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EXTREME VALUES OF POISSON'S RATIO AND OTHER ENGINEERING MODULI IN ANISOTROPIC MATERIALS

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Conditions for a maximum or minimum of Poisson's ratio of anisotropic elastic materials are derived. For a uniaxial stress in the 1-direction and Poisson's ratio ν defined by the contraction in the 2-direction, the following three quantities vanish at a stationary value: s_{14}, $[2\nu s_{15} + s_{25}]$ and $[(2\nu - 1)s_{16} + s_{26}]$, where s_{IJ} are the components of the compliance tensor. Analogous conditions for stationary values of Young's modulus and the shear modulus are obtained, along with second derivatives of the three engineering moduli at the stationary values. The stationary conditions and the hessian matrices are presented in forms that are independent of the coordinates, which lead to simple search algorithms for extreme values. In each case the global extremes can be found by a simple search over the stretch direction $\mathbf{n}$ only. Simplifications for stretch directions in a plane of orthotropic symmetry are also presented, along with numerical examples for the extreme values of the three engineering constants in crystals of monoclinic symmetry.

1. Introduction

Poisson's ratio ν, Young's modulus E and the shear modulus G, collectively called the engineering moduli, are of fixed value in isotropic materials and related by $2G(1 + \nu) = E$. No such connection holds in anisotropic elastic solids, and all three become dependent upon the directions of stretch, lateral strain, and the shear directions. Hayes [1972] derived some universal relations between values for certain pairs of orthogonal directions. However, apart from cubic symmetry [Norris 2006b], there is no general formula for the directions and values associated with the largest and smallest values of the engineering moduli. The purpose of this paper is to provide systematic methods which can be used to find the extreme values of the engineering moduli in any type of anisotropy.

The problem of finding the extreme values of Young's modulus is the simplest since E depends only on a single direction of stretch. Numerical searching is practical and straightforward; thus Cazzani and Rovati provide a detailed analysis of the extrema of Young's modulus for cubic and transversely isotropic materials

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[Cazzani and Rovati 2003] and for materials with tetragonal symmetry [Cazzani and Rovati 2005], with extensive illustrative examples. Boulanger and Hayes [1995] obtained analytic expressions related to extrema of Young's modulus. For stretch in the 1-direction, they showed that $E = 1/s_{11}$ achieves a stationary value if the two conditions $s_{15} = 0$ and $s_{16} = 0$ are satisfied. In a pair of complementary papers, Ting derived explicit expressions for the stress directions and the stationary values of Young's modulus for triclinic and monoclinic [Ting 2005b], orthotropic, tetragonal, trigonal, hexagonal and cubic materials [Ting 2005a]. We will rederive the stationary conditions for E below, along with conditions required for a local maximum or minimum.

Poisson's ratio and the shear modulus depend upon pairs of orthogonal directions, which makes their classification far more complicated than for E. At the same time, there is considerable interest in anisotropic materials which exhibit negative values of Poisson's ratio, also called auxetic materials [Yang et al. 2004]. In sharp contrast to isotropic solids for which $-1 < \nu < 1/2$, the value of ν is unrestricted in anisotropic materials and may achieve arbitrarily large positive and negative values in the same material. The first hint of this surprising possibility was given by Boulanger and Hayes [1998] who presented a theoretical set of elastic moduli for a material with orthorhombic symmetry which satisfy the positivity requirements, but exhibit simultaneous arbitrarily large positive and negative values of ν. Ting and Chen [2005] and Ting [2004] subsequently demonstrated that the same remarkable phenomenon can be obtained in any nonisotropic material symmetry, including cubic symmetry and transverse isotropy. Further explanation of the effect in cubic symmetry is provided in Section 6 below and in [Norris 2006b]. We note that Rovati presented extensive numerical examples of auxetic behavior in orthorhombic [Rovati 2003] and monoclinic materials [Rovati 2004], while Ting and Barnett [2005] derived general conditions required for the occurrence of negative values of ν.

The purpose of this paper is to provide a general framework for finding the maximum and minimum values of ν and G in anisotropic materials. Some progress in this regard is due to Ting [2005a] who discusses the conditions for extreme values of the shear modulus with particular attention to shear in planes of material symmetry. As far as I know, there are no results reported to date on conditions necessary for extreme values of the Poisson's ratio. Particular attention is given in this paper to the Poisson's ratio, with the emphasis on deriving conditions that are independent of the coordinate system used. It will become evident that there is a strong analogy between the problems for the shear modulus and the Poisson's ratio. In particular, by formulating the problems in a coordinate free manner, the task of searching for extreme values of both is similar.

The outline of the paper is as follows. The three engineering moduli are introduced in Section 2, along with the equations for the transformation of elastic moduli under rotation. These are used in Section 3 to derive the conditions required for stationary values of ν, E and G, and the values of the second derivatives (Hessian) at the stationary points are determined in Section 4. The various results are all cast in terms of stretch, strain and shearing along coordinate axes. The more general format for stationary conditions in general directions, independent of the coordinates, are presented in Section 5. The specific application to Poisson's ratio is considered in Section 6. The stationary conditions for stretch in a plane of orthotropic symmetry are derived, and it is shown that at most four stationary values of ν can occur, two for in-plane lateral strain, and two out-of-plane. These results are applied to the specific case of extreme values of ν in materials with cubic symmetry, recovering results of [Norris 2006b]. Applications to generally anisotropic materials are also discussed, and a fast procedure for searching for extreme values of ν is derived and demonstrated for some materials of monoclinic symmetry. Finally, in Section 7 we present a similar procedure for finding the global extreme values of G in generally anisotropic media, with numerical examples.

2. Definition of the engineering moduli and preliminary equations

Poisson's ratio measures lateral strain in the presence of uniaxial stress. For any orthonormal pair of vectors $\{\mathbf{n}, \mathbf{m}\}$, the Poisson's ratio $\nu_{nm} = \nu(\mathbf{n}, \mathbf{m})$ is defined by the ratio of the strains in the two directions for a uniaxial state of stress along one of them [Rovati 2004]:

$$\nu_{nm} = -\frac{\boldsymbol{\varepsilon} : \mathbf{mm}}{\boldsymbol{\varepsilon} : \mathbf{nn}} \qquad \text{for } \boldsymbol{\sigma} = \sigma\, \mathbf{nn},$$

where $\boldsymbol{\varepsilon}$ and $\boldsymbol{\sigma}$ are the symmetric tensors of strain and stress, respectively, and $\mathbf{ab}$ is the tensor product, sometimes denoted $\mathbf{a} \otimes \mathbf{b}$. The Young's modulus $E_n = E(\mathbf{n})$ relates the axial strain and stress,

$$E_n = \frac{\sigma}{\boldsymbol{\varepsilon} : \mathbf{nn}} \qquad \text{for } \boldsymbol{\sigma} = \sigma\, \mathbf{nn}.$$

The third engineering modulus is the shear modulus $G_{nm} = G(\mathbf{n}, \mathbf{m})$,

$$G_{nm} = \frac{\sigma}{\boldsymbol{\varepsilon} : (\mathbf{nm} + \mathbf{mn})} \qquad \text{for } \boldsymbol{\sigma} = \sigma\, (\mathbf{nm} + \mathbf{mn}).$$

Tensor components are defined relative to the fixed orthonormal basis $\{\mathbf{e}_1, \mathbf{e}_2, \mathbf{e}_3\}$,

$$\boldsymbol{\sigma} = \sigma_{ij}\, \mathbf{e}_i \mathbf{e}_j, \qquad \boldsymbol{\varepsilon} = \varepsilon_{ij}\, \mathbf{e}_i \mathbf{e}_j.$$

The stress σ_{ij} and strain ε_{ij} are related by

$$\varepsilon_{ij} = s_{ijkl} \sigma_{kl}.$$

(Lower case Latin suffixes take on the values 1, 2, and 3, and the summation convention on repeated indices is assumed unless noted otherwise.) Here s_{ijkl} denote the components of the fourth order compliance tensor. We use the Voigt notation for conciseness; compliance is $\mathbf{S} = [s_{IJ}]$, $I, J = 1, 2, \ldots, 6$, with $I = 1, 2, 3, 4, 5, 6$ corresponding to $ij = 11, 22, 33, 23, 31, 12$, and $s_{JI} = s_{IJ}$.

The goal is to find conditions for a maximum or minimum of the engineering moduli, with emphasis on Poisson's ratio. With no loss in generality assume that $\mathbf{n}$ is in the $\mathbf{e}_1$ direction, and $\mathbf{m}$ is in the $\mathbf{e}_2$ direction. Thus, we consider $\nu \equiv \nu_{12}$, $E \equiv E_1$ and $G \equiv G_{12}$, that is,

$$\nu = -\frac{s_{12}}{s_{11}}, \qquad E = \frac{1}{s_{11}}, \qquad G = \frac{1}{4s_{66}}. \tag{1}$$

(We take $s_{66} = s_{1212}$ although it is common to subsume the factor of 4 in the definition of s_{66} in eq. $(1)_3$.) Our objective is then to find conditions for a maximum or minimum of each engineering modulus under the assumption that the material is assumed to be free to orient in arbitrary directions with oriented moduli while the stress remains of fixed orientation. This is equivalent to stationarity conditions for ν_{nm}, E_n and G_{nm} for a fixed orientation material while $\{\mathbf{n}, \mathbf{m}\}$ range over all possible orthonormal pairs.

We therefore need to consider how ν, E and G of (1) vary under general rotation of the material. Define the rotation by angle θ about an arbitrary direction $\mathbf{q}$, $|\mathbf{q}| = 1$, as $\mathbf{Q}(\mathbf{q}, \theta) \in O(3)$, such that vectors (including the basis vectors) transform as $\mathbf{r} \to \mathbf{r}' = \mathbf{Qr}$. Under the change of basis associated with $\mathbf{Q}(\mathbf{q}, \theta)$, second order tensors (including stress and strain) transform as $\boldsymbol{\sigma} \to \boldsymbol{\sigma}'$, where $\sigma'_{ij} = Q_{ir} Q_{js} \sigma_{rs}$, or

$$\sigma'_{ij} = \mathfrak{Q}_{ijrs} \sigma_{rs}, \qquad \text{where} \quad \mathfrak{Q}_{ijrs} = \tfrac{1}{2}\big(Q_{ir} Q_{js} + Q_{is} Q_{jr}\big).$$

In order to simplify the algebra we use the connection between fourth order elasticity tensors in 3 dimensions and second order symmetric tensor of 6 dimensions [Mehrabadi and Cowin 1990]. Accordingly, the 6×6 matrix $\widehat{\mathbf{S}}$ with elements $\widehat{S}_{IJ}$ is defined as

$$\widehat{\mathbf{S}} = \mathbf{TST}, \qquad \text{where } \mathbf{T} \equiv \operatorname{diag}\big(1,\ 1,\ 1,\ \sqrt{2},\ \sqrt{2},\ \sqrt{2}\big).$$

Rotation of second and fourth order tensors is most simply presented in terms of the 6×6 rotation matrix $\widehat{\mathbf{Q}}$ which is the 6-dimensional version of the fourth order tensor $\mathfrak{Q}_{ijrs}$, introduced by Mehrabadi et al. [1995]. Fourth order tensors transform as $\widehat{\mathbf{S}} \to \widehat{\mathbf{S}}' = \widehat{\mathbf{Q}}\widehat{\mathbf{S}}\widehat{\mathbf{Q}}^T$, where $\widehat{\mathbf{Q}}(\mathbf{q}, \theta)$ is an orthogonal second order tensor of six dimensions, satisfying $\widehat{\mathbf{Q}}\widehat{\mathbf{Q}}^T = \widehat{\mathbf{Q}}^T\widehat{\mathbf{Q}} = \widehat{\mathbf{I}}$ =diag(1, 1, 1, 1, 1, 1). It satisfies

$$\frac{\partial \widehat{\mathbf{Q}}}{\partial \theta}(\mathbf{q}, \theta) = \widehat{\mathbf{R}}(\mathbf{q})\widehat{\mathbf{Q}}, \qquad \widehat{\mathbf{Q}}(\mathbf{q}, 0) = \widehat{\mathbf{I}}, \tag{2}$$

where $\widehat{\mathbf{R}}$ is a skew symmetric six dimensional tensor linear in $\mathbf{q}$,

$$\widehat{\mathbf{R}}(\mathbf{q}) = \begin{pmatrix} 0 & 0 & 0 & 0 & \sqrt{2}q_2 & -\sqrt{2}q_3 \\ 0 & 0 & 0 & -\sqrt{2}q_1 & 0 & \sqrt{2}q_3 \\ 0 & 0 & 0 & \sqrt{2}q_1 & -\sqrt{2}q_2 & 0 \\ 0 & \sqrt{2}q_1 & -\sqrt{2}q_1 & 0 & q_3 & -q_2 \\ -\sqrt{2}q_2 & 0 & \sqrt{2}q_2 & -q_3 & 0 & q_1 \\ \sqrt{2}q_3 & -\sqrt{2}q_3 & 0 & q_2 & -q_1 & 0 \end{pmatrix}.$$

Further details can be found in [Mehrabadi et al. 1995; Norris 2006a].

3. Extremal conditions

Consider any one of the engineering moduli, say f, as a function of both the underlying compliance and of the rotation $\widehat{\mathbf{Q}}$. A stationary value is obtained if f is unchanged with respect to additional small rotations. In order to formulate this more precisely, assume f is at a stationary point, and define

$$\widehat{\mathbf{S}}(\mathbf{q}, \theta) = \widehat{\mathbf{Q}}(\mathbf{q}, \theta)\widehat{\mathbf{S}}\widehat{\mathbf{Q}}^T(\mathbf{q}, \theta). \tag{3}$$

Define the rotational derivative,

$$f'(\mathbf{q}) \equiv \frac{\partial f}{\partial \theta}\big(\widehat{\mathbf{S}}(\mathbf{q}, \theta)\big)\Big|_{\theta=0} = \frac{\partial f}{\partial s_{IJ}}\, s'_{IJ}(\mathbf{q}). \tag{4}$$

The elements $s'_{IJ}(\mathbf{q})$ of the the rotational derivative of the compliance can be expressed by using the representation (2) with (3),

$$\widehat{\mathbf{S}}' = \widehat{\mathbf{R}}(\mathbf{q})\widehat{\mathbf{S}} + \widehat{\mathbf{S}}\widehat{\mathbf{R}}^T(\mathbf{q}). \tag{5}$$

Thus, we have the equality given on top of page 798, where the s_{IJ} are the values at $\theta = 0$ (which are independent of $\mathbf{q}$) and the derivatives are linear functions of the coordinates of $\mathbf{q}$. We may write

$$f'(\mathbf{q}) = \mathbf{d}^{(f)} \cdot \mathbf{q}, \tag{6}$$

where the vector $\mathbf{d}^{(f)}$ is independent of $\mathbf{q}$ and depends only on the compliances.

The engineering modulus f is stationary with respect to the direction $\mathbf{n}$, and the direction $\mathbf{m}$ where applicable, if $f'(\mathbf{q})$ vanishes for *all* axes of rotation $\mathbf{q}$. This is equivalent to requiring that all possible deviations in $\mathbf{n}$ and $\mathbf{m}$ leave f unchanged to first order in the rotation. The stipulation that this hold for all rotation axes covers all permissible transformations. The general condition for stationarity is therefore that the vector $\mathbf{d}^{(f)}$ must vanish, that is,

$$\mathbf{d}^{(f)} = 0 \quad \text{at a stationary point of } f.$$

$$\begin{pmatrix} s'_{11} \\ s'_{22} \\ s'_{33} \\ s'_{12} \\ s'_{23} \\ s'_{13} \\ s'_{14} \\ s'_{25} \\ s'_{36} \\ s'_{15} \\ s'_{16} \\ s'_{24} \\ s'_{26} \\ s'_{34} \\ s'_{35} \\ s'_{44} \\ s'_{55} \\ s'_{66} \\ s'_{45} \\ s'_{46} \\ s'_{56} \end{pmatrix} = \begin{pmatrix} 0 & 4s_{15} & -4s_{16} \\ -4s_{24} & 0 & 4s_{26} \\ 4s_{34} & -4s_{35} & 0 \\ -2s_{14} & 2s_{25} & 2s_{16}-2s_{26} \\ 2s_{24}-2s_{34} & -2s_{25} & 2s_{36} \\ 2s_{14} & 2s_{35}-2s_{15} & -2s_{36} \\ s_{12}-s_{13} & -s_{16}+2s_{45} & s_{15}-2s_{46} \\ s_{26}-2s_{45} & s_{23}-s_{12} & -s_{24}+2s_{56} \\ -s_{35}+2s_{46} & s_{34}-2s_{56} & s_{13}-s_{23} \\ s_{16} & -s_{11}+s_{13}+2s_{55} & -s_{14}-2s_{56} \\ -s_{15} & s_{14}+2s_{56} & s_{11}-s_{12}-2s_{66} \\ s_{22}-s_{23}-2s_{44} & -s_{26} & s_{25}+2s_{46} \\ -s_{25}-2s_{46} & s_{24} & -s_{22}+s_{12}+2s_{66} \\ -s_{33}+s_{23}+2s_{44} & -s_{36}-2s_{45} & s_{35} \\ s_{36}+2s_{45} & s_{33}-s_{13}-2s_{55} & -s_{34} \\ 2s_{24}-2s_{34} & -2s_{46} & 2s_{45} \\ 2s_{56} & 2s_{35}-2s_{15} & -2s_{45} \\ -2s_{56} & 2s_{46} & 2s_{16}-2s_{26} \\ s_{25}-s_{35}+s_{46} & -s_{14}+s_{34}-s_{56} & s_{55}-s_{44} \\ -s_{36}+s_{26}-s_{45} & s_{44}-s_{66} & s_{14}-s_{24}+s_{56} \\ s_{66}-s_{55} & s_{36}-s_{16}+s_{45} & -s_{25}+s_{15}-s_{46} \end{pmatrix} \begin{pmatrix} q_1 \\ q_2 \\ q_3 \end{pmatrix}.$$

We now apply this formalism to the three engineering moduli and derive $\mathbf{d}^{(\nu)}$, $\mathbf{d}^{(E)}$ and $\mathbf{d}^{(G)}$ in turn.

3.1. ***Poisson's ratio.*** For Poisson's ratio, Equation (4) becomes

$$\nu'(\mathbf{q}) = (s_{11})^{-2}\left[s_{12}\, s'_{11}(\mathbf{q}) - s_{11}\, s'_{12}(\mathbf{q})\right]. \tag{7}$$

Thus, from the display above and Equations (6) and (7), we have

$$\mathbf{d}^{(\nu)} = \frac{2}{s_{11}^2}\left[s_{11}s_{14}\mathbf{e}_1 + \big(2s_{12}s_{15} - s_{11}s_{25}\big)\mathbf{e}_2 + \big(s_{11}s_{26} - s_{11}s_{16} - 2s_{12}s_{16}\big)\mathbf{e}_3\right]. \tag{8}$$

Setting this to zero and using the definition of ν in (1), and the fact that $s_{11} > 0$, we obtain three conditions for a stationary value of Poisson's ratio:

$$s_{14} = 0, \qquad 2\nu s_{15} + s_{25} = 0, \qquad (2\nu - 1)s_{16} + s_{26} = 0. \tag{9}$$

These must be simultaneously satisfied at a maximum or minimum of ν. Note that the compliance elements appearing in (9) are all zero in isotropic materials.

3.2. ***Young's modulus.*** Proceeding in the same manner as for the Poisson's ratio, and using $E'(\mathbf{q}) = -(s_{11})^{-2} s'_{11}(\mathbf{q})$, gives

$$\mathbf{d}^{(E)} = 4(s_{11})^{-2}\,(-s_{15}\mathbf{e}_2 + s_{16}\mathbf{e}_3).$$

Setting this to zero implies the conditions for an extremum in Young's modulus

$$s_{15} = 0, \qquad s_{16} = 0. \tag{10}$$

These agree with two conditions determined by Boulanger and Hayes [1995] and by Ting [2005b].

3.3. ***Shear modulus.*** The rotational derivative of the shear modulus is

$$G'(\mathbf{q}) = -\tfrac{1}{4}(s_{66})^{-2} s'_{66}(\mathbf{q}),$$

and the gradient vector is

$$\mathbf{d}^{(G)} = \tfrac{1}{2}(s_{66})^{-2}\left[s_{56}\mathbf{e}_1 - s_{46}\mathbf{e}_2 + (s_{26} - s_{16})\mathbf{e}_3\right].$$

Hence, the shear modulus has an extreme value if the following conditions hold:

$$s_{56} = 0, \qquad s_{46} = 0, \qquad s_{16} - s_{26} = 0. \tag{11}$$

4. Second derivatives

The nature of a stationary value of the general engineering modulus f can be discerned, at least locally, by the second derivative. By analogy with Equation (4), we define the rotational second derivative,

$$f''(\mathbf{q}) \equiv \frac{\partial^2 f}{\partial s_{IJ}\,\partial s_{KL}}\, s'_{IJ}(\mathbf{q}) s'_{KL}(\mathbf{q}) + \frac{\partial f}{\partial s_{IJ}}\, s''_{IJ}(\mathbf{q}). \tag{12}$$

The elements $s''_{IJ}(\mathbf{q})$ of the rotational second derivative of the compliance follow from

$$\widehat{\mathbf{S}}''(\mathbf{q}) = \widehat{\mathbf{R}}^2\widehat{\mathbf{S}} + \widehat{\mathbf{S}}\widehat{\mathbf{R}}^{2T} + 2\widehat{\mathbf{R}}\widehat{\mathbf{S}}\widehat{\mathbf{R}}^T.$$

This is a direct consequence of Equation (5). We do not need all 21 elements, and for brevity only present the following three values which are necessary to evaluate the second derivatives of the engineering moduli,

$$s''_{11} = 4\big[(s_{13}-s_{11}+2s_{55})q_2^2+(s_{12}-s_{11}+2s_{66})q_3^2-2(s_{14}+2s_{56})q_2q_3 \\ +s_{15}q_3q_1+s_{16}q_1q_2\big],$$

$$s''_{12} = 2\big[(s_{13}-s_{12})q_1^2+(s_{23}-s_{12})q_2^2+(s_{11}+s_{22}-2s_{12}-4s_{66})q_3^2 \\ +(s_{14}-2s_{24}+4s_{56})q_2q_3+(s_{25}-2s_{15}+4s_{46})q_3q_1+(s_{16}+s_{26}-4s_{45})q_1q_2\big],$$

$$s''_{66} = 2\big[(s_{55}-s_{66})q_1^2+(s_{44}-s_{66})q_2^2+(s_{16}+s_{26}-2s_{36}-2s_{45})q_1q_2 \\ +(s_{11}+s_{22}-2s_{12}-4s_{66})q_3^2+(2s_{25}-2s_{15}+3s_{46})q_1q_3+(2s_{14}-2s_{24}+3s_{56})q_2q_3\big].$$

Before applying these to the three engineering moduli $f = \nu$, E and G, we note that in each case that f is a homogeneous function of degree 0 or -1 in the compliance elements. Consequently the second derivative f'' evaluated at the stationary point where $f' = 0$ simplifies because the first term in (12) vanishes, leaving

$$f''(\mathbf{q}) = \frac{\partial f}{\partial s_{IJ}}\, s''_{IJ}(\mathbf{q}) \qquad \text{at } f'(\mathbf{q}) = 0. \tag{13}$$

The terms $s''_{IJ}(\mathbf{q})$ are second order in $\mathbf{q}$, and we can write

$$f''(\mathbf{q}) = \mathbf{D}^{(f)} : \mathbf{qq} \qquad \text{at } f'(\mathbf{q}) = 0,$$

where $\mathbf{D}^{(f)} = \mathbf{D}^{(f)T}$ is a nondimensional symmetric 3×3 matrix which is independent of $\mathbf{q}$. Thus, $\mathbf{D}^{(f)}$ is positive (negative) semidefinite at a local minimum (maximum) of f. The condition for a local minimum (maximum) is therefore that the three eigenvalues of $\mathbf{D}^{(f)}$ are positive (negative). If the matrix is not definite and has eigenvalues of opposite sign, then the modulus has a locally saddle shaped behavior.

4.1. ***Poisson's ratio.*** The second derivative of the Poisson's ratio at a stationary point is, using (13),

$$\nu''(\mathbf{q}) = -(s_{11})^{-1}\left(s''_{12} + \nu s''_{11}\right) \qquad \text{at } \nu'(\mathbf{q}) = 0. \tag{14}$$

Thus, when $\nu'(\mathbf{q}) = 0$, Equation (14) gives

$$\nu''(\mathbf{q}) = \frac{2}{s_{11}^2}\Big\{s_{11}(s_{12}-s_{13})q_1^2 + \big[s_{11}(s_{12}-s_{13}) + 2s_{12}(s_{13}-s_{11}+2s_{55})\big]q_2^2 \\ + \big[s_{11}(2s_{12}+4s_{66}-s_{11}-s_{22}) + 2s_{12}(s_{12}-s_{11}+2s_{66})\big]q_3^2 \\ + 2\big[s_{11}(s_{24}-2s_{56}-\tfrac{1}{2}s_{14}) - 2s_{12}(s_{14}+2s_{56})\big]q_2q_3 \\ + 2\big[s_{11}(s_{15}-2s_{46}-\tfrac{1}{2}s_{25}) + s_{12}s_{15}\big]q_3q_1 \\ + 2\big[s_{11}(2s_{45}-\tfrac{1}{2}s_{16}-\tfrac{1}{2}s_{26}) + s_{12}s_{16}\big]q_1q_2\Big\}.$$

Since this is evaluated at the stationary value, we may use (9) to simplify and obtain

$$\mathbf{D}^{(\nu)} = \frac{2}{s_{11}} \begin{pmatrix} s_{12}-s_{13} & 2s_{45}-s_{16} & s_{15}-2s_{46} \\ 2s_{45}-s_{16} & \begin{array}{l} s_{12}-s_{13}- \\ \quad 2\nu(s_{13}-s_{11}+2s_{55}) \end{array} & s_{24}-2(1-2\nu)s_{56} \\ s_{15}-2s_{46} & s_{24}-2(1-2\nu)s_{56} & \begin{array}{l} s_{12}-s_{22}+2s_{66}+ \\ \quad (1-2\nu)(s_{12}-s_{11}+2s_{66}) \end{array} \end{pmatrix}, \quad (15)$$

where we have used the definition of ν to simplify the elements.

4.2. ***Young's modulus.*** At a stationary point we have $E''(\mathbf{q}) = -(s_{11})^{-2}\, s''_{11}$ and $E'(\mathbf{q}) = 0$. Using the extremal (10), we find

$$\mathbf{D}^{(E)} = \frac{1}{s_{11}^2} \begin{pmatrix} 0 & 0 & 0 \\ 0 & s_{11}-s_{13}-2s_{55} & s_{14}+2s_{56} \\ 0 & s_{14}+2s_{56} & s_{11}-s_{12}-2s_{66} \end{pmatrix}.$$

Note that $\mathbf{D}^{(E)}$ is rank deficient (of rank 2), which is a consequence of the fact that E is invariant under rotation about the $\mathbf{e}_1$ stretch axis. The local nature of the stationary value depends upon the two nonzero eigenvalues of the matrix.

4.3. ***Shear modulus.*** The shear modulus satisfies

$$G''(\mathbf{q}) = -\tfrac{1}{4}(s_{66})^{-2}\, s''_{66} \qquad \text{at } G'(\mathbf{q}) = 0,$$

and hence,

$$\mathbf{D}^{(G)} = \frac{1}{2s_{66}^2} \begin{pmatrix} s_{66}-s_{55} & s_{36}-s_{16}+s_{45} & s_{15}-s_{25} \\ s_{36}-s_{16}+s_{45} & s_{66}-s_{44} & s_{24}-s_{14} \\ s_{15}-s_{25} & s_{24}-s_{14} & 2s_{12}+4s_{66}-s_{11}-s_{22} \end{pmatrix}.$$

5. Coordinate invariant formulation

In this section we rephrase the results for the stationary conditions and for the second derivatives at the stationary conditions in coordinate invariant form. Let $\{\mathbf{n}, \mathbf{m}, \mathbf{p}\}$ be an orthonormal triad analogous to $\{\mathbf{e}_1, \mathbf{e}_2, \mathbf{e}_3\}$ before. Define the nondimensional symmetric second order tensors $\mathbf{A}$, $\mathbf{B}$, $\mathbf{C}$, $\mathbf{N}$, $\mathbf{M}$ and $\mathbf{P}$ by

$$A_{ij} = s_{nn}^{-1} s_{ijkl} n_k n_l, \qquad B_{ij} = s_{nn}^{-1} s_{ijkl} m_k m_l, \qquad C_{ij} = s_{nn}^{-1} s_{ijkl} p_k p_l,$$
$$N_{ij} = s_{nn}^{-1} s_{ikjl} n_k n_l, \qquad M_{ij} = s_{nn}^{-1} s_{ikjl} m_k m_l, \qquad P_{ij} = s_{nn}^{-1} s_{ikjl} p_k p_l,$$

where $s_{nn} = s_{ijkl} n_i n_j n_k n_l$. Thus,

$$\nu(\mathbf{n}, \mathbf{m}) = -\mathbf{A} : \mathbf{mm}, \qquad E(\mathbf{n}) = \frac{1}{s_{nn}}, \qquad G(\mathbf{n}, \mathbf{m}) = \frac{E(\mathbf{n})}{4\mathbf{N} : \mathbf{mm}}.$$

5.1. ***Poisson's ratio.*** The derivative of Poisson's ratio can be expressed in general form as

$$\mathbf{d}^{(\nu)} = \big[\mathbf{A} : (\mathbf{mp} + \mathbf{pm})\big]\mathbf{n} - \big[(2\nu\mathbf{A} + \mathbf{B}) : (\mathbf{pn} + \mathbf{np})\big]\mathbf{m} \\ + \big\{\big[(2\nu - 1)\mathbf{A} + \mathbf{B}\big] : (\mathbf{nm} + \mathbf{mn})\big\}\mathbf{p}, \quad (16)$$

which follows from (8), and may be checked by the substitutions $\mathbf{n} \to \mathbf{e}_1$, $\mathbf{m} \to \mathbf{e}_2$ and $\mathbf{p} \to \mathbf{e}_3$. This provides a local expansion of the Poisson's ratio for small rotation about the axis $\mathbf{q}$:

$$\nu(\mathbf{q}, \theta) = \nu(\mathbf{q}, 0) + \mathbf{d}^{(\nu)} \cdot \mathbf{q}\,\theta + \mathrm{O}(\theta^2).$$

In particular, $\mathbf{d}^{(\nu)} = 0$ at a stationary point.

The second order tensor $\mathbf{D}^{(\nu)}$ of (15) becomes, in general format,

$$\begin{aligned}\mathbf{D}^{(\nu)} = \big[\mathbf{A} : (\mathbf{mm} - \mathbf{pp})\big]\mathbf{nn} &+ \big\{\nu - [(1 + 2\nu)\mathbf{A} + 4\nu\mathbf{N}] : \mathbf{pp}\big\}\mathbf{mm} \\ &+ \big\{2\nu^2 - 1 + [4(1 - \nu)\mathbf{N} - \mathbf{M}] : \mathbf{mm}\big\}\mathbf{pp} \\ &+ \big[(2\mathbf{P} - \mathbf{N}) : (\mathbf{nm} + \mathbf{mn})\big]\tfrac{1}{2}(\mathbf{nm} + \mathbf{mn}) \\ &+ \big[(\mathbf{N} - 2\mathbf{M}) : (\mathbf{pn} + \mathbf{np})\big]\tfrac{1}{2}(\mathbf{pn} + \mathbf{np}) \\ &+ \big\{\big[\mathbf{M} - 2(1 - 2\nu)\mathbf{N}\big] : (\mathbf{mp} + \mathbf{pm})\big\}\tfrac{1}{2}(\mathbf{mp} + \mathbf{pm}). \end{aligned} \quad (17)$$

Hence, the local expansion near a stationary point is

$$\nu(\mathbf{q}, \theta) = \nu(\mathbf{q}, 0) + \tfrac{1}{2}\mathbf{D}^{(\nu)} : \mathbf{qq}\,\theta^2 + \mathrm{O}(\theta^3).$$

5.2. ***Young's modulus.*** In the same way as before we find that

$$\mathbf{d}^{(E)} = 2E(\mathbf{n})\big[-\mathbf{A} : (\mathbf{pn} + \mathbf{np})\,\mathbf{m} + \mathbf{B} : (\mathbf{nm} + \mathbf{mn})\,\mathbf{p}\big], \quad (18)$$

$$\mathbf{D}^{(E)} = E(\mathbf{n})\,\big\{\big[\mathbf{A} : (\mathbf{nn}{-}\mathbf{pp}) - 2\mathbf{P} : \mathbf{nn}\big]\,\mathbf{mm} + \big[\mathbf{A} : (\mathbf{nn}{-}\mathbf{mm}) - 2\mathbf{M} : \mathbf{nn}\big]\,\mathbf{pp} \\ + (\mathbf{A} + 2\mathbf{N}) : (\mathbf{mp}{+}\mathbf{pm})\tfrac{1}{2}(\mathbf{mp}{+}\mathbf{pm})\big\}. \quad (19)$$

5.3. ***Shear modulus.*** Similarly, for the shear modulus

$$\mathbf{d}^{(G)} = 4\frac{G^2(\mathbf{n})}{E(\mathbf{n})}\,\big[\mathbf{N} : (\mathbf{mp}{+}\mathbf{pm})\,\mathbf{n} - \mathbf{M} : (\mathbf{pn}{+}\mathbf{np})\,\mathbf{m} + (\mathbf{B}{-}\mathbf{A}) : (\mathbf{nm}{+}\mathbf{mn})\,\mathbf{p}\big] \quad (20)$$

$$\begin{aligned}\mathbf{D}^{(G)} = 8\frac{G^2(\mathbf{n})}{E(\mathbf{n})}\,\big\{&\mathbf{N} : (\mathbf{mm}{-}\mathbf{pp})\,\mathbf{nn} + \mathbf{M} : (\mathbf{nn}{-}\mathbf{pp})\,\mathbf{mm} + 4\mathbf{N} : \mathbf{mm}\,\mathbf{pp} \quad (21) \\ &+ (\mathbf{P}{+}\mathbf{C}{-}\mathbf{A}) : (\mathbf{nm}{+}\mathbf{mn})\tfrac{1}{2}(\mathbf{nm} + \mathbf{mn}) \\ &+ (\mathbf{A}{-}\mathbf{B}) : \big[(\mathbf{mm}{-}\mathbf{nn})\,\mathbf{pp} - (\mathbf{mp}{+}\mathbf{pm})\tfrac{1}{2}(\mathbf{mp}{+}\mathbf{pm}) + (\mathbf{pn}{+}\mathbf{np})\tfrac{1}{2}(\mathbf{pn}{+}\mathbf{np})\big]\big\}.\end{aligned}$$

6. Applications to Poisson's ratio

We now concentrate on general properties of the Poisson's ratio, applying the formalism for the stationary value to different situations. We begin with the general case of a plane of material symmetry in an orthotropic material.

6.1. ***Plane of symmetry in orthotropic material.*** We assume the stretch direction $\mathbf{n}$ lies in a plane of symmetry of an orthotropic material, and the direction of contraction $\mathbf{m}$ lies (a) perpendicular to the plane or (b) in the plane. This configuration includes all planes in hexagonal materials that contain the axis of symmetry, and therefore provides the stationary values of ν in materials with hexagonal symmetry (transverse isotropy).

With no loss in generality, let $\mathbf{e}_3^{(0)}$ be the normal to the plane of symmetry and let case (a) correspond to $\mathbf{m} = \mathbf{e}_3$ and case (b) corresponds to $\mathbf{m}$ in the plane of $\mathbf{e}_1^{(0)}, \mathbf{e}_2^{(0)}$. In both (a) and (b) $\mathbf{n}$ lies in the plane of $\mathbf{e}_1^{(0)}, \mathbf{e}_2^{(0)}$. Define the rotated axes

$$\mathbf{e}_1 = \cos\theta\, \mathbf{e}_1^{(0)} + \sin\theta\, \mathbf{e}_2^{(0)}, \qquad \mathbf{e}_2 = -\sin\theta\, \mathbf{e}_1^{(0)} + \cos\theta\, \mathbf{e}_2^{(0)}, \qquad \mathbf{e}_3 = \mathbf{e}_3^{(0)}.$$

Let S_{IJ} denote the compliances relative to the fixed set of axes $\{\mathbf{e}_1^{(0)}, \mathbf{e}_2^{(0)}, \mathbf{e}_3^{(0)}\}$, and s_{IJ} the compliances in the coordinates of the rotated axes. By definition of a symmetry plane, all coefficients s_{ijkl} with index 3 appearing once or thrice are zero. Then,

$$s_{11} = \frac{S_{11}S_{22} - S_0^2}{S_{11} + S_{22} - 2S_0} + \tfrac{1}{4}(S_{11} + S_{22} - 2S_0)\Big(\frac{S_{22} - S_{11}}{S_{11} + S_{22} - 2S_0} - \cos 2\theta\Big)^2, \tag{22}$$

$$s_{12} = S_{12} + \tfrac{1}{4}(S_{11} + S_{22} - 2S_0)\ \sin^2 2\theta, \tag{23}$$

$$s_{13} = \tfrac{1}{2}(S_{13} + S_{23}) - \tfrac{1}{2}(S_{23} - S_{13})\ \cos 2\theta, \tag{24}$$

$$s_{16} = \tfrac{1}{4}(S_{11} + S_{22} - 2S_0)\Big(\frac{S_{22} - S_{11}}{S_{11} + S_{22} - 2S_0} - \cos 2\theta\Big)\ \sin 2\theta, \tag{25}$$

$$s_{26} = \tfrac{1}{4}(S_{11} + S_{22} - 2S_0)\Big(\frac{S_{22} - S_{11}}{S_{11} + S_{22} - 2S_0} + \cos 2\theta\Big)\ \sin 2\theta, \tag{26}$$

$$s_{36} = \tfrac{1}{2}(S_{23} - S_{13})\ \sin 2\theta, \tag{27}$$

where $S_0 \equiv S_{12} + 2S_{66}$. Thus, in the two cases to be considered, we have $\mathbf{n} = \mathbf{e}_1$ and $s_{11} = 1/E(\theta)$.

Case (a): $\mathbf{m} = \mathbf{e}_3$ *perpendicular to the plane of symmetry.* We now consider stationary values of $\nu = \nu_{13}$, for which the three conditions for stationary ν are, instead of (9),

$$s_{14} = 0, \qquad 2\nu s_{16} + s_{36} = 0, \qquad (2\nu - 1)s_{15} + s_{35} = 0. \tag{28}$$

The first and last of these are automatically satisfied, based on the assumed material symmetry. Using s_{16} and s_{36} from (22)–(27), the second of (28) implies that

$\sin 2\theta = 0$, which is the exceptional case of prior symmetry, or that θ satisfies

$$\cos 2\theta = \frac{S_{22} - S_{11}}{S_{11} + S_{22} - 2S_0} + \frac{1}{\nu}\Big(\frac{S_{23} - S_{13}}{S_{11} + S_{22} - 2S_0}\Big).$$

Using this to eliminate $\cos 2\theta$ from the expression for $\nu = \nu_{13} = -s_{13}/s_{11}$ yields a quadratic equation for ν,

$$\nu^2 - \nu_a \nu - \tfrac{1}{4}\rho_a = 0,$$

where

$$\nu_a = \frac{(S_0 - S_{22})S_{13} + (S_0 - S_{11})S_{23}}{S_{11}S_{22} - S_0^2}, \qquad \rho_a = \frac{(S_{23} - S_{13})^2}{S_{11}S_{22} - S_0^2}.$$

Define E^* and θ^* by

$$E^* = \frac{S_{11} + S_{22} - 2S_0}{S_{11}S_{22} - S_0^2},$$

then we may identify E^* as the value of $E(\theta)$ when the second term on the RHS of (22) vanishes, that is, $E^* = E(\theta^*)$, where θ^* satisfies

$$\cos 2\theta^* = \frac{S_{22} - S_{11}}{S_{11} + S_{22} - 2S_0}. \tag{29}$$

The angle θ^* defines the direction at which E is stationary (maximum or minimum). It exists iff the RHS of (29) lies between -1 and 1. Regardless of whether or not the angle exists, it can be checked, $\nu_a = \nu_{13}(\theta^*) = -E^* s_{13}(\theta^*)$. The value of Young's modulus in the stretch direction θ for the stationary value of ν satisfies

$$\frac{E^*}{E} + \frac{\nu_a}{\nu} = 2.$$

In summary, the possible stationary values for stretch in the plane of symmetry and the strain measured in the direction perpendicular to the plane are

$$\nu_{a\pm} = \tfrac{1}{2}\nu_a \pm \tfrac{1}{2}\big(\nu_a^2 + \rho_a\big)^{1/2}, \tag{30}$$

and the stationary values occur if $-1 < \gamma_{a\pm} < 1$, where

$$\gamma_{a\pm} = \frac{S_{22} - S_{11}}{S_{11} + S_{22} - 2S_0} + \frac{1}{\nu_{a\pm}}\Big(\frac{S_{23} - S_{13}}{S_{11} + S_{22} - 2S_0}\Big),$$

in which case the direction of stretch is given by $\theta = \frac{1}{2}\cos^{-1}\gamma_{a\pm}$. Otherwise the stationary values occur at $\theta = 0$ and $\pi/2$.

Case (b): $\mathbf{m} = \mathbf{e}_2$ *in the plane of symmetry.* With $\mathbf{n} = \mathbf{e}_1$ again, conditions $(9)_1$ and $(9)_2$ are met and only $(9)_3$ is not automatically satisfied. Substituting the expressions for s_{16} and s_{26} from (22)–(27) into equation $(9)_3$ implies that either $\sin 2\theta = 0$, which is simply the axial case, or

$$\cos 2\theta = \frac{S_{22} - S_{11}}{S_{11} + S_{22} - 2S_0} + \frac{1}{\nu - 1}\left(\frac{S_{22} - S_{11}}{S_{11} + S_{22} - 2S_0}\right).$$

Substituting this into the relation for $\nu = \nu_{12}$, namely $\nu s_{nn} + s_{12} = 0$, and eliminating $\cos 2\theta$ produces a quadratic equation in ν. The equation is most simply expressed as a quadratic in the shifted Poisson's ratio $(\nu - 1)$:

$$(\nu - 1)^2 - (\nu_b - 1)(\nu - 1) - \tfrac{1}{4}\rho_b = 0,$$

where

$$\nu_b = -1 - E^*\big(S_{12} - S_0\big), \qquad \rho_b = \frac{(S_{11} - S_{22})^2}{S_{11}S_{22} - S_0^2}.$$

That is, $\nu_b = \nu_{12}(\theta^*) = -E^* s_{12}(\theta^*)$. Note that the value of Young's modulus E in the stretch direction θ satisfies

$$\frac{E^*}{E} + \frac{\nu_b - 1}{\nu - 1} = 2.$$

In summary, the possible stationary values for stretch and strain both in the plane of symmetry are

$$\nu_{b\pm} = \tfrac{1}{2}(\nu_b + 1) \pm \tfrac{1}{2}\big((\nu_b - 1)^2 + \rho_b\big)^{1/2}, \tag{31}$$

and the stationary values occur if $-1 < \gamma_{b\pm} < 1$, where

$$\gamma_{b\pm} = \frac{S_{22} - S_{11}}{S_{11} + S_{22} - 2S_0} + \frac{1}{\nu_{b\pm} - 1}\left(\frac{S_{22} - S_{11}}{S_{11} + S_{22} - 2S_0}\right),$$

in which case the direction of stretch is given by $\theta = \frac{1}{2}\cos^{-1}\gamma_{b\pm}$.

6.2. ***Example: cubic materials.*** The general coordinate invariant form of the compliance of a cubic material is [Walpole 1984]

$$\mathbf{S} = \left(\frac{1}{3\kappa} - \frac{1}{2\mu_2}\right)\mathbf{J} + \frac{1}{2\mu_1}\mathbf{I} + \left(\frac{1}{2\mu_2} - \frac{1}{2\mu_1}\right)\mathbf{D}, \tag{32}$$

where $\mathbf{I}$ and $\mathbf{J}$ are fourth order isotropic tensors, $I_{ijkl} = \frac{1}{2}(\delta_{ik}\delta_{jl} + \delta_{il}\delta_{jk})$, $J_{ijkl} = \frac{1}{3}\delta_{ij}\delta_{kl}$, and

$$\mathbf{D} = \mathbf{aaaa} + \mathbf{bbbb} + \mathbf{cccc}.$$

Here, the orthonormal triad $\{\mathbf{a},\ \mathbf{b},\ \mathbf{c}\}$ is coaxial with the cube axes. The condition that the elastic strain energy is always positive definite is that the three moduli κ, μ_1 and μ_2 are positive. We use, for simplicity, crystallographic-type notation for unit vectors, e.g., $pq\bar{r}$ where p, q and r are positive numbers, indicates the unit vector $(p\mathbf{a}+q\mathbf{b}-r\mathbf{c})/\sqrt{p^2+q^2+r^2}$.

We consider the stationary conditions (9) for stretch in the $\mathbf{e}_1$ direction and lateral strain in the $\mathbf{e}_2$ direction. Since s_{14}, s_{15}, s_{16}, s_{25} and s_{26} vanish for isotropic media, it follows that the only contribution to these quantities is from the tensor $\mathbf{D}$. We may therefore rewrite the stationary conditions (9) as

$$D_{14}=0, \qquad 2\nu D_{15}+D_{25}=0, \qquad (2\nu-1)D_{16}-D_{26}=0, \tag{33}$$

where $D_{14}=D_{1123}$, etc. The realm of stretch directions that needs to be considered may be reduced to those defining the irreducible $\frac{1}{48}$th of the surface of the unit sphere. This in turn is defined by $\frac{1}{48}$th of the surface of the cube (see figure), where the vertices of the triangle correspond to the directions 001, 110, and 111. In a separate paper [Norris 2006b] it is shown that the extreme values of ν do not occur within the interior of the triangle. It turns out that the extreme values are only possible for stretch direction $\mathbf{e}_1$ along 001, 110, or in certain cases, for $\mathbf{e}_1$ located along the edge between 110 and 111. In the case that $\mathbf{e}_1=001$, the lateral direction $\mathbf{e}_2$ may be any orthogonal direction, and when $\mathbf{e}_1=110$ the lateral directions are 001 or $1\bar{1}0$, each of which can correspond to the minimum or maximum for ν, depending on the elastic parameters κ, μ_1 and μ_2. It is clear from the symmetry of the situation that the quantities D_{14}, D_{15}, D_{16}, D_{25} and D_{26} vanish identically for $\mathbf{e}_1$ along 001 or 110 with $\mathbf{e}_2$ as described. A full description of the possible extreme values of ν in cubic materials is involved but complete, and we refer to [Norris 2006b] for details.

To summarize the findings of Norris [2006b] regarding solutions of Equations (33): all possible stretch directions which solve the three stationary conditions are confined to the symmetry plane with normal 110, and equivalent planes of

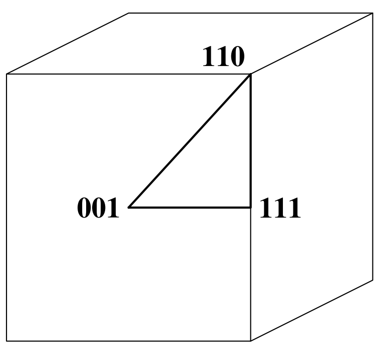

Figure 1. The irreducible $\frac{1}{48}$th of the cube surface is defined by the isosceles triangle with vertices as shown.

symmetry. We can therefore apply the results for a plane of orthotropic symmetry. Explicit calculation from (32) gives $S_{66} = (4\mu_1)^{-1}$, $S_{12} = S_{23} = (9\kappa)^{-1} - (6\mu_2)^{-1}$, $S_{13} = S_{12} + \chi/4$, $S_0 = S_{12} + 2S_{66}$, $S_{11} = S_0 + \chi/4$, $S_{22} = S_0 + \chi/2$, where $\chi = (\mu_2)^{-1} - (\mu_1)^{-1}$. Thus,

$$\nu_a = \nu_b = \nu_{111} \equiv \frac{3\kappa - 2\mu_1}{6\kappa + 2\mu_1}, \qquad \rho_a = \rho_b = \rho \equiv \tfrac{1}{6}(\nu_{111} + 1)\Big(\frac{\mu_1}{\mu_2} - 1\Big), \tag{34}$$

where $\nu_{111} = \nu(111, \mathbf{m})$ is the Poisson's ratio for stretch in the 111 direction, and is independent of the lateral direction $\mathbf{m}$.

The actual values of the possible extrema for ν can be obtained from equations and (30), (31) and (34). Skipping over the unedifying details, see [Norris 2006b], it can be shown that only the stationary values ν_{a-} and ν_{b+} are possible global extrema,

$$\nu_{a-} = \tfrac{1}{2}\nu_{111} - \tfrac{1}{2}\sqrt{\nu_{111}^2 + \rho}, \qquad \nu_{b+} = \tfrac{1}{2}\big(\nu_{111} + 1\big) + \tfrac{1}{2}\sqrt{\big(\nu_{111} - 1\big)^2 + \rho}.$$

Note that ν_{111} is independent of μ_2, which only enters these expressions via the term ρ. The extremely large values of Poisson's ratio discovered by Ting and Chen [2005] correspond to $\rho \gg 1$, which can occur if $\mu_2/\mu_1 \ll 1$. Under this circumstance ν_{a-} is large and negative, ν_{b+} is large and positive, and the magnitudes are, in principle, unbounded [Ting and Chen 2005; Ting and Barnett 2005; Norris 2006b].

The directions associated with the global extrema are given by

$$\cos 2\theta_{a-} = \tfrac{1}{3} - \frac{1}{3\nu_{a-}}, \qquad \cos 2\theta_{b+} = \tfrac{1}{3} + \frac{1}{3(\nu_{b+} - 1)}.$$

Both directions bifurcate from $\theta = 0$ [Norris 2006b], and therefore these extreme values only occur if $\nu < -\frac{1}{2}$ or $\nu > \frac{3}{2}$, respectively. A complete description of the extrema for all possible values of the elastic moduli is given by Norris [2006b].

6.3. ***Application to generally anisotropic materials.*** We first present a result that suggests a simple algorithm for searching for global extreme values of ν in generally anisotropic materials.

6.3.1. *A local min-max result for Poisson's ratio.* The tensor of second derivatives of $\nu(\mathbf{n}, \mathbf{m})$ at the stationary point $\mathbf{D}^{(\nu)}$ must be positive or negative definite in order that the stationary point be a minimum or a maximum, respectively. Consider a possible minimum, then a necessary although not sufficient condition is that the three diagonal elements of $\mathbf{D}^{(\nu)}$ are positive. In particular, Equation (17) gives

$$\mathbf{D}^{(\nu)} : \mathbf{nn} = \nu_{np} - \nu_{nm} \geq 0.$$

This implies that $\nu = \nu_{nm}$ must be strictly less than ν_{np}. At the same time, the stationary condition $\mathbf{d}^{(\nu)} = 0$ must hold, and in particular,

$$\mathbf{d}^{(\nu)} \cdot \mathbf{n} = 0 \qquad \Rightarrow \qquad \boldsymbol{\varepsilon} : \mathbf{mp} = 0 \qquad \text{for } \boldsymbol{\sigma} = \sigma\, \mathbf{nn}. \tag{35}$$

This implies that the shear strain ε_{mp} in the $\mathbf{m}$, $\mathbf{p}$-plane is zero. Hence, for any unit vector $\mathbf{r} \perp \mathbf{n}$, we have

$$\boldsymbol{\varepsilon} : \mathbf{rr} = (\mathbf{r} \cdot \mathbf{m})^2\, \varepsilon_{mm} + (\mathbf{r} \cdot \mathbf{p})^2\, \varepsilon_{pp},$$

or

$$\nu_{nr} = (\mathbf{r} \cdot \mathbf{m})^2\, \nu_{nm} + (\mathbf{r} \cdot \mathbf{p})^2\, \nu_{np} = \nu_{nm} + (\mathbf{r} \cdot \mathbf{p})^2 \left(\nu_{np} - \nu_{nm}\right) \geq \nu_{nm},$$

with equality only for $\mathbf{r} = \mathbf{m}$. Thus:

Lemma 1. *If ν_{nm} is a minimum* (*maximum*) *value*, *then it is also a minimum* (*maximum*) *among all possible ν_{nr} for* $\mathbf{r}$ *in the plane perpendicular to* $\mathbf{n}$.

This result is a direct consequence of the general expression for $\mathbf{D}^{(\nu)}$. It implies that if we can satisfy (35) then the values of ν_{nm} and ν_{np} are the extreme values for the given stretch direction $\mathbf{n}$. We next show how this single condition can be achieved.

6.3.2. *Satisfaction of one extremal condition.* The stationary values of Poisson's ratio occur, in general, for stretch directions at which the vector $\mathbf{d}^{(\nu)}$ of Equation (16) vanishes. We now show that one of the three components can be made to vanish; specifically, $\mathbf{d}^{(\nu)} \cdot \mathbf{n} = \mathbf{A} : (\mathbf{mp} + \mathbf{pm})$ is zero for an appropriate choice of the orthogonal directions $\mathbf{m}$ and $\mathbf{p}$.

We use the fact that the appropriate pair $\mathbf{m}$ and $\mathbf{p}$ correspond to stationary values of $\mathbf{A} : \mathbf{mm}$ and $\mathbf{A} : \mathbf{pp}$. These satisfy $\mathbf{A} : \mathbf{mm} + \mathbf{A} : \mathbf{pp} = \mathrm{tr}\mathbf{A} - 1$, so a maximum in one implies a minimum for the other. In order to find these directions for a given $\mathbf{n}$, consider the function of $\mathbf{m}$:

$$g(\mathbf{m}) \equiv \mathbf{A} : \mathbf{mm} - \lambda \mathbf{m} \cdot \mathbf{m} - 2\alpha \mathbf{m} \cdot \mathbf{n}.$$

Setting to zero the gradient with respect to $\mathbf{m}$ implies that $\mathbf{m}$ satisfies

$$\mathbf{m} = \alpha \left(\mathbf{A} - \lambda \mathbf{I}\right)^{-1} \mathbf{n}.$$

The scalars λ and α follow by requiring that $\mathbf{m} \cdot \mathbf{n} = 0$ and $\mathbf{m} \cdot \mathbf{m} = 1$, respectively. The former implies that λ satisfies

$$\mathbf{n} \cdot \left(\mathbf{A} - \lambda \mathbf{I}\right)^{-1} \mathbf{n} = 0.$$

This condition can be rewritten by expanding the inverse in terms of the cofactor matrix of $\left(\mathbf{A} - \lambda \mathbf{I}\right)$, and using the property $\mathbf{A} : \mathbf{nn} = 1$, which yields a quadratic in λ:

$$\lambda^2 + \lambda\left(1 - \mathrm{tr}\,\mathbf{A}\right) + \mathrm{adj}(\mathbf{A}) : \mathbf{nn} = 0. \tag{36}$$

Here adj($\mathbf{A}$) is the adjoint matrix. If $\mathbf{A}$ is invertible, then $\text{adj}(\mathbf{A}) = (\det\mathbf{A})\mathbf{A}^{-1}$, and more generally the adjoint is the transpose of the cofactor matrix. Thus for any type of anisotropy, and for any direction $\mathbf{n}$, it is a straightforward to determine the appropriate orthogonal pair $\mathbf{m}$, $\mathbf{p}$, which automatically give $\mathbf{d}^{(\nu)} \cdot \mathbf{n} = 0$. Finding the right axes requires solving the quadratic (36) for λ. The associated values of Poisson's ratio are the maximum and minimum for the given direction $\mathbf{n}$. In this way, finding extremal values of Poisson's ratio for all possible $\mathbf{n}$ is reduced to seeking values which satisfy the remaining two conditions:

$$(2\nu\mathbf{A} + \mathbf{B}) : \mathbf{np} = 0, \qquad \big[(2\nu - 1)\mathbf{A} + \mathbf{B}\big] : \mathbf{nm} = 0,$$

or equivalently, $2\nu s_{15} + s_{25} = 0$ and $(2\nu - 1)s_{16} + s_{26} = 0$, respectively. This is the strategy used to determine the global extrema of ν in materials with cubic symmetry [Norris 2006b].

6.3.3. *Algorithm for finding global extreme values of ν.* Rather than searching for directions $\mathbf{n}$ which satisfy the three stationary conditions on ν, Lemma 1 suggests that a simple search for maximum and minimum values of Poisson's ratio can be effected as follows. For a given $\mathbf{n}$ define the pair $\nu_\pm(\mathbf{n})$ by

$$\begin{aligned}
\nu_\pm(\mathbf{n}) &= -\mathbf{A} : \mathbf{m}_\pm^{(A)}\mathbf{m}_\pm^{(A)}, \\
\mathbf{m}_\pm^{(A)} &= \|\big(\mathbf{A} - \lambda_\pm^{(A)}\mathbf{I}\big)^{-1}\mathbf{n}\|^{-1}\,\big(\mathbf{A} - \lambda_\pm^{(A)}\mathbf{I}\big)^{-1}\mathbf{n}, \\
\lambda_\pm^{(A)} &= \tfrac{1}{2}\big(\operatorname{tr}\mathbf{A} - 1\big) \pm \tfrac{1}{2}\big[\big(\operatorname{tr}\mathbf{A} - 1\big)^2 - 4\,\text{adj}(\mathbf{A}) : \mathbf{nn}\big]^{1/2}.
\end{aligned}$$

The search for global extrema is then a matter of finding the largest and smallest values of $\nu_\pm(\mathbf{n})$ by searching over all possible directions $\mathbf{n}$. In practice, even for triclinic materials with no symmetry, the search only has to be performed over half of the unit sphere $\|\mathbf{n}\| = 1$, such as $\mathbf{n} \cdot \mathbf{e} \geq 0$ for some fixed direction $\mathbf{e}$. In this way, the numerical search is equivalent in complexity to that of finding the global extrema of Young's modulus.

This algorithm was applied to data for two crystals of monoclinic symmetry: Cesium dihydrogen phosphate and Lanthanum niobate, with the results in Table 1. The numerical results were obtained by using a 100×100 mesh for the hemisphere $\|\mathbf{n}\| = 1$, $\mathbf{n} \cdot \mathbf{e}_2 \geq 0$. It was found that the extreme values of the engineering moduli are not sensitive to the mesh size, although the values of the directions do change slightly.

7. Applications to the shear modulus

If we compare the vector derivative function for the shear modulus, $\mathbf{d}^{(G)}$ of (20), with $\mathbf{d}^{(\nu)}$ of (16), we note that the components in the $\mathbf{n}$ direction have a similar form, but with different matrices involved. Thus, it is $\mathbf{N}$ for $\mathbf{d}^{(G)} \cdot \mathbf{n}$, while for

Material	quantity	value	n_1	n_2	n_3
Cesium dihydrogen phosphate (CsH_2PO_4)	$E_{\max}$	19.3	0.44	0.76	0.47
	$E_{\min}$	0.53	0.99	0.00	0.06
	$G_{\max}$	12.2	0.42	0.71	−0.56
	$G_{\min}$	0.20	0.68	0.00	0.73
	$\nu_{\max}$	2.70	−0.23	0.82	0.52
	$\nu_{\min}$	−1.93	−0.49	0.85	−0.20
Lanthanum niobate ($LaNbO_4$)	$E_{\max}$	154.8	0.45	0.87	−0.21
	$E_{\min}$	2.27	−0.50	0.00	0.87
	$G_{\max}$	72.57	−0.28	0.71	−0.64
	$G_{\min}$	0.70	−0.96	0.00	0.27
	$\nu_{\max}$	3.95	0.00	1.00	0.00
	$\nu_{\min}$	-3.01	0.00	1.00	0.00

Table 2. Extreme values of E, G and ν for two materials of monoclinic symmetry with symmetry plane $n_2 = 0$. Units of E and G are GPa. Cesium dihydrogen phosphate: s_{11} = 1820.0, s_{22} = 103.0, s_{33} = 772.0, s_{44} = 33.25, s_{55} = 112.5, s_{66} = 29.25, s_{12} = −219.0, s_{13} = −1170.0, s_{23} = 138.0, s_{15} = 124.5, s_{25} = −75.0, s_{35} = −90.5, s_{46} = 8.25. Lanthanum niobate: s_{11} = 66.8, s_{22} = 14.8, s_{33} = 146.0, s_{44} = 5.7, s_{55} = 265.0, s_{66} = 4.675, s_{12} = 16.9, s_{13} = −94.8, s_{23} = −30.8, s_{15} = 118.0, s_{25} = 45.6, s_{35} = −186.5, s_{46} = 0.95. Units in $(\text{TPa})^{-1}$. (Data from Every and McCurdy [1992]).

$\mathbf{d}^{(\nu)} \cdot \mathbf{n}$ it is $\mathbf{A}$. The properties of the second derivatives $\mathbf{D}^{(G)} : \mathbf{nn}$ and $\mathbf{D}^{(\nu)} : \mathbf{nn}$ are similarly related. Proceeding with the same arguments as for the Poisson's ratio, we deduce:

Lemma 2. *If G_{nm} is a minimum* (*maximum*) *value*, *then it is also a minimum* (*maximum*) *among all possible G_{nr} for* $\mathbf{r}$ *in the plane perpendicular to* $\mathbf{n}$.

This in turn leads to a similar method for finding the global extrema of G.

7.1. ***Algorithm for finding global extreme values of G.*** Define the pair $G_\pm(\mathbf{n})$ by

$$
\begin{aligned}
G_\pm(\mathbf{n}) &= \frac{E(\mathbf{n})}{\mathbf{N} : \mathbf{m}_\pm^{(N)} \mathbf{m}_\pm^{(N)}}, \\
\mathbf{m}_\pm^{(N)} &= \left\| \left(\mathbf{N} - \lambda_\pm^{(N)} \mathbf{I}\right)^{-1} \mathbf{n} \right\|^{-1} \left(\mathbf{N} - \lambda_\pm^{(N)} \mathbf{I}\right)^{-1} \mathbf{n}, \\
\lambda_\pm^{(N)} &= \tfrac{1}{2}\left(\operatorname{tr} \mathbf{N} - 1\right) \pm \tfrac{1}{2}\left[\left(\operatorname{tr} \mathbf{N} - 1\right)^2 - 4 \operatorname{adj}(\mathbf{N}) : \mathbf{nn}\right]^{1/2}.
\end{aligned}
$$

Then the global extreme values of G can be found by searching over $\mathbf{n}$ only. Thus, the problem of finding the global extrema of the shear modulus is reduced to the same level of complexity as searching for the maximum and minimum Young's modulus. Table 1 summarizes the extreme values of G found using this algorithm for two crystals of monoclinic symmetry.

8. Conclusions

The results of this paper provide a consistent framework for determining the extreme values of the three engineering moduli in materials of any crystal symmetry or none. General conditions have been derived which must be satisfied at stationary values of ν, E and G. These are equations (9), (10) and (11), which have also been cast in forms that are independent of the coordinates used, in equations (16), (18) and (20), respectively. The associated three hessian matrices which determine the local nature of the stationary value, maximum, minimum or saddle, are given in equations (17), (19) and (21). The stationary conditions for Poisson's ratio simplify for stretch in a plane of orthotropic symmetry, for which there are at most 4 stationary values of ν. Two can occur for in-plane stretch and strain, and the other two for out-of-plane strain. This implies that transversely isotropic materials have at most four stationary values of Poisson's ratio. The results for the plane of symmetry also reproduce known results for cubic materials [Norris 2006b]. The hessian matrices for ν and G lead to algorithms for finding the extreme values. The key is to remove the dependence on the $\mathbf{m}$ direction by explicit representation of the maximum and minimum for a given $\mathbf{n}$ direction. The algorithms have been demonstrated by application to materials of low symmetry.

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