Spectral Analysis of Piezoelectric Tensors

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Abstract

A third order real tensor is called a piezoelectric-type tensor if it is partially symmetric with respect to its last two indices. The piezoelectric tensor is a piezoelectric-type tensor of dimension three. We introduce C-eigenvalues and C-eigenvectors for piezoelectric-type tensors. Here, “C” names after Curie brothers, who first discovered the piezoelectric effect. We show that C-eigenvalues always exist, they are invariant under orthonormal transformations, and for a piezoelectric-type tensor, the largest C-eigenvalue and its C-eigenvectors form the best rank-one piezoelectric-type approximation of that tensor. This means that for the piezoelectric tensor, its largest C-eigenvalue determines the highest piezoelectric coupling constant. We further show that for the piezoelectric tensor, the largest C-eigenvalue corresponds to the electric displacement vector with the largest 2-norm in the piezoelectric effect under unit uniaxial stress, and the strain tensor with the largest 2-norm in the converse piezoelectric effect under unit electric field vector. Thus, C-eigenvalues and C-eigenvectors have concrete physical meanings in piezoelectric effect and converse piezoelectric effect. Finally, we apply C-eigenvalues and associated C-eigenvectors for various piezoelectric crystals with different symmetries.

Key words. Piezoelectric tensor, piezoelectric effect, converse piezoelectric effect, eigenvalue, eigenvector, crystal.

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1 Introduction

Third order tensors have extensive applications in physics and engineering. Examples include piezoelectric tensors in crystal study \cite{2, 6, 11, 14, 15, 21}, third order symmetric traceless-tensors in liquid crystal study \cite{1, 5, 19} and third order susceptibility tensors in nonlinear optics study \cite{10, 12}. Among these third order tensors, the most popular one is the piezoelectric tensor, which plays the key role in piezoelectric effect and converse piezoelectric effect. Piezoelectricity was discovered by Jacques Curie and Pierre Curie in 1880 \cite{2}. In the next year, the converse piezoelectric effect was predicted by Lippmann \cite{13} and confirmed by Curies \cite{3} immediately. Now it has wide applications in the production and detection of sound, generation of high voltages, electronic frequency generation, microbalances, and ultra fine focusing of optical assemblies \cite{11}.

Eigenvalues of higher order tensors were introduced and studied in the recent years \cite{16, 17, 18}. Particularly, tensor eigenvalues were applied to third order symmetric traceless-tensors in liquid crystal study \cite{1, 5, 19}. Can we also apply tensor eigenvalues to piezoelectric tensors? We found that to make it physically meaningful, we may introduce some new eigenvalue definitions for piezoelectric tensors.

In the next section, we introduce C-eigenvalues and C-eigenvectors for piezoelectric-type tensors. Here, “C” names after Curie brothers. A third order real tensor is called a piezoelectric-type tensor if it is partially symmetric with respect to its last two indices. For solid materials, the last two indices of the piezoelectric tensor is symmetric since the stress tensor is symmetric. Thus, for solid materials, the piezoelectric tensor is a piezoelectric-type tensor of dimension three. This is not true for liquid crystal, where there is dissipation \cite{7, 8, 9}. We show that C-eigenvalues always exist, they are invariant under orthonormal transformations, and for a piezoelectric-type tensor, the largest C-eigenvalue and its C-eigenvectors form the best rank-one approximation of that tensor. This means that for the piezoelectric tensor, its largest C-eigenvalue determines the highest piezoelectric coupling constant.

In Section 3, we further show that for the piezoelectric tensor in solid crystal, the largest C-eigenvalue corresponds to the electric displacement vector with the largest 2-norm in the piezoelectric effect under unit uniaxial stress, and the strain tensor with the largest 2-norm in the converse piezoelectric effect under unit electric field vector. Thus, C-eigenvalues and C-eigenvectors have concrete physical meanings in piezoelectric effect and converse piezoelectric effect.

In Section 4, we compute C-eigenvalues and associated C-eigenvectors of typical piezoelectric tensors for various crystal classes.

Then, in Section 5, we show that the definition of C-eigenvalues for piezoelectric tensors is different from the definitions of matrix singular values if we look piezoelectric tensors as a $3 \times 6$ matrices \cite{15, 21}.

Our results are summarized in Section 6.

2 Spectral Analysis of Piezoelectric-Type Tensors

First, we introduce the definition of piezoelectric-type tensors.


Definition 2.1. Let $A = [a_{ijk}] \in \mathbb{R}^{n \times n \times n}$ be a third-order $n$ dimensional tensor. If the later two indices of $A$ are symmetric, i.e., $a_{ijk} = a_{ikj}$ for all $j$ and $k$, then $A$ is called a piezoelectric-type tensor.

Obviously, the number of independent elements of a piezoelectric-type tensor $A \in \mathbb{R}^{n \times n \times n}$ is $\frac{1}{2} n^2 (n+1)$. For $\alpha, \beta \in \mathbb{R}$ and $A = [a_{ijk}], B = [b_{ijk}] \in \mathbb{R}^{n \times n \times n}$, $\alpha A + \beta B = [\alpha a_{ijk} + \beta b_{ijk}] \in \mathbb{R}^{n \times n \times n}$. The inner product of $A$ and $B$ is $\langle A, B \rangle = \sum_{i,j,k} a_{ijk} b_{ijk}$. A nonnegative scalar $\|A\|_F = \sqrt{\langle A, A \rangle}$ is the Frobenius norm of $A$. For vectors $x \in \mathbb{R}^n$ and $y \in \mathbb{R}^n$, we denote a scalar $x A y^\top y = \sum_{i,j,k} a_{ijk} x_i y_j y_k \in \mathbb{R}$ as a product of the piezoelectric tensor $A$ with vectors $x$ and $y$. Moreover, we define $Ax y^\top y = \begin{pmatrix} \sum_{j,k} a_{ij} y_j y_k \\ \vdots \\ \sum_{j,k} a_{njk} y_j y_k \end{pmatrix} \in \mathbb{R}^n$ and $x A y = \begin{pmatrix} \sum_{i,j} x_i a_{ij} y_j \\ \vdots \\ \sum_{i,j} x_i a_{ijn} y_j \end{pmatrix} \in \mathbb{R}^n$.

Let $\lambda$ be a real number and $x, y \in \mathbb{R}^n$ be unit vectors, i.e., $x^\top x = 1$ and $y^\top y = 1$. Elements of a rank-one piezoelectric-type tensor $\lambda x \circ y \circ y \in \mathbb{R}^{n \times n \times n}$ are $[\lambda x \circ y \circ y]_{ijk} = \lambda x_i y_j y_k$ for $i, j, k = 1, 2, \ldots, n$. Here, "$\circ$" means the outer product. If a scalar $\lambda \in \mathbb{R}$ and vectors $x, y \in \mathbb{R}^n$ minimize the following optimization problem

$$\min \left\{ \|A - \lambda x \circ y \circ y\|_F^2 : \lambda \in \mathbb{R}, x^\top x = 1, y^\top y = 1 \right\},$$

then $\lambda x \circ y \circ y$ is called the best rank-one piezoelectric-type approximation of $A$.

Using these notations, we present the following definition of C-eigenvalues and C-eigenvectors of a piezoelectric tensor. Here, "C" names after Curie brothers.

Definition 2.2. Let $A \in \mathbb{R}^{n \times n \times n}$ be a piezoelectric-type tensor. If there exist a scalar $\lambda \in \mathbb{R}$, vectors $x \in \mathbb{R}^n$ and $y \in \mathbb{R}^n$ satisfying the following system

$$Ay y_{\top} y = \lambda x, \quad x A y = \lambda y, \quad x^\top x = 1, \quad \text{and} \quad y^\top y = 1,$$

then, $\lambda$ is called a C-eigenvalue of $A$, $x$ and $y$ are called associated left and right C-eigenvectors, respectively.

We have the following theorem.

Theorem 2.3. Let $A$ be a piezoelectric-type tensor. Then we have the following conclusions.

(a) There exist C-eigenvalues of $A$ and associated left and right C-eigenvectors.

(b) Suppose that $\lambda, x$ and $y$ are a C-eigenvalue and its associated left and right C-eigenvectors of $A$, respectively. Then

$$\lambda = x A y.$$
Furthermore, \((\lambda, x, -y), (-\lambda, -x, y), \) and \((-\lambda, -x, -y)\) are also C-eigenvalues and their associated C-eigenvectors of \(A\).

(c) Denote the largest C-eigenvalue of \(A\) and its associated left and right C-eigenvectors as \(\lambda^*, x^*\) and \(y^*\), respectively. Then

\[
\lambda^* = \max \{x^T A y : x^T x = 1, y^T y = 1\}.
\]

Furthermore, \(x^* y^* \circ y^*\) forms the best rank-one piezoelectric-type approximation of \(A\).

Proof. (a) We consider the following optimization problem

\[
\max \{x^T A y : x^T x = 1, y^T y = 1\}.
\]

On one hand, since the objective function \(x^T A y\) is continuous in variables \(x\) and \(y\) and the feasible region \(\{(x, y) \in \mathbb{R}^n \times \mathbb{R}^n : x^T x = 1, y^T y = 1\}\) is compact, there exist vectors \(x^*\) and \(y^*\) that solve (4) with the maximal objective value \(\lambda^*\).

On the other hand, we write the Lagrangian of (4):

\[
L(x, y, \mu_1, \mu_2) = -x^T A y + \frac{\mu_1}{2} (x^T x - 1) + \mu_2 (y^T y - 1).
\]

By the Lagrangian multiplier method, for the optimal solution \((x^*, y^*)\), there exist multipliers \(\mu_1^*\) and \(\mu_2^*\) such that

\[
\begin{align*}
\frac{\partial L}{\partial x} &= -A y^* + \mu_1^* x^* = 0, \\
\frac{\partial L}{\partial y} &= -2x^* A y^* + 2\mu_2^* y^* = 0, \\
\frac{\partial L}{\partial \mu_1} &= \frac{1}{2} (x^T x^* - 1) = 0, \\
\frac{\partial L}{\partial \mu_2} &= y^T y^* - 1 = 0.
\end{align*}
\]

By \(x^T x^* = y^T y^* = 1\), we have \(\mu_1^* = \mu_2^* = x^T A y^* y^* = \lambda^*\). Hence, \(\lambda^*, x^*\) and \(y^*\) satisfy (2) and hence a C-eigenvalue and its associated left and right C-eigenvectors of \(A\). This proves the existence.

(b) It is straightforward to verify the assertion (b).

(c) By some calculations, we find

\[
\|A - \lambda x \circ y \circ y\|_F^2 = \|A\|_F^2 - 2\lambda \langle A, x \circ y \circ y \rangle + \lambda^2 \|x\|^2 \|y\|^4.
\]

Minimizing this square-cost with respect to \(\lambda\), we get \(\lambda = \langle A, x \circ y \circ y \rangle\) because of \(\|x\| = \|y\| = 1\).

By substituting \(\lambda = \langle A, x \circ y \circ y \rangle\) to the square-cost, we have

\[
\|A - \lambda x \circ y \circ y\|_F^2 = \|A\|_F^2 - \langle A, x \circ y \circ y \rangle^2.
\]

Hence, there is a dual problem of (4) [20]:

\[
\max \{\langle A, x \circ y \circ y \rangle : x^T x = 1, y^T y = 1\}.
\]

Then, there exist vectors \(x^*\) and \(y^*\) such that

\[
\langle A, x^* \circ y^* \circ y^* \rangle = \max \{\langle A, x \circ y \circ y \rangle : x^T x = 1, y^T y = 1\}
\]

because a piezoelectric-type tensor \(A\) is partially symmetric with respect to the later two indices. This yields (4). Here, \(\langle A, x^* \circ y^* \circ y^* \rangle = x^T A y^* y^* = \lambda^*\) is the largest C-eigenvalue of \(A\), \(x^*\) and \(y^*\) are its associated left and right C-eigenvectors respectively. \(\square\)
By Theorem 2.3 (c), $\lambda^* \mathbf{x}^* \circ \mathbf{y}^* \circ \mathbf{y}^*$ forms the best rank-one piezoelectric type approximation of $\mathcal{A}$. This implies that for the piezoelectric tensor $\mathcal{A}$, its largest C-eigenvalue determines the highest piezoelectric coupling constant, and $\mathbf{y}^*$ is the corresponding direction of the stress where this appears. Thus, the largest C-eigenvalue of the piezoelectric tensor has concrete physical meaning. In the next section, we will further discuss its meanings.

Next, we show that C-eigenvalues of a piezoelectric-type tensor $A = [a_{ijk}]$ are invariant under orthogonal transformations. Let $Q \in \mathbb{R}^{n \times n}$ be an orthogonal matrix. We define a new tensor $AQ^3 \in \mathbb{R}^{n \times n \times n}$ in which elements are

$$[AQ^3]_{rst} = \sum_{i,j,k} a_{ijk}q_{ir}q_{js}q_{kt}$$

for $r, s, t = 1, 2, \ldots, n$. Obviously, $AQ^3$ is also a piezoelectric-type tensor.

**Theorem 2.4.** Suppose that $Q \in \mathbb{R}^{n \times n}$ is an orthogonal matrix. Let $\lambda$, $\mathbf{x}$ and $\mathbf{y}$ be a C-eigenvalue and its associated C-eigenvectors of a piezoelectric-type tensor $\mathcal{A} \in \mathbb{R}^{n \times n \times n}$. Then, $\lambda$, $Q^\top \mathbf{x}$ and $Q^\top \mathbf{y}$ are a C-eigenvalue and its associated C-eigenvectors of $AQ^3$.

**Proof.** We look at the $r$th component of a vector $(AQ^3)(Q^\top \mathbf{y})(Q^\top \mathbf{y})$:

$$[[AQ^3](Q^\top \mathbf{y})(Q^\top \mathbf{y})]_r = \sum_{s,t} [AQ^3]_{rst}[Q^\top \mathbf{y}]_s[Q^\top \mathbf{y}]_t$$

$$= \sum_{s,t} \left( \sum_{i,j,k} a_{ijk}q_{ir}q_{js}q_{kt} \right) \left( \sum_j q_{js}y_j \right) \left( \sum_k q_{kt}y_k \right)$$

$$= \sum_i q_{ir} \left( \sum_{j,k} a_{ijk} \left( \sum_j q_{js}y_j \right) \left( \sum_k q_{kt}y_k \right) \right)$$

$$= \sum_i q_{ir} \left( \sum_{j,k} a_{ijk} [QQ^\top \mathbf{y}]_j [QQ^\top \mathbf{y}]_k \right)$$

$$= \sum_i q_{ir} [\mathcal{A} \mathbf{y} \mathbf{y}]_i,$$

where the orthogonal matrix $Q$ satisfies $QQ^\top = I$. Then, we get $(AQ^3)(Q^\top \mathbf{y})(Q^\top \mathbf{y}) = Q^\top (A \mathbf{y} \mathbf{y})$. From $A \mathbf{y} \mathbf{y} = \lambda \mathbf{x}$, we immediately get an equation

$$(AQ^3)(Q^\top \mathbf{y})(Q^\top \mathbf{y}) = \lambda Q^\top \mathbf{x}.$$ 

Similarly, we have

$$(Q^\top \mathbf{x})(AQ^3)(Q^\top \mathbf{y}) = \lambda Q^\top \mathbf{y}. $$

In addition,

$$(Q^\top \mathbf{x})^\top (Q^\top \mathbf{x}) = (Q^\top \mathbf{y})^\top (Q^\top \mathbf{y}) = 1.$$

Hence, $\lambda$ is a C-eigenvalue of $AQ^3$, $Q^\top \mathbf{x}$ and $Q^\top \mathbf{y}$ are its associated C-eigenvectors. \qed
3 Applications in Piezoelectric Effect and Converse Piezoelectric Effect

In the last section, we showed that for the piezoelectric tensor, the largest C-eigenvalue of \( A \) determines the highest piezoelectric coupling constant, and \( y^* \) is the corresponding direction of the stress where this appears. We now further discuss its physical meanings.

For non-centrosymmetric materials, the linear piezoelectric equation is expressed as

\[
P_i = \sum_{j,k} a_{ijk} T_{jk},
\]

where \( A = [a_{ijk}] \in \mathbb{R}^{3 \times 3 \times 3} \) is a piezoelectric tensor, \( T \in \mathbb{R}^{3 \times 3} \) is the stress tensor, and \( P \) is the electric change density (polarization). Since \( A \) is a piezoelectric-type tensor, the last two indices of \( A \) are symmetric, i.e., \( a_{ijk} = a_{ikj} \) for all \( j \) and \( k \). Hence, there are 18 independent elements in \( A \).

What situations trigger the extreme piezoelectricity under unit uniaxial stress? An example of uniaxial stress is the stress in a long, vertical rod loaded by hanging a weight on the end [15, Page 90]. In this case, the stress tensor could be rewritten as \( T = yy^\top \) with \( y^\top y = 1 \). Then, we consider the following problem

\[
\begin{align*}
\max & \quad \|P\|_2 \\
\text{s.t.} & \quad P = Ayy, \\
& \quad y^\top y = 1.
\end{align*}
\]

Using a dual norm, we have \( \|P\|_2 = \max_{x^\top x = 1} x^\top P = \max_{x^\top x = 1} x^\top Ayy \). Hence, it suffices to consider the optimization problem

\[
\begin{align*}
\max & \quad x^\top Ayy \\
\text{s.t.} & \quad x^\top x = 1, \quad y^\top y = 1.
\end{align*}
\]

We denote \((x^*, y^*)\) as the optimal solution of the above optimization problem. Then, \( \lambda^* = x^* A y^* \) is the largest C-eigenvalue of the piezoelectric tensor \( A \), and \( y^* \) is the unit uniaxial direction that the extreme piezoelectric effect along took place. Then we have the following theorem.

**Theorem 3.1.** Suppose that \( \lambda^* \), \( x^* \) and \( y^* \) are the largest C-eigenvalue and its associated C-eigenvectors of the piezoelectric tensor \( A \). Then, \( \lambda^* \) is the maximum value of the 2-norm of the electric polarization under a unit uniaxial stress along direction \( y^* \).

The linear equation for the converse piezoelectric effect is

\[
S_{jk} = \sum_i a_{ijk} E_i,
\]

where \( S \) is the strain tensor and \( E \) is the electric field strength. Let \( \| \cdot \|_2 \) be the matrix spectral
norm, i.e., \( \|S\|_2 = \max_{y^\top y = 1} y^\top Sy \). Now, we maximize the spectral norm of \( S \):

\[
\begin{align*}
\max & \quad \|S\|_2 \\
\text{s.t.} & \quad S_{jk} = \sum_{i=1}^{3} E_i a_{ijk} \quad \forall j, k \in \{1, 2, 3\}, \\
& \quad \|E\| = 1.
\end{align*}
\]

(8)

Since \( \|S\|_2 = \max_{y^\top y = 1} y^\top Sy = \max_{y^\top y = 1} EAyy \), we rewrite (8) as follows

\[
\max \{EAyy : E^\top E = 1, y^\top y = 1\}.
\]

We denote \((E^*, y^*)\) as the optimal solution of the above optimization problem. Then, \( \lambda^* = E^* A y^* \) is the largest C-eigenvalue of \( A \), \( E^* \) and \( y^* \) are its associated left and right C-eigenvectors.

**Theorem 3.2.** Suppose that \( \lambda^*, x^* \) and \( y^* \) are the largest C-eigenvalue and its associated C-eigenvectors of the piezoelectric tensor \( A \). Then, \( \lambda^* \) is the largest spectral norm of a strain tensor generated by the converse piezoelectric effect under unit electric field strength \( \|x^*\| = 1 \).

### 4 C-Eigenvalues for Piezoelectric Tensors

Owing to the crystallographic symmetry of materials, there are 32 classes in crystals [6]. However, for 11 classes in crystals possessing the center of symmetry, piezoelectricity vanishes. For the class 432, piezoelectric changes cancel each other. Hence, piezoelectricity may exist in the remaining 20 crystallographic classes. We examine some typical crystals in these classes in this section.

By Theorem 2.3 (b), we know that \((-\lambda, -x, y), (\lambda, x, -y), \) and \((-\lambda, -x, -y)\) are C-eigenvalues and associated C-eigenvectors of a piezoelectric tensor if \((\lambda, x, y)\) are C-eigenvalue and associated C-eigenvectors of the piezoelectric tensor. In this section, we use \((\lambda, x, y)\) to present a group of these four C-eigenvalues and associated C-eigenvectors of the piezoelectric tensor for compactness.

Piezoelectric tensors of crystals have special structures owing to the symmetry. First, we consider crystals in 23 and 43m crystallographic point groups. There is only one independent parameter in the corresponding piezoelectric tensor \( A(\alpha) \):

\[
a_{123} = a_{213} = a_{312} = -\alpha,
\]

where \( \alpha \neq 0 \). Other elements of \( A(\alpha) \) are zeros. Then, we have the following proposition.

**Proposition 4.1.** There are 13 groups of C-eigenvalues and associated C-eigenvectors of \( A(\alpha) \).
Proof. We solve the polynomial system (2) for $\mathcal{A}(\alpha)$:

\[
\begin{align*}
-2\alpha y_2 y_3 &= \lambda x_1, \quad (9a) \\
-2\alpha y_1 y_3 &= \lambda x_2, \quad (9b) \\
-2\alpha y_1 y_2 &= \lambda x_3, \quad (9c) \\
-\alpha x_2 y_3 - \alpha x_3 y_2 &= \lambda y_1, \quad (9d) \\
-\alpha x_1 y_3 - \alpha x_3 y_1 &= \lambda y_2, \quad (9e) \\
-\alpha x_1 y_2 - \alpha x_2 y_1 &= \lambda y_3, \quad (9f) \\
x_1^2 + x_2^2 + x_3^2 &= 1, \quad (9g) \\
y_1^2 + y_2^2 + y_3^2 &= 1. \quad (9h)
\end{align*}
\]

If $\lambda = 0$, we know two of $y_1, y_2, y_3$ are zeros from (9a)-(9c) and (9d). Assume $y = (\pm 1, 0, 0)^\top$. By (9a)-(9h), we have $x_2 = x_3 = 0$. In addition, $x_1 = \pm 1$ by (9g). Hence, we get the solution

\[
\lambda_1^* = 0, \quad x_1^* = (1, 0, 0)^\top, \quad y_1^* = (1, 0, 0)^\top.
\]

Similarly, we have

\[
\begin{align*}
\lambda_2^* &= 0, \quad x_2^* = (0, 1, 0)^\top, \quad y_2^* = (0, 1, 0)^\top, \\
\lambda_3^* &= 0, \quad x_3^* = (0, 0, 1)^\top, \quad y_3^* = (0, 0, 1)^\top.
\end{align*}
\]

Next, we consider the case that $\lambda \neq 0$ and $y_1 = 0$. By (9a)-(9b), we get $x_1 = x_2 = 0$. In addition, by (9c), we obtain $x_3 = \pm 1$. From (9d)-(9e), we know $\mp \alpha y_2 = \lambda y_1$ and $\pm \alpha y_1 = \lambda y_2$. Then, $\lambda y_1 y_2 = \mp \alpha y_2^2 = \mp \alpha y_1^2$. Hence, $y_1^2 = y_2^2 = \frac{1}{2}$ by (9h). In short, we have two solutions

\[
\lambda_1^* = \alpha, \quad x_4^* = (0, 0, -1)^\top, \quad y_4^* = \left(\frac{1}{\sqrt{2}}, \frac{1}{\sqrt{2}}, 0\right)^\top,
\]

and

\[
\lambda_2^* = \alpha, \quad x_5^* = (0, 0, 1)^\top, \quad y_5^* = \left(\frac{1}{\sqrt{2}}, -\frac{1}{\sqrt{2}}, 0\right)^\top.
\]

Using a similar approach, we obtain four more solutions for the case of $\lambda \neq 0$ and $y_2 = 0$ and the case of $\lambda \neq 0$ and $y_1 = 1$:

\[
\begin{align*}
\lambda_3^* &= \alpha, \quad x_6^* = (0, -1, 0)^\top, \quad y_6^* = \left(\frac{1}{\sqrt{2}}, 0, \frac{1}{\sqrt{2}}\right)^\top, \\
\lambda_4^* &= \alpha, \quad x_7^* = (0, 1, 0)^\top, \quad y_7^* = \left(\frac{1}{\sqrt{2}}, 0, -\frac{1}{\sqrt{2}}\right)^\top, \\
\lambda_5^* &= \alpha, \quad x_8^* = (-1, 0, 0)^\top, \quad y_8^* = \left(0, \frac{1}{\sqrt{2}}, \frac{1}{\sqrt{2}}\right)^\top, \\
\lambda_6^* &= \alpha, \quad x_9^* = (1, 0, 0)^\top, \quad y_9^* = \left(0, \frac{1}{\sqrt{2}}, -\frac{1}{\sqrt{2}}\right)^\top.
\end{align*}
\]

Finally, we consider the case that $y_1 \neq 0$, $y_2 \neq 0$, $y_3 \neq 0$, and $\lambda \neq 0$. From (9a)-(9c), we know $x_1 \neq 0$, $x_2 \neq 0$, and $x_3 \neq 0$. By (9a)-(9d), we have

\[
\frac{x_1}{x_2} = \frac{y_2}{y_1} \equiv t \neq 0.
\]
Then, by multiplying $t$ to both sides of (9d), we get $-\alpha x_1 y_3 - \alpha x_3 y_1 t^2 = \lambda y_2$. Combining this equation and (9e), we get $-\alpha x_3 y_1 (t^2 - 1) = 0$. Hence,

$$t^2 = 1, \quad x_1^2 = x_2^2, \quad \text{and} \quad y_1^2 = y_2^2.$$ 

Similarly, we have $x_1^2 = x_3^2$ and $y_1^2 = y_3^2$. By (9g) and (9h), we have $x_1^2 = x_2^2 = x_3^2 = \frac{1}{3}$ and $y_1^2 = y_2^2 = y_3^2 = \frac{1}{3}$. In a word, we obtain four more solutions

$$\lambda_{10}^* = \frac{2\alpha}{\sqrt{3}}, \quad x_{10}^* = \left( -\frac{1}{\sqrt{3}}, -\frac{1}{\sqrt{3}}, -\frac{1}{\sqrt{3}} \right)^T, \quad y_{10}^* = \left( \frac{1}{\sqrt{3}}, \frac{1}{\sqrt{3}}, \frac{1}{\sqrt{3}} \right)^T,$$

$$\lambda_{11}^* = \frac{2\alpha}{\sqrt{3}}, \quad x_{11}^* = \left( -\frac{1}{\sqrt{3}}, -\frac{1}{\sqrt{3}}, \frac{1}{\sqrt{3}} \right)^T, \quad y_{11}^* = \left( \frac{1}{\sqrt{3}}, -\frac{1}{\sqrt{3}}, \frac{1}{\sqrt{3}} \right)^T,$$

$$\lambda_{12}^* = \frac{2\alpha}{\sqrt{3}}, \quad x_{12}^* = \left( -\frac{1}{\sqrt{3}}, \frac{1}{\sqrt{3}}, \frac{1}{\sqrt{3}} \right)^T, \quad y_{12}^* = \left( \frac{1}{\sqrt{3}}, -\frac{1}{\sqrt{3}}, \frac{1}{\sqrt{3}} \right)^T,$$

$$\lambda_{13}^* = \frac{2\alpha}{\sqrt{3}}, \quad x_{13}^* = \left( -\frac{1}{\sqrt{3}}, -\frac{1}{\sqrt{3}}, \frac{1}{\sqrt{3}} \right)^T, \quad y_{13}^* = \left( \frac{1}{\sqrt{3}}, \frac{1}{\sqrt{3}}, -\frac{1}{\sqrt{3}} \right)^T.$$ 

The proof is complete. \(\square\)

Now, we are presenting C-eigenvalues and associated C-eigenvectors of piezoelectric tensors arising from known piezoelectric materials with different symmetries. Here, coefficients of piezoelectric tensors are measured in [4] with unit (pC/N) that is omitted for convenience. We note that “p” means pico (10\(^{-12}\)), “C” stands for coulomb (electric), and “N” is newton (force).

**Example 1.** The compound VFeSb belongs to the $\bar{3}m$ crystallographic point group [4]. Nonzero coefficients of the piezoelectric tensor $A_{VFeSb}$ are

$$a_{123} = a_{213} = a_{312} = -3.68180667.$$ 

By Proposition [4], we find that the largest C-eigenvalue of $A_{VFeSb}$ is about 4.25138.

In remainder examples, the polynomial system [2] of C-eigenvalues are solved by the function `NSolve` in Mathematica.

**Example 2.** The piezoelectricity of $\alpha$-quartz ($SiO_2$) crystal were discovered by Curie brothers in 1880 [2]. The $\alpha$-quartz belongs to the 32 crystallographic point group [6]. Hence, there are two independent parameters in the piezoelectric tensor $A_{SiO2}$:

$$a_{111} = -a_{122} = -a_{212} = -0.13685 \quad \text{and} \quad a_{123} = -a_{213} = -0.009715.$$ 

Other elements of the piezoelectric tensor are zeros. Positive C-eigenvalue of $A_{SiO2}$ and associated C-eigenvectors are reported in Table [1]

**Example 3.** The compound Cr$_2$AgBiO$_8$ belongs to the $\bar{4}$ crystallographic point group [4]. There are four independent parameters in the piezoelectric tensor $A_{Cr2AgBiO8}$

$$a_{123} = a_{213} = -0.22163, \quad a_{113} = -a_{223} = 2.608665,$$

$$a_{311} = -a_{322} = 0.152485, \quad \text{and} \quad a_{312} = -0.37153.$$
Table 1: Positive C-eigenvalues of a piezoelectric tensor of $\alpha$-quartz.

| No. | $\lambda$  | $x^\top$       | $y^\top$       |
|-----|------------|----------------|----------------|
| 1   | 0.137536   | 1.0 0.0 0.0    | 0.0 0.997515 -0.0704604 |
| 2   | 0.137536   | -0.5 0.866025 0.0 | 0.863873 0.498757 0.0704604 |
| 3   | 0.137536   | -0.5 -0.866025 0.0 | 0.863873 -0.498757 -0.0704604 |
| 4   | 0.13685    | -1.0 0.0 0.0    | 1.0 0.0 0.0    |
| 5   | 0.13685    | 0.5 0.866025 0.0 | 0.5 0.866025 0.0    |
| 6   | 0.13685    | 0.5 -0.866025 0.0 | 0.5 -0.866025 0.0    |
| 7   | 0.000686228 | -1.0 0.0 0.0 0.0 | 0.0 0.0704604 0.997515 |
| 8   | 0.000686228 | 0.5 -0.866025 0.0 | 0.0610205 0.0352302 -0.997515 |
| 9   | 0.000686228 | 0.5 0.866025 0.0 | 0.0610205 -0.0352302 0.997515 |

Table 2: Positive C-eigenvalues of the piezoelectric tensor of $\text{Cr}_2\text{AgBiO}_8$.

| No. | $\lambda$  | $x^\top$       | $y^\top$       |
|-----|------------|----------------|----------------|
| 1   | 2.6258     | 0.872141 0.48317 0.0769254 | 0.589036 -0.394962 0.705012 |
| 2   | 2.6258     | -0.872141 -0.48317 -0.0769254 | 0.589036 -0.394962 -0.705012 |
| 3   | 2.6258     | 0.48317 -0.872141 -0.0769254 | 0.394962 0.589036 0.705012 |
| 4   | 2.6258     | -0.48317 0.872141 -0.0769254 | 0.394962 0.589036 -0.705012 |
| 5   | 2.61806    | 0.961197 -0.275862 0.0 | 0.693742 0.136827 0.707107 |
| 6   | 2.61806    | -0.961197 0.275862 0.0 | 0.693742 0.136827 -0.707107 |
| 7   | 2.61806    | 0.275862 0.961197 0.0 | 0.136827 -0.693742 0.707107 |
| 8   | 2.61806    | -0.275862 -0.961197 0.0 | 0.136827 -0.693742 -0.707107 |
| 9   | 0.401605   | 0.0 0.0 1.0 | 0.830569 -0.556916 0.0 |
| 10  | 0.401605   | 0.0 0.0 -1.0 | 0.556916 0.830569 0.0 |
Other elements of the piezoelectric tensor are zeros. Positive C-eigenvalue of $A_{Cr_2AgBiO_8}$ and associated C-eigenvectors are reported in Table 2.

**Example 4.** The compound RbTaO$_3$ belongs to the $3m$ crystallographic point group [4]. There are four independent parameters in the piezoelectric tensor $A_{RbTaO_3}$

$$
a_{113} = a_{223} = -8.40955, \quad a_{222} = -a_{212} = -a_{211} = -5.412525
$$

$$
a_{311} = a_{322} = -4.3031, \quad \text{and} \quad a_{333} = -5.14766.
$$

Other elements of the piezoelectric tensor are zeros. Positive C-eigenvalue of $A_{RbTaO_3}$ and associated C-eigenvectors are reported in Table 3.

**Table 3:** Positive C-eigenvalues of the piezoelectric tensor of RbTaO$_3$.

| No. | $\lambda$ | $\mathbf{x}^\top$ | $\mathbf{y}^\top$ |
|-----|-----------|---------------------|---------------------|
| 1   | 12.4234   | 0.804378 0.464408 -0.370541 | 0.695227 0.401389 -0.596277 |
| 2   | 12.4234   | -0.804378 0.464408 -0.370541 | 0.695227 -0.401389 0.596277 |
| 3   | 12.4234   | 0.0 -0.928816 -0.370541 | 0.0 0.802779 0.596277 |
| 4   | 7.82245   | 0.677808 -0.391333 -0.622442 | 0.49743 -0.287191 -0.81587 |
| 5   | 7.82245   | -0.677808 -0.391333 -0.622442 | 0.49743 0.287191 0.81587 |
| 6   | 7.82245   | 0.0 0.782666 -0.622442 | 0.0 0.574382 -0.81587 |
| 7   | 6.91463   | 0.677894 -0.391382 -0.622318 | 0.5 0.860025 0.0 |
| 8   | 6.91463   | -0.677894 -0.391382 -0.622318 | 0.5 -0.860025 0.0 |
| 9   | 6.91463   | 0.0 0.782764 -0.622318 | 1.0 0.0 0.0 |
| 10  | 5.14766   | 0.0 0.0 -1.0 | 0.0 0.0 1.0 |
| 11  | 4.38052   | 0.0247105 0.014266 -0.999593 | 0.826334 0.477084 0.299271 |
| 12  | 4.38052   | -0.0247105 0.014266 -0.999593 | 0.826334 -0.477084 -0.299271 |
| 13  | 4.38052   | 0.0 -0.0285332 -0.999593 | 0.0 0.954168 -0.299271 |

**Example 5.** The compound NaBiS$_2$ belongs to the $mm2$ crystallographic point group [4]. There are five independent parameters in the piezoelectric tensor $A_{NaBiS_2}$

$$
a_{113} = -8.90808, \quad a_{223} = -0.00842, \quad a_{311} = -7.11526,
$$

$$
a_{322} = -0.6222, \quad \text{and} \quad a_{333} = -7.93831.
$$

Other elements of the piezoelectric tensor are zeros. Positive C-eigenvalue of $A_{NaBiS_2}$ and associated C-eigenvectors are reported in Table 4.

**Example 6.** The compound LiBiB$_2$O$_5$ belongs to the $2$ crystallographic point group [4]. There are eight independent parameters in the piezoelectric tensor $A_{LiBiB_2O_5}$

$$
a_{123} = 2.35682, \quad a_{112} = 0.34929, \quad a_{211} = 0.16101, \quad a_{222} = 0.12562,
$$

$$
a_{233} = 0.1361, \quad a_{213} = -0.05587, \quad a_{323} = 6.91074, \quad \text{and} \quad a_{312} = 2.57812.
$$

Other elements of the piezoelectric tensor are zeros. Positive C-eigenvalue of $A_{LiBiB_2O_5}$ and associated C-eigenvectors are reported in Table 5.
Table 4: Positive C-eigenvalues of the piezoelectric tensor of NaBiS$_2$.

| No. | $\lambda$  | $x^{\top}$ | $y^{\top}$ |
|-----|-------------|-------------|-------------|
| 1   | 11.6674     | 0.762919    | -0.646494  |
| 2   | 11.6674     | -0.762919   | 0.693139   |
| 3   | 7.93831     | 0.0         | -1.0       |
| 4   | 7.11526     | 0.0         | 1.0        |
| 5   | 0.6222      | 0.0         | -1.0       |

Example 7. The compound KBi$_2$F$_7$ belongs to the 1 crystallographic point group [4]. There are eighteen independent parameters in the piezoelectric tensor $A_{KBiF7}$

\[
\begin{align*}
a_{111} &= 12.64393, & a_{122} &= 1.08802, & a_{133} &= 4.14350, & a_{123} &= 1.59052, \\
a_{113} &= 1.96801, & a_{112} &= 0.22465, & a_{211} &= 2.59187, & a_{222} &= 0.08263, \\
a_{233} &= 0.81041, & a_{223} &= 0.51165, & a_{213} &= 0.71432, & a_{212} &= 0.10570, \\
a_{311} &= 1.51254, & a_{322} &= 0.68235, & a_{333} &= -0.23019, & a_{323} &= 0.19013, \\
& & & a_{313} &= 0.39030, & a_{312} &= 0.08381.
\end{align*}
\]

Positive C-eigenvalue of $A_{KBiF7}$ and associated C-eigenvectors are reported in Table 6.

Example 8. The compound BaNiO$_3$ belongs to the 6 crystallographic point group [4]. There are three independent parameters in the piezoelectric tensor $A_{BaNiO3}$

\[
\begin{align*}
a_{113} &= a_{223} = 0.038385, & a_{311} &= a_{322} = 6.89822, & a_{333} &= 27.4628.
\end{align*}
\]

Other elements of the piezoelectric tensor are zeros. There are infinite C-eigenvalues of $A_{BaNiO3}$. We report positive C-eigenvalue of $A_{BaNiO3}$ and associated C-eigenvectors in Table 7.

Table 5: Positive C-eigenvalues of the piezoelectric tensor of LiBiB$_2$O$_5$.

| No. | $\lambda$  | $x^{\top}$ | $y^{\top}$ |
|-----|-------------|-------------|-------------|
| 1   | 7.73762     | 0.302351    | 0.953081   |
| 2   | 7.73762     | -0.302351   | -0.953081  |
| 3   | 0.499616    | 0.902379    | 0.320695   |
| 4   | 0.499616    | -0.902379   | 0.320695   |
| 5   | 0.205796    | 0.0         | 1.0        |
| 6   | 0.12562     | 0.0         | 1.0        |
| 7   | 0.0913135   | 0.0         | 1.0        |
Table 6: Positive C-eigenvalues of the piezoelectric tensor of \( \text{KBi}_2\text{F}_7 \).

| No. | \( \lambda \) | \( \mathbf{x}^\top \) | \( \mathbf{y}^\top \) |
|-----|----------------|----------------|----------------|
| 1   | 13.5021        | 0.970501       | 0.209737       |
|     |                | 0.118907       | 0.118907       |
| 2   | 4.46957        | 0.981961       | 0.189047       |
|     |                | -0.00361752    | -0.00361752    |
| 3   | 0.544863       | 0.759805       | -0.368785      |
|     |                | 0.535439       | 0.535439       |

Table 7: Positive C-eigenvalues of the piezoelectric tensor of \( \text{BaNiO}_3 \).

| No. | \( \lambda \) | \( \mathbf{x}^\top \) | \( \mathbf{y}^\top \) |
|-----|----------------|----------------|----------------|
| 1   | 27.4628        | 0.0 0.0 1.0   | 0.0 0.0 1.0   |
| 2   | 6.89822        | 0.0 0.0 1.0   | \( y_1 \pm \sqrt{1-y_2^2} \) \( 0.0 \)

5 Difference from Matrix Singular Values

An \( n \)-by-\( n \) symmetric matrix \( S = [s_{ij}] \) contains \( \frac{n(n+1)}{2} \) independent elements. Hence we may vectorize \( S \) as a vector

\[
\text{vec}(S) = (s_{11}, s_{22}, \ldots, s_{nn}, \sqrt{2}s_{(n-1)n}, \ldots, \sqrt{2}s_{12})^\top \in \mathbb{R}^{\frac{n(n+1)}{2}}.
\]

Here, we equip off-diagonal elements of \( S \) with coefficient \( \sqrt{2} \), while diagonal elements of \( S \) are with coefficient 1. Hence, we have \( \|S\|_F = \|\text{vec}(S)\|_2 \).

Let \( A \in \mathbb{R}^{n \times n \times n} \) be a piezoelectric-type tensor that contains \( \frac{n^2(n+1)}{2} \) independent elements. Owing to the symmetry of latter two indices of \( A \), we could represent each symmetric slice-matrix as a vector. Collecting these vectors, we obtain an \( n \)-by-\( \frac{n(n+1)}{2} \) matrix

\[
M(A) = \begin{pmatrix}
a_{111} & a_{122} & \cdots & a_{1nn} & \sqrt{2}a_{1(n-1)n} & \cdots & \sqrt{2}a_{12}
\vdots & \vdots & \ddots & \vdots & \vdots & \ddots & \vdots
\vdots & \vdots & \ddots & \vdots & \vdots & \ddots & \vdots
a_{n11} & a_{n22} & \cdots & a_{nn} & \sqrt{2}a_{n(n-1)n} & \cdots & \sqrt{2}a_{n12}
\end{pmatrix}. \tag{10}
\]

Here, each row of the above matrix corresponds to a symmetric slice-matrix of the piezoelectric tensor. Let \( \mathbf{y} = (y_1, \ldots, y_n)^\top \in \mathbb{R}^n \). By some calculations, we find that

\[
A\mathbf{y}\mathbf{y}^\top = M(A)\text{vec}(\mathbf{y}\mathbf{y}^\top).
\]

**Theorem 5.1.** Let \( \lambda^* \) and \( \mu^* \) be the largest C-eigenvalue of a piezoelectric-type tensor \( A \) and the largest singular value of the matrix \( M(A) \), respectively. Then,

\[
\lambda^* \leq \mu^*. \tag{11}
\]

*In the above inequality, strict inequality may hold in some cases.*

**Proof.** From Theorem 2.3 (c), \( \lambda^* \) is the optimal objective value of the following maximization problem

\[
\lambda^* = \max \{ \mathbf{x}^\top A\mathbf{y}\mathbf{y}^\top : \|\mathbf{x}\|_2 = 1, \|\mathbf{y}\|_2 = 1 \}.
\]
We denote the corresponding optimal solution as \((x^*, y^*)\). Obviously, \(\|\text{vec}(y^*y^*)\|_2 = \|y^*y^*\|_F = \|y^*\|_2^2 = 1\).

By matrix theory, \(\mu^* = \text{max} \{x^\top M(A)z : \|x\|_2 = 1, \|z\|_2 = 1\}\).

It is easy to see that \((x^*, \text{vec}(y^*y^*)^\top)\) is a feasible of this problem. Hence,

\[ \mu^* \geq x^\top M(A)\text{vec}(y^*y^*) = x^\top A y^* = \lambda^*. \]

We now give an example for which strict inequality holds in (11). Consider a piezoelectric tensor \(A_0\) with dimension 2. There are only two nonzero elements in \(A_0\):

\[ a_{112} = a_{222} = 1. \]

Hence,

\[ M(A_0) = \begin{pmatrix} 0 & 0 & \sqrt{2} \\ 0 & 1 & 0 \end{pmatrix}. \tag{12} \]

By some calculation, the largest singular value of \(M(A_0)\) is \(\sqrt{2}\), and the associated singular vectors are \((1, 0)^\top\) and \((0, 0, 1)^\top\).

Then, we turn to C-eigenvalues of \(A_0\). The system (2) reduces to

\[ 2y_1y_2 = \lambda x_1, \tag{13a} \]
\[ y_2^2 = \lambda x_2, \tag{13b} \]
\[ x_1y_2 = \lambda y_1, \tag{13c} \]
\[ x_1^2 + x_2^2 = 1, \tag{13d} \]
\[ y_1^2 + y_2^2 = 1. \tag{13e} \]

If \(\lambda = 0\), we know \(y_2 = 0\) by (13b). From (13b), we have \(y_1 = \pm 1\). Using (13d), we get \(x_1 = 0\). By (13c), we obtain \(x_2 = \pm 1\). Hence, we obtain a group of solution

\[ \lambda_1^* = 0, \quad x_1^* = (0, 1)^\top, \quad y_1^* = (1, 0)^\top. \]

In the case of \(\lambda \neq 0\) and \(y_2 = 0\), we get \(y_1 = 0\) by (13c), which contradicts (13b).

Now, we consider the case that \(\lambda \neq 0\) and \(y_2 \neq 0\). By (13b), we know \(x_2 \neq 0\). From (13a) and (13b), we have

\[ \frac{x_1}{x_2} = \frac{2y_1}{y_2} \equiv t. \]

Then, \(x_1 = tx_2\) and \(y_1 = \frac{1}{2}y_2\). From (13c) and (13d), we know

\[ \frac{t^2}{2} = \frac{y_1}{y_2} = \frac{x_1y_2}{x_1y_1 + x_2y_2} = \frac{tx_2y_2}{x_2^2y_2 + x_2y_2} = \frac{2t}{t^2 + 2}. \]

Solving this equation in \(t\), we get

\[ t_1 = \sqrt{2}, \quad t_2 = -\sqrt{2}, \quad \text{and} \quad t_3 = 0. \]
If \( t = \sqrt{2} \), by (13b), we know \( x_1 = \pm \frac{\sqrt{2}}{\sqrt{3}} \) and \( x_2 = \pm \frac{1}{\sqrt{3}} \). By (13d), we know \( y_1 = \frac{t}{2} y_2 \) and (13e), we have \( y_1 = \pm \frac{1}{\sqrt{3}} \) and \( y_2 = \pm \frac{\sqrt{2}}{\sqrt{3}} \). Then, by (13b), we know \( \lambda = \pm \frac{2}{\sqrt{3}} \). In sum, we have a solution
\[
\lambda^*_2 = \frac{2}{\sqrt{3}}, \quad x^*_2 = \left( \frac{\sqrt{2}}{\sqrt{3}}, \frac{1}{\sqrt{3}} \right)^\top, \quad y^*_2 = \left( \frac{1}{\sqrt{3}}, \frac{\sqrt{2}}{\sqrt{3}} \right)^\top.
\]

Using similar discussions, we get two more solutions
\[
\lambda^*_3 = \frac{2}{\sqrt{3}}, \quad x^*_3 = \left( -\frac{\sqrt{2}}{\sqrt{3}}, \frac{1}{\sqrt{3}} \right)^\top, \quad y^*_3 = \left( \frac{1}{\sqrt{3}}, -\frac{\sqrt{2}}{\sqrt{3}} \right)^\top,
\]
and
\[
\lambda^*_4 = 1, \quad x^*_4 = (0, 1)^\top, \quad y^*_4 = (0, 1)^\top.
\]

Hence, the largest C-eigenvalue of \( A_0 \) is \( \frac{2}{\sqrt{3}} \). Obviously, \( \frac{2}{\sqrt{3}} < \sqrt{2} \). Hence, strict inequality in \( \ref{eq:inequality} \) holds. The proof is complete.

6 Summary

We defined C-eigenvalues and C-eigenvectors for a piezoelectric tensor, where “C” names after Curie brothers. The existence of C-eigenvalues and its invariance under orthonormal transformations were also addressed. We argued that for a piezoelectric tensor, the largest C-eigenvalue corresponds to the electric displacement vector with the largest 2-norm in the piezoelectric effect under unit uniaxial stress, and the strain tensor with the largest 2-norm in the converse piezoelectric effect under unit electric field vector. Thus, C-eigenvalues and C-eigenvectors have concrete physical meanings in piezoelectric effect and converse piezoelectric effect. Finally, we present C-eigenvalues and associated C-eigenvectors of piezoelectric tensors for various crystal classes.

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