$$+ 2\alpha_4(\mathbf{PCQ} + \mathbf{QCP}) + \alpha_5\big(2\mathbf{QCQ} - (\mathbf{Q} \cdot \mathbf{C})\mathbf{Q}\big),$$

it is found that

$$\left.\begin{aligned} s_1 &= (\alpha_1\mathbf{P}\cdot\mathbf{C} + \alpha_3\mathbf{Q}\cdot\mathbf{C})z + 2\alpha_4\rho\mathbf{v}_1\cdot\mathbf{C}\mathbf{v}_2, \\ s_2 &= (\alpha_2\mathbf{Q}\cdot\mathbf{C} + \alpha_3\mathbf{P}\cdot\mathbf{C})\rho + 2\alpha_4 z\mathbf{v}_1\cdot\mathbf{C}\mathbf{v}_2 + \alpha_5\rho(2\mathbf{v}_2\cdot\mathbf{C}\mathbf{v}_2 - \mathbf{Q}\cdot\mathbf{C}), \\ s_3 &= 2(\alpha_4 z\mathbf{v}_1\cdot\mathbf{C}\mathbf{v}_3 + \alpha_5\rho\mathbf{v}_2\cdot\mathbf{C}\mathbf{v}_3). \end{aligned}\right\} \quad (28)$$

To calculate the maximum (17) with h as in (27) seems to be a difficult task in general and the following section deals with a natural special case.

4 The transversely isotropic displacement of the wells

We consider the case when $\mathbf{C}$ has the transversal symmetry, i.e.,

$$\mathbf{R}\mathbf{C}\mathbf{R}^T = \mathbf{C}$$

for each orthogonal tensor $\mathbf{R}$ such that $\mathbf{R}\mathbf{e} = \mathbf{e}$. Hence $\mathbf{C}$ must be of the form

$$\mathbf{C} = \beta_z\mathbf{P} + \beta_\rho\mathbf{Q} \quad (29)$$

for some real β_z, β_ρ. The insertion of (29) into (28) shows that

$$s_1 = \gamma_z z, \quad s_2 = \gamma_\rho, \quad s_3 = 0$$

where we define

$$\gamma_z = \alpha_1\beta_z + 2\alpha_3\beta_\rho, \quad \gamma_\rho = \alpha_3\beta_z + 2\alpha_2\beta_\rho. \quad (30)$$

Thus (27) provides

$$h(\mathbf{n}) = \frac{(\alpha_6\rho^2 + \alpha_4 z^2)\gamma_z^2 z^2 - 2\alpha_7\gamma_z\gamma_\rho\rho^2 z^2 + (\alpha_1 z^2 + \alpha_4\rho^2)\gamma_\rho^2\rho^2}{\omega}.$$

If we make a substitution $x = z^2$ and use $z^2 + \rho^2 = |\mathbf{n}|^2 = 1$, we find from (17) that

$$g = \max\{\hat{h}(x) : 0 \le x \le 1\} \quad (31)$$

where

$$\hat{h} = \frac{p}{q},$$

$$p = \big(\alpha_6(1-x)+\alpha_4 x\big)\gamma_z^2 x - 2\alpha_7\gamma_z\gamma_\rho(1-x)x + \big(\alpha_1 x + \alpha_4(1-x)\big)(1-x)\gamma_\rho^2, \quad (32)$$

$$q = \big(\alpha_1 x + \alpha_4(1-x)\big)\big(\alpha_6(1-x) + \alpha_4 x\big) - \alpha_7^2(1-x)x. \quad (33)$$

The above considerations show that $q(x) > 0$ for any $x \in [0,1]$. The maximum in (31) is realized either at the endpoints $0, 1$ or at some interior point of $[0,1]$ in which case $\hat{h}'(x) = 0$ which is equivalent to

$$M(x) = 0, \quad (34)$$

where

$$M = p'q - pq'.$$

One finds that

$$M(x) = \alpha_4(ax^2 + bx + c) \tag{35}$$

where

$$\begin{aligned} a &= ((\alpha_4 - \alpha_1 - \alpha_7)\gamma_\rho + (\alpha_6 - \alpha_4 + \alpha_7)\gamma_z) \\ &\quad \times ((\alpha_1 - \alpha_4 - \alpha_7)\gamma_\rho + (\alpha_6 - \alpha_4 - \alpha_7)\gamma_z) \\ b &= 2(\alpha_4^2 - \alpha_7^2 - \alpha_1\alpha_4)\gamma_\rho^2 + 2(\alpha_6\alpha_4 - \alpha_6^2)\gamma_z^2 + 4\alpha_6\alpha_7\gamma_\rho\gamma_z, \\ c &= \alpha_4(\alpha_4\gamma_\rho + \alpha_6\gamma_z - \alpha_7\gamma_\rho)(-\alpha_4\gamma_\rho + \alpha_6\gamma_z - \alpha_7\gamma_\rho). \end{aligned}$$

To discuss (34), assume first that $a \neq 0$ so that (34) is a quadratic equation. Its discriminant is

$$\Delta = 4\,\alpha_4^2\big(\alpha_6\alpha_7\gamma_z^2 + \alpha_1\alpha_7\gamma_\rho^2 + (\alpha_4^2 - \alpha_7^2 - \alpha_1\alpha_6)\gamma_z\gamma_\rho\big)^2$$

and hence (34) has always two real roots. We write

$$\Delta_{1/2} = 2\,\alpha_4\big(\alpha_6\alpha_7\gamma_z^2 + \alpha_1\alpha_7\gamma_\rho^2 + (\alpha_4^2 - \alpha_7^2 - \alpha_1\alpha_6)\gamma_z\gamma_\rho\big) \tag{36}$$

so that $\Delta_{1/2}^2 = \Delta$ but $\Delta_{1/2}$ can be both positive, zero, or negative. We denote the roots by $x_\pm$ and assign them by the convention

$$x_\pm = \frac{-b \pm \Delta_{1/2}}{2a};$$

explicitly,

$$\left.\begin{aligned} x_+ &= \frac{\alpha_6\gamma_z - \alpha_4\gamma_\rho - \alpha_7\gamma_\rho}{(\alpha_1 - \alpha_4 - \alpha_7)\gamma_\rho + (\alpha_6 - \alpha_4 - \alpha_7)\gamma_z}, \\ x_- &= \frac{\alpha_6\gamma_z + \alpha_4\gamma_\rho - \alpha_7\gamma_\rho}{(\alpha_4 - \alpha_1 - \alpha_7)\gamma_\rho + (\alpha_6 - \alpha_4 + \alpha_7)\gamma_z}. \end{aligned}\right\} \tag{37}$$

The values of h at these roots are

$$\left.\begin{aligned} h_+ &:= \hat{h}(x_+) = \frac{\alpha_6\gamma_z^2 - 2\alpha_7\gamma_z\gamma_\rho - 2\alpha_4\gamma_z\gamma_\rho + \alpha_1\gamma_\rho^2}{\alpha_6\alpha_1 - \alpha_7^2 - 2\alpha_7\alpha_4 - \alpha_4^2}, \\ h_- &:= \hat{h}(x_-) = \frac{\alpha_6\gamma_z^2 - 2\alpha_7\gamma_z\gamma_\rho + 2\alpha_4\gamma_z\gamma_\rho + \alpha_1\gamma_\rho^2}{\alpha_6\alpha_1 - \alpha_7^2 + 2\alpha_7\alpha_4 - \alpha_4^2}, \end{aligned}\right\} \tag{38}$$

respectively. The roots $x_\pm$ may but need not fall in the interval $[0, 1]$; this depends on the concrete values of γ_z, γ_ρ. This will be discussed below. Note further that if $x = x_\pm$ is a root then

$$\hat{h}''(x_\pm) = \frac{M'(x_\pm)}{q^2(x_\pm)} = \pm\frac{\Delta_{1/2}}{q^2(x_\pm)} \tag{39}$$

and hence only one of the roots can correspond to a local maximum of $\hat{h}$. We denote by t the root x for which $M'(x) \geq 0$ and note that this is unambiguous since $x_+ = x_-$ if $\Delta_{1/2} = 0$. We furthermore write h_t for the value of $\hat{h}$ at t, which is one of the two values in (38). Next assume that $a = 0$ but $b \neq 0$ so that (34) becomes a linear equation with the solution

$$t = \frac{\alpha_2\gamma_z - \alpha_3\gamma_\rho + \alpha_5\gamma_z}{\alpha_3\gamma_z + \alpha_5\gamma_z - \alpha_1\gamma_\rho + \alpha_2\gamma_z - \alpha_3\gamma_\rho}$$

and the corresponding value of h is

$$h_t = \frac{-2\alpha_3\gamma_z\gamma_\rho + \alpha_5\gamma_z^2 + \alpha_2\gamma_z^2 + \alpha_1\gamma_\rho^2}{\alpha_1\alpha_2 - \alpha_3^2 + \alpha_1\alpha_5}$$

To summarize, we have defined the quantity t in the cases $a \neq 0$ and $a = 0, b \neq 0$. Otherwise, we leave t undefined. Further, note that the values of h at $x = 0, 1$ are

$$h_0 = \frac{\gamma_\rho^2}{\alpha_6}, \quad h_1 = \frac{\gamma_z^2}{\alpha_1}$$

and denote by M_0, M_1 the values of M at $0, 1$, respectively:

$$M_0 = \alpha_4(\alpha_4\gamma_\rho + \alpha_6\gamma_z - \alpha_7\gamma_\rho)(\alpha_6\gamma_z - \alpha_4\gamma_\rho - \alpha_7\gamma_\rho) \tag{40}$$

$$M_1 = \alpha_4\left(\alpha_4\gamma_z - \alpha_1\gamma_\rho + \alpha_7\gamma_z\right)\left(\alpha_1\gamma_\rho + \alpha_4\gamma_z - \alpha_7\gamma_z\right). \tag{41}$$

The following proposition outlines a possible strategy for determining the maximum.

Proposition 4.1. *Assume that* (23) *hold. Then*
(i) *if*

$$M_0 \geq 0, \quad M_1 \leq 0 \tag{42}$$

then $t \in [0, 1]$ *and*

$$g = h_t; \tag{43}$$

(ii) *if at least one of the two inequalities in* (42) *does not hold and* $M_0M_1 \leq 0$ *then*

$$g = \max\{h_0, h_1\}; \tag{44}$$

(iii) *if* $M_0M_1 > 0$ *then either none or two roots are in* $(0, 1)$; *in the former case* (44) *holds, in the latter case*

$$g = \max\{h_b, h_t\} \tag{45}$$

where

$$h_b = \begin{cases} h_1 & \text{if } M_0 > 0, \\ h_0 & \text{if } M_0 < 0. \end{cases}$$

The procedure is based on determining the signs M_0 and M_1; in view of the factorized form of the expressions (40) and (41) this is relatively easy. Note that (i), (ii), and (iii) are mutually exclusive and cover all possibilities.

Proof. Note first that for any $x \in [0,1]$ we have

$$\hat{h}'(x) = \frac{M(x)}{q^2(x)}, \tag{46}$$

where we use that $q(x) \neq 0$ on $[0,1]$. (The function h may have singularities outside of $[0,1]$.) Assume first that $a \neq 0$ so that M is quadratic ad we have two possibly coinciding roots. (i): Assume that (42) hold. If $M_0 = M_1 = 0$ then the two roots are $0, 1$, and (43) follows. If $M_0 > 0, M_1 = 0$ then one of the two roots is 1. (a) If the other root w is in $(0,1)$ then $M_0 > 0, M_1 = 0$ imply that $M(x) > 0$ for $x \in (0,w)$ and $M(x) < 0$ for $x \in (w,1)$. From this we obtain that $M'(w) < 0$ and $\hat{h}(w) > h_0, \hat{h}(w) > h_1$. Thus $x = t$ and (43) follows. (b) If there is no root in $(0,1)$ then $M(x) \geq 0$ on $[0,1]$ and hence $M'(1) \leq 0$. Thus $t = 1$ and (43) follows again. The case $M_0 = 0, M_1 < 0$ and the case $M_0 > 0, M_1 < 0$ is similar. (ii): If at least one of the two inequalities in (42) does not hold and $M_0 M_1 \leq 0$ then either

$$M_0 < 0, \quad M_1 \geq 0, \tag{47}$$

or

$$M_1 > 0, \quad M_0 \leq 0. \tag{48}$$

Consider the case (47). There can be at most one root in $(0,1)$. If w is such a root then w is not a point of maximum of $\hat{h}$ since $M_0 < 0$ implies $M'(w) \geq 0$. Thus (44) follows. If there is no root in $(0,1)$, equation (44) follows as well. The case (48) is similar. (iii): By $M_0 M_1 > 0$ we have that M_0, M_1 are either both positive or both negative. Since M is quadratic, the assertion about the roots follows. If there are no roots, then (45) follows. Assume that the two roots are in $(0,1)$ and $M_0 > 0$. Denote them by x_m, x_M with $x_m \leq x_M$. Then $\hat{h}$ increases on $(0, x_m)$, decreases on (x_m, x_M) and increases on $(x_M, 1)$. Thus the only points of maximum can be $x_m, 1$ and the assertion follows. The case $M_0 < 0$ is similar. This completes the proof in the case $a \neq 0$. If $a = 0$ then M is linear and the above considerations simplify accordingly; the results are, however, formally the same. □

5 The positive definite displacement of the wells

Note that $\mathbf{C}$ as in (29) is positive semidefinite if and only if β_ρ, β_z are nonnegative. Proposition 5.1, below, gives an explicit form of g in this case. The following inequalities play role in the formulation of the result:

$$\left.\begin{aligned} \alpha_6\gamma_z - \alpha_4\gamma_\rho - \alpha_7\gamma_\rho \geq 0, \\ \alpha_4\gamma_z - \alpha_1\gamma_\rho + \alpha_7\gamma_z \leq 0. \end{aligned}\right\} \tag{49}$$

Proposition 5.1. *Assume that* (23) *hold and let* $\beta_\rho, \beta_z \geq 0$. *Then if*

$$\alpha_6\gamma_z - \alpha_3\gamma_\rho > 0, \tag{50}$$

we have

$$g = \begin{cases} \dfrac{\alpha_6\gamma_z^2 - 2\alpha_7\gamma_z\gamma_\rho - 2\alpha_4\gamma_z\gamma_\rho + \alpha_1\gamma_\rho^2}{\alpha_6\alpha_1 - \alpha_7^2 - 2\alpha_7\alpha_4 - \alpha_4^2} & \text{if (49) hold,} \\ \max\left\{\dfrac{\gamma_\rho^2}{\alpha_6}, \dfrac{\gamma_z^2}{\alpha_1}\right\} & \text{otherwise;} \end{cases} \tag{51}$$

if

$$\alpha_6\gamma_z - \alpha_3\gamma_\rho \leq 0, \tag{52}$$

then

$$g = \frac{\alpha_6\gamma_z^2 - 2\alpha_7\gamma_z\gamma_\rho + 2\alpha_4\gamma_z\gamma_\rho + \alpha_1\gamma_\rho^2}{\alpha_6\alpha_1 - \alpha_7^2 + 2\alpha_7\alpha_4 - \alpha_4^2}. \tag{53}$$

Proof. Let us first give the proof under the assumption $\beta_\rho > 0$. Then

$$\alpha_1\gamma_\rho - \alpha_3\gamma_z > 0 \tag{54}$$

since the left-hand side is equal to $2(\alpha_1\alpha_2 - \alpha_3^2)\beta_\rho$ and we have (23). Assume that (50) holds. By (37) we have

$$x_- = \frac{n}{d}$$

where $n = \alpha_6\gamma_z - \alpha_3\gamma_\rho > 0$ by (50) and $d = n - p$ where $p = \alpha_1\gamma_\rho - \alpha_3\gamma_z > 0$ by (54). From this we conclude that x_- is outside of the interval $[0, 1]$. Assume that the inequalities (49) hold. Then combining (40)–(41) with (49) we find that $M_0 \geq 0, M_1 \leq 0$ and Proposition 4.1(i) tells us that $t \in [0, 1]$ and $g = h_t$. As $x_- \notin [0, 1]$, necessarily $t = x_+$ and $(51)_1$ follows. If at least one of the inequalities in (49) does not hold and $M_0M_1 \leq 0$ then we have $(51)_2$ by Proposition 4.1(ii). If at least one of the inequalities in (49) does not hold and $M_0M_1 > 0$ then Proposition 4.1(iii) says that either none or both the two roots are in $(0, 1)$; as $x_- \notin [0, 1]$, necessarily the former case occurs and then we have $(51)_2$ by Proposition 4.1(iii). Assume that (52) holds. This reads

$$(\alpha_1\alpha_2 - \alpha_3^2)\beta_z + \alpha_5\gamma_z \leq 0;$$

combining (23) with $\beta_z \geq 0$ we conclude that

$$\gamma_z \leq 0. \tag{55}$$

Furthermore, let us prove that

$$\gamma_\rho > 0. \tag{56}$$

To prove it, note that (55) reads

$$\alpha_1\beta_z \le -2\alpha_3\beta_\rho, \tag{57}$$

while the opposite of (56) reads

$$2\alpha_2\beta_\rho \le -\alpha_3\beta_z. \tag{58}$$

From (57) we conclude that $\alpha_3 \le 0$ and thus we can multiply (57) and (58) to obtain, after canceling the positive term $\beta_\rho\beta_z$, that $\alpha_1\alpha_2 \le \alpha_3^2$ which contradicts (23). Thus (56) holds. Let us use this inequality to prove that $M_0 \ge 0$. This requires us to prove that

$$s := \alpha_6\gamma_z - \alpha_4\gamma_\rho - \alpha_7\gamma_\rho \le 0$$

and we have

$$s := (\alpha_6\gamma_z - \alpha_3\gamma_\rho) - 2\alpha_4\gamma_\rho;$$

the term in brackets is nonpositive by (52) and the second term is negative by (56). Next prove that $M_1 \le 0$. This requires to prove

$$s := \alpha_4\gamma_z - \alpha_1\gamma_\rho + \alpha_7\gamma_z \le 0.$$

We have

$$s := -(\alpha_1\gamma_\rho - \alpha_3\gamma_z) + 2\alpha_4\gamma_z;$$

the term in the brackets is nonnegative by (54) and the second term is nonpositive by (55). Thus since $M_0 \le 0, M_1 \ge 0$, Proposition 4.1(i) says that $g = h_t$. We have

$$x_+ = \frac{n}{d}$$

where $n = \alpha_6\gamma_z - \alpha_3\gamma_\rho - 2\alpha_4\gamma_\rho$ which is negative by (52) and $\gamma_\rho > 0$. The denominator is $d = n + p$ where

$$p = \alpha_1\gamma_\rho - (\alpha_4 + \alpha_7)\gamma_z = (\alpha_1\gamma_\rho - \alpha_3\gamma_z) - 2\alpha_4\gamma_z > 0$$

where we use (54) and $\gamma_z \le 0$. Thus $x_+ \notin [0,1]$. Hence $t = x_-$ and (53) follows from $g = h_t$. This completes the proof in the case $\beta_\rho > 0$.

The case $\beta_\rho = 0$ is much simpler since we have $\mathbf{C} = \beta_z\mathbf{P}$ and thus $\mathbf{C}$ is compatible with $\mathbf{0}$. We have the solution given by Remark 2.3: $g = C = \mathbf{C}\cdot\mathbb{C}\mathbf{C}$ and hence

$$g = \beta_z^2\alpha_1 \tag{59}$$

and the only thing we have to prove is that the description in the proposition gives the same value. We have

$$\gamma_z = \alpha_1, \quad \gamma_\rho = \alpha_3.$$

Using this, one finds that (50) holds while $(49)_2$ is violated. Thus by (51),

$$g = \max\left\{\frac{\gamma_\rho^2}{\alpha_6}, \frac{\gamma_z^2}{\alpha_1}\right\}$$

and this coincides with (59). □

We conclude this section with calculations of g in some particular cases. Note that when g is considered as a function of $\mathbf{C}$, written then g is a homogeneous function of degree 2, i.e., for any $\lambda \in \mathbb{R}$ we have $g(\lambda\mathbf{C}) = \lambda^2 g(\mathbf{C})$. A direct specialization of Proposition 5.1 gives the following examples.

Special Case 1: $\mathbf{C} = \mathbf{P}$. Then

$$g = \alpha_1.$$

Special Case 2: $\mathbf{C} = \mathbf{Q}$. Note that for $\mathbf{C} = \mathbf{Q}$ we have $\beta_z = 0, \beta_\rho = 1$ in (29) and hence $\gamma_z = 2\alpha_3, \gamma_\rho = 2\alpha_2$ by (30). Distinguish the cases whether or not the inequalities

$$\alpha_3\alpha_5 > 2\alpha_2\alpha_4, \quad \alpha_1\alpha_2 - \alpha_3^2 > 2\alpha_3\alpha_4, \tag{60}$$

hold. For $\alpha_3 > 0$,

$$g = 4\begin{cases} \dfrac{\alpha_1\alpha_2^2 - 4\alpha_2\alpha_3\alpha_4 - \alpha_3^2\alpha_2 + \alpha_3^2\alpha_5}{\alpha_1\alpha_2 + \alpha_1\alpha_5 - 4\alpha_4^2 - 4\alpha_3\alpha_4 - \alpha_3^2} & \text{if (60) hold,} \\ \max\left\{\dfrac{\alpha_2^2}{\alpha_2 + \alpha_5}, \dfrac{\alpha_3^2}{\alpha_1}\right\} & \text{otherwise,} \end{cases}$$

while for $\alpha_3 \le 0$,

$$g = 4\frac{\alpha_1\alpha_2^2 + \alpha_3^2\alpha_5 - \alpha_2\alpha_3^2}{\alpha_1\alpha_2 + \alpha_1\alpha_5 - \alpha_3^2}.$$

Special Case 3: $\mathbf{C} = \mathbf{1}$. The following inequalities will play role in the formulation of the result:

$$\left.\begin{aligned} \alpha_1\alpha_2 - \alpha_3^2 &\ge 4\alpha_2\alpha_4 + 2\alpha_3\alpha_4 - \alpha_1\alpha_5 - 2\alpha_3\alpha_5, \\ \alpha_1\alpha_2 - \alpha_3^2 &\ge \alpha_1\alpha_4 + 2\alpha_3\alpha_4. \end{aligned}\right\} \tag{61}$$

The result reads: if

$$\alpha_1\alpha_2 - \alpha_3^2 + \alpha_1\alpha_5 + 2\alpha_3\alpha_5 > 0$$

then

$$g = \begin{cases} \dfrac{(\alpha_9 + 2\alpha_{10})\alpha_8^2 + \alpha_5\alpha_9^2 - 4\alpha_4\alpha_9\alpha_{10}}{\alpha_8^2 - 4\alpha_4^2 - 4\alpha_3\alpha_4 + \alpha_1\alpha_5} & \text{if (61) holds,} \\ \max\left\{\dfrac{(\alpha_3 + 2\alpha_2)^2}{\alpha_2 + \alpha_5}, \dfrac{(\alpha_1 + 2\alpha_3)^2}{\alpha_1}\right\} & \text{otherwise,} \end{cases}$$

while if

$$\alpha_1\alpha_2 - \alpha_3^2 + \alpha_1\alpha_5 + 2\alpha_3\alpha_5 \le 0$$

then

$$g = \frac{4\alpha_2\alpha_8^2 + (\alpha_1 + 4\alpha_3)(\alpha_8^2 + \alpha_1\alpha_5) + 4\alpha_5\alpha_3^2}{\alpha_8^2 + \alpha_1\alpha_5}$$

where we abbreviate

$$\alpha_8^2 = \alpha_1\alpha_2 - \alpha_3^2, \quad \alpha_9 = \alpha_1 + 2\alpha_3, \quad \alpha_{10} = 2\alpha_2 + \alpha_3.$$

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