Tensor Properties of Materials
—problems—

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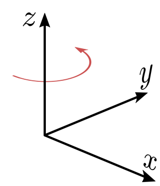
Note: All rotations are understood according to the right-hand rule and rotation matrices rotate column vectors via pre-multiplication as $\vec{v}' = \mathbf{L}\vec{v}$. The axes $\vec{x}_1$, $\vec{x}_2$ and $\vec{x}_3$ form a right-handed 3D Cartesian coordinate system and indexes take up values in the range $i, j, k, l, m, n \in \{1, 2, 3\}$.



Problem 1 *Tensors*

Expand the below expressions as summations using the Einstein convention. Evaluate the sum assuming that all tensors are constant tensors (every entry in the tensor is the same number). What is the rank of the resulting tensor?

(i) $v_i w_i$, where $v_i = 1$ and $w_i = 2$ for all i. Hint: this is the scalar product between the vectors $\vec{v} = (1, 1, 1)^T$ and $\vec{w} = (2, 2, 2)^T$.

(ii) $S_{ij}T_{jk}$, where $S_{ij} = 2$ and $T_{jk} = 1$ for all i, j and k. Hint: this is a matrix-matrix product and every matrix entry in $\mathbf{T}$ is 1 while every matrix entry in $\mathbf{S}$ is 2.

(iii) $T_{ij}T_{ij}$, where $T_{ij} = 1$ for all i and j.

(iv) $S_{ijkl}T_{ij}$, where $S_{ijkl} = 5$ and $T_{ij} = 2$ for all i, j, k and l

(v) write the following matrix operations as Einstein summations: $\mathbf{AB}$, $\mathbf{A}^T\mathbf{B}$, $\mathrm{Tr}[\mathbf{A}]$, $\mathrm{Tr}[\mathbf{A}^T\mathbf{B}]$. Here $\mathbf{A}$ and $\mathbf{B}$ are 3×3 real matrices, $\mathrm{Tr}[\cdot]$ is the trace operation (sum of diagonals) and $(\cdot)^T$ is the transpose operation.

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Problem 2 *Active and Passive Rotations*

Suppose the homogeneous electric field between two large parallel charged plates is described by the column vector $\vec{E} = (\sqrt{3}/2, -1/2, 0)^T$. Suppose we want to find the rotation matrix that simplifies this vector such that after the transformation $\vec{E}' = (1, 0, 0)^T$. The basic rotation matrix around the z axis is defined as

$$\mathbf{R}_z(\theta) = \begin{bmatrix} \cos\theta & -\sin\theta & 0 \\ \sin\theta & \cos\theta & 0 \\ 0 & 0 & 1 \end{bmatrix},$$

and the transformation it performs can be interpreted either as an active or a passive rotation.

(i) **Active rotation:** Imagine we physically rotate the two parallel plates and thus the electric field rotates as $\vec{E}' = \mathbf{R}_z(\theta)\vec{E}$. Draw this transformation and calculate the angle of rotation θ.

(ii) The rotation matrix can also be used to rotate the coordinate axes. Draw the rotated coordinate axes but using the *inverse* rotation matrix as $\vec{x}_i' = \mathbf{R}_z^T(\theta)\vec{x}_i$.

(iii) **Passive rotation:** Show that if we leave the charged plates unchanged and calculate vector entries using the new axes $\vec{x}_i'$ we obtain the desired vector $\vec{E}' = (1, 0, 0)^T$. Hint: the vector entries in the new coordinate system are calculated using the scalar products as $E_i' = \vec{E} \cdot \vec{x}_i'$, where we use the unchanged vector $\vec{E} = (\sqrt{3}/2, -1/2, 0)^T$.

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Problem 3 *Calculating rotation matrices*

Compute the 3×3 matrices for the following rotations and draw how the coordinate axes are rotated $\vec{x}_i' = \mathbf{L}\vec{x}_i$. Hint: the rotated vectors $\vec{x}_i'$ form column vectors of $\mathbf{L}$.

(i) $-30°$ around the $\vec{x}_3$ axis. Hint: you can verify the result by comparing to the definition of the basic rotation matrix in Problem 2.

(ii) $45°$ around the $\vec{x}_2$ axis

(iii) rotation (i) followed by rotation (ii)

(iv) rotation (ii) followed by rotation (i). Is it is the same as (iii)? Why?

(v) $120°$ about the [111] direction in a cubic crystal

(vi) from the crystal axes of a tetragonal crystal with $a = b = 5$ and $c = 6$ (with $\vec{x}_3$ parallel to the c-axis) rotating around $\vec{x}_1$ so that $\mathbf{L}\vec{x}_3$ becomes parallel with the [011] direction

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(vii) $90°$ about the [110] direction in a cubic crystal

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Problem 4 *Crystal symmetry*

(i) Explain how anisotropy in a crystal can lead to electrical conductivity whereby a current flows in a direction that is not parallel to the applied electric field. Describe how the anisotropic conductivity can be visualised using the representation quadric.

(ii) The electrical conductivity of a uniaxial crystal when measured along its axis of symmetry is twice that when measured perpendicular to the axis. In what direction will the current flow through the crystal if an electric field is applied at $45°$ to the axis of symmetry? (hint: we have a freedom in defining the electric field vector, so it simplifies the argument if we choose a simple arrangement)

(iii) A uniaxial crystal has principal electrical conductivities

$$\sigma_1^{PAS} = \sigma_2^{PAS} = 5.6 \times 10^4\,\Omega^{-1}\text{m}^{-2}, \qquad \sigma_3^{PAS} = 8.2 \times 10^4\,\Omega^{-1}\text{m}^{-2}.$$

A rod of the crystal of cross sectional area $1\,\text{mm}^2$ has its axis of symmetry $60°$ from the crystal axis (as defined by the rotation below). A current of $5\,\text{mA}$ passes down the rod such that

$$\begin{bmatrix} 0 \\ 0 \\ J'_3 \end{bmatrix} = \vec{J}' = \boldsymbol{\sigma}'\vec{E}', \qquad \text{with } J'_3 = 5 \times 10^3\,\text{A}\,\text{m}^{-1}$$

As we translate between this coordinate system and the principal axis system, the vector entries transform according to $\vec{J}' = \mathbf{L}\vec{J}$ and $\vec{E}' = \mathbf{L}\vec{E}$ where $\mathbf{L} = \mathbf{R}_x(60°)$ is the basic rotation matrix around the $\vec{x}_1$ axis with an angle $60°$. Find the electric field components (a) parallel to and (b) perpendicular to the axis of the rod. Would it have made any difference if the rotation were performed around $\vec{x}_2$ instead?

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Problem 5 *Orthogonal matrices*

The axes of two Cartesian coordinate systems $\vec{x}_1$, $\vec{x}_2$, $\vec{x}_3$ and $\vec{x}'_1 = \mathbf{L}\vec{x}_1$, $\vec{x}'_2 = \mathbf{L}\vec{x}_2$, $\vec{x}'_3 = \mathbf{L}\vec{x}_3$ have the following angular relationships

$$\measuredangle(\vec{x}_1 O \vec{x}'_1) = 60°, \qquad \measuredangle(\vec{x}_1 O \vec{x}'_2) = 90°,$$
$$\measuredangle(\vec{x}_2 O \vec{x}'_1) > 90°, \qquad \measuredangle(\vec{x}_2 O \vec{x}'_2) < 90°,$$
$$\measuredangle(\vec{x}_3 O \vec{x}'_1) = 45°.$$

Here $\measuredangle(AOB)$ denotes the angle specified by three points A, O and B where $O = (0,0,0)$ is the origin.

(i) Calculate all entries of the rotation matrix using the direction cosines $L_{ij} = \cos\theta_{ij}$ where θ_{ij} is the angle between $\vec{x}_i$ and $\vec{x}'_j$. Exploit the condition that column (and row) vectors of $\mathbf{L}$ are mutually orthogonal and normalised as

$$\sum_i L_{ij} L_{ik} = \begin{cases} 1 & \text{if } j = k \\ 0 & j \neq k \end{cases},$$

and the fact that both coordinate systems are right-handed.

(ii) Verify that the orthonormality relationships above are valid for all possible indices, and that the determinant $|\mathbf{L}|$ is equal to $+1$.

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Problem 6 *Thermal conductivity*

In a certain crystal the principal thermal conductivities are

$$K_{11} = 3\,\mathrm{W\,m^{-1}\,K^{-1}}, \quad K_{22} = 4\,\mathrm{W\,m^{-1}\,K^{-1}}, \quad K_{33} = 1\,\mathrm{W\,m^{-1}\,K^{-1}}.$$

The original axes $\vec{x}_1$, $\vec{x}_2$ and $\vec{x}_3$ are the principal axes and we transform our coordinate system using the *inverse rotation* as $\vec{x}'_1 = \mathbf{L}^T \vec{x}_1$, $\vec{x}'_2 = \mathbf{L}^T \vec{x}_2$, $\vec{x}'_3 = \mathbf{L}^T \vec{x}_3$. Here $\mathbf{L}$ is the basic rotation matrix around the $\vec{x}_2$ axis with an angle $\pi/4$.

(i) A vector $\vec{v}$ has vector entries

$$v_1 = 3, \qquad v_2 = 4, \qquad v_3 = 1,$$

in the old coordinate system. Calculate the vector entries v'_i in the new coordinate system. Hint: recall that an inverse rotation of the coordinate system has the same effect on the vector entries as an active rotation of the vector.

(ii) Calculate the nine components K'_{ij} of the thermal conductivity tensor in the new coordinate system.

(iii) What is the volume enclosed by the representation quadric $\vec{x}^T \mathbf{K} \vec{x} = 1$?

(iv) Calculate the sum of the diagonal components (trace of the matrix $\mathbf{K}$) (a) before the transformation and (b) after the transformation, and show that they are equal. Are they always identical?

(v) Calculate the sum of squares of all matrix entries as $K_{ij} K_{ij}$ (a) before the transformation and (b) after the transformation, and show that they are equal. Could this quantity be used as a measure of the "magnitude" of a tensor variable? Hint: expressing the sum of squares $K_{ij} K_{ij}$ as the trace of a product of two matrices from Problem 1 helps because the trace is the same in all coordinate systems.

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(vi) A thin plate of this crystal is cut perpendicular to the new coordinate axis $\vec{x}'_3$, and a temperature gradient of $1000\,\mathrm{K\,m^{-1}}$ is maintained between its faces. Calculate the rate of flow of heat (a) perpendicular to its faces, and (b) parallel to its faces. **Note:** The heat flow equation is $\vec{Q} = -\mathbf{K}\overrightarrow{\nabla T}$ where $\vec{Q}$ is the heat flow vector, and $\overrightarrow{\nabla T}$ is the temperature gradient vector as

$$\overrightarrow{\nabla T} = \frac{\partial T}{\partial x_1}\vec{x_1} + \frac{\partial T}{\partial x_2}\vec{x_2} + \frac{\partial T}{\partial x_3}\vec{x_3}.$$

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Problem 7 *Stress tensor*

Given the rank-2 stress tensor as the following matrix

$$\boldsymbol{\sigma} = \begin{bmatrix} 4 & 0 & -3 \\ 0 & 2 & 0 \\ -3 & 0 & -1 \end{bmatrix}$$

(i) Compute explicitly the cubic polynomial whose roots λ_i are the three principal values of the tensor.

(ii) By plotting the value of the cubic expression for several different values of λ, estimate the three principal values of the tensor.

(iii) Diagonalize $\boldsymbol{\sigma}$ and compare the principal values to those estimated in part (ii).

(iv) Recall that the stress tensor expresses the linear relation between a unit vector and a corresponding traction vector $\vec{T}$ (force vector per unit area). What is the direction of the unit vector $\vec{n}$ for which we obtain the largest possible traction vector $|T|$? Is it always this direction?

(v) The stresses acting on a body have the following components σ_{ij} in the coordinate system spanned by $\vec{x}_1$, $\vec{x}_2$ and $\vec{x}_3$ as

$$\boldsymbol{\sigma} = \begin{bmatrix} \sigma & 0 & 0 \\ 0 & -\sigma & 0 \\ 0 & 0 & 0 \end{bmatrix}.$$

We transform our coordinate system to $\vec{x}'_1$, $\vec{x}'_2$, and $\vec{x}'_3$ by a rotation of 45° about $\vec{x}_3$ such that $\vec{x}'_1$ bisects the angle between $\vec{x}_1$ and $-\vec{x}_2$. Calculate the rotation matrix $\mathbf{L}$ that transforms vector entries as $\vec{V}' = \mathbf{L}\vec{V}$. Calculate the entries σ'_{ij} of the stress tensor in the new coordinate system. Comment on your results.

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Problem 8 *Thermal expansion*

A 1 cm cube of material with principal thermal expansion coefficients

$$\alpha_{11} = \alpha_{22} = 5.1 \times 10^{-5}\,\mathrm{K}^{-1}, \qquad \alpha_{33} = 1.3 \times 10^{-5}\,\mathrm{K}^{-1},$$

is placed on a flat surface. The axis of crystal symmetry is parallel to the diagonal of one of the vertical faces of the cube. At what angle to the vertical are each of the edges of the cube after it is heated by 1000 °C? What is its new volume? (hint: don't forget to include any rotation of the cube as it stays resting on the flat surface)

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Problem 9 *Refractive index*

A monoclinic crystal has an electrical susceptibility given by the tensor

$$\boldsymbol{\chi} = \begin{bmatrix} 3 & 0 & 2 \\ 0 & 5 & 0 \\ 2 & 0 & 8 \end{bmatrix}.$$

Find the principal values of the refractive index for the material.

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