3.012 Fund of Mat Sci: Structure – Lecture 20

SYMMETRIES AND TENSORS

Photograph removed for copyright reasons.

Einstein explaining the Einstein convention

Homework for Mon Nov 28

- Study: 3.3 Allen-Thomas (Symmetry constraints)
- Read all of Chapter 1 Allen-Thomas

Last time:

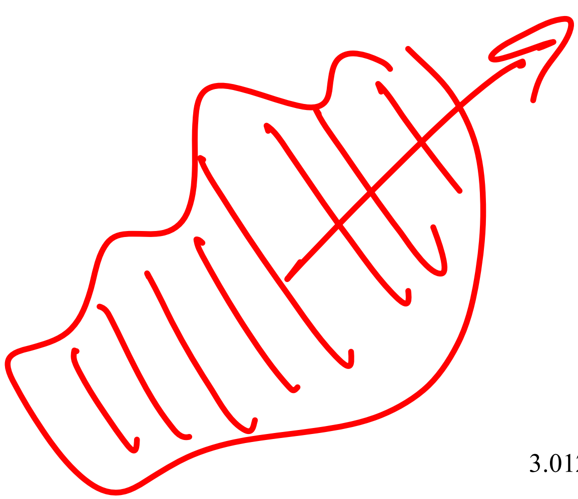
1. Atoms as spherical scatterers
2. Huygens construction → Laue condition
3. Ewald construction
4. Debye-Scherrer experiments

Scalars, vectors, tensors

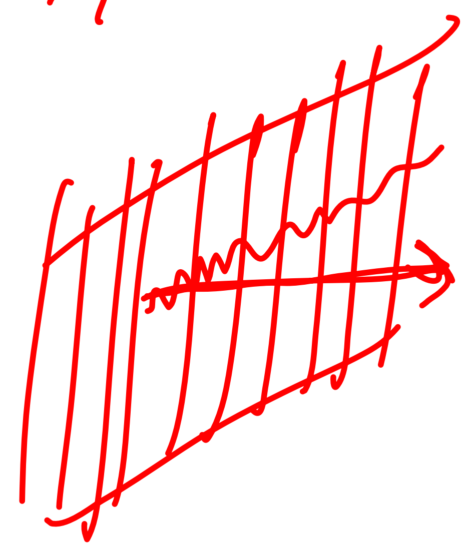
$\rho(\vec{x})$ SCALAR $\rightarrow$ TENSOR OF RANK "0"

$\vec{j}(\vec{x}) = \left(j_1(\vec{x}),\ j_2(\vec{x}),\ j_3(\vec{x}) \right)$

TENSOR OF RANK "1"



$$\underbrace{j = \sigma E}_{\text{LINEAR APPROXIMATION}} + \sigma_2 E^2$$



Scalars, vectors, tensors

$\vec{E} = (E_1, 0, 0)$ $\vec{j} = (j_1, j_2, j_3)$

$j_1 = \sigma_{11} E_1$ $j_2 = \sigma_{21} E_1$ $j_3 = \sigma_{31} E_1$

$j_1 = \sum_{k=1}^{3} \sigma_{1k} E_k$

$j_2 = \sum_k \sigma_{2k} E_k$

$j_3 = \sum_k \sigma_{3k} E_k$

$$\boxed{\begin{aligned} j_1 &= \sigma_{11}E_1 + \sigma_{12}E_2 + \sigma_{13}E_3 \\ j_2 &= \sigma_{21}E_1 + \sigma_{22}E_2 + \sigma_{23}E_3 \\ j_3 &= \sigma_{31}E_1 + \sigma_{32}E_2 + \sigma_{33}E_3 \end{aligned}}$$

LINEAR

$\Rightarrow \vec{j} = \underline{\underline{\sigma}}\, \vec{E}$

$\Downarrow$

2nd RANK TENSOR

Einstein's convention

$$\boxed{J_i = \sum_k \sigma_{ik} E_k}$$

$$J_i = \sigma_{ik} E_k = \sigma_{il} E_l \neq$$

DUMMY INDEX $\neq \sigma_{li} E_l$

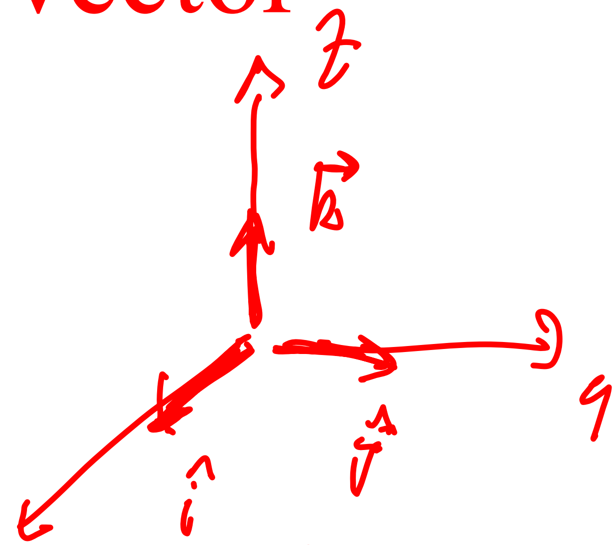
Transformation of a vector

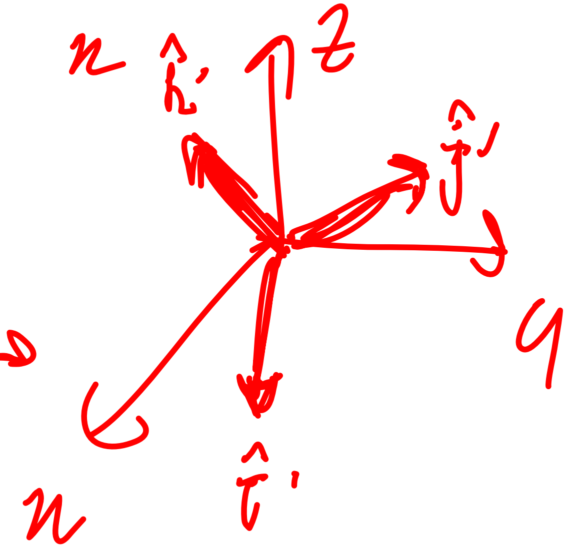
$$\vec{P} = (x, y, z) = x\hat{i} + y\hat{j} + z\vec{k}$$

$$\hat{i} = (1, 0, 0)$$

$$\hat{j} = (0, 1, 0)$$

$$\hat{k} = (0, 0, 1)$$





$$\hat{i}' = \underbrace{(\hat{i}' \cdot \hat{i})}_{\cos\alpha_1}\hat{i} + \underbrace{(\hat{i}' \cdot \hat{j})}_{\cos\alpha_2}\hat{j} + \underbrace{(\hat{i}' \cdot \hat{k})}_{\cos\alpha_3}\vec{k}$$

DIRECTION COSINES

Transformation of a vector

$$\hat{i}' = \overset{a_{11}}{\cos\alpha_1}\,\hat{i} + \overset{a_{12}}{\cos\alpha_2}\,\hat{j} + \overset{a_{13}}{\cos\alpha_3}\,\hat{k}$$

$$\hat{j}' = \overset{a_{21}}{\cos\beta_1}\,\hat{i} + \overset{a_{22}}{\cos\beta_2}\,\hat{j} + \overset{a_{23}}{\cos\beta_3}\,\hat{k}$$

$$\hat{k}' = \overset{a_{31}}{\cos\gamma_1}\,\hat{i} + \overset{a_{32}}{\cos\gamma_2}\,\hat{j} + \overset{a_{33}}{\cos\gamma_3}\,\hat{k}$$

TENSOR RANK 2

$$\vec{P} = (x, y, z) = x\hat{i} + y\hat{j} + z\hat{k}$$

$$\vec{P}' = (x', y', z') = (x_1', x_2', x_3')$$

$$\boxed{x_i' = a_{ij}\, x_j}$$

$$\vec{x}' = A\,\vec{x}$$

$$\sum_i a_{ik} a_{ij} = \delta_{jk}$$

$A = (a_{ij})$

$A^T = (a_{ji})$

$AA^T = \mathbb{I}$

$\Downarrow$

$A^T = A^{-1}$

Orthogonal Matrices

WHAT IS THE MOST GENERAL TRANSFORMATION A SUCH THAT

$$\|P\| = \|P'\| \Rightarrow \sum_i x_i^2 = \sum_i (x_i')^2$$

$$\sum_i x_i^2 = \sum_i \left(\sum_k a_{ik} x_k\right)^2 = \sum_i \left(\sum_j \sum_k a_{ik} x_k a_{ij} x_j\right)$$

$\Downarrow$

$$\sum_i x_i^2 = \sum_i \left(\sum_{j,k} a_{ik} a_{ij}\right) x_k x_j = \sum_{jk} \left(\underbrace{\sum_i a_{ik} a_{ij}}_{=\delta_{jk}}\right) x_k x_j$$

Transformation of a tensor

ORTHOGONAL TRANSF.

$$\underline{\underline{A}}$$

$$\underline{\underline{A}}\,\underline{\underline{A}}^T = \underline{\underline{1}}$$

$$\underline{\underline{A}}^T\underline{\underline{A}} = \underline{\underline{1}}$$

$$\vec{J} = \underline{\underline{\sigma}}\,\vec{E}$$

$$\underline{\underline{A}}\vec{J} = \underline{\underline{A}}\,\underline{\underline{\sigma}}\,\vec{E} = \underline{\underline{A}}\,\underline{\underline{\sigma}}\,\underline{\underline{1}}\,\vec{E} = \underline{\underline{A}}\,\underline{\underline{\sigma}}\,\underline{\underline{A}}^T\underline{\underline{A}}\,\vec{E}$$

$$\vec{J}' = \underline{\underline{\sigma}}' \vec{E}'$$

$$\underline{\underline{A}}\vec{J} = \left(\underline{\underline{A}}\,\underline{\underline{\sigma}}\,\underline{\underline{A}}^T\right)\underline{\underline{A}}\,\vec{E}$$

TENSOR OF 2nd RANK IN THE NEW REF. SYST.

$x_i' x_j' x_k' = a_{il} a_{jm} a_{kn} x_l x_m x_n$

γ'_{ijk} γ_{lmn}

Transformation law for products of coordinates

$\underline{\underline{\sigma}} = \sigma_{ij} \quad 3^2 = 9$ ELEMENTS

$\underline{\underline{\underline{\gamma}}} = \sigma_{ijk} \quad 3^3 = 27$ ELEMENTS

$\underline{\underline{\underline{\underline{C}}}} = C_{ijkl} \quad 3^4 = 81$ ELEMENTS

FIRST CONV FIRST CONV

$$\underbrace{x_i' x_j'}_{\sigma_{ij}'} = (a_{ik} x_k)(a_{jl} x_l) = a_{ik} a_{jl} \underbrace{x_k x_l}$$

$$\underbrace{a_{ik} a_{jl}}_{A \sigma A^T} \sigma_{kl}$$

Neumann's principle

- *the symmetry elements of any physical property of a crystal must include all the symmetry elements of the point group of the crystal*

$$\sigma_{ij} = \sigma'_{ij}$$

TRANSFORMATION IS A POINT-GROUP SYMMETRY OPERATOR

Symmetry constraints

$\frac{2}{m}$

- Determine the crystallographic point group
- Choose a generator group (set of symmetry operation which fully generates the complete point group symmetry)
- Transform all components of a tensor by each of the symmetry elements
- Impose Neumann's principle that a tensor component and its transformed remain identical for a symmetry operation

Symmetry constraints

$\frac{2}{n}$

2 i

$x_1 \rightarrow -x_1$

$x_2 \rightarrow -x_2$

$x_3 \rightarrow -x_3$

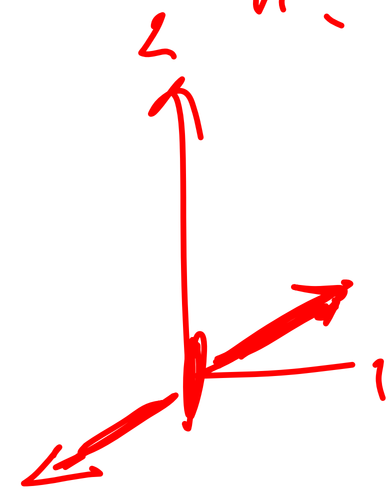
INVERSION

$x_1 \rightarrow -x_1$

$x_2 \rightarrow -x_2$

$x_3 \rightarrow x_3$

2-FOLD



Symmetry constraints

$$(x_1' x_1') = (-x_1)(-x_1) = x_1 x_1$$

$$(\ldots)$$

$$(\ldots)$$

$$(\ldots)$$

$$(x_2' x_3') = (-x_2)(x_3) \Rightarrow a_{23}' = -a_{23}$$

$$a_{11}' = a_{11}$$

$$a_{12}' = a_{12}$$

$$\vdots$$

$$a_{33}' = a_{33}$$

$$a_{13}' = -a_{13}$$

$$a_{23} = 0 = a_{13} = a_{31} = a_{32}$$

Scalar, vector, tensor properties

- Mass (0), polarization (1), strain (2)

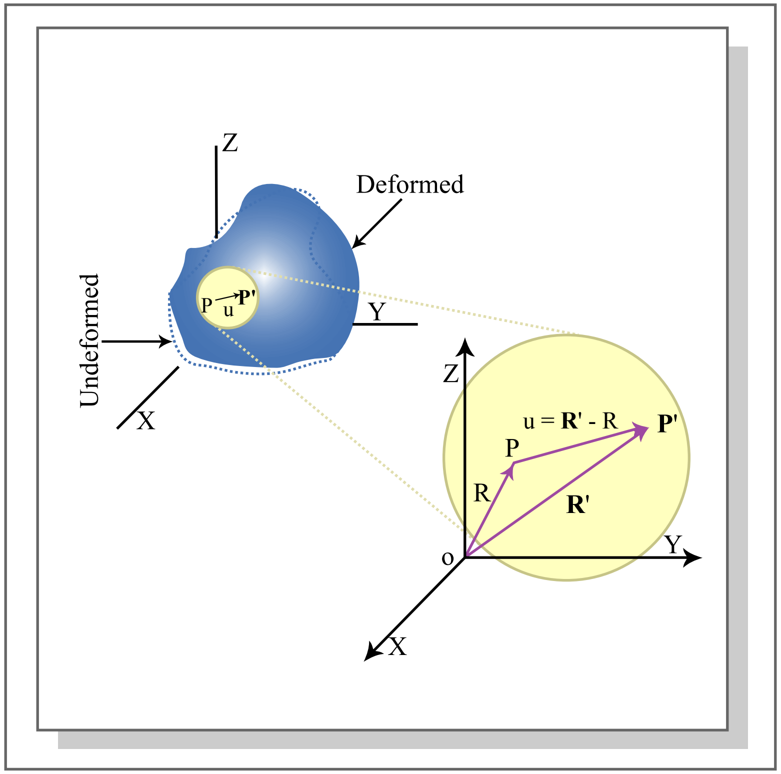


Figure by MIT OCW.

$$\varepsilon_{ij} = \frac{1}{2}\left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i}\right)$$

Physical properties and their relation to symmetry

- Density (mass, from a certain volume)
- Pyroelectricity (polarization from temperature)
- Conductivity (current, from electric field)
- Piezoelectricity (polarization, from stress)
- Stiffness (strain, from stress)

Curie's Principle

- *a crystal under an external influence will exhibit only those symmetry elements that are common to both the crystal and the perturbin influence*