# Symmetry Implementation for Pair Distribution Function

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**Abstract**

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# Introduction

## Mathematical Description of Crystals

### Lattice

A lattice is a collection of points in three dimensional space which fulfill three (linearly independent) translation symmetries. If $\boldsymbol{a}, \boldsymbol{b}, \boldsymbol{c} \in \mathbb{R}^3$ are the translation vectors of the lattice, a basis for i can be given in terms of these vectors. Thus with the origin $O$ set at a lattice point any lattice point can be described as a linear combination of the translation vectors.

$$\overrightarrow{O\,X} = \boldsymbol{a}x + \boldsymbol{b}y + \boldsymbol{c}z = (\boldsymbol{a}\ \ \boldsymbol{b}\ \ \boldsymbol{c})\begin{pmatrix} x \\ y \\ z \end{pmatrix}; x, y, z \in \mathbb{Z} \tag{1}$$

To describe any point in space this defintion can be extended by allowing $x, y, z \in \mathbb{R}$ giving us $P = \left\{ \begin{pmatrix} x \\ y \\ z \end{pmatrix}; x, y, z \in \mathbb{R} \right\}$ the set of all points.

The Metric on this space is given by:

$$\begin{aligned} d(\cdot,\cdot) : P \times P &\longrightarrow \mathbb{R} \\ (X, Y) &\longmapsto \left|\overrightarrow{XY}\right| = \sqrt{\overrightarrow{XY}^T G \overrightarrow{XY}} \end{aligned} \tag{2}$$

Where $G$ is the metric tensor given by:

$$G = \begin{pmatrix} \boldsymbol{a}\cdot\boldsymbol{a} & \boldsymbol{a}\cdot\boldsymbol{b} & \boldsymbol{a}\cdot\boldsymbol{c} \\ \boldsymbol{b}\cdot\boldsymbol{a} & \boldsymbol{b}\cdot\boldsymbol{b} & \boldsymbol{b}\cdot\boldsymbol{c} \\ \boldsymbol{c}\cdot\boldsymbol{a} & \boldsymbol{c}\cdot\boldsymbol{b} & \boldsymbol{c}\cdot\boldsymbol{c} \end{pmatrix} = \begin{pmatrix} a^2 & ab\cos(\gamma) & ac\cos(\beta) \\ ba\cos(\gamma) & b^2 & bc\cos(\alpha) \\ ca\cos(\beta) & cb\cos(\alpha) & c^2 \end{pmatrix} \tag{3}$$

The coefficients of the metric tensor on the left are given in $a, b, c$ and $\alpha, \beta, \gamma$ the length of the basis vectors and the angles between them. This is the most common format used for the lattice parameters.

### Lattice Isomerties

Lattice isometries are distance and angle preserving transformations on the lattice. Isometries can be represented as affine transformation, which consist of a matrix and a translation vector. Following the convention in the International Table for Crystallography, the transformation will be notated like this:

$$\mathcal{Q} = (\boldsymbol{Q}, \boldsymbol{q}) \tag{4}$$

$$\overrightarrow{O\tilde{X}} = \overrightarrow{O\mathcal{Q}X} = \boldsymbol{Q}\overrightarrow{OX} + \boldsymbol{q} \tag{5}$$

By simple symbol manipulation the following formulas for composition and inversion can be proven.

$$\mathcal{Q}\mathcal{P} = (\boldsymbol{Q}, \boldsymbol{q})(\boldsymbol{P}, \boldsymbol{p}) = (\boldsymbol{Q}\boldsymbol{P}, \boldsymbol{Q}\boldsymbol{p} + \boldsymbol{q}) \tag{6}$$

$$\mathcal{Q}^{-1} = (\boldsymbol{Q}^{-1}, -\boldsymbol{Q}^{-1}\boldsymbol{q}) \tag{7}$$

For this transformation to be an isometry the following statement must hold for all $a, b \in P$:

$$\begin{aligned} d(X, Y) &= d(\mathcal{Q}X, \mathcal{Q}Y) \\ \left|\overrightarrow{XY}\right| &= \left|\overrightarrow{\mathcal{Q}X\mathcal{Q}Y}\right| \\ &= \left|\boldsymbol{Q}\overrightarrow{OY} + \boldsymbol{q} - \boldsymbol{Q}\overrightarrow{OX} - \boldsymbol{q}\right| \\ &= \left|\boldsymbol{Q}\left(\overrightarrow{OY} - \overrightarrow{OX}\right)\right| \\ &= \left|\boldsymbol{Q}\overrightarrow{XY}\right| \end{aligned} \tag{8}$$

As expected the translation vector $q$ is free as a translation doesn't affect the distance between two points.

Since X and Y are arbitrary points the vector $v$ between the is too. Using the definition of the metric in Equation 2:

$$\begin{aligned} |\boldsymbol{v}| &= |\boldsymbol{Q}\boldsymbol{v}| \\ |\boldsymbol{v}|^2 &= |\boldsymbol{Q}\boldsymbol{v}|^2 \\ \boldsymbol{v}^T\boldsymbol{G}\boldsymbol{v} &= (\boldsymbol{Q}\boldsymbol{v})^T\boldsymbol{G}(\boldsymbol{Q}\boldsymbol{v}) \\ &= \boldsymbol{v}^T\boldsymbol{Q}^T\boldsymbol{G}\boldsymbol{Q}\boldsymbol{v} \end{aligned} \tag{9}$$

Since v is arbitrary this equation leads to the following condition on $\boldsymbol{Q}$:

$$\boldsymbol{G} = \boldsymbol{Q}^T\boldsymbol{G}\boldsymbol{Q} \tag{10}$$

Which might me more familiar to the reader in the standard basis where $\boldsymbol{G} = \boldsymbol{I}$

$$\boldsymbol{I} = \boldsymbol{Q}^T\boldsymbol{Q} \tag{11}$$

Which is the condition for $\boldsymbol{Q}$ to be orthagonal. Orthagonal matrices have determinant $\pm 1$ the same is the case for the transformation matrix by:

$$\begin{aligned} \det(\boldsymbol{G}) = \det(\boldsymbol{Q}^T\boldsymbol{G}\boldsymbol{Q}) &= \det(\boldsymbol{Q}^T)\det(\boldsymbol{G})\det(\boldsymbol{Q}) \\ 1 = \det(\boldsymbol{Q}^T)\det(\boldsymbol{Q}) &= \det(\boldsymbol{Q})^2 \\ \Rightarrow \det(\boldsymbol{Q}) &= \pm 1 \end{aligned} \tag{12}$$

### Additional Restictions

## Pairs

## Yell

# Programm

## Spacegroup implementation

**Definition** Quotient group

group extension

## Pair implementation

# Results

# Discussion

# Appendix

**Definition** $H$ is a normal subgroup of $G$ if $ghg^{-1} \in H$ for all $g \in G$ and $h \in H$.

**Claim** Let $\mathfrak{H}$ be a spacegroup and $\mathfrak{T} = \{(\boldsymbol{I}, \boldsymbol{v}); \boldsymbol{v} \in \mathbb{Z}^3\}$ the group of interger translation. Then $\mathfrak{T}$ is a normal subgroup of $\mathfrak{H}$.

**Proof** Let $\mathcal{H} \in \mathfrak{H}$ be an arbitrary symmetry element and $\mathcal{T} \in \mathfrak{T}$ be an arbitrary interger translation.

$$\begin{aligned} \mathcal{H}\mathcal{T}\mathcal{H}^{-1} &= (\boldsymbol{H}, \boldsymbol{h})(\boldsymbol{I}, \boldsymbol{t})(\boldsymbol{H}^{-1}, -\boldsymbol{H}^{-1}\boldsymbol{q}) \\ &= (\boldsymbol{H}, \boldsymbol{h})(\boldsymbol{H}^{-1}, -\boldsymbol{H}^{-1}\boldsymbol{q} + \boldsymbol{t}) \\ &= (\boldsymbol{H}\boldsymbol{H}^{-1}, \boldsymbol{H}(-\boldsymbol{H}^{-1}\boldsymbol{q} + \boldsymbol{t}) + \boldsymbol{q}) \\ &= (\boldsymbol{I}, \boldsymbol{H}\boldsymbol{T}) \end{aligned} \tag{13}$$