Reciprocal space

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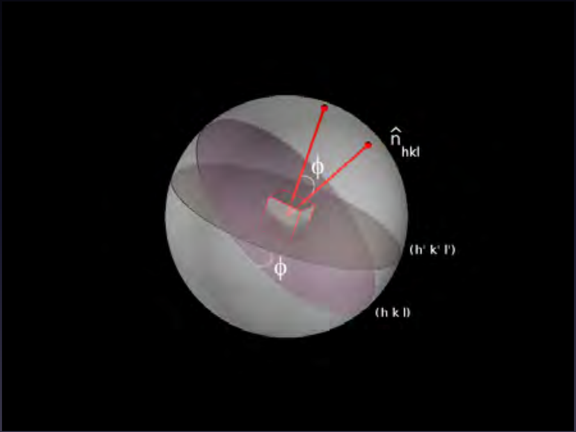
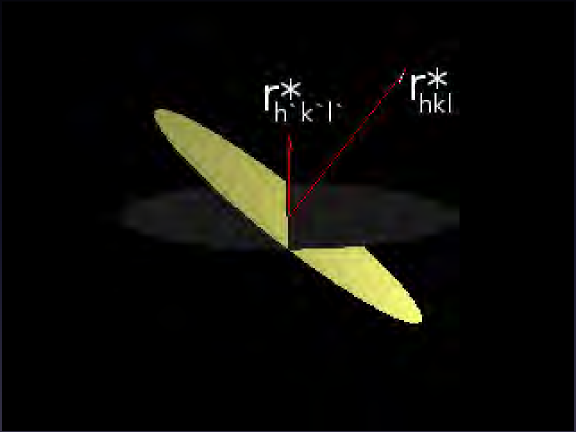
Definition



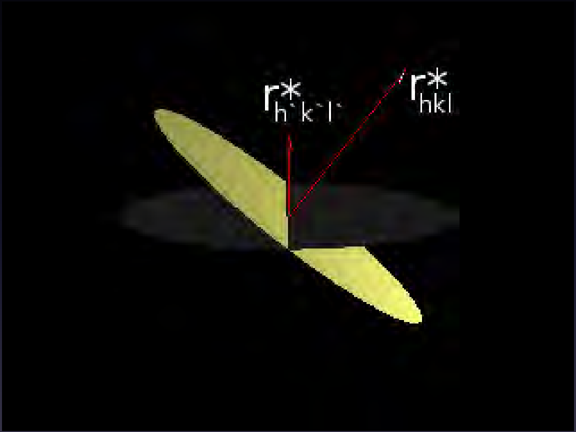
While constructing the stereographic projection we saw that the angle between planes could be also measured as the angles between the corresponding normal.

Definition



We can add metric information to the normals by asociating the norm of the vector somehow to the interplanar distance.

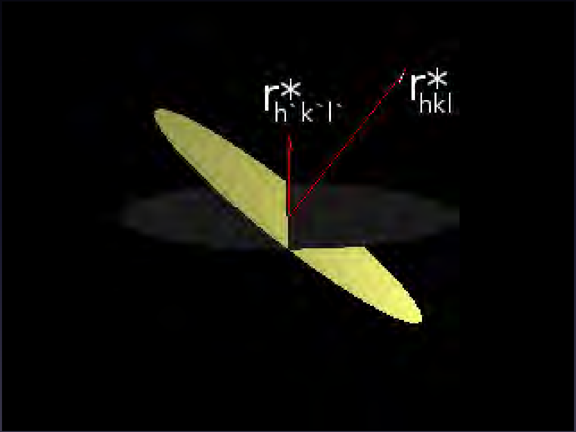
Definition



We can add metric information to the normals by asociating the norm of the vector somehow to the interplanar distance.

The reciprocal vector $\vec{r^*_{hkl}}$ is defined as a vector normal to plane (hkl) with length $1/d_{hkl}$

Definition



$$\vec{r^*_{hkl}} || \hat{n_{hkl}}$$

$$|\vec{r^*_{hkl}}| = \frac{1}{d_{hkl}}$$

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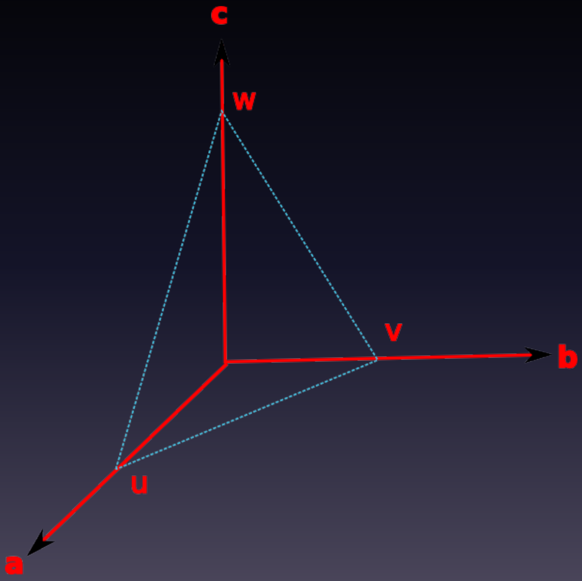
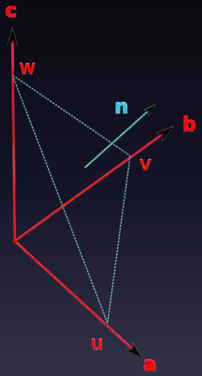
Equation of a plane



$$(u, 0, 0)\ (0, v, 0)\ (0, 0, w)$$

$$\vec{u} = u\vec{a}$$
$$\vec{v} = v\vec{b}$$
$$\vec{w} = w\vec{c}$$

Equation of a plane



$$\vec{n} = (\vec{u} - \vec{v}) \times (\vec{v} - \vec{w})$$

$$\vec{n} = (\vec{v} \times \vec{w}) + (\vec{w} \times \vec{u}) + (\vec{u} \times \vec{v})$$

$$\vec{n} = vw(\vec{b} \times \vec{c}) + uw(\vec{c} \times \vec{a}) + uv(\vec{a} \times \vec{b})$$

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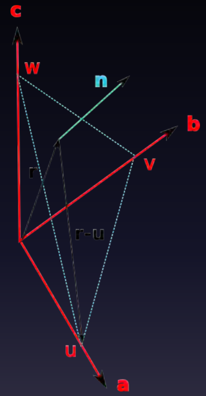
Equation of a plane



$$\vec{n} \cdot (\vec{r} - \vec{u}) = 0$$

$$\vec{n} \cdot \vec{r} = \vec{n} \cdot \vec{u}$$

$$\vec{n} = vw(\vec{b} \times \vec{c}) + uw(\vec{c} \times \vec{a}) + uv(\vec{a} \times \vec{b})$$
$$\vec{r} = x\vec{a} + y\vec{b} + z\vec{c}$$

$$vwx(\vec{b} \times \vec{c}) \cdot \vec{a} + uwy(\vec{c} \times \vec{a}) \cdot \vec{b} + uvz(\vec{a} \times \vec{b}) \cdot \vec{c} = uvw(\vec{b} \times \vec{c}) \cdot \vec{a}$$

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Equation of a plane

$$vwx(\vec{b} \times \vec{c}) \cdot \vec{a} + uwy(\vec{c} \times \vec{a}) \cdot \vec{b} + uvz(\vec{a} \times \vec{b}) \cdot \vec{c} = uvw(\vec{b} \times \vec{c}) \cdot \vec{a}$$

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Equation of a plane

$$vwx(\vec{b} \times \vec{c}) \cdot \vec{a} + uwy(\vec{c} \times \vec{a}) \cdot \vec{b} + uvz(\vec{a} \times \vec{b}) \cdot \vec{c} = uvw(\vec{b} \times \vec{c}) \cdot \vec{a}$$

$$\frac{x}{u}\left[\frac{\vec{b} \times \vec{c}}{\vec{a} \cdot (\vec{b} \times \vec{c})}\right] \cdot \vec{a} + \frac{y}{v}\left[\frac{\vec{c} \times \vec{a}}{\vec{a} \cdot (\vec{b} \times \vec{c})}\right] \cdot \vec{b} + \frac{z}{w}\left[\frac{\vec{a} \times \vec{b}}{\vec{a} \cdot (\vec{b} \times \vec{c})}\right] \cdot \vec{c} = 1$$

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Equation of a plane

$$vwx(\vec{b} \times \vec{c}) \cdot \vec{a} + uwy(\vec{c} \times \vec{a}) \cdot \vec{b} + uvz(\vec{a} \times \vec{b}) \cdot \vec{c} = uvw(\vec{b} \times \vec{c}) \cdot \vec{a}$$

$$\frac{x}{u}\left[\frac{\vec{b} \times \vec{c}}{\vec{a} \cdot (\vec{b} \times \vec{c})}\right] \cdot \vec{a} + \frac{y}{v}\left[\frac{\vec{c} \times \vec{a}}{\vec{a} \cdot (\vec{b} \times \vec{c})}\right] \cdot \vec{b} + \frac{z}{w}\left[\frac{\vec{a} \times \vec{b}}{\vec{a} \cdot (\vec{b} \times \vec{c})}\right] \cdot \vec{c} = 1$$

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

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

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

Equation of a plane

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

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

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

$$\vec{a} \cdot \vec{a^*} = 1 \qquad \vec{b} \cdot \vec{a^*} = 0 \qquad \vec{c} \cdot \vec{a^*} = 0$$

$$\vec{a} \cdot \vec{b^*} = 0 \qquad \vec{b} \cdot \vec{b^*} = 1 \qquad \vec{c} \cdot \vec{b^*} = 0$$

$$\vec{a} \cdot \vec{c^*} = 0 \qquad \vec{b} \cdot \vec{b^*} = 0 \qquad \vec{c} \cdot \vec{b^*} = 1$$

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Equation of a plane

$$\frac{x}{u}\left[\frac{\vec{b}\times\vec{c}}{\vec{a}\cdot(\vec{b}\times\vec{c})}\right]\cdot\vec{a}+\frac{y}{v}\left[\frac{\vec{c}\times\vec{a}}{\vec{a}\cdot(\vec{b}\times\vec{c})}\right]\cdot\vec{b}+\frac{z}{w}\left[\frac{\vec{a}\times\vec{b}}{\vec{a}\cdot(\vec{b}\times\vec{c})}\right]\cdot\vec{c}=1$$

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Equation of a plane

$$\frac{x}{u}\left[\frac{\vec{b}\times\vec{c}}{\vec{a}\cdot(\vec{b}\times\vec{c})}\right]\cdot\vec{a}+\frac{y}{v}\left[\frac{\vec{c}\times\vec{a}}{\vec{a}\cdot(\vec{b}\times\vec{c})}\right]\cdot\vec{b}+\frac{z}{w}\left[\frac{\vec{a}\times\vec{b}}{\vec{a}\cdot(\vec{b}\times\vec{c})}\right]\cdot\vec{c}=1$$

$$(x\vec{a})\cdot(h\vec{a^*})+(y\vec{b})\cdot(k\vec{b^*})+(z\vec{c})\cdot(l\vec{c^*})=1$$

Equation of the plane

$$hx+ky+lz=1$$

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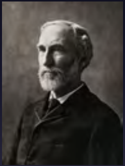
Some history

Gibbs (1839-1903)



Gibbs introduced the reciprocal base $\{\vec{a_j^*}\}$ from the condition $\vec{a_i} \cdot \vec{a_j^*} =^K \delta_{ij}$

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Reciprocal vector

$$(x\vec{a}) \cdot (h\vec{a^*}) + (y\vec{b}) \cdot (k\vec{b^*}) + (z\vec{c}) \cdot (l\vec{c^*}) = 1$$

$$hx + ky + lz = 1$$

can be written as

$$\vec{r_{xyz}} \cdot \vec{r^*_{hkl}} = 1$$

where

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

if

$$\vec{r^*_{hkl}} || n\hat{_{hkl}} \qquad |\vec{r^*_{hkl}}| = \frac{1}{d_{hkl}}$$

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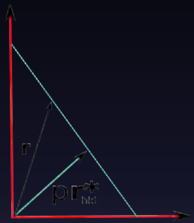
Reciprocal vector



$$\vec{r^*_{hkl}} \cdot (\vec{r} - p\vec{r^*_{hkl}}) = 0$$

$$p|\vec{r^*_{hkl}}|^2 = \vec{r} \cdot \vec{r^*_{hkl}} = 1$$

$$p = \frac{1}{|\vec{r^*_{hkl}}|^2}$$

Now by construction

$$p|\vec{r^*_{hkl}}| = d_{hkl} \Rightarrow |\vec{r^*_{hkl}}| = \frac{1}{d_{hkl}}$$

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Coordinates transformations

$$\begin{pmatrix} x' \\ y' \\ z' \end{pmatrix} = F \cdot \begin{pmatrix} x \\ y \\ z \end{pmatrix}$$

$$\vec{r} = (\vec{a}\,\vec{b}\,\vec{c}) \cdot \begin{pmatrix} x \\ y \\ z \end{pmatrix} = (\vec{a'}\,\vec{b'}\,\vec{c'}) \cdot \begin{pmatrix} x' \\ y' \\ z' \end{pmatrix} = (\vec{a'}\,\vec{b'}\,\vec{c'}) \cdot F \cdot \begin{pmatrix} x \\ y \\ z \end{pmatrix}$$

from where

Basis transformation

$$(\vec{a'}\,\vec{b'}\,\vec{c'}) = (\vec{a}\,\vec{b}\,\vec{c}) \cdot F^{-1}$$

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Metric tensor transformations

$$\vec{r}\cdot\vec{r} = (x\,y\,z)\cdot G\cdot\begin{pmatrix} x \\ y \\ z \end{pmatrix} = (x'\,y'\,z')\cdot G'\cdot\begin{pmatrix} x' \\ y' \\ z' \end{pmatrix} =$$

$$(x\,y\,z)\cdot F^T\cdot G'\cdot F\cdot\begin{pmatrix} x \\ y \\ z \end{pmatrix}$$

from where calling $M = (F^T)^{-1}$

Metric tensor transformation

$$G' = M\cdot G\cdot M^T$$

Metric tensor transformations

Consider the transformation

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

Metric tensor transformations

Consider the transformation

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

from where

$$\begin{pmatrix} \vec{a^*} \\ \vec{b^*} \\ \vec{c^*} \end{pmatrix} \cdot (\vec{a}\,\vec{b}\,\vec{c}) = M \cdot \begin{pmatrix} \vec{a} \\ \vec{b} \\ \vec{c} \end{pmatrix} \cdot (\vec{a}\,\vec{b}\,\vec{c})$$

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Metric tensor transformations

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

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Metric tensor transformations

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

$$\begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} = M \cdot \begin{pmatrix} \vec{a}\cdot\vec{a} & \vec{a}\cdot\vec{b} & \vec{a}\cdot\vec{c} \\ \vec{b}\cdot\vec{a} & \vec{b}\cdot\vec{b} & \vec{b}\cdot\vec{c} \\ \vec{c}\cdot\vec{a} & \vec{c}\cdot\vec{b} & \vec{c}\cdot\vec{c} \end{pmatrix} = M \cdot G$$

$$M = G^{-1} \quad F = G$$

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Metric tensor transformations

$$\begin{pmatrix} \vec{a^*} \\ \vec{b^*} \\ \vec{c^*} \end{pmatrix} = G^{-1} \cdot \begin{pmatrix} \vec{a} \\ \vec{b} \\ \vec{c} \end{pmatrix}$$

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Metric tensor transformations

$$\begin{pmatrix} \vec{a^*} \\ \vec{b^*} \\ \vec{c^*} \end{pmatrix} = G^{-1} \cdot \begin{pmatrix} \vec{a} \\ \vec{b} \\ \vec{c} \end{pmatrix}$$

and

$$\begin{aligned} G = F^T \cdot G^* \cdot F = G^T \cdot G^* \cdot G \\ G^{-1} \cdot G = G^{-1} \cdot G \cdot G^* \cdot G \\ I = G^* \cdot G \end{aligned}$$

Metric tensor transformations

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Reciprocal tensor

$$G^* = G^{-1}$$

Transformation in reciprocal space

$$\vec{r^*} = (h\,k\,l) \cdot \begin{pmatrix} \vec{a^*} \\ \vec{b^*} \\ \vec{c^*} \end{pmatrix} = (h'\,k'\,l') \cdot \begin{pmatrix} \vec{a^*}' \\ \vec{b^*}' \\ \vec{c^*}' \end{pmatrix} =$$

$$(h\,k\,l) \cdot G^{-1} \cdot \begin{pmatrix} \vec{a} \\ \vec{b} \\ \vec{c} \end{pmatrix} = (h\,k\,l) \cdot G^{-1} \cdot F^T \begin{pmatrix} \vec{a'} \\ \vec{b'} \\ \vec{c'} \end{pmatrix} =$$

$$(h\,k\,l) \cdot G^{-1} \cdot F^T \cdot G' \begin{pmatrix} \vec{a^*}' \\ \vec{b^*}' \\ \vec{c^*}' \end{pmatrix}$$

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Transformation in reciprocal space

$$\vec{r^*} = (h\,k\,l) \cdot \begin{pmatrix} \vec{a^*} \\ \vec{b^*} \\ \vec{c^*} \end{pmatrix} = (h\,k\,l) \cdot G^{-1} \cdot F^T \cdot G' \begin{pmatrix} \vec{a^*}' \\ \vec{b^*}' \\ \vec{c^*}' \end{pmatrix}$$

Now

$$G' = M \cdot G \cdot M^T = (F^T)^{-1} \cdot G \cdot F^{-1}$$

and finally

Reciprocal coordinates

$$(h'\,k'\,l') = (h\,k\,l) \cdot M^T = (h\,k\,l) \cdot F^{-1}$$

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Point symmetry transformation in reciprocal space

Let R be a point symmetry operation acting over the coordinates of the atoms, then according to the transformation rules already derived

$$(h^e\, k^e\, l^e) = (h\, k\, l) \cdot R^{-1}$$

and $(h^e\, k^e\, l^e)$ is a plane symmetry related to $(h\, k\, l)$. Therefore:

Point symmetry in reciprocal space

$$R^* = R^{-1}$$

Point symmetry transformation in reciprocal space

Example:
Three fold axis $3_{[0\,0\,1]}$:

$$(x\,y\,z) \longrightarrow (-y \quad x-y \quad z) \longrightarrow (y-x \quad -x \quad z)$$

Point symmetry transformation in reciprocal space

Example:
Three fold axis $3_{[0\,0\,1]}$:

$$(x\,y\,z) \longrightarrow (-y \quad x-y \quad z) \longrightarrow (y-x \quad -x \quad z)$$

$$R = \begin{pmatrix} 0 & \bar{1} & 0 \\ 1 & \bar{1} & 0 \\ 0 & 0 & 1 \end{pmatrix}$$

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Point symmetry transformation in reciprocal space

Example:
Three fold axis $3_{[0\,0\,1]}$:

$$(x\,y\,z) \longrightarrow (-y \quad x-y \quad z) \longrightarrow (y-x \quad -x \quad z)$$

$$R = \begin{pmatrix} 0 & \bar{1} & 0 \\ 1 & \bar{1} & 0 \\ 0 & 0 & 1 \end{pmatrix} \qquad R^* = \begin{pmatrix} \bar{1} & 1 & 0 \\ \bar{1} & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix}$$

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Point symmetry transformation in reciprocal space

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Three fold axis $3_{[0\,0\,1]}$:

$$(x\,y\,z) \longrightarrow (-y \quad x-y \quad z) \longrightarrow (y-x \quad -x \quad z)$$

$$R = \begin{pmatrix} 0 & \bar{1} & 0 \\ 1 & \bar{1} & 0 \\ 0 & 0 & 1 \end{pmatrix} \qquad R^* = \begin{pmatrix} \bar{1} & 1 & 0 \\ \bar{1} & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix}$$

$$(h\,k\,l) \longrightarrow (-h-k \quad h \quad l) \longrightarrow (k \quad -h-k \quad l)$$

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Symmetry group in reciprocal space

Symmetry group in reciprocal space

$$\{R^*\} = \{R\}$$

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Fourier transform and reciprocal vectors

Fourier transform

$$\Gamma[f(\vec{r})] = \widehat{f}(\vec{r^*}) = F(\vec{r^*}) \equiv \int_{-\infty}^{\infty} f(\vec{r}) \exp\left(-2\pi i \vec{r^*} \cdot \vec{r}\right) d\vec{r}$$

where

$$\vec{r^*} = x^* \vec{a^*} + y^* \vec{b^*} + z^* \vec{c^*}$$
$$\vec{r} = x\vec{a} + y\vec{b} + z\vec{c}$$

and therefore

$$\vec{r^*} \cdot \vec{r} = x^* \, x + y^* \, y + z^* \, z$$

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Fourier transform of the lattice

Definition (Dirac comb)

$L = \sum_{u,v,w=-\infty}^{\infty} \delta(\vec{r} - u\vec{a} - v\vec{b} - w\vec{c})$

$$\Gamma[L(\vec{r})] = \int \cdots \int_{-\infty}^{\infty} \sum_{u,v,w=-\infty}^{\infty} \delta(\vec{r} - u\vec{a} - v\vec{b} - w\vec{c}) \exp\left(-2\pi i \vec{r^*} \cdot \vec{r}\right) d\vec{r}$$

$$= \sum_{u,v,w=-\infty}^{\infty} \exp\left(-2\pi i \vec{r^*} \cdot (u\vec{a} + v\vec{b} + w\vec{c})\right)$$

$$= \sum_{u=-\infty}^{\infty} e^{(-2\pi i u \vec{r^*} \cdot \vec{a})} \sum_{v=-\infty}^{\infty} e^{(-2\pi i v \vec{r^*} \cdot \vec{b})} \sum_{w=-\infty}^{\infty} e^{(-2\pi i w \vec{r^*} \cdot \vec{c})}$$

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Fourier transform of the lattice

Dirac comb

$\frac{1}{|a|}\sum_{n=-\infty}^{\infty}\exp\left(2\pi inx/a\right)=\sum_{m=-\infty}^{\infty}\delta(x-ma)$

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Fourier transform of the lattice

Dirac comb

$\frac{1}{|a|}\sum_{n=-\infty}^{\infty}\exp\left(2\pi i n x/a\right)=\sum_{m=-\infty}^{\infty}\delta(x-ma)$

$$\Gamma[L(\vec{r})]=\sum_{u=-\infty}^{\infty}e^{(-2\pi i u \vec{r^*}\cdot\vec{a})}\sum_{v=-\infty}^{\infty}e^{(-2\pi i v \vec{r^*}\cdot\vec{b})}\sum_{w=-\infty}^{\infty}e^{(-2\pi i w \vec{r^*}\cdot\vec{c})}$$

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Fourier transform of the lattice

Dirac comb

$\frac{1}{|a|}\sum_{n=-\infty}^{\infty}\exp\left(2\pi i n x/a\right) = \sum_{m=-\infty}^{\infty}\delta(x-ma)$

$$\Gamma[L(\vec{r})] = \sum_{u=-\infty}^{\infty} e^{(-2\pi i u \vec{r^*}\cdot\vec{a})} \sum_{v=-\infty}^{\infty} e^{(-2\pi i v \vec{r^*}\cdot\vec{b})} \sum_{w=-\infty}^{\infty} e^{(-2\pi i w \vec{r^*}\cdot\vec{c})}$$

$$L^*(\vec{r^*}) = \sum_{h,k,l=-\infty}^{\infty} \delta(\vec{r^*}\cdot\vec{a}-h)\delta(\vec{r^*}\cdot\vec{b}-k)\delta(\vec{r^*}\cdot\vec{c}-l)$$

$$= \sum_{h,k,l=-\infty}^{\infty} \delta(\vec{r^*}-h\vec{a^*})\delta(\vec{r^*}-k\vec{b^*})\delta(\vec{r^*}-l\vec{c^*})$$

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