PERGAMON

International Journal of Solids and Structures 38 (2001) 943–965

INTERNATIONAL JOURNAL OF SOLIDS and STRUCTURES

www.elsevier.com/locate/ijsolstr

Rank 1 perturbations of deformation gradients

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Received 10 December 1998

Abstract

Rank 1 connections, i.e., pairs $\boldsymbol{F},\boldsymbol{G}$ of tensors (matrices) differing by a rank 1 tensor, $\boldsymbol{G} = \boldsymbol{F} + \boldsymbol{f} \otimes \boldsymbol{n}$, play an important role in the nonlinear elasticity and in particular in the theory of solid-to-solid phase transformations. If $\boldsymbol{F}$, $\boldsymbol{G}$ are rank 1 connected, $\boldsymbol{G}$ is said to be a rank 1 perturbation of $\boldsymbol{F}$. This paper describes the set of all rank 1 perturbations of $\boldsymbol{F}$ with prescribed singular values. In an n-dimensional space, this set is shown to consist of 2^n families of dimension $n-1$ and within each family, $\boldsymbol{G}$ and $\boldsymbol{f}$ may be expressed as functions of the unit vector $\boldsymbol{n}$, given by explicit formulas. These are then specialized to dimensions $n = 2$ and 3. Some illustrative examples are given. © 2001 Elsevier Science Ltd. All rights reserved.

Keywords: Rank 1 perturbations; Deformation gradients

1. Introduction

Let Lin denote the linear space of all second-order tensors on an n-dimensional real vector space Vect with scalar product. (If Vect is identified with $\mathbb{R}^n$, then Lin may be identified with the set of all n by n matrices.) The tensor $\boldsymbol{G} \in \mathsf{Lin}$ is said to be a rank 1 perturbation of the tensor $\boldsymbol{F} \in \mathsf{Lin}$ if $\boldsymbol{G} = \boldsymbol{F} + \boldsymbol{f} \otimes \boldsymbol{n}$ for some $\boldsymbol{f} \in \mathsf{Vect}$, $\boldsymbol{n} \in \mathsf{Sph} := \{\boldsymbol{n} \in \mathsf{Vect} : |\boldsymbol{n}| = 1\}$, with $|\cdot|$ the euclidean norm. In indices, $G_{ij} = F_{ij} + \boldsymbol{f}_i n_j$. Rank 1 perturbations play important roles in the theory of coherent phase transitions in crystalline solids, and, through the definition of rank 1 convexity, in the nonlinear (thermo) elasticity of isotropic materials. [1] The underlying reason is the Hadamard lemma for a continuous deformation with a discontinuity of the deformation gradient across a singular surface S. The limiting values of the deformation gradients from the two sides of S must be rank 1 connected.

In the last 15 years, a theory of martensitic transformations in crystalline materials based on energy minimization has been intensively studied (Ball and James, 1987, 1992; Fonseca, 1987; Chipot and Kinderlehrer, 1988; Bhattacharya, 1991, 1992, 1993; Bhattacharya, 1994; Dolzmann and Müller, 1995; Abeyaratne et al., 1996; Ball and Carstensen, 1997). The microstructures can often be analysed by solving algebraic problems of finding matrices on energy wells having appropriate rank 1 connections. Similarly, in the

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[1] See Dacorogna (1990) and Šilhavý (1997) for the book expositions of the background material.

0020-7683/01/$ - see front matter
PII: S0020-7683(00)00068-8

isotropic nonlinear elasticity, the rank 1 convexity notion and the associated rank 1 perturbations are helpful in analysing stored energy functions (Ball, 1977) and in particular in the problems associated with the relaxation and rank 1 convexification of the nonelliptic energy functions (Dacorogna, 1990; Kohn and Strang, 1983, 1986a,b,c; Dacorogna and Koshigoe, 1993; Buttazzo et al., 1994; Dacorogna and Tanteri, 1998).

Here, a more systematic approach to rank 1 perturbations is presented inasmuch as this paper describes all rank 1 perturbations $\boldsymbol{G}$ of a given $\boldsymbol{F}$ subject to the condition that $\boldsymbol{G}$ has prescribed singular values. [2] Recall that the singular values of a tensor $\boldsymbol{G}$ are defined as the eigenvalues of $\sqrt{\boldsymbol{G}\boldsymbol{G}^{\mathrm{T}}}$ arranged nonincreasingly, with appropriate multiplicities. In view of the polar decomposition theorem, it suffices to consider the case when $\boldsymbol{F} \equiv \boldsymbol{V}$ is positive definite symmetric. It turns out that if $v = (v_1, \dots, v_n)$ are the singular values of $\boldsymbol{F}$ then $w = (w_1, \dots, w_n)$ are the singular values of some rank 1 perturbation of $\boldsymbol{G}$ if and only if w, v satisfy the following system of inequalities

$$w_1 \geqslant v_2, \quad v_1 \geqslant w_2 \geqslant v_3, \dots, v_{n-1} \geqslant w_n,$$

which I propose to call bilateral interlacing inequalities (Šilhavý, 1999). It is shown that for a given n-tuple $w = (w_1, \dots, w_n)$ subject to the bilateral interlacing inequalities, and in the absence of degeneracies, the set of all rank 1 perturbations $\boldsymbol{G} = \boldsymbol{V} + \boldsymbol{f} \otimes \boldsymbol{n}$ with the prescribed singular values w consists of 2^n families in Lin, each of dimension $n-1$, parametrized by $\boldsymbol{n}$ from a certain set $\mathsf{A} \subset \mathsf{Sph}$ that depends on $\boldsymbol{V}$ and w. For each of the 2^n families, the value $\boldsymbol{f}$ is a function of $\boldsymbol{n}$ given by rather explicit formulas involving the roots $h_1, \dots, h_{n-1}$ of a certain polynomial of degree $n-1$, related to the characteristic polynomial of $\boldsymbol{V}^2 - \boldsymbol{V}\boldsymbol{n} \otimes \boldsymbol{V}\boldsymbol{n}$. It turns out that provided these are known, all the substantial information about $\boldsymbol{G}$ is derivable from explicit formulas. Such is the case of the amplitude $\boldsymbol{f}$, of the members $\boldsymbol{R}, \boldsymbol{H}, \boldsymbol{K}$ of the polar decomposition $\boldsymbol{G} = \boldsymbol{H}\boldsymbol{R} = \boldsymbol{R}\boldsymbol{K}$, and of the diagonalization of $\boldsymbol{H} = \sqrt{\boldsymbol{G}\boldsymbol{G}^{\mathrm{T}}}$ in the basis of eigenvectors of $\boldsymbol{V}$. For $n = 2, 3$ the roots $h_1, \dots, h_{n-1}$ are easily determined by $\boldsymbol{V}, \boldsymbol{n}$ and the formulas become completely explicit.

The general rank 1 perturbations are approached through *symmetric rank 1 perturbations* $\boldsymbol{B} = \boldsymbol{A} + \boldsymbol{m} \otimes \boldsymbol{m}$, where $\boldsymbol{A}, \boldsymbol{B}$ are symmetric and $\boldsymbol{m} \in \mathsf{Vect}$. The polarization formula (4.6) shows that a general rank 1 perturbation may be treated as a superposition of two symmetric rank 1 perturbations. Following an earlier work (Donoghue, 1974), in Šilhavý (1999), formulas for the components of $\boldsymbol{m}$ in the basis of eigenvectors of $\boldsymbol{A}$ have been derived, including the degenerate case. Here, I furthermore provide an orthogonal matrix giving the diagonalization of $\boldsymbol{B}$ in the basis of eigenvectors of $\boldsymbol{A}$ and apply these facts do derive the results on the general rank 1 perturbations described above.

The results provide a simple way to the particular results known previously. I choose to illustrate that briefly on the formulas for mechanical twinning [3] and on the rank 1 perturbations of identity, [4] playing an important role in determining the orientation of the austenite/martensite interface, both classical and nonclassical. [5]

2. Elementary systems and Cauchy matrices

Let $\mathbb{D}^n = \{x \in \mathbb{R}^n : x_1 \geqslant \cdots \geqslant x_n\}$; we furthermore denote by $\mathbb{R}_+ (\mathbb{R}_{++})$ the nonnegative (positive) half-axis and write $\mathbb{R}^n_+$, $\mathbb{R}^n_{++}$ for the nth cartesian powers of $\mathbb{R}_+$, $\mathbb{R}_{++}$. Throughout, the indices i, j, k, m range the interval $\{1, \dots, n\}$ unless stated otherwise. If $a \in \mathbb{R}^n$, we say that a has distinct components if $a_i \neq a_j$ for all $i, j, i \neq j$. We say that $x \in \mathbb{R}^n$ is nonnegative (positive) if $x \in \mathbb{R}^n_+$ $(x \in \mathbb{R}^n_{++})$. If $a, b \in \mathbb{R}^n$ then ab denotes the n-

[2] Rosakis (1990) gave a particular rank 1 perturbation with the prescribed singular values if $n = 3$; another set of particular rank 1 perturbations is given in (Šilhavý, 1999) arbitrary dimension.

[3] See Ericksen (1981, 1985) and Gurtin (1983).

[4] See Khachaturyan (1983, p. 176) and Ball and James (1987, Proposition 4).

[5] See Wechsler et al. (1953), Ball and James (1987) and Ball and Carstensen (1997).

tuple $ab = (a_1b_1, \dots, a_nb_n)$. If $f : \mathbb{R} \to \mathbb{R}$ is a *scalar-valued* function of a *scalar variable* and $a \in \mathbb{R}^n$, then $f(a)$ denotes the n-tuple $f(a) := (f(a_1), \dots, f(a_n))$. In particular, $a^2 = (a_1^2, \dots, a_n^2)$ and if a is nonnegative then $\sqrt{a} = (\sqrt{a_1}, \dots, \sqrt{a_n})$. Furthermore, $e_1, \dots, e_n$ denotes the canonical basis in $\mathbb{R}^n$ and $\{-1, 1\}^n$ denotes the set of all n-tuples $\omega = (\omega_1, \dots, \omega_n)$ where $\omega_i \in \{-1, 1\}$. For each $a \in \mathbb{R}^n$, p_a denotes the polynomial

$$p_a(z) = \prod_{i=1}^n (a_i - z) \equiv \sum_{k=0}^n S^k(a)(-z)^{n-k}, \quad z \in \mathbb{R}, \tag{2.1}$$

where S^k is the kth elementary symmetric function of n variables,

$$S^0(a_1, \dots, a_n) = 1, \qquad S^k(a_1, \dots, a_n) = \sum_{1 \leqslant i_1 < \cdots < i_k \leqslant n} a_{i_1} \dots a_{i_k}, \quad a \in \mathbb{R}^n, \qquad k > 0.$$

For each $a \in \mathbb{R}^n$, we define

$$d_j(a) := \prod_{\substack{i=1 \\ i \neq j}}^n (a_i - a_j).$$

Let $S : \mathbb{R}^n \to \mathbb{R}^n$ be defined by $S(a) = (S^1(a), \dots, S^n(a))$, $a \in \mathbb{R}^n$, and let $\nabla S(a) = [M_{ij}]$ be the matrix of the derivatives of S at a, where $M_{ij} = S^i_j(a) := \partial S^i(a)/\partial a_j$.

2.1. Elementary systems

The *elementary system* corresponding to $a, b \in \mathbb{R}^n$ is the linear system for the unknown $x \in \mathbb{R}^n$ of the form

$$S(b) - S(a) = \nabla S(a)x,$$

explicitly,

$$S^k(b) - S^k(a) = \sum_{j=1}^n S^k_j(a)x_j, \quad k = 1, \dots, n. \tag{2.2}$$

The matrix $\nabla S(a)$ of the elementary system is nonsingular if and only if a has distinct components (Šilhavý, 1999, Lemma 2.4); hence in this case, the system is uniquely solvable for each $b \in \mathbb{R}^n$. If some of the components of a coincide, then the system is solvable only for certain b (Šilhavý, 1999). However, for our purposes it completely suffices to describe the solution when a, b or b, a satisfy the interlacing inequalities. We say that $a, b \in \mathbb{D}^n$ satisfy the *interlacing inequalities* if

$$b_1 \geqslant a_1 \geqslant b_2 \geqslant a_2 \geqslant \cdots \geqslant b_n \geqslant a_n. \tag{2.3}$$

If $c \in \mathbb{R}^n$ and $z \in \mathbb{R}$, we denote by $m(z; c) \geqslant 0$ the *multiplicity* of z in the sequence $c_1, \dots, c_n$. An index $i \in \{1, \dots, n\}$ is said to be the *beginning of an interval of constancy* of $a \in \mathbb{D}^n$ if either $i = 1$ or $i > 1$ and $a_{i-1} > a_i$. An *interval of constancy* of a is an interval of positive integers of the form $\{j : i \leqslant j < i + m(a_i; a)\}$ where i is the beginning of an interval of constancy of a. The *end of an interval of constancy* of a is $i - 1 + m(a_i, a)$. Note that if the components of a are distinct, then each $i \in \{1, \dots, n\}$ is the beginning and end of an interval of constancy of a.

Proposition 2.1. *If a, b satisfy the interlacing inequalities then*

(1) *the elementary system corresponding to a, b has a particular solution given by*

$$x_j = (b_j - a_j) \prod_{i \in P(j)} \frac{b_i - a_j}{a_i - a_j}, \quad \text{where } P(j) := \{i : a_i \neq a_j\}; \tag{2.4}$$

(2) *we have* $x_j \geqslant 0$ *for each* j; *moreover*, $x_j > 0$ *only if* j *is the beginning of an interval of constancy of* a *and the end of an interval of constancy of* b;

(3) *the general solution is the sum of this particular solution with any n-tuple* $u \in \mathbb{R}^n$ *such that*

$$\sum_{i_\gamma \leqslant j < i_{\gamma+1}} u_j = 0, \quad \gamma = 1, \dots, r,$$

where $i_1, i_2, \dots, i_r$ *is the increasingly ordered set of all beginnings of the intervals of constancy of* a, $i_{r+1} := n + 1$, (*and necessarily* r *is the number of all distinct values in the sequence* a);

(4) *if* a *has distinct components the elementary system corresponding to* a, b *has a unique solution* x *given by*

$$x_j = p_b(a_j)/d_j(a). \tag{2.5}$$

Solution (2.4) is called the *particular solution* of the elementary system corresponding to a, b.

Proof. For the proof of (1), (3), (4), see (Šilhavý, 1999, Section 3). Let us prove (2). If i is the beginning of an interval of constancy of a with the interval of constancy $\{j : i \leqslant j < m(a_i; a)\}$ and with the multiplicity $m(a_i; a) > 1$, one finds that the interlacing inequalities give $b_j = a_j$ for all j, $i < j < m(a_i; a)$ and thus (2.5) implies $x_j = 0$ for all j, $i < j < m(a_i; a)$. The assertion about the end of an interval of constancy is proved similarly. □

In the absence of degeneracies, the elementary system reduces to a Cauchy system to be now introduced. Let $a, b \in \mathbb{R}^n$ be such that

$$b_i \neq a_j \quad \text{for all} \quad i, j \in \{1, \dots, n\}. \tag{2.6}$$

If, moreover, a, b have each distinct components, the *Cauchy matrix* corresponding to a, b is the matrix $C = [C_{ij}]$ with elements $C_{ij} = (b_i - a_j)^{-1}$, and the *Cauchy system* corresponding to a, b (or corresponding to the Cauchy matrix C) is the n by n linear system for the unknown $x \in \mathbb{R}^n$:

$$\sum_{j=1}^{n} C_{ij} x_j = 1, \quad i = 1, \dots, n. \tag{2.7}$$

Proposition 2.2. *If* $a, b \in \mathbb{R}^n$ *have each distinct components and satisfy condition* (2.6) *then* $x \in \mathbb{R}^n$ *is a solution of the elementary system corresponding to a,b if and only if x is a solution of the Cauchy system corresponding to a,b.*

Proof. It has been shown in (Šilhavý, 1999, Section 3), that x satisfies the elementary system corresponding to a, b if and only if

$$p_a(z) f(z) = p_b(z), \quad z \in \mathbb{R} \setminus \{a_1, \dots, a_n\}, \tag{2.8}$$

where f is a rational function defined by

$$f(z) = 1 + \sum_{j=1}^{n} x_j/(a_j - z).$$

Thus, if x is a solution of the elementary system, Eq. (2.8) implies $p_a(b_i) f(b_i) = p_b(b_i) = 0$. By Eq. (2.6) $p_a(b_i) \neq 0$ and so $f(b_i) = 0$ which means that x satisfies the Cauchy system. The converse implication is obtained by reversing the arguments. □

The *reciprocal elementary system* corresponding to $a, b \in \mathbb{R}^n$ is the system

$$S(b) - S(a) = \nabla S(b)y$$

for the unknown $y \in \mathbb{R}^n$. Since $S^k(-b) = (-1)^k S^k(b),\ \nabla S^k(-b) = (-1)^{k+1}\nabla S^k(b)$, the reciprocal elementary system corresponding to a, b is the elementary system corresponding to $-b, -a$. If a, b satisfy the interlacing inequalities, the reciprocal elementary system corresponding to a, b has a *particular solution* given by

$$y_j = (b_j - a_j) \prod_{i \in Q(j)} \frac{b_j - a_i}{b_j - b_i}, \quad \text{where } Q(j) := \{i : b_i \neq b_j\}. \tag{2.9}$$

Moreover, y is nonnegative and $y_j > 0$ only if j is the beginning of an interval of constancy of a and the end of an interval of constancy of b. If b has distinct components then Eq. (2.9) reduces to

$$y_j = -p_a(b_j)/d_j(b). \tag{2.10}$$

If $a, b \in \mathbb{R}^n$ have each distinct components and satisfy condition (2.6) then the reciprocal elementary system is equivalent to the *reciprocal Cauchy system* corresponding to a, b, which is the system

$$\sum_{j=1}^{n} C_{ji} y_j = 1, \quad i = 1, \ldots, n$$

for the unknown $y \in \mathbb{R}^n$. This is the Cauchy system corresponding to $-b, -a$.

The following proposition shows that the particular solution of the elementary system can always be obtained by solving a 'reduced' Cauchy system.

Proposition 2.3. *Let a, b satisfy the interlacing inequalities, let x, y be the particular solutions of the elementary and reciprocal elementary systems corresponding to a,b, let*

$$\mathsf{X}^0 = \{i : x_i = 0\}, \quad \mathsf{X}^+ = \{i : x_i > 0\}, \quad \mathsf{Y}^0 = \{i : y_i = 0\}, \quad \mathsf{Y}^+ = \{i : y_i > 0\},$$

and note that since x,y are nonnegative, we have $\mathsf{X}^0 \cup \mathsf{X}^+ = \mathsf{Y}^0 \cup \mathsf{Y}^+ = \{1, \ldots, n\}$. Then,

1. *X^0 and Y^0 have the same number of elements and therefore there exists a unique increasing mapping s from Y^0 onto X^0;*
2. *if $(i, j) \in \mathsf{X}^+ \times \mathsf{Y}^+$ then $a_i \neq b_j$ and $a^+ := \{a_i : i \in \mathsf{X}^+\}$, $b^+ := \{b_i : i \in \mathsf{Y}^+\}$ have each distinct components;*
3. *the restrictions $x^+ := \{x_i : i \in \mathsf{X}^+\}$, $y^+ := \{y_i : i \in \mathsf{Y}^+\}$ are the unique solutions of the Cauchy and reciprocal Cauchy systems corresponding to a^+, b^+, i.e.,*

$$x_i = p_{b^+}(a_i)/d_i(a^+), \quad i \in \mathsf{X}^+, \tag{2.11a}$$

$$y_j = -p_{a^+}(a_j)/d_j(b^+), \quad j \in \mathsf{Y}^+, \tag{2.11b}$$

where

$$p_{a^+}(z) = \prod_{k \in \mathsf{X}^+} (a_k - z), \qquad d_i(a^+) = \prod_{k \in \mathsf{X}^+,\, k \neq i} (a_k - a_i), \quad i \in \mathsf{X}^+,$$

and $p_{b^+}(z)$, $d_j(b^+)$ are defined analogously with X^+ replaced by Y^+.

Proof. Let q be the greatest common divisor of p_a, p_b and denote by $\tilde{p}_a = p_a/q, \tilde{p}_b = p_b/q$. Let $\mathsf{V},\ \mathsf{W}$ be the sets of all roots of $\tilde{p}_a, \tilde{p}_b$, respectively, taken with the corresponding multiplicities. The construction implies that $\mathsf{V},\ \mathsf{W}$ have the same number of elements, counting the multiplicities. Let us show that the multiplicity of each element of V and of each element of W is actually 1. To see it, let $c_\gamma, 1 \leqslant g \leqslant p$, be an increasingly ordered set of all points common to a and b, i.e., c_γ are such that $c_1 < c_2 < \cdots < c_p$, for each γ there exist i, j such that $c_\gamma = a_i = b_j$, and if $a_j = b_j$ for some i, j then $c_\gamma = a_j = b_j$ for some γ. Then,

$$p_a(z) = q_a^0(z)\prod_{\gamma=1}^{p}(c_\gamma - z)^{m_\gamma}, \qquad p_b(z) = q_b^0(z)\prod_{\gamma=1}^{p}(c_\gamma - z)^{n_\gamma}, \tag{2.12}$$

where $m_\gamma = m(c_\gamma; a), n_\gamma = m(c_\gamma; b)$, and the polynomials q_a^0, q_b^0 are as follows. The set of roots of q_a^0 is exactly the set of elements of a that are not in b and the set of roots of q_b^0 is exactly the set of elements of b that are not in a, with the corresponding multiplicities. If ξ is an element of a not contained in b then the interlacing inequalities imply that $m(\xi, a) = 1$; thus the multiplicity of the roots of q_a^0 is 1 and the same is true for q_b^0. Both $q_a^0,\ q_b^0$ contribute to $\tilde{p}_a,\ \tilde{p}_b$. Finally, it remains to see how the products containing c_γ in Eq. (2.12) enter $\tilde{p}_a,\ \tilde{p}_b$. The interlacing inequalities imply that $m_\gamma - 1 \leqslant n_\gamma \leqslant m_\gamma + 1,\ 1 \leqslant \gamma \leqslant p$, and thus, if $m_\gamma = n_\gamma + 1$, the factor $c_\gamma - z$ (in the power 1) goes to $\tilde{p}_a$ but does not go to $\tilde{p}_b$. If $m_\gamma = n_\gamma$ then c_γ is neither the root of $\tilde{p}_a$ nor the root of $\tilde{p}_b$ and if $m_\gamma = n_\gamma - 1$, the factor $c_\gamma - z$ goes to $\tilde{p}_b$ but does not go to $\tilde{p}_a$. This completes the proof of the assertion about the simple multiplicity of the roots of $\tilde{p}_a,\ \tilde{p}_b$. Also the roots of $\tilde{p}_a,\ \tilde{p}_b$ are disjoint. Thus since there are no multiplicities in V, for each $\alpha \in \mathsf{V}$ there exists a unique i such that $\alpha = a_i$ and i is the beginning of an interval of constancy of a, and for each $\beta \in \mathsf{W}$ there exists a unique j such that $\beta = b_j$ and j is the end of an interval of constancy of b. Let us show that

$$\mathsf{V} = \{a_i : i \in \mathsf{X}^+\}, \tag{2.13a}$$

$$\mathsf{W} = \{b_j : j \in \mathsf{Y}^+\}. \tag{2.13b}$$

The elementary system reads (cf. the proof of Proposition 2.2)

$$p_b(z) = p_a(z)\left[1 + \sum_{i\in\mathsf{X}^+} x_i/(a_i - z)\right], \quad z \in \mathbb{R}\setminus\{a_i : i \in \mathsf{X}^+\},$$

which is equivalent to

$$\tilde{p}_b(z) = \tilde{p}_a(z)\left[1 + \sum_{i\in\mathsf{X}^+} x_i/(a_i - z)\right], \quad z \in \mathbb{R}\setminus\{a_i : i \in \mathsf{X}^+\}. \tag{2.14}$$

Since each element of X^+ is the beginning of an interval of constancy of a (see Proposition 2.4) we have $a_i \neq a_j$ for each $i, j \in \mathsf{X}^+,\ i \neq j$. Thus, the singularities in the square brackets in Eq. (2.14) cannot cancel each other. The left-hand side of Eq. (2.14) has no singularities, and thus the absence of singularities of the right-hand side implies that $\tilde{p}_a(a_i) = 0$ for each $i \in \mathsf{X}^+$ which gives $\{a_i : i \in \mathsf{X}^+\} \subset \mathsf{V}$. Conversely, we have $\tilde{p}_b(\alpha) \neq 0$ for each $\alpha \in \mathsf{V}$ and since $\tilde{p}_a(\alpha) = 0$, the square bracket in Eq. (2.14) must have a singularity, which proves $\mathsf{V} \subset \{a_i : i \in \mathsf{X}^+\}$ and hence Eq. (2.13a). Eq. (2.13b) is proved similarly. Since V and W have the same number of elements, we see that $\mathsf{X}^+,\ \mathsf{Y}^+$ have the same number of elements, which proves (1). Also (2) has been proved on the way. Finally, from Eq. (2.14), we deduce that

$$\sum_{i\in\mathsf{X}^+} x_i/(b_j - a_i) = 1, \quad j \in \mathsf{Y}^+,$$

and the fact that $\mathsf{X}^+,\ \mathsf{Y}^+$ have the same number of elements and (2) show that x^+ is the solution of the Cauchy system corresponding to $a^+,\ b^+$ and hence x^+ is given by Eq. (2.5), which here reads as Eq. (2.11a). Eq. (2.11b) is proved similarly. □

Proposition 2.4. *Let $a, b \in \mathbb{R}^n$ have each distinct components and satisfy condition* (2.6). *Then the Cauchy matrix C corresponding to a, b is nonsingular and*

$$C^{-1} = \operatorname{diag}(x)C^{\mathrm{T}}\operatorname{diag}(y),$$

where x, y are the solutions of the Cauchy and Cauchy reciprocal systems corresponding to a, b, respectively. Schechter (1959) and Vavřín (1997, Lemma 12) gives a generalization to the confluent Cauchy matrices. (The formula also follows from the general result in Heinig and Rost (1984, Theorem 2.7, p. 161)) once the solution of the Cauchy system is known (Finck et al., 1993, Corollary 3.1).

3. Symmetric rank 1 perturbations with prescribed spectrum

Direct vector notation is used throughout (Gurtin, 1981; Šilhavý, 1997). In addition to the notation explained in Introduction, we write $\boldsymbol{u} \cdot \boldsymbol{w}$ for the scalar product in Vect and recall that a second-order tensor $\boldsymbol{A}$ is a linear transformation from Vect into Vect, with the product of two tensors defined as the composition of the linear transformations. Furthermore, Sym and Sym^+ denote the sets of symmetric and positive definite symmetric tensors, respectively, and $\mathsf{Orth} \subset \mathsf{Lin}$ and $\mathsf{Orth}^+ \subset \mathsf{Lin}$ the orthogonal and the proper orthogonal groups. By a basis of Vect we always mean an orthonormal basis. If $\mathsf{E} = \{\boldsymbol{e}_i\}$ is an basis and Q an orthogonal matrix, then $Q\mathsf{E} := \{\boldsymbol{f}_i\}$ denotes the basis given by

$$\boldsymbol{f}_i = \sum_{j=1}^{n} Q_{ij}\boldsymbol{e}_j.$$

If E, F are two bases, we say that an orthogonal matrix Q realizes the passage from E to C if $\mathsf{F} = Q\mathsf{E}$. We have $Q(R\mathsf{E}) = (QR)\mathsf{E}$ for any two orthogonal matrices Q, R and any basis E.

We say that $\boldsymbol{A} \in \mathsf{Sym}$ has the eigenvalues $a \in \mathbb{D}^n$ if the components of a are the eigenvalues of $\boldsymbol{A}$ occurring with appropriate multiplicities and in a nonincreasing order; we also say that a is the spectrum of $\boldsymbol{A}$. By a basis of eigenvectors of $\boldsymbol{A}$, we always mean a basis $\{\boldsymbol{e}_i\}$ of eigenvectors of $\boldsymbol{A}$ ordered in such a way that $\boldsymbol{e}_i$ corresponds to the eigenvalue a_i, with a_i ordered as above. Thus, if the components of a are distinct, a permutation of the elements of $\{\boldsymbol{e}_i\}$ is no longer a basis of eigenvectors of $\boldsymbol{A}$. We say that $\boldsymbol{G} \in \mathsf{Lin}$ has the *singular values* $w \in \mathbb{D}^n \cap \mathbb{R}^n_+$ if $\sqrt{\boldsymbol{G}\boldsymbol{G}^{\mathrm{T}}}$ has the eigenvalues w. We say that $\boldsymbol{A} \in \mathsf{Lin}$ has distinct singular values $w \in \mathbb{D}^n$ if w are the singular values of $\boldsymbol{A}$ and the components of w are distinct. The same convention applies to the eigenvalues.

The tensor $\boldsymbol{B} \in \mathsf{Lin}$ is said to be a *rank 1 perturbation* of $\boldsymbol{A} \in \mathsf{Lin}$ if $\boldsymbol{B} = \boldsymbol{A} + \boldsymbol{f} \otimes \boldsymbol{b}$ for some $\boldsymbol{f}, \boldsymbol{b} \in \mathsf{Vect}$. The tensor $\boldsymbol{B}$ is said to be a *symmetric rank 1 perturbation* of $\boldsymbol{A}$ if $\boldsymbol{B} = \boldsymbol{A} + \boldsymbol{m} \otimes \boldsymbol{m}$ for some $\boldsymbol{m} \in \mathsf{Vect}$.

Proposition 3.1. *If $\boldsymbol{A} \in \mathsf{Sym}$ has the spectrum $a \in \mathbb{D}^n$ then $b \in \mathbb{D}^n$ is the spectrum of some symmetric rank* 1 *perturbation of $\boldsymbol{A}$ if and only if a, b satisfy the interlacing inequalities* (Šilhavý, 1999, Section 4).

Proposition 3.2. *Let $\boldsymbol{A} \in \mathsf{Sym}$ have the spectrum $a \in \mathbb{D}^n$; $\boldsymbol{B} = \boldsymbol{A} + \boldsymbol{m} \otimes \boldsymbol{m}$, $\boldsymbol{m} \in \mathsf{Vect}$; E be a basis of eigenvectors of $\boldsymbol{A}$ and $m \in \mathbb{R}^n$ the components of $\boldsymbol{m}$ in E and $\hat{\mathsf{E}}$ be a basis of eigenvectors of $\boldsymbol{B}$ and $\hat{m} \in \mathbb{R}^n$ the components of $\boldsymbol{m}$ in $\hat{\mathsf{E}}$, then the following three conditions are equivalent*:

(1) *$b \in \mathbb{D}^n$ is the spectrum of $\boldsymbol{B}$*;

(2) *the squares $m^2 = (m_1^2, \ldots, m_n^2)$ satisfy the elementary system corresponding to a, b; i.e.,*

$$m_i = \omega_i \sqrt{x_i}, \tag{3.1}$$

for some $\omega \in \{-1, 1\}^n$ and some nonnegative solution $x \in \mathbb{R}^n$ of the elementary system corresponding to a, b; equivalently,

$$\sum_{i_\gamma \leqslant j < i_{\gamma+1}} m_j^2 = x_{i_\gamma}, \quad \gamma = 1, \ldots, r,$$

where $i_1, i_2, \ldots, i_r$ *is the increasingly ordered set of all beginnings of intervals of constancy of* a, $i_{r+1} := n+1$, *and* x *is the particular solution of the elementary system corresponding to* a, b;

(3) *the squares* $\hat{m}^2 = (\hat{m}_1^2, \ldots, \hat{m}_n^2)$ *satisfy the reciprocal elementary system corresponding to* a, b; *i.e.*,

$$\hat{m}_i = \tau_i \sqrt{y_i},$$

for some $\tau \in \{-1, 1\}^n$ *and some nonnegative solution* y *of the reciprocal elementary system corresponding to* a, b; *equivalently*

$$\sum_{j_{\delta-1} < j \leqslant j_\delta} \hat{m}_j^2 = y_{j_\delta}, \quad \delta = 1, \ldots, s,$$

where $j_1, j_2, \ldots, j_s$ *is the increasingly ordered set of all ends of intervals of constancy of* b, $j_0 := 0$, *and* y *is the particular solution of the reciprocal elementary system corresponding to* a, b.

Moreover, if these conditions are satisfied, then in E, $\boldsymbol{B}$ *is represented by the matrix*

$$B := \operatorname{diag}(a) + \omega\sqrt{x} \otimes \omega\sqrt{x}, \tag{3.2}$$

where $x \in \mathbb{R}^n$ *is the nonnegative solution of the elementary system corresponding to* a, b *as in (2) and in* $\hat{\mathsf{E}}$, $\boldsymbol{A}$ *is represented by the matrix*

$$A := \operatorname{diag}(b) - \tau\sqrt{y} \otimes \tau\sqrt{y},$$

where $y \in \mathbb{R}^n$ *is the nonnegative solution of the reciprocal elementary system corresponding to* a, b *as in (3).*

Proof. This follows from Šilhavý (1999, Proposition 4.2). □

Remark 3.3. *If the spectrum* a *of* $\boldsymbol{A} \in \mathsf{Sym}$ *has distinct components and if* $b \in \mathbb{D}^n$ *has distinct components and is such that* a, b *satisfy the interlacing inequalities and condition* (2.6) *then there are* 2^{n-1} *different symmetric rank* 1 *perturbations* $\boldsymbol{B}$ *of* $\boldsymbol{A}$ *with the spectrum* b.

Proof. Under the hypotheses, the elementary system corresponding to a, b has a unique solution x and the components of x are strictly positive. Thus, Eq. (3.1) gives 2^n different values of $\boldsymbol{m}$ that lead to $\boldsymbol{B}$ with the spectrum b. The assertion then follows from the immediate fact that $\boldsymbol{A} + \boldsymbol{m} \otimes \boldsymbol{m} = \boldsymbol{A} + \boldsymbol{n} \otimes \boldsymbol{n}$ for some $\boldsymbol{m}, \boldsymbol{n} \in \mathsf{Vect}$ if and only if either $\boldsymbol{m} = \boldsymbol{n}$ or $\boldsymbol{m} = -\boldsymbol{n}$. □

Let us show that in an appropriately chosen basis of eigenvectors of $\boldsymbol{A}$, the components of $\boldsymbol{m}$ are given by Eq. (3.1) with $\omega = (1, \ldots, 1) \in \{-1, 1\}^n$ and with x the *particular solution* of the elementary system corresponding to a, b.

Remark 3.4. *If* $\boldsymbol{A}, \boldsymbol{B} \in \mathsf{Sym}$ *have the spectra* a, b, *respectively, and* $\boldsymbol{B}$ *is a symmetric rank* 1 *perturbation of* $\boldsymbol{A}$, *then there exists a basis* E *of eigenvectors of* $\boldsymbol{A}$ *such that the components* m *of* $\boldsymbol{m}$ *in* E *are* $m_i = \sqrt{x_i}$ *and the matrix* B *of* $\boldsymbol{B}$ *in* E *is*

$$B = \operatorname{diag}(a) + \sqrt{x} \otimes \sqrt{x}, \tag{3.3}$$

where x *is the particular solution* (2.4) *of the elementary system corresponding to* a, b.

Proof. Indeed, one can always find a basis of eigenvectors of $\boldsymbol{A}$ such that the component m_i of $\boldsymbol{m}$ in this basis are nonzero only if i is the beginning of an interval of constancy of a. Then m^2 necessarily coincides with x and hence we have Eq. (3.2) for some $\omega \in \{-1, 1\}^n$. An appropriate change of the signs of the elements of this basis then leads to a basis in which Eq. (3.3) holds. □

Let us now proceed to the diagonalization of the perturbed transformation. Let

$$\rho_{ij} := \begin{cases} 1 & \text{if } i \geqslant j, \\ -1 & \text{if } i < j. \end{cases}$$

Theorem 3.5. *Let a, b satisfy the interlacing inequalities, let x, y be the particular solutions of the elementary and reciprocal elementary systems corresponding to a, b, let $\omega \in \{-1, 1\}^n$, define B by Eq.* (3.2), *let X^0, X^+, Y^0, Y^+ and s be as in Proposition 2.3, and define an n by n matrix Q by*

$$Q_{ij} = \begin{cases} \dfrac{\omega_i\sqrt{x_i y_j}}{b_j - a_i} & \text{if } (i,j) \in \mathsf{X}^+ \times \mathsf{Y}^+, \\ \omega_i \rho_{ij} \delta_{i,s(j)} & \text{if } (i,j) \in \mathsf{X}^0 \times \mathsf{Y}^0, \\ 0 & \text{otherwise}, \end{cases} \tag{3.4}$$

and note that Proposition 2.3(2) guarantees that the denominator in Eq. (3.4) (first equation) is nonzero. Then Q is orthogonal and

$$B = Q \operatorname{diag}(b) Q^{\mathrm{T}}, \tag{3.5a}$$

$$\omega\sqrt{x} = Q\sqrt{y}. \tag{3.5b}$$

If additionally $a, b \in \mathbb{D}^n$ have each distinct components and satisfy condition (2.6) *then*

$$Q = \operatorname{diag}(\omega\sqrt{x}) C^{\mathrm{T}} \operatorname{diag}(\sqrt{y}), \tag{3.6}$$

where C is the Cauchy matrix corresponding to a, b.

The matrix Q with various choices of a, b and with $\omega = (1, \ldots, 1) \in \{-1, 1\}^n$ will play important role in the description of the general rank 1 perturbations in Section 4, and we write $Q = \mathsf{Q}(a, b)$.

Proof. To simplify notation, let $\omega = (1, \ldots, 1)$. It is convenient to consider first the nondegenerate case mentioned at the end of the theorem. Thus let a, b have each distinct components and satisfy condition (2.6), which by Eqs. (2.5) and (2.10) implies that all the components of x and y are positive. Let Q be given by Eqs. (3.5a) and (3.5b). The inversion formula in Proposition 2.4 can be rewritten as

$$\left(\operatorname{diag}(\sqrt{y}) C \operatorname{diag}(\sqrt{x})\right)^{-1} = \operatorname{diag}(\sqrt{x}) C^{\mathrm{T}} \operatorname{diag}(\sqrt{y}),$$

i.e., $(Q^{\mathrm{T}})^{-1} = Q$, which proves that Q is orthogonal. Furthermore, we have

$$(BQ)_{ik} = \frac{a_i\sqrt{x_i}\sqrt{y_k}}{b_k - a_i} + \sqrt{x_i}\sum_{j=1}^{n} \frac{x_j\sqrt{y_k}}{b_k - a_j} = \frac{a_i\sqrt{x_i}\sqrt{y_k}}{b_k - a_i} + \sqrt{x_i}\sqrt{y_k} = (Q\operatorname{diag}(b))_{ik},$$

where we have used that x satisfies the Cauchy system. This proves Eqs. (3.5a) and (3.5b) is proved similarly. In the general case, let t be the number of elements of X^+. Let $\mathbb{R}(\mathsf{X}^+)$ denote the t-dimensional space of all sequences $\xi = \{\xi_i \in \mathbb{R} : i \in \mathsf{X}^+\}$ indexed by the indices from the set X^+, let $\mathbb{M}(\mathsf{X}^+)$ denote the t^2-dimensional space of all matrices $\Gamma = [\Gamma_{ij} \in \mathbb{R} : i, j \in \mathsf{X}^+]$ indexed by the indices from the set X^+, and let finally $\mathbb{M}(\mathsf{X}^+, \mathsf{Y}^+)$ be the matrices with the first index from X^+ and the second from Y^+. Let $a^+,\ x^+ \in \mathsf{X}^+,\ b^+,\ y^+ \in \mathsf{Y}^+$ be as in Proposition 2.3, let $B^+ \in \mathbb{M}(\mathsf{X}^+)$ be defined by

$$B^+ = \operatorname{diag}(a^+) + \sqrt{x^+} \otimes \sqrt{x^+}$$

and let $Q^+ \in \mathbb{M}(\mathsf{X}^+, \mathsf{Y}^+)$ be defined by $Q^+_{ij} = Q_{ij},\ i \in \mathsf{X}^+,\ j \in \mathsf{Y}^+$, where Q is as in Eq. (3.6). By Proposition 2.3, the pair a^+, b^+ satisfies the hypotheses of the special case and the matrix Q is Q^+, from which we learn that

$$B^+ = Q^+ \operatorname{diag}(b^+) Q^{+\mathrm{T}}, \quad \sqrt{x^+} = Q^+ \sqrt{y^+},$$

and Q^+ is orthogonal. The last implies that also Q is orthogonal and that it satisfies Eqs. (3.5a) and (3.5b). □

Remark 3.6. (1) *In the general degenerate case, the diagonalizing matrix is not unique, and in particular, any orthogonal matrix in the block* $\mathsf{X}^0 \times \mathsf{Y}^0$ *would lead to a matrix* Q *satisfying Eqs.* (3.5a) *and* (3.5b)*. The form* (3.4) (*second equation*) *is to make a unique choice, with s obviously the most natural. The occurrence of* ρ_{ij} *in Eq.* (3.4) (*second equation*) *is a convenient choice as seen from the following assertion*: *If* $\omega = (1, \ldots, 1)$ *then the elements of* Q *are nonpositive above the main diagonal and nonnegative on or below the main diagonal. This follows from Eq.* (3.4), *the interlacing inequalities*, *and the definition of* ρ.

(2) *Example: In the situation of Theorem* 3.5, *let* $\omega = (1, \ldots, 1)$, *let* $a \in \mathbb{D}^n$ *have distinct components*, *let* $b_1 > a_1$ *and define* $b_k = a_{k-1}$ *for* $k = 2, \ldots, n$. *Then* $b \in \mathbb{D}^n$ *and* a, b *satisfy the interlacing inequalities. One finds that* $x_1 = x_2 = \cdots = x_{n-1} = 0$, $x_n = b_1 - a_n > 0$, $y_1 = b_1 - a_n$, $y_2 = \cdots = y_n = 0$,

$$\mathsf{X}^0 = \{1, \ldots, n-1\}, \qquad \mathsf{X}^+ = \{n\}, \qquad \mathsf{Y}^0 = \{2, \ldots, n\}, \qquad \mathsf{Y}^+ = \{1\}, \qquad s(i) = i - 1, \qquad i \in \mathsf{Y}^0,$$

$$Q = \begin{bmatrix} 0 & -1 & 0 & \cdots & 0 \\ 0 & 0 & -1 & \cdots & 0 \\ & & \vdots & & \\ 0 & 0 & 0 & \cdots & -1 \\ 1 & 0 & 0 & \cdots & 0 \end{bmatrix},$$

$$B = \operatorname{diag}(a) + \sqrt{x} \otimes \sqrt{x} = \operatorname{diag}(a_1, a_2, \ldots, a_{n-1}, b_1) \quad \textit{and} \quad Q^{\mathrm{T}} B Q = \operatorname{diag}(b_1, a_1, \ldots, a_{n-1}).$$

4. Rank 1 perturbations with prescribed singular values

We consider a general rank 1 perturbation $\boldsymbol{G} = \boldsymbol{F} + \boldsymbol{f} \otimes \boldsymbol{n}$ of $\boldsymbol{F} \in \mathsf{Lin}$, $\det \boldsymbol{F} \neq 0$, and assume throughout that $\boldsymbol{n} \in \mathsf{Sph}$. With this choice of $\boldsymbol{n}$, the vector $\boldsymbol{f}$ is called the amplitude of $\boldsymbol{G}$. In view of the polar decomposition theorem it suffices to consider the case when $\boldsymbol{F} = \boldsymbol{V} \in \mathsf{S}ym^+$. The pair w, v, where $w, v \in \mathbb{D}^n \cap \mathbb{R}^n_+$ is said to satisfy the *bilateral interlacing inequalities* if

$$w_1 \geqslant v_2, \quad v_1 \geqslant w_2 \geqslant v_3, \ldots, v_{n-1} \geqslant w_n. \tag{4.1}$$

If the pair w, v satisfies the bilateral interlacing inequalities then also the pair v, w satisfies the bilateral interlacing inequalities.

Proposition 4.1. *If* $\boldsymbol{V} \in \mathsf{S}ym^+$ *has the eigenvalues* $v \in \mathbb{D}^n \cap \mathbb{R}^n_{++}$ *then a necessary and sufficient condition that* $w \in \mathbb{D}^n \cap \mathbb{R}^n_{++}$ *be the singular values of some rank* 1 *perturbation of* $\boldsymbol{V}$ *is that* w, v *satisfy the bilateral interlacing inequalities* (Šilhavý, 1999, Section 4).

In the rest of the paper, $\boldsymbol{V}$ is always a tensor in $\mathsf{S}ym^+$ and v is its spectrum; moreover, let

$$\boldsymbol{D} = \boldsymbol{V}^2 - \boldsymbol{V}\boldsymbol{n} \otimes \boldsymbol{V}\boldsymbol{n}, \tag{4.2}$$

where $\boldsymbol{V}$, $\boldsymbol{n} \in \mathsf{Sph}$ have the current local meaning specified by the surrounding text. In the same situation, let $h \in \mathbb{D}^n \cap \mathbb{R}^n_+$ be an n-tuple such that h^2 is the spectrum of $\boldsymbol{D}$, and $\bar{x}, \bar{y}$ the particular solutions of the elementary and reciprocal elementary systems corresponding to h^2, v^2.

Lemma 4.2. (1) *If* $\boldsymbol{n} \in \mathsf{Sph}$ *then* $\boldsymbol{D}$ *is positive semidefinite, 0 is its eigenvalue corresponding to the eigenvector* $\boldsymbol{V}^{-1}\boldsymbol{n}$ *and* $h_i > 0$ *for all* i, $1 \leqslant i < n$; *moreover,*

$$|\boldsymbol{V}^{-1}\boldsymbol{n}| = \frac{h_1 \dots h_{n-1}}{v_1 \dots v_n}; \tag{4.3}$$

(2) *a necessary and sufficient condition that* $\bar{h}^2 \in \mathbb{D}^n$, *where* $\bar{h} \in \mathbb{D}^n \cap \mathbb{R}^n_+$, *is the spectrum of* $\boldsymbol{D}$ *for some* $\boldsymbol{n} \in \mathsf{Sph}$ *is that* $\bar{h}_n = 0$ *and* $v, \bar{h}$ *satisfy the interlacing inequalities.*

Proof. (1) If $\boldsymbol{x} \in \mathsf{Vect}$ the Schwarz's inequality implies

$$\boldsymbol{Dx} \cdot \boldsymbol{x} = \boldsymbol{V}^2\boldsymbol{x} \cdot \boldsymbol{x} - (\boldsymbol{n} \cdot \boldsymbol{Vx})^2 \geqslant \boldsymbol{V}^2\boldsymbol{x} \cdot \boldsymbol{x} - |\boldsymbol{Vx}|^2 = 0,$$

which proves the positive semidefiniteness of $\boldsymbol{D}$. The assertion that $\boldsymbol{V}^{-1}\boldsymbol{n}$ is an eigenvector corresponding to 0 is immediate. To prove Eq. (4.3), let us calculate $\operatorname{cof}\boldsymbol{D}$ in two ways. First, since $h_n = 0$, in the basis of eigenvectors of $\boldsymbol{D}$, $\operatorname{cof}\boldsymbol{D}$ is represented by $\operatorname{diag}(0, \dots, 0, [h_1 \cdots h_{n-1}]^2)$; since the normalized eigenvector corresponding to $h_n = 0$ is $\boldsymbol{V}^{-1}\boldsymbol{n}/|\boldsymbol{V}^{-1}\boldsymbol{n}|$ one finds that

$$\operatorname{cof}\boldsymbol{D} = (h_1 \dots h_{n-1})^2 \frac{\boldsymbol{V}^{-1}\boldsymbol{n} \otimes \boldsymbol{V}^{-1}\boldsymbol{n}}{|\boldsymbol{V}^{-1}\boldsymbol{n}|^2}. \tag{4.4}$$

On the other hand, $\boldsymbol{D} = \boldsymbol{V}(\boldsymbol{1} - \boldsymbol{n} \otimes \boldsymbol{n})\boldsymbol{V}$ and hence,

$$\operatorname{cof}\boldsymbol{D} = \operatorname{cof}\boldsymbol{V} \operatorname{cof}(\boldsymbol{1} - \boldsymbol{n} \otimes \boldsymbol{n}) \operatorname{cof}\boldsymbol{V} = (\det \boldsymbol{V})^2 \boldsymbol{V}^{-1}\boldsymbol{n} \otimes \boldsymbol{n}\boldsymbol{V}^{-1} = (\det \boldsymbol{V})^2 \boldsymbol{V}^{-1}\boldsymbol{n} \otimes \boldsymbol{n}\boldsymbol{V}^{-1}\boldsymbol{n}, \tag{4.5}$$

and a comparison of Eqs. (4.4) and (4.5) gives Eq. (4.3).

(2): If $\bar{h}^2$ is the spectrum of $\boldsymbol{D}$ then $\bar{h}_n = 0$ follows from (1) and since $\boldsymbol{V}^2$ is a symmetric rank 1 perturbation of $\boldsymbol{D}$, $v^2, \bar{h}^2$ satisfy the interlacing inequalities. Conversely, if $\bar{h} \in \mathbb{D}^n$ satisfies the conditions stated in (2), then $\bar{h}^2$ is the spectrum of some symmetric rank 1 perturbation $\boldsymbol{D}$ of $\boldsymbol{V}^2$ of the form $\boldsymbol{D} := \boldsymbol{V}^2 - \boldsymbol{m} \otimes \boldsymbol{m}$, where $\boldsymbol{m} \in \mathsf{Vect}$. As $\bar{h}_n = 0$, one has $\det \boldsymbol{D} = \det(\boldsymbol{V}^2 - \boldsymbol{m} \otimes \boldsymbol{m}) = 0$, i.e., $\det \boldsymbol{V}^2(1 - \boldsymbol{V}^{-2}\boldsymbol{m} \cdot \boldsymbol{m}) = 0$. This gives $|\boldsymbol{V}^{-1}\boldsymbol{m}|^2 = 1$ and setting $\boldsymbol{n} := \boldsymbol{V}^{-1}\boldsymbol{m}$ one has $\boldsymbol{n} \in \mathsf{Sph}$ and $\boldsymbol{D} = \boldsymbol{V}^2 - \boldsymbol{Vn} \otimes \boldsymbol{Vn}$. □

We shall use the identity

$$\boldsymbol{GG}^{\mathrm{T}} = \boldsymbol{V}^2 + (\boldsymbol{f} + \boldsymbol{Vn}) \otimes (\boldsymbol{f} + \boldsymbol{Vn}) - \boldsymbol{Vn} \otimes \boldsymbol{Vn}; \tag{4.6}$$

to determine all rank 1 perturbations $\boldsymbol{G} = \boldsymbol{V} + \boldsymbol{f} \otimes \boldsymbol{n}$ with the prescribed singular values. That identity shows that $\boldsymbol{GG}^{\mathrm{T}}$ is a superposition of two symmetric rank 1 perturbations of $\boldsymbol{V}^2$ so that the results of Section 3 will be applicable. The following theorem describes the set of all rank 1 perturbations of a general positive definite tensor, including the amplitude and the polar decomposition. It deals with a general, possibly degenerate case. The result simplifies in the nondegenerate case as the treatment that follows shows.

We say that a basis $\mathsf{E} = \{\boldsymbol{e}_i\}$ is a basis of eigenvectors of $\boldsymbol{V}$ special with respect to $\boldsymbol{n}$ if $\mathsf{Q}(h^2, v^2)^{\mathrm{T}}\mathsf{E}$ is a basis of eigenvectors of $\boldsymbol{D}$. When h, v have each distinct components and condition (4.14) is satisfied, then there are exactly two bases of eigenvectors of $\boldsymbol{V}$ special with respect to $\boldsymbol{n}$, namely those in which either all components of $\boldsymbol{Vn}$ are positive or all negative; see Remark 4.5. In the degenerate case, the components of $\boldsymbol{n}$ in a special basis are all nonnegative or all nonpositive, but the notion of a special basis is more restrictive. Recall the orthogonal matrix $\mathsf{Q}(a, b)$ defined after Theorem 3.5.

Theorem 4.3. *Let* $v, w \in \mathbb{D}^n \cap \mathbb{R}^n_{++}$, $\boldsymbol{V} \in \mathsf{Sym}^+$, $\boldsymbol{n} \in \mathsf{Sph}$, $\boldsymbol{f} \in \mathsf{Vect}$ *and set* $\boldsymbol{G} = \boldsymbol{V} + \boldsymbol{f} \otimes \boldsymbol{n}$. *Then*

(1) $\boldsymbol{G}$ *has the singular values* w *if and only if* h^2, w^2 *satisfy the interlacing inequalities and there exists a basis* E *of eigenvectors of* $\boldsymbol{V}$ *special with respect to* $\boldsymbol{n}$ *such that the components* f *of* $\boldsymbol{f}$ *in* E *are given by*

$$f = -Vn + \mathsf{Q}(h^2, v^2)^{\mathrm{T}} P\sqrt{x}, \tag{4.7}$$

where $V = \operatorname{diag}(v)$, *n are the components of* $\boldsymbol{n}$ *in* E, *x is the particular solution of the elementary system corresponding to* h^2, w^2, *and P is an orthogonal matrix such that*

$$P \operatorname{diag}(h) P^{\mathrm{T}} = \operatorname{diag}(h). \tag{4.8}$$

If condition (1) *is satisfied then*

(2) *in* E, $\sqrt{\boldsymbol{G}\boldsymbol{G}^{\mathrm{T}}}$ *is represented by the matrix*

$$H = S \operatorname{diag}(w) S^{\mathrm{T}}, \tag{4.9}$$

where $S = \mathsf{Q}(h^2, v^2)^{\mathrm{T}} P \mathsf{Q}(h^2, w^2)$, *and the polar decomposition of* $\boldsymbol{G} = \boldsymbol{H}\boldsymbol{R} = \boldsymbol{R}\boldsymbol{K}$ *is represented by* $G = HR = RK$, *where*

$$\begin{aligned} R &= H^{-1}\Big[V(1 - n\otimes n) + \mathsf{Q}(h^2, v^2)^{\mathrm{T}} P\sqrt{x}\otimes n\Big], \\ K &= \Big[(1 - n\otimes n)V + n\otimes \mathsf{Q}(h^2, v^2)^{\mathrm{T}} P\sqrt{x}\Big] H^{-1}\Big[V(1 - n\otimes n) + \mathsf{Q}(h^2, v^2)^{\mathrm{T}} P\sqrt{x}\otimes n\Big]; \end{aligned} \tag{4.10}$$

(3) *in an appropriate basis of eigenvectors of* $\boldsymbol{G}\boldsymbol{G}^{\mathrm{T}}$, *the components* $\bar{f}$ *of* $\boldsymbol{f}$ *are given by*

$$\bar{f} = -\bar{V}\bar{n} + \sqrt{y},$$

where $\bar{V} = S^{\mathrm{T}} \operatorname{diag}(v) S$, *is the matrix of* $\boldsymbol{V}$ *in this basis,* $\bar{n} = S^{\mathrm{T}} n$ *are the components of* $\boldsymbol{n}$ *and y is the solution of the reciprocal elementary system corresponding to* h^2, w^2; *the orthogonal tensor* $\boldsymbol{R}$ *from the polar decomposition of* $\boldsymbol{G}$ *is represented by the matrix*

$$\bar{R} = \operatorname{diag}(w^{-1})[\bar{V}(I - \bar{n}\otimes\bar{n}) + \sqrt{y}\otimes\bar{n}].$$

Since, for a fixed $\boldsymbol{V}$, h is a function of $\boldsymbol{n}$, the condition that h^2, w^2 satisfy the interlacing inequalities determines all possible $\boldsymbol{n}$ for which there exists an $\boldsymbol{f}$ such that $\boldsymbol{G}$ has the singular values w.

Proof. (1) Let $\boldsymbol{G}$ have the singular values w. The tensor $\boldsymbol{V}^2$ is a symmetric rank 1 perturbation of $\boldsymbol{D}$. Let G be any basis of eigenvectors of $\boldsymbol{D}$ and define $\mathsf{E} := \mathsf{Q}(h^2, v^2)\mathsf{G}$. Then by Theorem 3.5, E is a basis of eigenvectors of $\boldsymbol{V}$ special with respect to $\boldsymbol{n}$. By Eq. (4.6), $\boldsymbol{G}\boldsymbol{G}^{\mathrm{T}}$ is a rank 1 perturbation of $\boldsymbol{D}$, and hence, first, h^2, w^2 satisfy the interlacing inequalities and second, by Remark 3.4, there exists a basis $\bar{\mathsf{G}}$ of eigenvectors of $\boldsymbol{D}$ such that the components of $\boldsymbol{c} := \boldsymbol{f} + \boldsymbol{V}\boldsymbol{n}$ in $\bar{\mathsf{G}}$ are $\sqrt{x}$. Let P denote the matrix of the passage from G to $\bar{\mathsf{G}}$ so that from the condition that both of them are bases of eigenvectors of $\boldsymbol{D}$ we have Eq. (4.8). Then $\mathsf{Q}(h^2, v^2)^{\mathrm{T}} P$ realizes the passage from $\bar{\mathsf{G}}$ to E and hence the components of $\boldsymbol{c}$ in E are $\mathsf{Q}(h^2, v^2)^{\mathrm{T}} P\sqrt{x}$ which gives Eq. (4.7). Conversely, let there be a basis E of eigenvectors of $\boldsymbol{V}$ special with respect to $\boldsymbol{n}$ such that the components of $\boldsymbol{f}$ are given as in (1). Then $\mathsf{G} = \mathsf{Q}(h^2, v^2)\mathsf{E}$ is a basis of eigenvectors of $\boldsymbol{D}$. In G, $\boldsymbol{D}$ is represented by diag (h^2) and $\boldsymbol{f}$ by $-\mathsf{Q}(h^2, v^2)Vn + P\sqrt{x}$. Then $\boldsymbol{G}\boldsymbol{G}^{\mathrm{T}}$ as in (4.6) is represented by $\operatorname{diag}(h^2) + P\sqrt{x}\otimes P\sqrt{x}$ and in the basis $P\mathsf{G}$ by $\operatorname{diag}(h^2) + \sqrt{x}\otimes\sqrt{x}$. The latter is a symmetric rank 1 perturbation of $\operatorname{diag}(h^2)$ with the spectrum w^2.

(2): In the basis of eigenvectors of $\boldsymbol{G}\boldsymbol{G}^{\mathrm{T}}$, $\sqrt{\boldsymbol{G}\boldsymbol{G}^{\mathrm{T}}}$ is represented by $\operatorname{diag}(w)$ and the matrix S realizes the passage from the basis of eigenvectors of $\boldsymbol{G}\boldsymbol{G}^{\mathrm{T}}$ to E, which proves Eq. (4.9). The rest is just a calculation based on $R = H^{-1}G$ and $K = R^{\mathrm{T}}HR$. □

Remark 4.4. *In the situation and notation of Theorem* 4.3, *let* $\boldsymbol{G}$ *have the singular values w. Then*

(1) *there exists a* $\delta \in \{-1, 1\}$ *such that* $Pe_n = \delta e_n$ *and in the basis* E, *either all components of n are nonnegative or nonpositive. In the first case,* $\operatorname{sgn}\det\boldsymbol{G} = \delta$; *in the second,* $\operatorname{sgn}\det\boldsymbol{G} = -\delta$;

(2) *we have*

$$R = H^{-1}V(I - n \otimes n) + \eta \frac{v_1 \dots v_n}{w_1 \dots w_n} HV^{-1} n \otimes n, \quad \eta = \operatorname{sgn} \det \boldsymbol{G}. \tag{4.11}$$

Proof. (1) the assertion $Pe_n = \delta e_n$ follows from Eq. (4.8) and the fact that $h_n = 0$ is a simple eigenvalue of $\boldsymbol{D}$. Let us prove the assertion about the components of $\boldsymbol{n}$. Since $\mathsf{Q}(h^2, v^2)^{\mathrm{T}}$ realizes the passage from the basis of eigenvectors of $\boldsymbol{V}$ to the basis of eigenvectors of $\boldsymbol{D}$ and $\boldsymbol{V}^{-1}\boldsymbol{n}/|\boldsymbol{V}^{-1}\boldsymbol{n}|$ is an eigenvector of $\boldsymbol{D}$ corresponding to the simple eigenvalue $h_n = 0$, we have

$$\mathsf{Q}(h^2, v^2)V^{-1}n/|V^{-1}n| = \gamma e_n \tag{4.12}$$

for some $\gamma \in \{-1, 1\}$; then $n = \gamma |V^{-1}n| V \mathsf{Q}(h^2, v^2)^{\mathrm{T}} e_n$, i.e.,

$$n_i = \gamma |V^{-1}n| v_i \mathsf{Q}(h^2, v^2)_{ni},$$

and it suffices to recall (see Remark 3.6(1)) that the last row of $\mathsf{Q}(h^2, v^2)$ is nonnegative. The assertion about the sign of determinant of $\boldsymbol{G}$: By Eq. (4.7), we have

$$\det \boldsymbol{G} = \det \boldsymbol{V}(1 + \boldsymbol{V}^{-1}\boldsymbol{f} \otimes \boldsymbol{n}) = \det \boldsymbol{V}\left[\mathsf{Q}(h^2, v^2)^{\mathrm{T}} P\sqrt{x} \cdot V^{-1}n\right],$$

and thus from Eq. (4.12) and $Pe_n = \delta e_n$,

$$\det \boldsymbol{G} / \det \boldsymbol{V} = \left[\sqrt{x} \cdot P^{\mathrm{T}} \mathsf{Q}(h^2, v^2)V^{-1}n\right] = \gamma\,\delta\,|V^{-1}n|\,\sqrt{x_n}.$$

Hence $\gamma\delta$ determines the sign of the determinant of $\boldsymbol{G}$.

(2) To prove Eq. (4.11), note that

$$\boldsymbol{f} + \boldsymbol{V}\boldsymbol{n} = \eta \frac{v_1 \dots v_n}{w_1 \dots w_n} \boldsymbol{G}\boldsymbol{G}^{\mathrm{T}} \boldsymbol{V}^{-1}\boldsymbol{n}. \tag{4.13}$$

Indeed, applying $\boldsymbol{V}^{-1}\boldsymbol{n}$ to Eq. (4.6) we obtain $(\boldsymbol{f} + \boldsymbol{V}\boldsymbol{n})(\boldsymbol{f} \cdot \boldsymbol{V}^{-1}\boldsymbol{n} + 1) = \boldsymbol{G}\boldsymbol{G}^{\mathrm{T}}\boldsymbol{V}^{-1}\boldsymbol{n}$ and from $\det \boldsymbol{G} = \det \boldsymbol{V}(\boldsymbol{f} \cdot \boldsymbol{V}^{-1}\boldsymbol{n} + 1)$, further, $\boldsymbol{f} \cdot \boldsymbol{V}^{-1}\boldsymbol{n} + 1 = \eta w_1 \dots w_n / v_1 \dots v_n$. Comparing Eq. (4.13) with Eq. (4.7) one sees that

$$\mathsf{Q}(h^2, v^2)^{\mathrm{T}} P\sqrt{x} = \eta \frac{v_1 \dots v_n}{w_1 \dots w_n} GG^{\mathrm{T}} V^{-1} n = \eta \frac{v_1 \dots v_n}{w_1 \dots w_n} H^2 V^{-1} n$$

and Eq. (4.10) reduces to Eq. (4.11). □

Remark 4.5. *Let v have distinct components, $\boldsymbol{n} \in \mathsf{Sph}$, and let E be any basis of eigenvectors. Then the components of $\boldsymbol{n}$ in E are all nonzero if and only if the components of h are distinct and*

$$h_i \neq v_j, \quad 1 \leqslant i, j \leqslant n. \tag{4.14}$$

If these conditions are satisfied then the components of $\bar{x}$ and $\bar{y}$ are all positive. Moreover, there are exactly two bases of eigenvectors of $\boldsymbol{V}$ special with respect to $\boldsymbol{n}$: that in which all components of $\boldsymbol{n}$ are positive and that in which all components of $\boldsymbol{n}$ are negative.

Proof. Assume that the components of $\boldsymbol{n}$ in E are all nonzero. By Remark 3.4, there is a basis E_0 of eigenvectors of $\boldsymbol{V}$ such that the components of $\boldsymbol{V}\boldsymbol{n}$ are $\sqrt{\bar{y}}$. Since $\boldsymbol{V}$ has a nondegenerate spectrum, the passage from E to E_0 is realized by a diagonal matrix $\operatorname{diag}(\omega)$, $\omega \in \{-1, 1\}^n$, and thus $\sqrt{\bar{y}} = \operatorname{diag}(\omega)\operatorname{diag}(v)n \neq 0$ where n are the components of $\boldsymbol{n}$ in E. Hence all the components of $\bar{y}$ are positive. Eq. (2.9) then shows that Eq. (4.14) holds. Proposition 3.5(1) says that also all components of $\bar{x}$ are positive. Proposition 2.1(2) then says that all $i \in \{1, \dots, n\}$ are the beginnings of an interval of constancy of h^2 which proves that the components of h are distinct. The converse implications are proved similarly. To show that there are exactly two bases of eigenvectors of $\boldsymbol{V}$ special with respect to $\boldsymbol{n}$ let $\mathsf{E}_1, \mathsf{E}_2$ be special bases, and let

$$\mathsf{G}_\alpha := \mathsf{Q}(h^2, v^2)^{\mathrm{T}} \mathsf{E}_\alpha, \quad \alpha = 1, 2, \tag{4.15}$$

so that these are the bases of eigenvectors of $\boldsymbol{D}$. Since the spectra of $\boldsymbol{V}$ and $\boldsymbol{D}$ have distinct components, we have $\mathsf{E}_2 = \mathrm{diag}(\eta)\mathsf{E}_1$, $\mathsf{G}_2 = \mathrm{diag}(\sigma)\mathsf{G}_1$ for some $\eta, \sigma \in \{-1, 1\}^n$ and Eq. (4.15) provides

$$\mathrm{diag}(\sigma)\mathsf{Q}(h^2, v^2)^{\mathrm{T}} = \mathsf{Q}(h^2, v^2)^{\mathrm{T}}\,\mathrm{diag}(\eta), \quad \text{i.e.,} \ \ (\sigma_i - \eta_j)\mathsf{Q}(h^2, v^2)^{\mathrm{T}}_{ij} = 0. \tag{4.16}$$

Combining Eq. (3.4) with the fact that $\bar{x}, \bar{y}$ have all components strictly positive, one finds that $\mathsf{Q}(h^2, v^2)^{\mathrm{T}}_{ij} \neq 0$ for all i, j and hence Eq. (4.16) implies $\sigma_i = \eta_j$. This implies that η is constant, i.e., either $\eta = (1, \ldots, 1)$ or $\eta = (-1, \ldots, -1)$, i.e. either $\mathsf{E}_1 = \mathsf{E}_2$ or $\mathsf{E}_1 = -\mathsf{E}_2$. □

Proposition 4.6. *In the situation of Theorem 4.3, assume additionally that v has distinct components and let E be any basis of eigenvectors of $\boldsymbol{V}$. If all components of $\boldsymbol{n}$ in E are nonzero then $\boldsymbol{G}$ has the singular values w if and only if h^2, w^2 satisfy the interlacing inequalities and there exist an $\omega \in \{-1, 1\}^n$ such that the components f of $\boldsymbol{f}$ in E are given by*

$$f_i = v_i n_i \left[\sum_{j=1}^{n} \frac{(-1)^{n-j}\omega_j \sqrt{p_{v^2}(h_j^2) p_{w^2}(h_j^2)}}{(v_i^2 - h_j^2) d_j(h^2)} - 1 \right], \tag{4.17}$$

where n are the components of $\boldsymbol{n}$ in E. Moreover, these satisfy

$$n_i = \tau_i v_i^{-1} \sqrt{-p_{h^2}(v_i^2)/d_i(v^2)} \tag{4.18}$$

with some $\tau \in \{-1, 1\}^n$. By Remark 4.5, the denominators in the last two formulas are nonzero.

Proof. By Remark 4.5, there is a basis E_0 special with respect to $\boldsymbol{n}$ in which the components of $\boldsymbol{n}$ are positive. Let us first prove Eq. (4.17) in this basis. By Eq. (4.7), we have to evaluate $\mathsf{Q}(h^2, v^2)^{\mathrm{T}} P \sqrt{x}$. By Remark 4.5, we have Eq. (4.14), the components of h are distinct, and $\bar{x}, \bar{y}$ have all components different from 0, and thus, we can use Eq. (3.6) to find

$$\mathsf{Q}(h^2, v^2)^{\mathrm{T}}_{ij} = \frac{1}{h_j^2 - v_i^2} \sqrt{-\frac{p_{h^2}(v_i^2) p_{v^2}(h_{j^2})}{d_i(v^2) d_j(h^2)}}, \qquad x_j = p_{w^2}(h_j^2)/d_j(h^2). \tag{4.19}$$

Moreover, Eq. (4.8) implies that $P = \mathrm{diag}(\omega)$ for some $\omega \in \{-1, 1\}^n$. Then,

$$\left(\mathsf{Q}(h^2, v^2)^{\mathrm{T}} P \sqrt{x}\right)_i = \sum_{j=1}^{n} \frac{(-1)^{n-j}\omega_j \sqrt{p_{v^2}(h_j^2) p_{w^2}(h_j^2)}}{(h_j^2 - v_i^2) d_j(h^2)} \sqrt{-p_{h^2}(v_i^2)/d_i(v^2)}, \tag{4.20}$$

where we have used that $(-1)^{n-j} d_j(h^2) > 0$. With our choice of itE_0, we have

$$v_i n_i = \sqrt{-p_{h^2}(v_i^2)/d_i(v^2)}, \tag{4.21}$$

which gives Eq. (4.18) with $\tau = (1, \ldots, 1)$; eliminating the second square root in Eq. (4.20) via Eq. (4.21) then provides Eq. (4.17). To prove Eq. (4.17) and (4.18) in an arbitrary basis itE, it suffices to note that i$tE = \mathrm{diag}(\tau)$itE_0 for some $\tau \in \{-1, 1\}^n$ and to transform the components in itE_0 into the components in itE. Under this operation, Eq. (4.17) remains invariant (with the same ω) while Eq. (4.18) takes the general form. □

Remark 4.7. Consider the situation of Proposition 4.6.

(1) Let $\boldsymbol{n}$ be fixed and $\omega, \bar{\omega} \in \{-1,1\}^n$. If Eq. (4.17) with ω and $\bar{\omega}$ gives the same f and $\omega_j \neq \bar{\omega}_j$ for some j then $h_j = w_i$ for some i; if

$$h_i \neq w_j, \quad 1 \leqslant i, j \leqslant n, \tag{4.22}$$

then ω as in Eq. (4.17) is uniquely determined by f and independent of the choice of the basis of eigenvectors of $\boldsymbol{V}$; moreover,

$$\operatorname{sgn} \det \boldsymbol{G} = \omega_n. \tag{4.23}$$

Thus, in contrast to τ as in Eq. (4.18), ω cannot be transformed out. The reader is referred to Section 6.2, where two different choices of ω distinguish between Type I and Type II twins. To prove these assertions, let us first show that ω is uniquely determined by f in a fixed basis. Write Eq. (4.17) with ω and with $\bar{\omega}$, then subtract the equations, and cancel the nonzero factor $v_i n_i$. What results is an equation of the form $C\xi = 0$, where C is the Cauchy matrix corresponding to h^2, v^2 and

$$\xi_j = \frac{(-1)^{n-j}(\omega_j - \bar{\omega}_j)\sqrt{p_{v^2}(h_j^2)p_{w^2}(h_j^2)}}{d_j(h^2)}.$$

Under the hypotheses of Proposition 4.6, C is nonsingular by Proposition 2.4, and hence $\xi = 0$. When combined with $p_{v^2}(h_j^2) \neq 0$ this gives $(\omega_j - \bar{\omega}_j)p_{w^2}(h_j^2) = 0$. Thus, if Eq. (4.22) holds, we have the uniqueness of ω in a fixed basis. Next, we invoke the independence of Eq. (4.17) of the basis of eigenvectors of $\boldsymbol{V}$ demonstrated in the proof of Proposition 4.6. To prove Eq. (4.23), we take a basis of eigenvectors of $\boldsymbol{V}$ in which the components of $\boldsymbol{n}$ are positive, use Remark 4.4(1) and note that $\delta = \omega_n$.

(2) Since the n-tuple h with $h_n = 0$ is a function of $\boldsymbol{n}$, we see from Eq. (4.17) that there are 2^n families of $\boldsymbol{f}$ leading to rank 1 perturbations $\boldsymbol{G}$ with the prescribed singular values. These families are distinguished by ω, and for each fixed ω, the family is parametrized by $\boldsymbol{n}$. Of these 2^n families, 2^{n-1} lead to $\boldsymbol{G}$ with positive determinant by Eq. (4.23). By (1), two families can intersect at those $\boldsymbol{n}$ for which some components of h coincide with some components of w. In Sections 5 and 6, we shall give more explicit expressions of $\boldsymbol{f}$ as functions of $\boldsymbol{n}$ when $n = 2$ or 3.

The following proposition gives a tensor form of the above results. Let $I_k(\boldsymbol{A})$ be the kth principal invariant of $\boldsymbol{A} \in \mathsf{Sym}$, i.e., $I_k(\boldsymbol{A}) = S^k(a)$, where a is the spectrum of $\boldsymbol{A}$, or equivalently, $I_k(\boldsymbol{A})$ is defined by the expansion

$$\det(\boldsymbol{A} - z\boldsymbol{1}) = \sum_{i=0}^{n} I_i(\boldsymbol{A})(-z)^{n-i}, \quad z \in \mathbb{R}. \tag{4.24}$$

Let $DI_k(\boldsymbol{A}) \in \mathsf{S}ym$ be the derivative of I_k with respect to $\boldsymbol{A}$. If we differentiate Eq. (4.24) with respect to $\boldsymbol{A}$, we obtain

$$\operatorname{cof}(\boldsymbol{A} - z\boldsymbol{1}) = \sum_{i=1}^{n} DI_i(\boldsymbol{A})(-z)^{n-i}, \tag{4.25}$$

and this expansion determines $DI_i(\boldsymbol{A})$ uniquely. In the basis of eigenvectors of $\boldsymbol{A}$, $DI_i(\boldsymbol{A})$ is represented by $\operatorname{diag}(\nabla S^k(a))$.

Proposition 4.8. *In the situation of Proposition* 4.6, *if* $\boldsymbol{G}$ *has the singular values* w, *then*

$$\boldsymbol{f} + \boldsymbol{V}\boldsymbol{n} = \sum_{i=1}^{n} g_i DI_i(\boldsymbol{V}^2)\boldsymbol{V}\boldsymbol{n}, \tag{4.26}$$

where

$$g_i = \sum_{j=1}^{n} \omega_j c_j (-h_j^2)^{n-i} / d_j(h^2), \quad c_j = \sqrt{p_{w^2}(h_j^2)/p_{v^2}(h_j^2)}.$$

Proof. Formula (4.17) can be written as

$$\boldsymbol{f} + \boldsymbol{V}\boldsymbol{n} = \sum_{j=1}^{n} \frac{\omega_j c_j}{d_j(h^2)} \operatorname{cof}(\boldsymbol{V}^2 - h_j^2 \mathbf{1}) \boldsymbol{V}\boldsymbol{n}. \tag{4.27}$$

Eliminating the cofactors from Eq. (4.27) via Eq. (4.25) provides Eq. (4.26). □

5. Dimension two

The purpose of this section is specialize the results of Section 4 to the case $n = 2$. Let $w \in \mathbb{D}^2 \cap \mathbb{R}^2_{++}$ satisfy the bilateral interlacing inequalities

$$w_1 \geqslant v_2, \quad v_1 \geqslant w_2,$$

and let us seek rank 1 perturbations of $\boldsymbol{V}$ with the singular values w.

5.1. General solutions

Let the eigenvalues of $\boldsymbol{V}$ be distinct and specialize the formulas of Proposition 4.8 assuming Eq. (4.14) to hold. We have $h = (h_1, h_2)$ where $h_2 = 0$ and write h for h_1. From Eq. (4.3),

$$h = |(\operatorname{cof} \boldsymbol{V})\boldsymbol{n}|, \tag{5.1}$$

and one finds that

$$g_1 = \omega_1 \gamma, \quad g_2 = \frac{1}{h^2}\left(\frac{w_1 w_2}{v_1 v_2}\omega_2 - \omega_1 \gamma\right), \qquad \gamma := c_1 = \sqrt{\frac{(w_1^2 - h^2)(w_2^2 - h^2)}{(v_1^2 - h^2)(v_2^2 - h^2)}},$$

and hence, from Eq. (4.26),

$$\boldsymbol{f} = \left(\omega_2 \frac{w_1 w_2}{v_1 v_2} - \omega_1 \gamma\right) \frac{\boldsymbol{V}^{-1}\boldsymbol{n}}{|\boldsymbol{V}^{-1}\boldsymbol{n}|^2} - (1 - \omega_1 \gamma)\boldsymbol{V}\boldsymbol{n}. \tag{5.2}$$

For a given $\boldsymbol{n}$, there exists an $\boldsymbol{f}$ such that $\boldsymbol{G}$ has the singular values w if and only if h^2, w^2 satisfy the interlacing inequalities which by Eq. (5.1) gives

$$w_2 \leqslant |\operatorname{cof} \boldsymbol{V}\boldsymbol{n}| \leqslant w_2. \tag{5.3}$$

Condition (4.14) holds if and only if $\boldsymbol{n}$ is not an eigenvector of $\boldsymbol{V}$. To summarize, for a given $\boldsymbol{n} \in \mathsf{Sph}$ there exists an $\boldsymbol{f} \in \mathsf{Vect}$ such that $\boldsymbol{V} + \boldsymbol{f} \otimes \boldsymbol{n}$ has the singular values w if and only if Eq. (5.3) holds; if this is the case, and $\boldsymbol{n}$ is not an eigenvector of $\boldsymbol{V}$, then $\boldsymbol{f}$ is given by Eq. (5.2) where $\omega_1, \omega_2 \in \{-1, 1\}$ are arbitrary. In the case $\det \boldsymbol{G} > 0$, i.e., $\omega_2 = 1$, the polar decomposition of $\boldsymbol{G}$ reads (Šilhavý, 1998; Dacorogna and Tanteri, 1998) $\boldsymbol{G} = \boldsymbol{H}\boldsymbol{R} = \boldsymbol{R}\boldsymbol{K}$ where

$$\boldsymbol{K} = \frac{1}{w_1 + w_2}(\boldsymbol{G}^{\mathrm{T}}\boldsymbol{G} + w_1 w_2 \mathbf{1}), \qquad \boldsymbol{H} = \frac{1}{w_1 + w_2}(\boldsymbol{G}\boldsymbol{G}^{\mathrm{T}} + w_1 w_2 \mathbf{1}),$$

$$\boldsymbol{R} = \frac{1}{w_1 + w_2}(\boldsymbol{V} + w_1 w_2 \boldsymbol{V}^{-1} + \boldsymbol{f} \otimes \boldsymbol{n} - v_1 v_2 \boldsymbol{V}^{-1}\boldsymbol{n} \otimes \boldsymbol{V}^{-1}\boldsymbol{f}).$$

5.2. Expressions in the basis of eigenvectors

Let $\boldsymbol{V}$ have distinct eigenvalues, let $\boldsymbol{n} \in \mathsf{Sph}$, $\boldsymbol{f} \in \mathsf{Vect}$, $w \in \mathbb{D}^2 \cap \mathbb{R}^2_{++}$, and let E be any basis of eigenvectors of $\boldsymbol{V}$. Then $\boldsymbol{G} := \boldsymbol{V} + \boldsymbol{f} \otimes \boldsymbol{n}$ has the singular values w and positive determinant if and only if Eq. (5.3) holds and the components of $\boldsymbol{f}$ in E are given by

$$f_1 = \frac{(w_1 w_2 v_2 - v_1 h^2)n_1 + \omega v_1 n_2 r}{h^2}, \qquad f_2 = \frac{(v_1 w_1 w_2 - v_2 h^2)n_2 - \omega v_2 n_1 r}{h^2} \tag{5.4}$$

with some $\omega \in \{-1, 1\}$ where $r = \sqrt{(w_1^2 - h^2)(h^2 - w_2)}$. If this condition holds then the rotation from the polar decomposition theorem is represented by the matrix

$$R = \begin{bmatrix} c_R & -s_R \\ s_R & c_R \end{bmatrix}, \text{ where } \begin{cases} c_R = \dfrac{\left(v_1 n_2^2 + v_2 n_1^2\right)(h^2 + w_1 w_2) + \omega(v_1 - v_2)n_1 n_2 r}{h^2(w_1 + w_2)}, \\ s_R = \dfrac{(v_1 - v_2)(h^2 + w_1 w_2)n_1 n_2 - \omega\left(v_1 n_2^2 + v_2 n_1^2\right)r}{h^2(w_1 + w_2)}. \end{cases} \tag{5.5}$$

If w has distinct components, then $\boldsymbol{G}\boldsymbol{G}^{\mathrm{T}}$ is represented by $\bar{S}\,\mathrm{diag}(w^2)\bar{S}$, where

$$\bar{S} = \begin{bmatrix} c_S & -s_S \\ s_S & c_S \end{bmatrix}, \quad \begin{cases} c_S = \dfrac{\omega v_2 w_2 n_1 \sqrt{w_1^2 - h^2} + v_1 w_1 n_2 \sqrt{h^2 - w_2^2}}{h^2 \sqrt{w_1^2 - w_2^2}}, \\ s_S = \dfrac{\omega v_1 w_2 n_2 \sqrt{w_1^2 - h^2} - w_1 v_2 n_1 \sqrt{h^2 - w_2^2}}{h^2 \sqrt{w_1^2 - w_2^2}}; \end{cases} \tag{5.6}$$

$\boldsymbol{G}$ is represented by $G = \bar{S}\,\mathrm{diag}(w)O$, where

$$O = \begin{bmatrix} c_O & -s_O, \\ s_O & c_O \end{bmatrix}, \tag{5.7a}$$

$$c_O = \frac{\omega n_1 \sqrt{w_1^2 - h^2} + n_2 \sqrt{h^2 - w_2^2}}{\sqrt{w_1^2 - w_2^2}}, \tag{5.7b}$$

$$s_O = \frac{n_1 \sqrt{h^2 - w_2^2} - \omega n_2 \sqrt{w_1^2 - h^2}}{\sqrt{w_1^2 - w_2^2}} \tag{5.7c}$$

and $\boldsymbol{H} = \sqrt{\boldsymbol{G}\boldsymbol{G}^{\mathrm{T}}}$ is represented by

$$H = \frac{1}{2}(w_1 + w_2)I + \frac{1}{2}(w_1 - w_2)\begin{bmatrix} \lambda & \mu \\ \mu & -\lambda \end{bmatrix}, \tag{5.8}$$

$$\lambda = \frac{\left[(w_1^2 + w_2^2)h^2 - 2w_1^2 w_2^2\right](v_1^2 n_2^2 - v_2^2 n_1^2) + 4\omega v_1 v_2 w_1 w_2 n_1 n_2 r}{h^4(w_1^2 - w_2^2)},$$

$$\mu = 2\frac{\omega w_1 w_2 (v_1^2 n_2^2 - v_2^2 n_1^2) r - v_1 v_2 n_1 n_2 \left[(w_1^2 + w_2^2)h^2 - 2w_1^2 w_2^2\right]}{h^4(w_1^2 - w_2^2)}.$$

Proof. Assume first that the components of w are distinct and that the components n_i of $\boldsymbol{n}$ are both nonzero in E. Then in some basis of eigenvectors of $\boldsymbol{V}$ the components of $\boldsymbol{n}$ are positive and let us first determine the objects in this basis. The amplitude can be calculated via Eq. (4.17), with $\omega_1 \in \{-1, 1\}$, $\omega_2 = 1$; if we write ω for ω_1, we obtain Eq. (5.4). Further, in the notation of Theorem 4.3, we have $P = \mathrm{diag}(\omega, 1)$, and the diagonalizing matrix from that theorem is $S = \mathsf{Q}(h^2, v^2)^{\mathrm{T}} P \mathsf{Q}(h^2, w^2)$. Using $n_1 > 0$, $n_2 > 0$, one finds from Eq. (3.6) that

$$\mathsf{Q}(h^2, v^2)^{\mathrm{T}} = \frac{1}{h}\begin{bmatrix} v_1 n_2 & v_2 n_1 \\ -v_2 n_1 & v_1 n_2 \end{bmatrix}, \quad \mathsf{Q}(h^2, w^2) = \frac{1}{h\sqrt{w_1^2 - w_2^2}}\begin{bmatrix} w_1\sqrt{h^2 - w_2^2} & -w_2\sqrt{w_1^2 - h^2} \\ w_2\sqrt{w_1^2 - h^2} & w_1\sqrt{h^2 - w_2^2} \end{bmatrix},$$

and a calculation gives

$$S = \begin{bmatrix} \omega c_S & -s_S \\ \omega s_S & c_S \end{bmatrix}, \tag{5.9}$$

where c_S, s_S are as above. If $\omega = -1$ then S is improper orthogonal and it is noted that then $\bar{S} := SP$ is a proper orthogonal diagonalizing matrix, i.e., $GG^{\mathrm{T}} = \bar{S}\,\mathrm{diag}(w^2)\bar{S}^{\mathrm{T}}$. From Eq. (5.9), we find that $\bar{S}$ is given by Eq. (5.6). To calculate $\boldsymbol{H}$, we use $H = \bar{S}\,\mathrm{diag}(w)\bar{S}^{\mathrm{T}}$ and note that

$$\mathrm{diag}(w) = w_+ I + w_- J \quad \text{where } J = \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}, \quad w_+ = \tfrac{1}{2}(w_1 + w_2), \quad w_- = \tfrac{1}{2}(w_1 - w_2)$$

to obtain

$$H = \bar{S}\,\mathrm{diag}(w)\bar{S}^{\mathrm{T}} = w_+ I + w_- \bar{S} J \bar{S}^{\mathrm{T}} = w_+ I + w_- \bar{S}^2 J \tag{5.10}$$

since $J\bar{S}^{\mathrm{T}} = \bar{S}J$. One finds that

$$\bar{S}^2 = \begin{bmatrix} \lambda & -\mu \\ \mu & \lambda \end{bmatrix}$$

and Eq. (5.10) leads to Eq. (5.8). We define $O := \bar{S}^{\mathrm{T}} R$ and note that with this definition $G = \bar{S}\,\mathrm{diag}(w) O$. In the notation Eq. (5.7a), we have

$$c_O = \bar{S}^{\mathrm{T}} R n \cdot n, \quad s_O = \bar{S}^{\mathrm{T}} R n \cdot n^{\perp} \quad \text{where } n^{\perp} = (-n_2, n_1). \tag{5.11}$$

Using Eqs. (4.10) and (3.5), one finds

$$m := \bar{S}^{\mathrm{T}} H^{-1} \mathsf{Q}(h^2, v^2)^{\mathrm{T}} P \sqrt{x} = \mathrm{diag}(w^{-1}) \bar{S}^{\mathrm{T}} \mathsf{Q}(h^2, v^2)^{\mathrm{T}} P \,\mathrm{diag}(w^{-1}) \sqrt{y}$$

and a calculation gives

$$m_1 = \omega\sqrt{\frac{w_1^2 - h^2}{w_1^2 - w_2^2}}, \qquad m_2 = \sqrt{\frac{h^2 - w_2^2}{w_1^2 - w_2^2}}.$$

A combination with Eq. (5.11) gives Eq. (5.7a). Then R is calculated as the product $R = \bar{S}O$ which leads to Eq. (5.5). Let us now consider an arbitrary basis E of eigenvectors of $\boldsymbol{V}$, let n_1, n_2 be the components of $\boldsymbol{n}$ in E and denote $\sigma_1 = \mathrm{sgn}\, n_1, \sigma_2 = \mathrm{sgn}\, n_2$. Then in the basis $\mathsf{E}_0 = \mathrm{diag}(\sigma)\mathsf{E}$ the components of $\boldsymbol{n}$ are $|n_1|, |n_2|$, and the above expressions with n_1, n_2 replaced by $|n_1|, |n_2|$ give the objects in E_0. These may be transformed back to E. It turns out that the expressions for f, R are still of the form (5.4) and (5.5) except that one has to redefine ω to be now $\omega\sigma_1\sigma_2$. On the contrary, $\bar{S}, O$ transform to $\sigma_2\bar{S}', \sigma_2 O'$ where $\bar{S}', O'$ are as in Eqs. (5.6) and (5.7a)–(5.7c) with the new ω. But then also $\bar{S}', O'$ provide $G = \bar{S}'\mathrm{diag}(w)O'$ in the basis E, and thus redefining $\bar{S}, O$ to be $\bar{S}', O'$ we have Eqs. (5.6) and (5.7a)–(5.7c). To summarize, we have proved the proposition under the additional restriction that the components of w are distinct and the components of $\boldsymbol{n}$ both different from 0. For the remaining cases, one has to use Theorem 4.3 and it is found that the results hold also in this case. □

As an illustration, let $\boldsymbol{V}$ have distinct eigenvalues and determine all $\boldsymbol{f}, \boldsymbol{n}, \boldsymbol{R} \in \mathsf{Orth}^+$ such that [6]

$$\boldsymbol{V} + \boldsymbol{f} \otimes \boldsymbol{n} = \boldsymbol{R}.$$

We apply Section 5.2 with $w = (1, 1)$. Condition (5.3) gives $h = 1$, and the interlacing inequalities for h^2, v^2 give that $v_1 \geqslant 1 \geqslant v_2$ which is a necessary and sufficient condition for the solution to exist. The case $v_1 = v_2$ being trivial, we assume $v_1 > v_2$. The equality $h = 1$ gives $v_1^2 n_2^2 + v_2^2 n_1^2 = 1$ from which

$$n_1 = \tau_1 \sqrt{\frac{v_1^2 - 1}{v_1^2 - v_2^2}}, \qquad n_2 = \tau_2 \sqrt{\frac{1 - v_2^2}{v_1^2 - v_2^2}}$$

for some $\tau_1, \tau_2 \in \{-1, 1\}$. Then formulas (5.4) reduce to

$$f_1 = -\tau_1 (v_1 - v_2) \sqrt{\frac{v_1^2 - 1}{v_1^2 - v_2^2}}, \qquad f_2 = \tau_2 (v_1 - v_2) \sqrt{\frac{1 - v_2^2}{v_1^2 - v_2^2}},$$

$$R = \begin{bmatrix} c_R & -s_R \\ s_R & c_R \end{bmatrix} \quad \text{where } c_R = \frac{1 + v_1 v_2}{v_1 + v_2}, \ s_R = \tau_1 \tau_2 \frac{\sqrt{(v_1^2 - 1)(1 - v_2^2)}}{v_1 + v_2}.$$

Thus, there are four solutions $\boldsymbol{n}, \boldsymbol{f}, \boldsymbol{R}$; however, only two of them are substantially different, since any solution $\boldsymbol{n}, \boldsymbol{f}, \boldsymbol{R}$ produces a new solution of the form $-\boldsymbol{n}, -\boldsymbol{f}, \boldsymbol{R}$. Note also that the factor ω has disappeared, the two families coincide and each of these families degenerate to a single point.

6. Dimension three

The purpose of this section is specialize the results of Section 4 to the case $n = 3$. Let $\boldsymbol{V}$ and $w \in \mathbb{D}^3 \cap \mathbb{R}^3_{++}$ be given. The bilateral interlacing inequalities read

$$w_1 \geqslant v_2, \quad v_1 \geqslant w_2 \geqslant v_3, \quad v_2 \geqslant w_3.$$

6.1. General solutions

We use Propositions 4.6 and 4.8 and assume that their hypotheses are satisfied. Formula (4.26) reads

$$\boldsymbol{f} = (g_1 + g_2 \operatorname{tr} \boldsymbol{V}^2 - 1) \boldsymbol{V}\boldsymbol{n} + g_2 \boldsymbol{V}^3 \boldsymbol{n} + \bar{g}_3 \frac{\boldsymbol{V}^{-1}\boldsymbol{n}}{|\boldsymbol{V}^{-1}\boldsymbol{n}|^2}, \tag{6.1}$$

where

$$g_1 = \frac{\omega_1 c_1 h_1^2 - \omega_2 c_2 h_2^2}{h_1^2 - h_2^2}, \qquad g_2 = -\frac{\omega_1 c_1 - \omega_2 c_2}{h_1^2 - h_2^2}, \qquad \bar{g}_3 = \frac{\omega_1 c_1 h_2^2 - \omega_2 c_2 h_1^2}{h_1^2 - h_2^2} + \frac{\omega_3 w_1 w_2 w_3}{v_1 v_2 v_3},$$

and

$$c_1 = \sqrt{p_{w^2}(h_1^2)/p_{v^2}(h_1^2)}, \qquad c_2 = \sqrt{p_{w^2}(h_2^2)/p_{v^2}(h_2^2)}.$$

The parameters h_1, h_2 can be calculated from $\boldsymbol{n}$ by

[6] Cf. Khachaturyan (1983, p. 176) and Ball and James (1987, Proposition 4).

$$h_1^2 + h_2^2 = \operatorname{tr} \boldsymbol{V}^2 - |\boldsymbol{Vn}|^2, \qquad h_1^2 h_2^2 = |\operatorname{cof} \boldsymbol{Vn}|^2,$$

which are obtained by taking the trace of Eq. (4.2) and by Eq. (4.3), respectively. Hence

$$h_{1,2}^2 = \frac{1}{2}\left[\operatorname{tr} \boldsymbol{V}^2 - |\boldsymbol{Vn}|^2 \pm \sqrt{(\operatorname{tr} \boldsymbol{V}^2 - |\boldsymbol{Vn}|^2)^2 - 4|\operatorname{cof} \boldsymbol{Vn}|^2}\right]. \tag{6.2}$$

Note that generally $\operatorname{tr} \boldsymbol{V}^2 - |\boldsymbol{Vn}|^2 \geqslant 2|\operatorname{cof} \boldsymbol{Vn}|$; thus Eq. (6.2) gives two nonnegative numbers, which, being the eigenvalues of $\boldsymbol{V}^2 - \boldsymbol{Vn} \otimes \boldsymbol{Vn}$, satisfy automatically $v_1 \geqslant h_1 \geqslant v_2 \geqslant h_2 \geqslant v_3$. Thus, for a given $\boldsymbol{n}$, there exists a $\boldsymbol{f} \in \mathsf{Vect}$ such that $\boldsymbol{G} = \boldsymbol{V} + \boldsymbol{f} \otimes \boldsymbol{n}$ has the singular values w if and only if h_1, h_2 given by Eq. (6.2) satisfy

$$w_1 \geqslant h_1 \geqslant w_2 \geqslant h_2 \geqslant w_3, \tag{6.3}$$

and if this is the case, then $\boldsymbol{f}$ is given by Eq. (6.1). For given $\boldsymbol{V}$ and w, the system of inequalities (6.3) determines a subset A of Sph of all possible $\boldsymbol{n}$ for which there exists an $\boldsymbol{f}$ such that $\boldsymbol{G}$ has the singular values w. Note also that Eq. (6.1) may be further simplified by eliminating $\boldsymbol{V}^3$ via the Cayley–Hamilton theorem.

6.2. Twinning

A tensor $\boldsymbol{G} \in \mathsf{Lin}$ with positive determinant is said to be a twin of $\boldsymbol{V}$ if $\boldsymbol{G}$ is a rank 1 perturbation of $\boldsymbol{V}$ and $\boldsymbol{G}$ has the same singular values as $\boldsymbol{V}$. Write $\boldsymbol{G} = \boldsymbol{V} + \boldsymbol{f} \otimes \boldsymbol{n}$. The basic assertion about twinning is that each twin is either type I twin or a type II twin, [7] where by definition the type I twin satisfies

$$\boldsymbol{f} = 2(\boldsymbol{V}^{-1}\boldsymbol{n}/|\boldsymbol{V}^{-1}\boldsymbol{n}|^2 - \boldsymbol{Vn}), \tag{6.4}$$

and type II twin satisfies

$$\boldsymbol{n} = 2(\boldsymbol{V}^{-1}\boldsymbol{f}/|\boldsymbol{V}^{-1}\boldsymbol{f}|^2 - \boldsymbol{Vf}/|\boldsymbol{f}|^2). \tag{6.5}$$

Moreover, the polar decomposition of $\boldsymbol{G}$ is $\boldsymbol{G} = \boldsymbol{HR}$, where

$$\boldsymbol{H} = \bar{\boldsymbol{S}}\boldsymbol{V}\bar{\boldsymbol{S}}^{\mathrm{T}}, \quad \boldsymbol{R} = \bar{\boldsymbol{S}}\bar{\boldsymbol{T}} \tag{6.6}$$

where the tensors $\bar{\boldsymbol{S}}, \bar{\boldsymbol{T}} \in \mathsf{Orth}^+$ may be chosen as 180° rotations:

$$\bar{\boldsymbol{S}} = 2\boldsymbol{o} \otimes \boldsymbol{o} - \boldsymbol{1}, \quad \bar{\boldsymbol{T}} = 2\boldsymbol{h} \otimes \boldsymbol{h} - \boldsymbol{1}, \quad \bar{\boldsymbol{S}}^2 = \bar{\boldsymbol{T}}^2 = \boldsymbol{1}, \tag{6.7}$$

where the axes of rotation are determined as follows:

for a type I twin $\quad \boldsymbol{o} = \boldsymbol{V}^{-1}\boldsymbol{n}/|\boldsymbol{V}^{-1}\boldsymbol{n}|, \quad \boldsymbol{h} = \boldsymbol{n};$
for a type II twin $\quad \boldsymbol{o} = \boldsymbol{f}/|\boldsymbol{f}|, \quad \boldsymbol{h} = \boldsymbol{V}^{-1}\boldsymbol{f}/|\boldsymbol{V}^{-1}\boldsymbol{f}|.$

Let us derive these assertions by using the general solution, under the assumption that $\boldsymbol{V}$ has distinct eigenvalues and condition (4.14) holds. In the present case $w = v$. Let us use the basis E of eigenvectors of $\boldsymbol{V}$ in which the components of $\boldsymbol{n}$ are nonnegative. Denoting $Q = \mathsf{Q}(h^2, v^2)$, $P = \operatorname{diag}(\omega)$, the diagonalizing matrix S from Theorem 4.3 is found to be

$$S = Q \operatorname{diag}(\omega) Q^{\mathrm{T}}, \quad \text{hence,} \quad S = S^{\mathrm{T}}, \quad S^2 = I.$$

Since Q realizes the passage from E to the basis of eigenvectors of $\boldsymbol{D}$, in E, $\boldsymbol{D}$ is represented by $D = Q \operatorname{diag}(h^2) Q^{\mathrm{T}}$ and from this

$$SDS^{\mathrm{T}} = QPQ^{\mathrm{T}}DQPQ^{\mathrm{T}} = QP \operatorname{diag}(h^2) PQ^{\mathrm{T}} = Q \operatorname{diag}(h^2) Q^{\mathrm{T}} = D,$$

[7] Ericksen (1981, 1985) and Gurtin (1983).

i.e., S commutes with D. Moreover, $\det \boldsymbol{G} > 0$ gives (see Remark 4.7(1)) $\omega_3 = 1$. We have $x = \bar{x}$, $y = \bar{y}$ and $Vn = \sqrt{\bar{y}}$. Thus from Eq. (4.7), $f = -Vn + QP\sqrt{x} = -Vn + QPQ^{\mathrm{T}}Q\sqrt{\bar{x}} = -Vn + S\sqrt{\bar{y}} = -Vn + SVn$, and hence,

$$f = (S - I)Vn, \tag{6.8}$$

which implies

$$Sf = (S^2 - S)Vn = (I - S)f = -f. \tag{6.9}$$

Furthermore,

$$SV^{-1}n/|V^{-1}n| = Q\,\mathrm{diag}(\omega)Q^{\mathrm{T}}V^{-1}n/|V^{-1}n| = Q\,\mathrm{diag}(\omega)e_3 = Q\omega_3 e_3 = Qe_3 = V^{-1}n/|V^{-1}n|.$$

Thus, $f/|f|$ and $V^{-1}n/|V^{-1}n|$ are two normalized eigenvectors of the symmetric orthogonal matrix S corresponding to the eigenvalues $-1, 1$. Hence, the system $\{P_1, P_2, P_3\}$, where

$$P_2 := \frac{f \otimes f}{|f|^2}, \qquad P_3 := \frac{V^{-1}n \otimes V^{-1}n}{|V^{-1}n|^2}, \qquad P_1 := I - P_2 - P_3$$

is a complete system of eigenprojectors of S. Denoting the third eigenvalue of S by $\eta \in \{-1, 1\}$, we have

$$S = \eta P_1 - P_2 + P_3 = \eta I - (\eta + 1)\frac{f \otimes f}{|f|^2} + (1 - \eta)\frac{V^{-1}n \otimes V^{-1}n}{|V^{-1}n|^2}. \tag{6.10}$$

Using $Q\sqrt{x} = Q\sqrt{\bar{x}} = \sqrt{\bar{y}} = Vn$, Eq. (4.11) reduces to

$$R = S\left[V^{-1}S^{\mathrm{T}}V(I - n \otimes n) + n \otimes n\right]. \tag{6.11}$$

If $\eta = -1$, then by Eq. (6.10)

$$S = 2\frac{V^{-1}n \otimes V^{-1}n}{|V^{-1}n|^2} - I, \tag{6.12}$$

Eq. (6.8) leads to Eq. (6.4) and the resulting twin is type I. With Eq. (6.12), one finds that for type I twin, $S^{\mathrm{T}}V(I - n \otimes n) = V(n \otimes n - I)$ and thus by Eq. (6.11), $R = ST$ where $T = 2n \otimes n - I$; defining $\bar{S} = S, \bar{T} = T$, we have Eqs. (6.6) and (6.7) in this case. If $\eta = 1$ then by Eq. (6.10),

$$S = I - 2\frac{f \otimes f}{|f|^2},$$

S has a double eigenvalue 1 and a simple eigenvalue -1, with the corresponding eigenvector f. Since S commutes with D, the eigenvector f corresponding to the simple eigenvalue of S must also be an eigenvector of D, i.e.,

$$(V^2 - Vn \otimes Vn)f = \lambda f \tag{6.13}$$

for some $\lambda \in \mathbb{R}$. Multiplying Eq. (6.8) by f and using Eq. (6.9), one obtains $|f|^2 = -2f \cdot Vn$; hence,

$$V^2 f + \tfrac{1}{2}|f|^2 Vn = \lambda f, \tag{6.14}$$

moreover, from $\det \boldsymbol{G} = \det \boldsymbol{V}$ one obtains $f \cdot V^{-1}n = 0$. Multiplying Eq. (6.13) by $V^{-2}f$ and using the last two formulas one finds that $\lambda = |f|^2/|V^{-1}f|^2$. Inserting this value into Eq. (6.14) and rearranging, we obtain Eq. (6.5) and the resulting twin is type II. Further,

$$
\begin{aligned}
S^{\mathrm{T}} V(I - n \otimes n) &= V(1 - n \otimes n) - 2\frac{f \otimes Vf}{|f|^2} + 2(Vf \cdot n)\frac{f \otimes n}{|f|^2} \\
&= V(1 - n \otimes n) + f \otimes \left(n - 2V^{-1}f/|V^{-1}f|^2\right) - f \otimes n \text{ (by Eq. (6.5))} \\
&= V(1 - n \otimes n) - 2f \otimes V^{-1}f/|V^{-1}f|^2,
\end{aligned}
$$

and thus,

$$
R = ST \quad \text{where } T = I - 2\frac{V^{-1}f \otimes V^{-1}f}{|V^{-1}f|^2};
$$

defining $\bar{S} = -S$, $\bar{T} = -T$, we have Eqs. (6.6) and (6.7) in this case. Note also that for Type I twins, with the knowledge $\omega_1 = \omega_2 = -1, \omega_3$ formula (6.1) leads directly to Eq. (6.4). It suffices to note that $c_1 = c_2 = 1$, and hence $g_1 = -1$, $g_2 = 0$, $\bar{g}_3 = 2$.

Acknowledgements

This work was supported by Grant No. A2019603 of the AVČR. The support is gratefully acknowledged.

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