Non linear Affine Transformations

Examples : Translation, Screw, Glide

NOTE: Can shear be represented as a combination of rotation + translation?

these are linear transformations that don't change distances

Answer is No

(But shear still is a linear transformation)

this is a non-length preserving linear transformation

In general, a linear transformation W is :

$$W(\vec{a}+\vec{b}) = W(\vec{a}) + W(\vec{b})$$
$$W(k\vec{a}) = k\,W(\vec{a})$$

from here we can see that by taking $k=0$:

$$W(\vec{0}) = \vec{0}$$

(and so there is at least one fixed point)

NOTE:

Rotation, Rotoinversion are Linear

Shear is also Linear

Translation, Screw and Glide are Non-linear

these all are affine

{however, we are not considering shear in this course}

LECTURE 8 (29/01/2024)

42] Geometrical Interpretation of Coordinate Triplet of a General Position

eg: General position of block $(0,0,0)+$ of space group no 230 ($Ia\bar{3}d$)

$$y+\frac{1}{4},\ \bar{x}+\frac{1}{4},\ z+\frac{3}{4}$$

i.e. $(x,y,z) \xrightarrow[W,\vec{w}]{} (\tilde{x},\tilde{y},\tilde{z})$

where, $\tilde{x} = y+\frac{1}{4}$

$\tilde{y} = \bar{x}+\frac{1}{4}$

$\tilde{z} = z+\frac{3}{4}$

{NOTE: $(W,\vec{w})\vec{x} = W\vec{x}+\vec{w}$ }

$\Downarrow$ this means

$$(W,\vec{w})\vec{0} = W\vec{0}+\vec{w} = \vec{w}$$

* Hence, $\vec{w}$ represents the mapping of the origin O, by the isometry $(W,\vec{w})$

Alternatively, we could have written:

$$\left.\begin{aligned}\tilde{x} &= y+\tfrac{1}{4} = 0x+1y+0z+\tfrac{1}{4}\\ \tilde{y} &= \bar{x}+\tfrac{1}{4} = -1x+0y+0z+\tfrac{1}{4}\\ \tilde{z} &= z+\tfrac{3}{4} = 0x+0y+1z+\tfrac{3}{4}\end{aligned}\right] \Rightarrow W = \begin{pmatrix} 0 & 1 & 0\\ \bar{1} & 0 & 0\\ 0 & 0 & 1\end{pmatrix} \quad \vec{w} = \begin{pmatrix} 1/4\\ 1/4\\ 3/4\end{pmatrix}$$

43] Analysis of $(W, \vec{w})$

(A) Analysis of the linear part W

Rotation or Rotoinversion

(A1) $\boxed{\text{Determinant } W = \pm 1}$ < +1 (Proper) ⇒ Rotation ; −1 (Improper) ⇒ Rotoinversion

eg: $\text{Det}\,W = \begin{vmatrix} 0 & 1 & 0\\ \bar{1} & 0 & 0\\ 0 & 0 & 1\end{vmatrix} = -1\begin{vmatrix} -1 & 0\\ 0 & 1\end{vmatrix}$

$= -1(-1) = +1$

(A2) Fold of Rotation :

$\text{Trace}\,W = \underbrace{W_{ii}}_{\text{Einstein's convention}} = W_{11} + W_{22} + W_{33}$ (sum of principle diagonal terms)

[Sum over repeated indices]

{ NOTE:
Actually we should write this as:
$\text{Det}\,W \cdot \text{Trace}\,W = 2\cos\phi + 1$ }

we see that, $\boxed{\pm\text{Trace}\,W = 2\cos\phi + 1}$

(where ϕ is the rotation angle)

eg: $\text{Trace}\,W = 0+0+1 = 1$

and, $2\cos\phi + 1 = 2\cos 90^\circ + 1$

$= 2(0) + 1$

$= 1$

⇓

Actually, we will solve for ϕ:

$1 = 2\cos\phi + 1$

$\Rightarrow \cos\phi = 0$

$\Rightarrow \phi = 90^\circ$

⇒ thus, this is a 4-fold rotation.

{ **NOTE:** These properties remain true, even upon the change of coordinate system. }

(A3) Orientation of the Rotation Axis (or the mirror plane in case of $\bar{2}$) { i.e., in general, the orientation of the symmetry element }

(i) Eigenvalue approach

$$W\vec{u} = \vec{u} \quad \text{for } \vec{u} \text{ along axis of } W$$

{ **NOTE:** For rotoinversion we use: $W\vec{u} = -\vec{u}$ }

eg: $\begin{pmatrix} 0 & 1 & 0 \\ \bar{1} & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix}\begin{pmatrix} u \\ v \\ w \end{pmatrix} = \begin{pmatrix} u \\ v \\ w \end{pmatrix}$

$$\Rightarrow \left.\begin{aligned} v &= u \\ -u &= v \end{aligned}\right\} \Rightarrow \therefore u = 0,\ v = 0$$
$$w = w$$

Hence we get $\begin{pmatrix} 0 \\ 0 \\ w \end{pmatrix}$

and the unit vector is $\begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix}$

So, our rotation axis is:

$$\vec{u} = \begin{pmatrix} 0 \\ 0 \\ w \end{pmatrix} \text{ or } \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix}$$

(ii) $Y(W)$ approach:

Let k be the order of W

Define $Y(W) = W^{k-1} + W^{k-2} + \ldots + W + I$

Consider an arbitrary vector $\vec{v}$

This is transformed to another vector $\vec{u}$ by $Y(W)$

{ **NOTE:** For rotoinversion, use $Y(-W)$ instead }

i.e. $\Rightarrow \vec{u} = Y(W)\vec{v}$

$$= (W^{k-1} + W^{k-2} + \ldots + W + I)\vec{v}$$

From here we see that:

$$W\vec{u} = \vec{u} \qquad \{ \text{since } W^k = I \text{ as } k \text{ is the order} \}$$

Thus, $Y(W)$ transforms any arbitrary vector $\vec{v}$ to a vector $\vec{u}$ along the rotation axis.

* **NOTE!** For $\det W = -1$, use $Y(-W)$

eg: For our case, we get

$$Y(W) = W^3 + W^2 + W + I$$
$$= \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 4 \end{pmatrix}$$

Let $\vec{v} = \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix}$, $Y(W)\vec{v} = \begin{pmatrix} 0 \\ 0 \\ 0 \end{pmatrix}$ $\rightsquigarrow$ This DOES NOT give the axis

[The reason being that we have selected a $\vec{v}$ that is perpendicular to the rotation axis]

for such a case, choose another $\vec{v}$

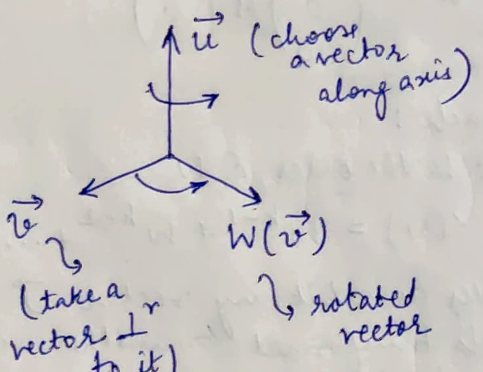
LECTURE 9 (01/02/2024)

Let $\vec{v} = \begin{pmatrix} 1 \\ 1 \\ 1 \end{pmatrix}$

then, $Y(W)\vec{v} = \begin{pmatrix} 0 \\ 0 \\ 4 \end{pmatrix} \Rightarrow \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix}$

(this is the reqd. vector along the axis)

44] (A4) Sense of Rotation



$\therefore$ Right Hand (RH) Rotation
$\equiv$ Counter clockwise Rotation
(Looking down $-\vec{u}$)
$\equiv$ +ve Rotation

Now, construct a matrix:

$$Z = \left[\, \vec{u} \;\vdots\; \vec{v} \;\vdots\; W(\vec{v}) \,\right]$$

Here, $\text{Det } Z = \begin{cases} +\text{ve} \Rightarrow \text{RH Rotation (i.e. +ve Rotation)} \\ -\text{ve} \Rightarrow \text{LH Rotation (i.e. −ve Rotation)} \end{cases}$

eg: For a given rotation 4_{001}
(i.e. 4-fold where axis is along $\begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix}$)

Here, $\vec{u} = \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix}$

Take a simple $\vec{v} = \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix} \underset{\text{thus}}{\Rightarrow} Z = \begin{pmatrix} 0 & 1 & 0 \\ 0 & 0 & \bar{1} \\ 1 & 0 & 0 \end{pmatrix}$

$\Rightarrow \text{Det } Z = -1 \Rightarrow 4^{-}_{001}$ (i.e. for (−ve rotation))

45] (B) Analysis of translation part $\vec{w}$

$$\vec{w} = \underbrace{\vec{w}_g}_{\substack{\text{intrinsic} \\ \text{translation}}} + \underbrace{\vec{w}_l}_{\substack{\text{location} \\ \text{part}}}$$

intrinsic translation (eg: in screw, glide)

location part (i.e. location of the axis)

Intrinsic Translation $\vec{w}_g$

$\vec{w}_g = 0 \Rightarrow$ Pure rotation

$\vec{w}_g \neq 0 \Rightarrow$ Screw or glide

Let k be the order of W, i.e. $W^k = I$

We need to find $(W, \vec{w})^2 \equiv (W, \vec{w})(W, \vec{w})$

* { NOTE: $(A, \vec{a})(B, \vec{b})\vec{x}$

$$= (A, \vec{a})\{B\vec{x} + \vec{b}\}$$

$$= A(B\vec{x} + \vec{b}) + \vec{a}$$

$$= AB\vec{x} + A\vec{b} + \vec{a}$$

$$\Rightarrow (A, \vec{a})(B, \vec{b}) \equiv (AB, A\vec{b} + \vec{a})$$ }

Thus : $(W, \vec{w})^2 = (W^2, W\vec{w} + \vec{w})$

Similarly, $(W, \vec{w})^3 = (W^2, W\vec{w} + \vec{w})(W, \vec{w})$

$$= (W^3, W^2\vec{w} + W\vec{w} + \vec{w})$$

$\vdots$ in general :

$$\therefore (W, \vec{w})^k = (W^k, W^{k-1}\vec{w} + W^{k-2}\vec{w} + \dots + W\vec{w} + \vec{w})$$

$$= (\underbrace{I}_{\substack{\text{since rotation} \\ \text{is Identity}}}, Y(W)\vec{w})$$

{ since $W^k = I$; and from our definition for $Y(W)$ }

since rotation is Identity

$\downarrow$

thus, this means

* k^{th} power of $(W, \vec{w})$ is always a pure translation

Now, let $\vec{w}_g$ be the intrinsic translation associated with $(W, \vec{w})$

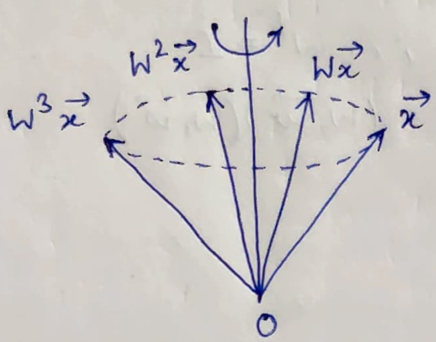
So we can write :

$$Y(W)\vec{w} = k\,\vec{w_g}$$

{i.e., after k applications of $(W, \vec{w})$ we have a pure translation, which is k times the intrinsic translation}

$$\Rightarrow \boxed{\vec{w_g} = \frac{Y(W)\vec{w}}{k}}$$

46] Geometrical Interpretation of Y(W)



If we add up all these vectors, we can see that we will get a vector along the axis

$$W^{k-1}\vec{x} + \dots + I\vec{x}$$

$$\equiv Y(W)\vec{x}$$

$$=$$ Translation along the axis

For eg: Using our initial $W = \begin{pmatrix} 0 & 1 & 0 \\ \bar{1} & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix}$, $\vec{w} = \begin{pmatrix} 1/4 \\ 1/4 \\ 3/4 \end{pmatrix}$ $\underset{\text{we saw}}{\Rightarrow}$ $Y(W) = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 4 \end{pmatrix}$

Here $\Rightarrow \vec{w_g} = \frac{1}{4}\begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 4 \end{pmatrix}\begin{pmatrix} 1/4 \\ 1/4 \\ 3/4 \end{pmatrix} = \frac{1}{4}\begin{pmatrix} 0 \\ 0 \\ 3 \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ 3/4 \end{pmatrix}$

$\therefore \Rightarrow$ We have a four-fold screw axis with a $3/4$ translation along the axis

$\downarrow$

i.e. $\bar{4}_3$ screw axis

The translation is obtained by: dividing smaller subscript by larger number (i.e. here, $3/4$)

(however earlier we also represented the orientation, in $\bar{4}_{001}$)

$\downarrow$

So we could say (for now) :

$\bar{4}_3$ operation along [001]

47] **Location of the axis**

Location part and reduced operation

$\vec{w}_l = \vec{w} - \vec{w}_g$ ($\vec{w}_l$ is the location part, and it fixes the axis)

Reduced operation $\equiv (W, \vec{w}_l)$

$$\underset{\text{Original isometry}}{(W, \vec{w})} \longrightarrow \underset{\text{Reduced operation}}{(W, \vec{w}_l)}$$

We can use the multiplication property to split the reduced operation as follows:

$$(W, \vec{w}_l) = (W, \vec{w} - \vec{w}_g)$$
$$= (I, -\vec{w}_g)(W, \vec{w})$$

As intrinsic translation is removed, $(W, \vec{w}_l)$ is a pure rotation, and the fixed points of $(W, \vec{w}_l)$ give the location of the axis.

So, solving the eigenvalue eqⁿ:

$(W, \vec{w}_l)\,\vec{x}_F = \vec{x}_F$, will give us the location of the axis

eg: $\vec{w} = \begin{pmatrix} 1/4 \\ 1/4 \\ 3/4 \end{pmatrix}$, $\vec{w}_g = \begin{pmatrix} 0 \\ 0 \\ 3/4 \end{pmatrix} \Rightarrow \vec{w}_l = \begin{pmatrix} 1/4 \\ 1/4 \\ 0 \end{pmatrix}$

So our reduced operator is:

$$\left\{ \begin{pmatrix} 0 & 1 & 0 \\ \bar{1} & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix}, \begin{pmatrix} 1/4 \\ 1/4 \\ 0 \end{pmatrix} \right\}$$

So fixed points are solved from:

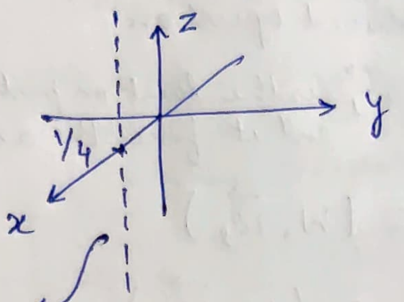
$$\begin{pmatrix} x_F \\ y_F \\ z_F \end{pmatrix} = \begin{pmatrix} 0 & 1 & 0 \\ \bar{1} & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix}\begin{pmatrix} x_F \\ y_F \\ z_F \end{pmatrix} + \begin{pmatrix} 1/4 \\ 1/4 \\ 0 \end{pmatrix}$$

$$\Rightarrow \left.\begin{aligned} x_F &= y_F + 1/4 \\ y_F &= -x_F + 1/4 \end{aligned}\right] \Rightarrow x_F = 1/4,\ y_F = 0$$

$$z_F = z_F$$

i.e. there is "no control" on z_F

Now we have a complete picture of our screw axis:



this is the axis {given by set of points $(\frac{1}{4}, 0, z)$}

48] International (IT) notation of resulting symmetry operation

{NOTE: We saw, that all this information we obtained

↓

Come from the original coordinate triplet

eg: $y+\frac{1}{4}, \bar{x}+\frac{1}{4}, z+\frac{3}{4}$

⟹ So this coord. triplet is equivalent to the IT notation}

Now, the internation notation will be in the following form:

$$\underbrace{4^-}_{\text{rotation with its dir}^n} \underbrace{(0,0,\tfrac{3}{4})}_{\text{intrinsic translation}} \underbrace{\tfrac{1}{4}, 0, z}_{\text{axis}}$$

LECTURE 10 (05/02/2024)

49] An example of solving for the case of rotoinversion (eg: glide):

Here, $|W| = -1$ (thus, rotoinversion)

Also, $-\text{Trace } W = 2\cos\phi + 1$ {eg: $\phi = 0°$ or $360° \Rightarrow \bar{1}$

$\phi = 180° \Rightarrow \bar{2}$

⋮ so on}

Now, let's say we get $\bar{2}$.

↓

to check whether it is a mirror or glide

↓

we need to determine using $\vec{w}$

From $\vec{w} \Rightarrow$ get $\vec{w}_g$ $\begin{cases} \vec{w}_g = \vec{0} \Rightarrow \text{mirror} \\ \vec{w}_g \neq \vec{0} \Rightarrow \text{glide} \end{cases}$ i.e.

$(\vec{\tilde{x}} = (W,\vec{w})(W,\vec{w})\vec{x})$

$P \xrightarrow{2\vec{w}_g} P''$ glide plane

$\xrightarrow{\vec{w}_g} P'(\vec{\tilde{x}} = (W,\vec{w})\vec{x})$

Here, $(W, \vec{w})^2 = (W, \vec{w})(W, \vec{w})$

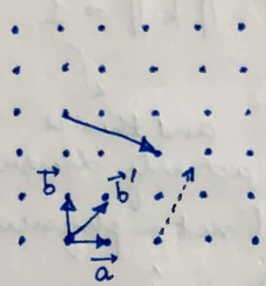
$$= (W^2, W\vec{w} + \vec{w})$$
$$= (I, \underbrace{W\vec{w} + \vec{w}}_{2\vec{w}_g})$$

$$\Rightarrow \boxed{2\vec{w}_g = (W+I)\vec{w}}$$

$$Y(-W) = (-W)^{2-1} + I = -W + I$$

$Y(-W)\vec{v} = \vec{u}$ along rotoinversion axis (i.e. $\bar{2}$ axis)

50] Crystallographic Computations



Lattice points : A period set of points

Lattice translation : A translation vector joining any two lattice points

The solid vectors ($\rightarrow$) are translation vectors

But dotted vector ($\dashrightarrow$) is NOT.

Basis vectors : Any two/set of (in higher dimensions) linearly independent vectors, are basis vectors.

Crystallographic Basis : A set of linearly independent lattice translations.

(In the above diagram:
$\vec{a}$ and $\vec{b}$ form an orthogonal basis ;
But instead, we could also use $\vec{a}$ and $\vec{b}'$ which form a non-orthogonal basis)

51] Calculations of lengths & angles in crystallographic basis

eg: What is the length of [1,1] vector in the basis $\{\vec{a}, \vec{b}\}$ shown above ?

* The meaning of [1,1] is essentially a shorthand for $1\vec{a} + 1\vec{b}$

Now, these are basis vectors
+
But that need not
mean that they are of length 1

Thus, for orthogonal basis vectors $\vec{a}$ and $\vec{b}$:

$$\| [1,1] \| = \sqrt{a^2+b^2}$$

Here, since $a=b \Rightarrow \| [1,1] \| = \sqrt{2}\,a$

52] Important distinction between orthonormal basis (i.e. cartesian basis), and general crystallographic basis
↓

Orthonormal basis: $\{\hat{i}, \hat{j}, \hat{k}\}$

where $\|\hat{i}\| = \|\hat{j}\| = \|\hat{k}\| = 1$

and this is actually dimensionless (not a physical length)

We write, $\vec{r} = \underbrace{x\hat{i} + y\hat{j} + z\hat{k}}$

Here, x, y, z have dimensions of length

Crystallographic basis: $\{\underbrace{\vec{a}, \vec{b}, \vec{c}}\}$
↓
Here, the basis vectors themselves have a physical length dimension! *

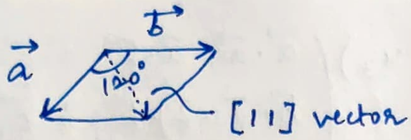
{and to thus maintain a length dimension for $\vec{r}$, the components here will be dimensionless} *

$$\vec{r} = x\vec{a} + y\vec{b} + z\vec{c} \qquad (x, y, z \text{ are dimensionless})$$

eg: ∴ $\| [111] \| \neq \sqrt{3}$ in a cubic crystal with lattice parameter a

instead it will be $\sqrt{3}\,a$.

eg: Consider [11] vector in the hexagonal basis
(i.e. $a=b$, $\gamma = 120°$)



$$[11] = 1\vec{a} + 1\vec{b} = \vec{a} + \vec{b}$$

So, here from the diagram we see that:

$$\|\vec{a}+\vec{b}\| = \|\vec{a}\| = a$$

(since they form parts of an equilateral triangle)

53] Dot product of two vectors in crystallographic basis

Let's say we have two vectors:

$$\vec{u} = [u_1, u_2, u_3]$$
$$\vec{v} = [v_1, v_2, v_3]$$

in orthonormal basis.

Then: $$\vec{u}\cdot\vec{v} = u_1 v_1 + u_2 v_2 + u_3 v_3$$

Now, let these vectors $\vec{u}$ and $\vec{v}$ be represented by their components in a crystallographic basis:

$$\vec{u} = u_1\vec{a} + u_2\vec{b} + u_3\vec{c}$$
$$\vec{v} = v_1\vec{a} + v_2\vec{b} + v_3\vec{c}$$

{**NOTE**: This $\vec{u}$ and $\vec{v}$ is NOT the same as before}

Then: $$\vec{u}\cdot\vec{v} = (u_1\vec{a} + u_2\vec{b} + u_3\vec{c})\cdot(v_1\vec{a} + v_2\vec{b} + v_3\vec{c})$$

$$\begin{aligned} &= u_1 v_1\,\vec{a}\cdot\vec{a} + u_1 v_2\,\vec{a}\cdot\vec{b} + u_1 v_3\,\vec{a}\cdot\vec{c} \\ &\quad + u_2 v_1\,\vec{b}\cdot\vec{a} + u_2 v_2\,\vec{b}\cdot\vec{b} + u_2 v_3\,\vec{b}\cdot\vec{c} \\ &\quad + u_3 v_1\,\vec{c}\cdot\vec{a} + u_3 v_2\,\vec{c}\cdot\vec{b} + u_3 v_3\,\vec{c}\cdot\vec{c} \end{aligned}$$

{i.e., here we will have 9 terms instead of just 3, as we saw for orthonormal}

In order to simplify this, we use matrix notation:

$$\vec{u}\cdot\vec{v} = (u_1\ u_2\ u_3)\begin{pmatrix} v_1\,\vec{a}\cdot\vec{a} + v_2\,\vec{a}\cdot\vec{b} + v_3\,\vec{a}\cdot\vec{c} \\ v_1\,\vec{b}\cdot\vec{a} + v_2\,\vec{b}\cdot\vec{b} + v_3\,\vec{b}\cdot\vec{c} \\ v_1\,\vec{c}\cdot\vec{a} + v_2\,\vec{c}\cdot\vec{b} + v_3\,\vec{c}\cdot\vec{c} \end{pmatrix}$$

$$= (u_1\ u_2\ u_3)\underbrace{\begin{pmatrix} \vec{a}\cdot\vec{a} & \vec{a}\cdot\vec{b} & \vec{a}\cdot\vec{c} \\ \vec{b}\cdot\vec{a} & \vec{b}\cdot\vec{b} & \vec{b}\cdot\vec{c} \\ \vec{c}\cdot\vec{a} & \vec{c}\cdot\vec{b} & \vec{c}\cdot\vec{c} \end{pmatrix}}\begin{pmatrix} v_1 \\ v_2 \\ v_3 \end{pmatrix}$$

Matrix of dot products of the basis vectors

↓

called the

"<u>METRIC TENSOR</u>", G

(or metric matrix)

$$= (u_1\ u_2\ u_3)\,(G)\begin{pmatrix} v_1 \\ v_2 \\ v_3 \end{pmatrix}$$

From the definition of G, it is clear that :

$$G^T = G$$, i.e. G <u>is a symmetric matrix</u> *

<u>Special case</u> :

↓

for Orthonormal basis :

$$G_{\text{orthonormal}} = \begin{pmatrix} \hat{i}\cdot\hat{i} & \hat{i}\cdot\hat{j} & \hat{i}\cdot\hat{k} \\ \hat{j}\cdot\hat{i} & \hat{j}\cdot\hat{j} & \hat{j}\cdot\hat{k} \\ \hat{k}\cdot\hat{i} & \hat{k}\cdot\hat{j} & \hat{k}\cdot\hat{k} \end{pmatrix} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} = I$$

(identity matrix)

Then:
$$\vec{u}\cdot\vec{v} = (u_1\ u_2\ u_3)\,(I)\begin{pmatrix} v_1 \\ v_2 \\ v_3 \end{pmatrix}$$

$$= (u_1\ u_2\ u_3)\begin{pmatrix} v_1 \\ v_2 \\ v_3 \end{pmatrix} = u_1v_1 + u_2v_2 + v_3v_3$$

54] <u>Length</u> :

$$\|\vec{u}\| = (\vec{u}\cdot\vec{u})^{1/2}$$

$$= \left[(u_1\ u_2\ u_3)\,(G)\begin{pmatrix} u_1 \\ u_2 \\ u_3 \end{pmatrix}\right]^{1/2}$$

<u>Angle between two vectors</u> :

$$\cos\theta = \frac{\vec{u}\cdot\vec{v}}{\|\vec{u}\|\,\|\vec{v}\|} = \frac{\left[(u_1\ u_2\ u_3)\,(G)\begin{pmatrix} v_1 \\ v_2 \\ v_3 \end{pmatrix}\right]}{\|\vec{u}\|\ \|\vec{v}\|}$$

use length formula above for these

Volume of a unit cell

$$(a, b, c, \alpha, \beta, \gamma)$$

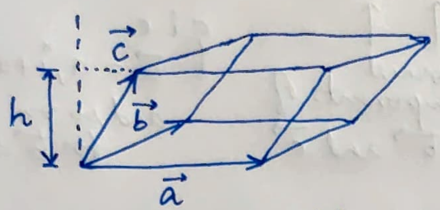
angle b/w $\vec{b}$ and $\vec{c}$

$V_{cubic} = a^3 \quad (a=b=c,\ \alpha=\beta=\gamma=90°)$

$V_{Tetragonal} = a^2 c \quad (a=b\neq c,\ \alpha=\beta=\gamma=90°)$

Now, we want to find the volume for triclinic case:

(i.e. $a\neq b\neq c,\ \alpha\neq\beta\neq\gamma$)



$$V = \text{Area of base } (\vec{a}, \vec{b}) \times \text{height}$$

$$= |\vec{a}\times\vec{b}| \cdot h$$

$$= (\vec{a}\times\vec{b})\cdot\vec{c}$$

steps left as an exercise

Let us introduce an orthonormal basis $(\hat{i}, \hat{j}, \hat{k})$

Then: $\begin{vmatrix} a_1 & a_2 & a_3 \\ b_1 & b_2 & b_3 \\ c_1 & c_2 & c_3 \end{vmatrix} = \vec{a}\cdot(\vec{b}\times\vec{c}) = V$

{These are the components of $\vec{a}$, $\vec{b}$ and $\vec{c}$ in $(\hat{i}, \hat{j}, \hat{k})$ basis}

LECTURE 11 (12/02/2024)

55] Metric Tensor (continued.)

Review: We have seen that: for orthonormal basis, the dot product is

i.e. $\{\hat{i}, \hat{j}, \hat{k}\}$

$$\vec{u}\cdot\vec{v} = (u_1\ u_2\ u_3)\begin{pmatrix} v_1 \\ v_2 \\ v_3 \end{pmatrix} = u_1v_1 + u_2v_2 + u_3v_3$$

In a general basis $\{\vec{a}, \vec{b}, \vec{c}\}$: the above relation is not true

Instead we observe:

$$\vec{u}\cdot\vec{v} = (u_1\ u_2\ u_3)\,(G)\begin{pmatrix} v_1 \\ v_2 \\ v_3 \end{pmatrix}$$

Based on which we get:

$$G = \begin{pmatrix} \vec{a}\cdot\vec{a} & \vec{a}\cdot\vec{b} & \vec{a}\cdot\vec{c} \\ \vec{b}\cdot\vec{a} & \vec{b}\cdot\vec{b} & \vec{b}\cdot\vec{c} \\ \vec{c}\cdot\vec{a} & \vec{c}\cdot\vec{b} & \vec{c}\cdot\vec{c} \end{pmatrix}$$

Also, for Volume we saw:

$$V = (\vec{a}\times\vec{b})\cdot\vec{c} = \begin{vmatrix} a_1 & b_1 & c_1 \\ a_2 & b_2 & c_2 \\ a_3 & b_3 & c_3 \end{vmatrix}$$

orthonormal components of $\vec{a}$, $\vec{b}$ and $\vec{c}$

{ i.e. $\vec{a} = a_1\hat{i} + a_2\hat{j} + a_3\hat{k}$ and so on for $\vec{b}$ & $\vec{c}$ }

56] Based on this, we can define:

$$A \equiv \begin{bmatrix} a_1 & b_1 & c_1 \\ a_2 & b_2 & c_2 \\ a_3 & b_3 & c_3 \end{bmatrix}$$, and then we know that: $V = \det(A)$

We can now find A^TA (just to see what we get):

$$A^TA = \begin{pmatrix} a_1 & a_2 & a_3 \\ b_1 & b_2 & b_3 \\ c_1 & c_2 & c_3 \end{pmatrix}\begin{pmatrix} a_1 & b_1 & c_1 \\ a_2 & b_2 & c_2 \\ a_3 & b_3 & c_3 \end{pmatrix}$$

$$= \begin{pmatrix} a_1^2+a_2^2+a_3^2 & a_1b_1+a_2b_2+a_3b_3 & a_1c_1+a_2c_2+a_3c_3 \\ a_1b_1+a_2b_2+a_3b_3 & b_1^2+b_2^2+b_3^2 & b_1c_1+b_2c_2+b_3c_3 \\ c_1a_1+c_2a_2+c_3a_3 & c_1b_1+c_2b_2+c_3b_3 & c_1^2+c_2^2+c_3^2 \end{pmatrix}$$

$$= \begin{pmatrix} \vec{a}\cdot\vec{a} & \vec{a}\cdot\vec{b} & \vec{a}\cdot\vec{c} \\ \vec{b}\cdot\vec{a} & \vec{b}\cdot\vec{b} & \vec{b}\cdot\vec{c} \\ \vec{c}\cdot\vec{a} & \vec{c}\cdot\vec{b} & \vec{c}\cdot\vec{c} \end{pmatrix}$$

$$= G$$

Thus we see the result that: $\boxed{G = A^TA}$

This means that: $\mathrm{Det}(G) = \mathrm{Det}(A^TA) = \mathrm{Det}(A^T)\cdot\mathrm{Det}(A)$
$= [\mathrm{Det}\,A]^2 = V^2$

Thus, we have: $\boxed{V = \sqrt{\mathrm{Det}\,G}}$

57] <u>G in terms of lattice parameters</u> (i.e., $a, b, c, \alpha, \beta, \gamma$)

$G_{11} = \vec{a}\cdot\vec{a} = a^2$
$G_{22} = \vec{b}\cdot\vec{b} = b^2$
$G_{33} = \vec{c}\cdot\vec{c} = c^2$

$G_{12} = \bar{a} \cdot \bar{b} = ab \cos\gamma$
$G_{13} = \bar{a} \cdot \bar{c} = ac \cos\beta$
$G_{23} = \bar{b} \cdot \bar{c} = bc \cos\alpha$

$$G = \begin{pmatrix} a^2 & ab\cos\gamma & ac\cos\beta \\ ab\cos\gamma & b^2 & bc\cos\alpha \\ ac\cos\beta & bc\cos\alpha & c^2 \end{pmatrix}$$

From here, we can see:

$$V = (\det G)^{1/2}$$
$$= abc\left[1 - \cos^2\alpha - \cos^2\beta - \cos^2\gamma + 2\cos\alpha\cos\beta\cos\gamma\right]^{1/2}$$

58] <u>Demystification of $\det W = \pm 1$</u>

(where W is an isometry)

We have:
$$\vec{\tilde{x}} = W\vec{x}$$

Here, W is an isometry
i.e. no change in length occurs

(Also, here $\vec{0}$ will remain fixed)

thus $\Rightarrow \|\vec{x}\| = \|\vec{\tilde{x}}\|$

$\Rightarrow \|\vec{x}\| = \|W\vec{x}\|$

$\Rightarrow \vec{x}\cdot\vec{x} = W\vec{x}\cdot W\vec{x}$

$\Rightarrow x^T G x = (Wx)^T G (Wx)$

$\Rightarrow x^T G x = x^T W^T G W x$

Since x is an arbitrary vector, thus this implies:
$$W^T G W = G$$

Taking the determinant:
$$\text{Det}(W^T G W) = \text{Det}\, G$$

$$\Rightarrow (\text{Det}\, W^T)(\text{Det}\, G)(\text{Det}\, W) = \text{Det}\, G$$

The determinant of the metric is equal to the square of the volume

$\downarrow$

Thus, it cannot be zero

$\downarrow$

So we can divide both sides by Det G :

$$(\text{Det } W^T)(\text{Det } W) = 1$$

$$\Rightarrow (\text{Det } W)^2 = 1$$

$$\Rightarrow \boxed{\text{Det } W = \pm 1}$$

59] Reciprocal Basis

We have been currently using a crystallographic basis:

$$\mathcal{B} = \{\vec{a}, \vec{b}, \vec{c}\}$$

Now, for every basis $\mathcal{B}$, we define another basis $\mathcal{B}^*$ such that:

$$\mathcal{B}^* = \{\vec{a}^*, \vec{b}^*, \vec{c}^*\}$$

defined by relations:

$$\begin{cases} \vec{a}^* \cdot \vec{a} = 1, & \vec{a}^* \cdot \vec{b} = 0, & \vec{a}^* \cdot \vec{c} = 0 \\ \vec{b}^* \cdot \vec{a} = 0, & \vec{b}^* \cdot \vec{b} = 1, & \vec{b}^* \cdot \vec{c} = 0 \\ \vec{c}^* \cdot \vec{a} = 0, & \vec{c}^* \cdot \vec{b} = 0, & \vec{c}^* \cdot \vec{c} = 1 \end{cases}$$

in shorthand

This can be expressed in the following manner:

$$\begin{pmatrix} \vec{a}^* \\ \vec{b}^* \\ \vec{c}^* \end{pmatrix} \cdot \begin{pmatrix} \vec{a} & \vec{b} & \vec{c} \end{pmatrix} = I$$

NOTE: {Here, the elements of the vector are themselves vectors}

60] Explicit definitions of $\vec{a}^*, \vec{b}^*, \vec{c}^*$

$$\vec{a}^* \cdot \vec{a} = 1 \,, \quad \underbrace{\vec{a}^* \cdot \vec{b} = 0}_{} \,, \quad \underbrace{\vec{a}^* \cdot \vec{c} = 0}_{}$$

i.e. $\vec{a}^* \perp \vec{b}$ $\quad \vec{a}^* \perp \vec{c}$

this means that:

$\vec{a}^* \perp \text{Plane}(\vec{b}, \vec{c})$

i.e. the plane in which both $\vec{b}$ & $\vec{c}$ lie

$$\Rightarrow \vec{a}^* \parallel \vec{b} \times \vec{c}$$

$$\Rightarrow \vec{a}^* = k(\vec{b} \times \vec{c})$$, for some k

Since we know that $\vec{a}^* \cdot \vec{a} = 1$:

$$\therefore k(\vec{b} \times \vec{c}) \cdot \vec{a} = 1$$

$$\Rightarrow kV = 1$$

$$\Rightarrow \boxed{k = \frac{1}{V}}$$

Hence we get that:

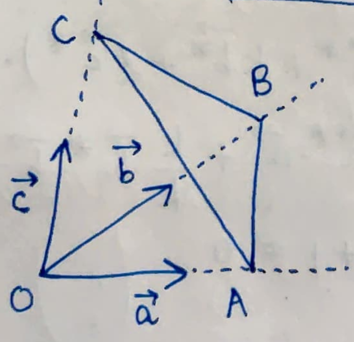
{after doing the same for $\vec{b}^*$ and $\vec{c}^*$} :

$$\boxed{\vec{a}^* = \frac{\vec{b} \times \vec{c}}{V} \,, \quad \vec{b}^* = \frac{\vec{c} \times \vec{a}}{V} \,, \quad \vec{c}^* = \frac{\vec{a} \times \vec{b}}{V}}$$

(from this we see that the dimension of $\vec{a}^*$, $\vec{b}^*$ and $\vec{c}^*$ is $\frac{1}{L}$)

which is why we call them reciprocal basis

61] Demystification of definition of Miller indices of Planes



Miller indices of plane ABC :

intercepts :	OA	OB	OC
dimensionless intercepts :	$\frac{OA}{a}$	$\frac{OB}{b}$	$\frac{OC}{c}$
Take the reciprocals :	$\frac{a}{OA}$	$\frac{b}{OB}$	$\frac{c}{OC}$

we know that we simply define these reciprocals as Miller indices

↓

i.e. $h = \frac{a}{OA}$, $k = \frac{b}{OB}$, $l = \frac{c}{OC}$

{ The question is, we could have directly chosen OA and OB and OC, and defined that as Miller indices (since they also identify the plane equivalently)

↓

So what is the advantage of this reciprocal definition? }

Let's say we construct a vector in "reciprocal space" with components h, k, l :

$$\vec{g}^*_{hkl} \equiv h\vec{a}^* + k\vec{b}^* + l\vec{c}^*$$

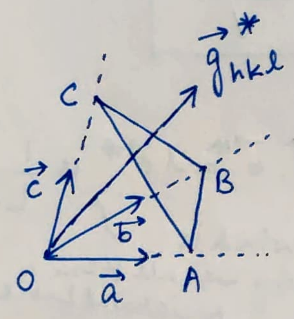
From our diagram now, we know :

$$\vec{AB} = \vec{OB} - \vec{OA}$$

where, $\vec{OB} = OB\ \widehat{OB} = OB\ \frac{\vec{b}}{b} = \frac{b}{k}\frac{\vec{b}}{b} = \frac{\vec{b}}{k}$

and similarly:

$\vec{OA} = \frac{\vec{a}}{h}$, $\vec{OC} = \frac{\vec{c}}{l}$



Thus :

$$\vec{AB} = \frac{\vec{b}}{k} - \frac{\vec{a}}{h}$$

What is the relation b/w $\vec{g}^*_{hkl}$ and $\vec{AB}$?

$$\vec{g}^*_{hkl} \cdot \vec{AB} = (h\vec{a}^* + k\vec{b}^* + l\vec{c}^*) \cdot \left(\frac{\vec{b}}{k} - \frac{\vec{a}}{h}\right)$$

$$= -\frac{h}{h}\vec{a}^* \cdot \vec{a} + \frac{k}{k}\vec{b}^* \cdot \vec{b}$$

$$= -1 + 1 = 0$$

$$\Rightarrow \vec{g}^*_{hkl} \cdot \vec{AB} = 0$$

Similarly, if we try for the others (BC and AC) we will get the same:

$$\vec{g}^{\,*}_{hkl} \cdot \vec{BC} = 0 \quad , \quad \vec{g}^{\,*}_{hkl} \cdot \vec{AC} = 0$$

And thus, we get that:

$$\vec{g}^{\,*}_{hkl} \perp \underbrace{\text{plane } (\vec{AB}, \vec{BC}, \vec{CA})}_{\text{OR}}$$

plane ABC

$\Downarrow$

i.e.

The vector in reciprocal space with components h, k, l identifies the normal to a plane having miller indices h, k, l.

*{**NOTE:** $d_{hkl} \equiv$ distance of (hkl) plane from origin

$=$ Projection of OA on normal

$= \dfrac{\vec{OA} \cdot \vec{g}^{\,*}_{hkl}}{|\vec{g}^{\,*}_{hkl}|}$

$= \dfrac{1}{|\vec{g}^{\,*}_{hkl}|} \underset{\text{i.e.}}{\Rightarrow} |\vec{g}^{\,*}_{hkl}| = \dfrac{1}{d_{hkl}}$ }

LECTURE 12 (15/02/2024)

62] Coord. system = Origin (O) + Basis vectors $B = \{\vec{a}, \vec{b}, \vec{c}\}$

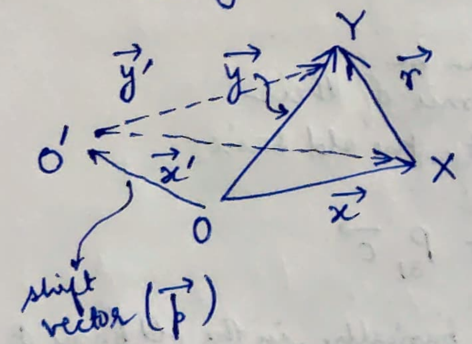
Vectors change upon coord. transformation

$\downarrow$

New coord. components. $= f($old coord. components$)$

Coordinate Transformation:
- Only origin shift $O \to O'$
- Only change of basis vectors $\{\vec{a}, \vec{b}, \vec{c}\} \to \{\vec{a}', \vec{b}', \vec{c}'\}$
- Both origin shift and basis change

63] 1. Origin Shift



$$\vec{x} = \begin{pmatrix} x_1 \\ x_2 \\ x_3 \end{pmatrix} \quad \vec{y} = \begin{pmatrix} y_1 \\ y_2 \\ y_3 \end{pmatrix}$$

$$\vec{r} = \vec{y} - \vec{x} = \begin{pmatrix} y_1 - x_1 \\ y_2 - x_2 \\ y_3 - x_3 \end{pmatrix}$$

Now, $\vec{p}$ = origin shift vector $= \vec{OO'}$

$$\therefore \vec{p} + \vec{x}' = \vec{x}$$

$$* \Rightarrow \vec{x}' = \vec{x} - \vec{p} = \begin{pmatrix} x_1 \\ x_2 \\ x_3 \end{pmatrix} - \begin{pmatrix} p_1 \\ p_2 \\ p_3 \end{pmatrix} = \boxed{\begin{pmatrix} x_1 - p_1 \\ x_2 - p_2 \\ x_3 - p_3 \end{pmatrix}}$$

$$\Rightarrow \vec{x}' = I\vec{x} - \vec{p} = (I, -\vec{p})\,\vec{x}$$
$$= (I, \vec{p})^{-1}\,\vec{x}$$

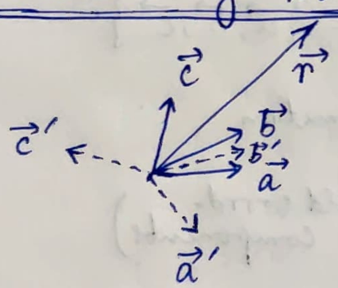
$\Big\{$ Since we know that :
$$(W, \vec{w})^{-1} = (W^{-1}, -W^{-1}\vec{w}) \Big\}$$

Thus we have :
$$\boxed{\vec{x}' = (I, \vec{p})^{-1}\,\vec{x}}$$

i.e. the coordinates will change due to origin shift

But the components of a "distance vector" $\overrightarrow{XY}$ do NOT change on origin shift :
$$\boxed{\overrightarrow{XY} = \vec{r} = \vec{y} - \vec{x} = \vec{y}' - \vec{x}'}$$

64] 2. **Basis change with fixed origin**



Here, $\vec{r} = x_1\vec{a} + x_2\vec{b} + x_3\vec{c}$
$= x_1'\vec{a}' + x_2'\vec{b}' + x_3'\vec{c}'$

i.e. $\begin{pmatrix} x_1' \\ x_2' \\ x_3' \end{pmatrix} = f\begin{pmatrix} x_1 \\ x_2 \\ x_3 \end{pmatrix}$

what is this f ?

To find the function f, we need the relationship of the new basis to the old basis

↓

New basis vectors can be expressed in terms of their components w.r.t. the old basis

$$\vec{a}' = P_{11}\vec{a} + P_{21}\vec{b} + P_{31}\vec{c}$$

$\Big\{$ i.e, basically, in the old basis $\mathcal{B}$:
$$(\vec{a}')_{\mathcal{B}} = \begin{pmatrix} P_{11} \\ P_{21} \\ P_{31} \end{pmatrix} \Big\}$$

Similarly, we can say:

$$\vec{b}' = P_{12}\vec{a} + P_{22}\vec{b} + P_{32}\vec{c}$$

$$\vec{c}' = P_{13}\vec{a} + P_{23}\vec{b} + P_{33}\vec{c}$$

which gives us:

$$(\vec{a}' \ \vec{b}' \ \vec{c}') = (\vec{a} \ \vec{b} \ \vec{c})\begin{pmatrix} P_{11} & P_{12} & P_{13} \\ P_{21} & P_{22} & P_{23} \\ P_{31} & P_{32} & P_{33} \end{pmatrix}$$

$$= (\vec{a} \ \vec{b} \ \vec{c})\, P$$

this is essentially the "relationship matrix"

However, we want to find the relationship for $x_1', x_2' x_3'$ in terms of x_1, x_2, x_3:

$$\vec{r} = x_1\vec{a} + x_2\vec{b} + x_3\vec{c} = (\vec{a} \ \vec{b} \ \vec{c})\begin{pmatrix} x_1 \\ x_2 \\ x_3 \end{pmatrix}$$

$$= x_1'\vec{a}' + x_2'\vec{b}' + x_3'\vec{c}' = (\vec{a}' \ \vec{b}' \ \vec{c}')\begin{pmatrix} x_1' \\ x_2' \\ x_3' \end{pmatrix}$$

From this, we get:

$$(\vec{a} \ \vec{b} \ \vec{c})\begin{pmatrix} x_1 \\ x_2 \\ x_3 \end{pmatrix} = (\vec{a}' \ \vec{b}' \ \vec{c}')\begin{pmatrix} x_1' \\ x_2' \\ x_3' \end{pmatrix}$$

$$= (\vec{a} \ \vec{b} \ \vec{c})(P)\begin{pmatrix} x_1' \\ x_2' \\ x_3' \end{pmatrix}$$

Thus,

$$\begin{pmatrix} x_1 \\ x_2 \\ x_3 \end{pmatrix} = P\begin{pmatrix} x_1' \\ x_2' \\ x_3' \end{pmatrix}$$

{here, the old components are being expressed in terms of new}

$$\Rightarrow \boxed{\begin{pmatrix} x_1' \\ x_2' \\ x_3' \end{pmatrix} = P^{-1}\begin{pmatrix} x_1 \\ x_2 \\ x_3 \end{pmatrix}}$$

Since P^{-1} is just some matrix itself, so we can give it another name:

Let, $P^{-1} \equiv Q \Rightarrow \boxed{\begin{pmatrix} x_1' \\ x_2' \\ x_3' \end{pmatrix} = Q\begin{pmatrix} x_1 \\ x_2 \\ x_3 \end{pmatrix}}$

{ or in other words :
$$\begin{pmatrix} x' \\ y' \\ z' \end{pmatrix} = Q \begin{pmatrix} x \\ y \\ z \end{pmatrix}$$
}

*** NOTE :** For this course, we will use the name "<u>Basis Transformation matrix</u>" for P, and "<u>Coordinate Transformation matrix</u>" for Q

In terms of matrix-column representation :
$$\vec{x}\,' = Q\,\vec{x}$$
$$= (Q, \vec{0})\,\vec{x}$$
$$= (P^{-1}, \vec{0})\,\vec{x}$$
$$= (P, \vec{0})^{-1}\,\vec{x}$$

65] Algorithm to find Q

Method I : ① Express the components of i^{th} ($i = 1, 2, 3$) new basis vector in terms of its components in old basis as the i^{th} column of matrix $\equiv P$

② $Q = P^{-1}$

Method II :
$$\begin{pmatrix} x_1' \\ x_2' \\ x_3' \end{pmatrix} = \begin{pmatrix} Q_{11} & Q_{12} & Q_{13} \\ Q_{21} & Q_{22} & Q_{23} \\ Q_{31} & Q_{32} & Q_{33} \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \\ x_3 \end{pmatrix}$$

* { **NOTE :** In this course, for clarity, we will always use W for symmetry transformations & P, Q will be for basis, coord. transformations

with W → the vector itself changes (basis is same)

with Q → vector remains SAME (only coord.s change due to new basis) }

i.e. here :
$$\begin{pmatrix} x_1' \\ x_2' \\ x_3' \end{pmatrix}_{B'} = Q \begin{pmatrix} x_1 \\ x_2 \\ x_3 \end{pmatrix}_{B}$$

Now, $\vec{a} = 1\vec{a} + 0\vec{b} + 0\vec{c}$

$$\therefore \Rightarrow \quad \vec{a}\,' = \begin{pmatrix} Q_{11} \\ Q_{21} \\ Q_{31} \end{pmatrix} = \begin{pmatrix} Q_{11} & Q_{12} & Q_{13} \\ Q_{21} & Q_{22} & Q_{23} \\ Q_{31} & Q_{32} & Q_{33} \end{pmatrix} \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix}$$

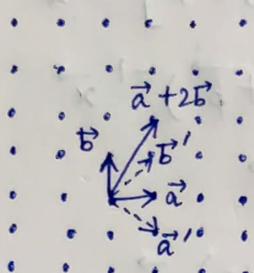
* Thus, we get:

$\vec{a}\,'$ = First column of Q
$\vec{b}\,'$ = Second column of Q
$\vec{c}\,'$ = Third column of Q

66] **For example:**

$\mathcal{B} \equiv \{\vec{a}, \vec{b}\}$ and $\mathcal{B}' \equiv \{\vec{a}\,', \vec{b}\,'\}$

Method I:



Here, $\vec{r} = \vec{a} + 2\vec{b} = \begin{pmatrix} 1 \\ 2 \end{pmatrix}_{\mathcal{B}}$; $\vec{a}\,' = 1\vec{a} - 1\vec{b}$, $\vec{b}\,' = 1\vec{a} + 1\vec{b}$

Now,

$$P = \begin{array}{c} \begin{array}{cc} \vec{a}\,' & \vec{b}\,' \\ \downarrow & \downarrow \end{array} \\ \begin{pmatrix} 1 & 1 \\ -1 & 1 \end{pmatrix} \end{array}$$

Thus:

$$Q = P^{-1} = \frac{1}{\det P}\begin{pmatrix} 1 & -1 \\ 1 & 1 \end{pmatrix}$$

$$= \frac{1}{2}\begin{pmatrix} 1 & -1 \\ 1 & 1 \end{pmatrix} = \begin{pmatrix} 1/2 & -1/2 \\ 1/2 & 1/2 \end{pmatrix}$$

Using this:

$$\begin{pmatrix} x' \\ y' \end{pmatrix} = \begin{pmatrix} 1/2 & -1/2 \\ 1/2 & 1/2 \end{pmatrix}\begin{pmatrix} 1 \\ 2 \end{pmatrix} = \begin{pmatrix} -1/2 \\ 3/2 \end{pmatrix} \rightsquigarrow \text{New components}$$

Method II:

↓

Direct method for Q

$$Q = \begin{pmatrix} 1/2 & -1/2 \\ 1/2 & 1/2 \end{pmatrix}$$

we write these by finding $\vec{a}$ in terms of $\vec{a}\,', \vec{b}\,'$ and $\vec{b}$ in terms of $\vec{a}\,', \vec{b}\,'$

3. Shift of origin as well as change of basis

67]

$$\begin{tikzcd} \vec{x} \arrow[r, "\text{Origin shift}", "(I,\vec{p})^{-1}"'] \arrow[rr, bend right, "(?)"'] & \vec{x}' \arrow[r, "\text{Basis change}", "(P,\vec{0})^{-1}"'] & \vec{x}'' \end{tikzcd}$$

Now,
$$\begin{aligned}
\vec{x}'' &= (P,\vec{0})^{-1}\vec{x}' \\
&= (P,\vec{0})^{-1}(I,\vec{p})^{-1}\vec{x} \\
&= \left[(I,\vec{p})(P,\vec{0})\right]^{-1}\vec{x} \\
&= (IP,\ I\vec{0}+\vec{p})^{-1}\vec{x} \\
&= (P,\vec{p})^{-1}\vec{x} \\
&= (P^{-1}, -P^{-1}\vec{p})\vec{x} \\
&= (Q, -Q\vec{p})\vec{x}
\end{aligned}$$

So the combined transformation can be written as:

$$\boxed{(P,\vec{p})^{-1} \quad \text{or} \quad (Q, -Q\vec{p})}$$

{where $\vec{p}$ gives shift of origin and P represents basis transformation}

68] **Revisiting the metric tensor**

Metric tensor can be also thought of as a basis transformation matrix from the real basis to the reciprocal basis

$$\vec{x}\cdot\vec{y} = (x_1\ x_2\ x_3)(G)\begin{pmatrix} y_1 \\ y_2 \\ y_3 \end{pmatrix}$$

Now, $\mathcal{B} = \{\vec{a}, \vec{b}, \vec{c}\} \Rightarrow$ "real" basis

$\mathcal{B}^* = \{\vec{a}^*, \vec{b}^*, \vec{c}^*\} \Rightarrow$ "reciprocal" basis

We know that:

$$\begin{pmatrix} \vec{a}^* & \vec{b}^* & \vec{c}^* \end{pmatrix} \cdot \begin{pmatrix} \vec{a} \\ \vec{b} \\ \vec{c} \end{pmatrix} \equiv I$$

{definition of $\vec{a}^*, \vec{b}^*$ and $\vec{c}^*$}

Now, any vector $\vec{r}$ can be expressed either in real basis, or the reciprocal basis

$$\vec{r} = x_1 \vec{a} + x_2 \vec{b} + x_3 \vec{c}$$
$$= x_1^* \vec{a}^* + x_2^* \vec{b}^* + x_3^* \vec{c}^*$$

So we can say:

$$\begin{pmatrix} x_1^* \\ x_2^* \\ x_3^* \end{pmatrix} = Q^* \begin{pmatrix} x_1 \\ x_2 \\ x_3 \end{pmatrix}$$

where,
$$Q^* = \begin{pmatrix} Q_{11}^* & Q_{12}^* & Q_{13}^* \\ Q_{21}^* & Q_{22}^* & Q_{23}^* \\ Q_{31}^* & Q_{32}^* & Q_{33}^* \end{pmatrix}$$

this will be $\vec{a}$ in terms of $\vec{a}^*, \vec{b}^*, \vec{c}^*$

and so on ...

i.e., $\vec{a} = Q_{11}^* \vec{a}^* + Q_{21}^* \vec{b}^* + Q_{31}^* \vec{c}^*$

$$\Rightarrow \underbrace{\vec{a} \cdot \vec{a}}_{G_{11}} = Q_{11}^* \underbrace{\vec{a}^* \cdot \vec{a}}_{1} + Q_{21}^* \overbrace{\cancel{\vec{b}^* \cdot \vec{a}}}^{0} + Q_{31}^* \overbrace{\cancel{\vec{c}^* \cdot \vec{a}}}^{0}$$

$$\therefore \Rightarrow \boxed{G_{11} = Q_{11}^*}$$

and similarly for all Q_{ij}^*.

$$\text{thus} \Rightarrow \boxed{Q^* = G}$$

*

METRIC TENSOR IS THE COORDINATE TRANSFORMATION MATRIX TO RECIPROCAL COORDINATES