Methods of

Computational Materials Science

Part One

Mathematical and Computational Foundations

Group Theory and Symmetry

Numerical Algorithms

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download: **http://tph.tuwien.ac.at/~rdirl/CMS.html**

Content of Lecture:

[1] Basic concepts of group theory:

Point group = subgroup of rotation group

Space group = subgroup of Euclidean group

Bloch states = symmetry adapted functions

[2] Representation theory:

Non-singular mappings of vector spaces

Special case: Linear representations

Reducible and irreducible representations

[3] Applications in quantum mechanics:

Schur's Lemma

Symmetry adaptation of states

Wigner Eckart Theorem

[4] Applications in solid state physics:

Wyckoff positions – Structure Analysis

Structural phase transitions – Domains

Symmetries of energy bands

Localized states – Wannier functions

Remarks on Group Theory and Applications in Physics

Aim: to disentangle the involved concepts

- algebraic structure of groups
- representations of groups
- physical applications

■ what is proper to group theory itself and what is proper to the physical application in question

[1] Groups: POSTULATES

$$\mathbf{G} = \left\{ g_1, g_2, g_3, \cdots \right\}$$

Composition law:	$g_i * g_j = g_k$
Associative law:	$(g_i * g_j) * g_k = g_i * (g_j * g_k)$
Identity element:	$e * g = g * e = g$
Inverse element:	$g * g^{-1} = g^{-1} * g = e$

Gross classification of groups:
Distinction by order of group and by commuting properties of composition law

Order of group: $|\mathbf{G}| =$ FINITE
$|\mathbf{G}| =$ COUNTABLE
$|\mathbf{G}| =$ CONTINUOUS

Commutativity: ABELIAN
$g_j * g_k = g_k * g_j$
for **all** g_j, g_k

NON-ABELIAN
$g_j * g_k \neq g_k * g_j$
for **some** g_j, g_k

Subgroups of Groups:

$$
\begin{aligned}
\mathbf{H} &= \{h_1, h_2, h_3, \dots\} \subseteq \mathbf{G} \\
h_1 &= g_1 = e = \text{unit element} \\
\mathbf{H} &= \mathbf{H} * \mathbf{H}^{-1}
\end{aligned}
$$

$$
\begin{aligned}
\mathbf{H}^g &= g * \mathbf{H} * g^{-1} \\
&= \textbf{conjugate}\ \text{subgroup} \\
\mathbf{H}^g &\neq \mathbf{H} \quad \text{for } \textbf{some } g \in \mathbf{G}, \text{ but } \mathbf{H}^g \sim \mathbf{H} \\
\mathbf{H}^g &= \mathbf{H} \quad \text{for } \textbf{all } g \in \mathbf{G} \\
&\Rightarrow \textbf{normal}\ \text{subgroup}
\end{aligned}
$$

Notion:

$$
\begin{aligned}
\mathbf{H} &\subset \mathbf{G} \quad \textbf{arbitrary}\ \text{subgroup} \\
\mathbf{N} &\triangleleft \mathbf{G} \quad \textbf{normal}\ \text{subgroup}
\end{aligned}
$$

Digression: Equivalence Relations and Equivalence Classes in Sets

An **equivalence relation** exists between any pair of elements $a, a' \in \mathcal{A}$, i.e. $a \sim a'$ iff the following conditions are satisfied:

$$\begin{aligned} \textbf{Reflexivity:} &\quad a \sim a \quad \forall a \in \mathcal{A} \\ \textbf{Symmetry:} &\quad a \sim a' \Longleftrightarrow a' \sim a \\ \textbf{Transitivity:} &\quad a \sim a'\,,\, a' \sim a'' \Longleftrightarrow a \sim a'' \end{aligned}$$

An **equivalence class** of a is denoted by the symbol $[a]$.

$$[a] = \left\{ a' \in \mathcal{A} \middle| a' \sim a \right\}$$

where $[a] = [a']$ iff $a \sim a'$ is valid. Conversely, if a and a'' are not equivalent elements, then the classes $[a]$ and $[a'']$ are disjoint, ie.

$$\begin{array}{ccccc} [a] \cap [a'] & = & [a] & \Longleftrightarrow & a \sim a' \\ [a] \cap [a'] & = & \emptyset & \Longleftrightarrow & a \not\sim a' \end{array}$$

Equivalence Relation: Coset decomposition of G w.r.t. H (left & right)

$$\begin{aligned} g &\sim g' \quad \text{if } \exists h \in \mathbf{H} \\ & \qquad\quad \text{such that } g' = g * h \\ \mathbf{G} &= \bigcup_{s=1}^{m} \left\{\bar{g}_s\right\} * \mathbf{H} = \bigcup_{s=1}^{m} \left[\bar{g}_s\right] \\ m &= |\mathbf{G}| : |\mathbf{H}| \end{aligned}$$

Note: The index m can be **finite** even if **G** and **H** are countable infinite groups.

Example: Space groups (3-dimensional)

$$\begin{aligned} \mathbf{G} &= \{\mathbf{T}, \mathbf{P} | \mathcal{O}, \mathrm{w}_{\mathsf{P}}\} \\ \mathbf{T} & \ \ldots \ \texttt{Translation group} \\ \mathbf{P} & \ \ldots \ \texttt{Point group} \\ \mathcal{O} & \ \ldots \ \texttt{Origin} \\ \mathrm{w}_{\mathsf{P}} &= \{\mathrm{n}(R) | R \in \mathbf{P}\} \ \ldots \\ & \quad \texttt{Set of Fractional translations} \\ \mathbf{T} & \lhd \mathbf{G} \end{aligned}$$

Equivalence Relation: Classes of conjugate elements of the group G

$$
\begin{aligned}
g \quad \sim \quad g' &\quad \text{if} \quad \exists \hat{g} \in \mathbf{G} \\
&\quad \text{such that } g' = \hat{g} * g * \hat{g}^{-1} \\
\left[g_n \right] &= \left\{ \hat{g} * g_n * \hat{g}^{-1} \middle| \hat{g} \in \mathbf{G} \right\} \\
\mathbf{G} &= \bigcup_{n=1}^{K} \left[g_n \right] \\
K &= \text{Divisor of } |\mathbf{G}|
\end{aligned}
$$

Note: The special case $\left[e\right] = \left\{e\right\}$ is valid for all groups. Moreover $K < |\mathbf{G}|$ if $\mathbf{G}$ is non-abelian, whereas $K = |\mathbf{G}|$ if $\mathbf{G}$ is abelian.

Digression: Mapping (function) of set $\mathcal{S}_1$ into (onto) $\mathcal{S}_2$

$$
\begin{aligned}
f &: \mathcal{S}_1 \longrightarrow \mathcal{S}_2 \\
f(\mathcal{S}_1) &= \text{image of } \mathcal{S}_1 \\
f(\mathcal{S}_1) &\subset \mathcal{S}_2 \quad \ldots \quad \textbf{INTO} \\
f(\mathcal{S}_1) &= \mathcal{S}_2 \quad \ldots \quad \textbf{ONTO}
\end{aligned}
$$

injective: $\forall a, a' \in \mathcal{S}_1$ with $a \neq a' \Rightarrow f(a) \neq f(a')$

surjective: $f : \mathcal{S}_1 \longrightarrow \mathcal{S}_2$ with $f(\mathcal{S}_1) = \mathcal{S}_2$

bijective: iff $f : \mathcal{S}_1 \longrightarrow \mathcal{S}_2$ is injective and surjective $\Rightarrow$ inverse mapping f^{-1} exists

Relations between Groups:

Homomorphism :

$$h : \mathbf{G} \longrightarrow \mathbf{G}'$$

$$h(\mathbf{G}) \subset \mathbf{G}' \quad \ldots \quad \textbf{INTO}$$

$$h(\mathbf{G}) = \mathbf{G}' \quad \ldots \quad \textbf{ONTO}$$

$$h(g) \circ h(g') = h(g * g')$$

Kernel of Homomorphism:

$$\mathbf{ker}_h = \mathbf{K}$$

$$= \left\{ g \in \mathbf{G} \middle| h(g) = e' \in \mathbf{G}' \right\}$$

$$\mathbf{K} \lhd \mathbf{G}$$

$$h(\mathbf{G}) = \mathbf{G}'$$

$$\mathbf{G} = \bigcup_{s=1}^{m} \left\{ \bar{g}_s * \mathbf{K} \right\}$$

Factor Group:

$$\mathbf{G}/\mathbf{K} = \left\{ \bar{g}_s * \mathbf{K} \middle| \bar{g}_s \in \mathbf{G}\!:\!\mathbf{K} \right\}$$

$$\left(\bar{g}_r * \mathbf{K} \right) * \left(\bar{g}_s * \mathbf{K} \right)$$

$$= \left(\bar{g}_{rs} * \mathbf{K} \right)$$

$$\mathbf{G}/\mathbf{K} \sim \mathbf{G}'$$

Isomorphism :

$$i : \mathbf{G} \longrightarrow \mathbf{G}'$$
$$i(\mathbf{G}) = \mathbf{G}' \Longleftrightarrow i^{-1}(\mathbf{G}') = \mathbf{G}$$
$$i(g) \circ i(g') = i(g * g')$$
$$\mathbf{G} \sim \mathbf{G}'$$

Automorphism :

$$a : \mathbf{G} \longrightarrow \mathbf{G}$$
$$a(\mathbf{G}) = \mathbf{G}$$
$$a(g) \circ a(g') = a(g * g')$$
$$a(e) = e$$

Automorphism Group:

$$\mathbf{Aut}(\mathbf{G}) = \left\{ a \middle| a(\mathbf{G}) = \mathbf{G} \right\}$$
$$a_j(a_k(g)) = \left[a_j \diamond a_k \right](g) = a_{jk}(g)$$
$$a(g) \circ a(g') = a(g * g') \quad \forall a$$

Inner Automorphism Group:

$$\mathbf{Aut}_o(\mathbf{G}) \sim \mathbf{G}/\mathbf{C}(\mathbf{G})$$

$\mathbf{C}(\mathbf{G})$ ... Center of $\mathbf{G}$

$$\mathbf{Aut}_o(\mathbf{G}) \subseteq \mathbf{Aut}(\mathbf{G})$$

Examples: Automorphism Groups

1. Automorphism Group of $\mathbb{Z}^m$

$$
\begin{array}{rcl}
\mathbb{Z} & \ldots & \text{Ring of Integers} \\
\mathbf{G} & = & \mathbb{Z}^m = \mathbb{Z} \otimes \mathbb{Z} \otimes \mathbb{Z} \otimes \cdots \otimes \mathbb{Z} \\
\underline{z} & = & (z_1, z_2, \ldots z_m)^{\mathrm{T}} \in \mathbb{Z}^m \\
\underline{z} * \underline{z}' & = & \underline{z} + \underline{z}' \in \mathbb{Z}^m \\
a_\xi(\underline{z}) & = & \mathbb{M}(\xi) \cdot \underline{z} = \underline{z}'' \in \mathbb{Z}^m \\
\mathbb{M}(\xi) & : & \mathbb{Z}^m \longrightarrow \mathbb{Z}^m \\
\mathbb{M}(\xi) & \in & \mathbb{GL}(m, \mathbb{Z}) \ \ldots \ \texttt{General Matrix Group} \\
 & & \qquad\qquad\quad \texttt{over Ring of Integers}
\end{array}
$$

2. Automorphism Group of $\mathbb{R}^m$

$$
\begin{array}{rcl}
\mathbb{R} & \ldots & \text{Field of Reals} \\
\mathbf{G} & = & \mathbb{R}^m = \mathbb{R} \otimes \mathbb{R} \otimes \mathbb{R} \otimes \cdots \otimes \mathbb{R} \\
\underline{x} & = & (x_1, x_2, \ldots x_m)^{\mathrm{T}} \in \mathbb{R}^m \\
a_\xi(\underline{x}) & = & \mathbb{M}(\xi) \cdot \underline{x} = \underline{x}'' \in \mathbb{R}^m \\
\mathbb{M}(\xi) & \in & \mathbb{GL}(m, \mathbb{R}) \ \ldots \ \texttt{General Matrix Group} \\
 & & \qquad\qquad\quad \texttt{over Field of Reals}
\end{array}
$$

Product Groups:

1. Direct Product Groups:

$$\begin{aligned}
\mathbf{G} \otimes \mathbf{H} &= \Big\{(g, h) \Big| g \in \mathbf{G}, h \in \mathbf{H}\Big\} \\
(g, h) * (g', h') &= (g \circ g', h \diamond h') \\
&\quad \forall g, g' \in \mathbf{G}, \forall h, h' \in \mathbf{H} \\
|\mathbf{G} \otimes \mathbf{H}| &= |\mathbf{G}| \cdot |\mathbf{H}|
\end{aligned}$$

2. Semi-Direct Product Groups:

$$\begin{aligned}
\phi &: \mathbf{H} \longrightarrow \mathbf{Aut}(\mathbf{N}) \\
\phi(h) &= a_h \in \mathbf{Aut}(\mathbf{N})
\end{aligned}$$

$$\begin{aligned}
\mathbf{N} \circledS \mathbf{H} &= \Big\{(n, h) \Big| g \in \mathbf{N}, h \in \mathbf{H}\Big\} \\
(n, h) * (n', h') &= (n \circ a_h(n'), h \diamond h') \\
&\quad \forall n, n' \in \mathbf{N}, \forall h, h' \in \mathbf{H} \\
|\mathbf{N} \circledS \mathbf{H}| &= |\mathbf{N}| \cdot |\mathbf{H}| \\
\mathbf{N} &\ \ldots\ \text{Normal Subgroup} \\
\phi(\mathbf{H}) &\subseteq \mathbf{Aut}(\mathbf{N}) \\
\mathbf{N} \cap \mathbf{H} &= \Big\{(e_N, e_H)\Big\}
\end{aligned}$$

3. More complicated Extensions:

a. Beyond Split Extensions:

Non-symmorphic SPACE Groups do not form semi-direct Product Groups. Their structure is more complicated, but they can be understood relatively easily when considering Space Groups as Subgroups of the **Euclidean Group**, which is a locally compact continuous group that is contained as proper subgroup in the **Affine Group**.

$$\begin{aligned} \mathbf{G} &= \{\mathsf{T}, \mathsf{P} | \mathcal{O}, \mathbf{w}_{\mathsf{P}}\} \\ \mathbf{G} &\subset \mathbf{E}(3, \mathbb{R}) \subset \mathbf{A}(3, \mathbb{R}) \end{aligned}$$

b. Cohomology Groups:

Cohomology Groups allow one to classify systematically SPACE Groups Types into so-called Arithmetic Classes.

Examples: Groups

1a. Group of INTEGERS and beyond (Periodic Boundary Conditions):

$$\begin{aligned} \mathbf{G} &= \mathbb{Z} = \left\{ z \,\middle|\, z \in \mathbb{Z} \right\} \\ z * z' &= z + z' \end{aligned}$$

$$\begin{aligned} \mathbf{N} &= N\mathbb{Z} = \left\{ Nz \,\middle|\, z \in \mathbb{Z} \right\} \\ Nz * Nz' &= Nz + Nz' = N(z + z') \\ \mathbf{G} &= \bigcup_{z=0}^{N-1} \{ z + \mathbf{N} \} \end{aligned}$$

Note the paradox $\mathbf{N} \triangleleft \mathbf{G}$ but $\mathbf{N} \sim \mathbf{G}$. Such paradoxa are only possible for countable groups.

$$\begin{aligned} \mathbf{G}/\mathbf{N} &= \left\{ \{ z + \mathbf{N} \} \,\middle|\, z = 0,1,\ldots \mathrm{N}{-}1 \right\} \\ \{ z + \mathbf{N} \} * \{ z' + \mathbf{N} \} &= \{ z + z' + \mathbf{N} \} \\ z * z' &= z + z' \qquad \text{mod N} \\ \mathbf{G}/\mathbf{N} &= \mathbb{Z}/(N\mathbb{Z}) \sim \mathbf{C}_N \\ \mathbf{C}_N &\ldots \text{ Cyclic Group of Order } N \end{aligned}$$

Examples: Groups

1b. Group of REALS and beyond (Periodic Boundary Conditions):

$$\begin{aligned} \mathbf{G} &= \mathbb{R} = \left\{ x \,\middle|\, x \in \mathbb{R} \right\} \\ x * x' &= x + x' \end{aligned}$$

$$\begin{aligned} \mathbf{N} &= a\mathbb{Z} = \left\{ az \,\middle|\, z \in \mathbb{Z} \right\} \\ az * az' &= az + az' = a(z + z') \\ \mathbf{G} &= \bigcup_{y \in [0,a)} \{ y + \mathbf{N} \} \end{aligned}$$

Note that the group-subgroup relation $\mathbf{N} \triangleleft \mathbf{G}$ is valid, whereas $\mathbf{N} \sim \mathbf{G}$ is not satisfied.

$$\begin{aligned} \mathbf{G}/\mathbf{N} &= \left\{ \{ y + \mathbf{N} \} \,\middle|\, y \in [0,a) \right\} \\ \{ y + \mathbf{N} \} * \{ y' + \mathbf{N} \} &= \{ y + y' + \mathbf{N} \} \\ y * y' &= y + y' \qquad \mathrm{mod}\ [0,a) \\ \mathbf{G}/\mathbf{N} &= \mathbb{R}/(a\mathbb{Z}) \sim \mathbf{C}_\infty \\ \mathbf{C}_\infty &\sim \mathbf{U}(1) \\ &\ldots \text{ Primitive Unit Cell} \end{aligned}$$

2. Cyclic Group of order N

$$\begin{aligned} \mathbf{C}_N &= \left\{ e^{im\varphi} \,\middle|\, m = 1,2,3,\ldots \mathrm{N}, \quad \varphi = \frac{2\pi}{N} \right\} \\ m * n &= m + n \quad \bmod N \end{aligned}$$

3. Group of INTEGERS and beyond (Closure of Product Sets):

$$\begin{aligned} \mathbf{G}_1 &= \left\{ \left[\begin{smallmatrix} 1 & 0 \\ a & 1 \end{smallmatrix} \right] \,\middle|\, a \in \mathbb{Z} \right\} \sim \mathbb{Z} \quad (\det \mathbb{A} = 1) \\ \mathbf{G}_2 &= \left\{ \left[\begin{smallmatrix} 1 & b \\ 0 & 1 \end{smallmatrix} \right] \,\middle|\, b \in \mathbb{Z} \right\} \sim \mathbb{Z} \quad (\det \mathbb{B} = 1) \end{aligned}$$

Closure of Product Sets $\mathbf{G}_1 * \mathbf{G}_2$ and $\mathbf{G}_2 * \mathbf{G}_1$:

$$\begin{aligned} \left[\begin{smallmatrix} 1 & 0 \\ a & 1 \end{smallmatrix} \right] \left[\begin{smallmatrix} 1 & b \\ 0 & 1 \end{smallmatrix} \right] &= \left[\begin{smallmatrix} 1 & b \\ a & 1+ab \end{smallmatrix} \right] = \mathbb{A}\mathbb{B} \\ \left[\begin{smallmatrix} 1 & b \\ 0 & 1 \end{smallmatrix} \right] \left[\begin{smallmatrix} 1 & 0 \\ a & 1 \end{smallmatrix} \right] &= \left[\begin{smallmatrix} 1+ab & b \\ a & 1 \end{smallmatrix} \right] = \mathbb{B}\mathbb{A} \\ \mathbb{A}\mathbb{B} &\neq \mathbb{B}\mathbb{A} \end{aligned}$$

$$\begin{aligned} \text{Closure} &= \left\{ \mathbf{G}_1 * \mathbf{G}_2 \cup \mathbf{G}_2 * \mathbf{G}_1 \right\} \\ \text{Closure} &\subseteq \mathbb{SL}(2, \mathbb{Z}) \\ \mathbb{SL}(2, \mathbb{Z}) &\ldots \text{ Special Matrix Group over} \\ & \quad\ \text{Ring of } \textbf{Integers} \end{aligned}$$

4. Special Orthogonal Group $\mathbb{SO}(2,\mathbb{R})$

$$
\begin{aligned}
\mathbb{SO}(2,\mathbb{R}) &= \left\{\mathbb{R}(\varphi) \,\middle|\, \varphi \in [0,2\pi)\right\} \\
\mathbb{R}(\varphi) &= \begin{bmatrix} \cos\varphi & -\sin\varphi \\ \sin\varphi & \cos\varphi \end{bmatrix} \\
\mathbb{R}(\varphi)\,\mathbb{R}(\varphi') &= \mathbb{R}(\varphi+\varphi') \\
\varphi * \varphi' &= \varphi + \varphi' \qquad \mathtt{mod}\ [0,2\pi)
\end{aligned}
$$

$\mathcal{E}^2_{\mathbb{R}}$ ... Euclidean Vector Space

$$
\begin{aligned}
\mathbf{x} &= x_1\mathbf{e}_1 + x_2\mathbf{e}_2 = \vec{\mathbf{e}}\cdot \underline{x} \in \mathcal{E}^2_{\mathbb{R}} \\
\underline{x} &= \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} \\
\vec{\mathbf{e}} &= (\mathbf{e}_1, \mathbf{e}_2)
\end{aligned}
$$

$$
\begin{aligned}
\mathcal{R}_\varphi \mathbf{e}_j &= \textstyle\sum_{k=1}^{2} \mathbb{R}_{kj}(\varphi)\,\mathbf{e}_k \\
\mathbf{x}' = \mathcal{R}_\varphi \mathbf{x} &\iff \underline{x}' = \mathbb{R}(\varphi)\,\underline{x}
\end{aligned}
$$

$\left\{\mathbb{R}(\varphi)\right\}$ ... Matrix Group

$\left\{\mathcal{R}_\varphi\right\}$ ... Linear Transformation Group of Euclidean Space $\mathcal{E}^2_{\mathbb{R}} \sim \mathbb{R}^2$ (norm & angle preserving)

$$
\mathbf{x}\cdot\mathbf{x}' = (\mathcal{R}_\varphi \mathbf{x})\cdot(\mathcal{R}_\varphi \mathbf{x}')
$$

5. AFFINE GROUP $\mathbf{A}(3,\mathbb{R})$

$$
\begin{aligned}
\mathbf{A}(3,\mathbb{R}) &= \mathbf{T}(3,\mathbb{R}) \circledS \mathbf{GL}(3,\mathbb{R}) \\
\mathbf{T}(3,\mathbb{R}) &\sim \mathbb{R}^3 \quad \ldots \quad \texttt{Continuous} \\
& \ \texttt{Translation Group} \\
& \ \texttt{over Field } \mathbb{R} \\
\mathbf{GL}(3,\mathbb{R}) &\ \ldots \ \texttt{General Linear Matrix} \\
& \ \texttt{Group over Field } \mathbb{R}
\end{aligned}
$$

$$
\begin{aligned}
\mathbb{D}^{aug}(\mathbf{A}(3,\mathbb{R})) &= \left\{ \mathbb{D}^{aug}(g) \,\middle|\, g \in \mathbf{A}(3,\mathbb{R}) \right\} \\
g &= (A|\mathbf{t}) \\
A &\in \mathbf{GL}(3,\mathbb{R}) \\
\mathbf{t} &= \vec{\mathbf{e}} \cdot \underline{t} \in \mathbf{T}(3,\mathbb{R}) \\
\underline{t} &= \begin{bmatrix} t_1 \\ t_2 \\ t_3 \end{bmatrix} \in \mathbb{R}^3 \\
\vec{\mathbf{e}} &= (\mathbf{e}_1, \mathbf{e}_2, \mathbf{e}_3) \\
\vec{\mathbf{e}} &\ \ldots \ \text{ONB of Space } \mathbb{R}^3
\end{aligned}
$$

5. AFFINE GROUP (cont'd)

Augmented Matrix Group (4-dimensional):

$$\begin{aligned}
\mathbb{D}^{aug}(A|\mathbf{t}) &= \begin{bmatrix} \mathbb{D}(A) & \underline{t} \\ 0\,0\,0 & 1 \end{bmatrix} \\
\mathbb{D}(A) &\in \mathbb{GL}(3,\mathbb{R}) \\
\mathbb{D}^{aug}(A|\mathbf{t})\,\mathbb{D}^{aug}(B|\mathbf{v}) &= \mathbb{D}^{aug}(AB|\mathbf{t}+\mathcal{A}\mathbf{v}) \\
\begin{bmatrix} \mathbb{D}(A) & \underline{t} \\ 0\,0\,0 & 1 \end{bmatrix} \begin{bmatrix} \mathbb{D}(B) & \underline{v} \\ 0\,0\,0 & 1 \end{bmatrix} &= \begin{bmatrix} \mathbb{D}(AB) & \underline{t}+\mathbb{D}(A)\underline{v} \\ 0\,0\,0 & 1 \end{bmatrix}
\end{aligned}$$

$$\begin{aligned}
\mathcal{A}\,\mathbf{e}_j &= \sum_{k=1}^{3} \mathbb{D}_{kj}(A)\,\mathbf{e}_k \\
\mathbf{v} &= \vec{\mathbf{e}} \cdot \underline{v} \\
\mathbf{v}' &= \mathcal{A}\,\mathbf{v} = \vec{\mathbf{e}} \cdot \underline{v}' \\
\underline{v}' &= \mathbb{D}(A)\,\underline{v} \\
\mathbf{t}+\mathcal{A}\mathbf{v} &\longmapsto \underline{t}+\mathbb{D}(A)\underline{v} \\
\mathbb{D}^{aug}(A|\mathbf{t})^{-1} &= \mathbb{D}^{aug}(A^{-1}|-\mathcal{A}^{-1}\mathbf{t}) \\
\begin{bmatrix} \mathbb{D}(A) & \underline{t} \\ 0\,0\,0 & 1 \end{bmatrix}^{-1} &= \begin{bmatrix} \mathbb{D}(A)^{-1} & -\mathbb{D}(A)^{-1}\underline{t} \\ 0\,0\,0 & 1 \end{bmatrix}
\end{aligned}$$

5. AFFINE GROUP (cont'd)

Transformation Group of Space $\mathbb{R}^3$:

$$
\begin{aligned}
\mathcal{E}^3_{\mathbb{R}} &\quad \ldots \quad \text{Euclidean Vector Space} \\
\mathbf{x} &= \vec{\mathbf{e}} \cdot \underline{x} \in \mathcal{E}^3_{\mathbb{R}} \sim \mathbb{R}^3 \\
\underline{x} &= \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} \in \mathbb{R}^3 \\
\mathbf{x} \cdot \mathbf{x}' &= \textstyle\sum_{j=1}^3 x_j x'_j = \|\mathbf{x}\| \, \|\mathbf{x}'\| \cos \Theta \\
d(\mathbf{x}, \mathbf{x}') &= \|\mathbf{x} - \mathbf{x}'\| \\
\|\mathbf{x}\| &= \sqrt{\mathbf{x} \cdot \mathbf{x}}
\end{aligned}
$$

$$
\begin{aligned}
\mathcal{M}(\mathbf{A}(3, \mathbb{R})) &= \left\{ \mathcal{M}(g) \,\middle|\, g \in \mathbf{A}(3, \mathbb{R}) \right\} \\
\mathcal{M}(g) &: \mathbb{R}^3 \longrightarrow \mathbb{R}^3 \\
\mathcal{M}(g)\, \mathbf{x} &= \mathbf{x}_g = \mathcal{A}\mathbf{x} + \mathbf{t} = \vec{\mathbf{e}} \cdot \underline{x}_g \\
\mathcal{M}(A|\mathbf{0})\, \mathbf{e}_j &= \mathcal{A}\mathbf{e}_j = \textstyle\sum_{k=1}^3 \mathbb{D}_{kj}(A)\, \mathbf{e}_k \\
\underline{x}_g &= \mathbb{D}(A)\, \underline{x} + \underline{t} = \underline{x}_{(A|\mathbf{t})}
\end{aligned}
$$

Note: The transformations $\mathcal{M}(A|\mathbf{t})$ are non-linear transformations iff $\mathbf{t} \neq \mathbf{0}$ is valid, whereas all $\mathcal{M}(A|\mathbf{0})$ represent linear transformations.

5. AFFINE GROUP (cont'd)

Transformation Group of Space $\mathbb{R}^3$:

$$
\begin{aligned}
g_o &= (A|\mathbf{0}) \\
A &\in \mathbf{GL}(3,\mathbb{R}) \setminus \mathbf{O}(3,\mathbb{R}) \\
\mathbf{x}_{g_o} \cdot \mathbf{x}'_{g_o} &= \mathcal{A}\mathbf{x} \cdot \mathcal{A}\mathbf{x}' \neq \mathbf{x} \cdot \mathbf{x}' \\
d(\mathbf{x}_g, \mathbf{x}'_g) &= \|\mathcal{A}\mathbf{x} - \mathcal{A}\mathbf{x}'\| \neq d(\mathbf{x}, \mathbf{x}') \\
\|\mathbf{x}_{g_o}\| &= \sqrt{\mathcal{A}\mathbf{x} \cdot \mathcal{A}\mathbf{x}} \neq \|\mathbf{x}\|
\end{aligned}
$$

6. EUCLIDEAN GROUP $\mathbf{E}(3,\mathbb{R})$

$$
\begin{aligned}
\mathbf{E}(3,\mathbb{R}) &= \mathbf{T}(3,\mathbb{R}) \circledS \mathbf{O}(3,\mathbb{R}) \\
\mathbf{T}(3,\mathbb{R}) &\sim \mathbb{R}^3 \\
\mathbf{O}(3,\mathbb{R}) &\ldots \text{Rotation Group} \\
\mathbf{O}(3,\mathbb{R}) &= \mathbf{SO}(3,\mathbb{R}) \times \{E, J\} \\
J &\longleftrightarrow \mathbb{D}(J) = \begin{bmatrix} -1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & -1 \end{bmatrix} \\
J &\ldots \text{Inversion}
\end{aligned}
$$

6. EUCLIDEAN GROUP (cont'd)

Augmented Matrix Group:

$$
\begin{aligned}
\mathbb{D}^{aug}(\mathbf{E}(3,\mathbb{R})) &= \left\{ \mathbb{D}^{aug}(\varepsilon) \,\middle|\, \varepsilon \in \mathbf{E}(3,\mathbb{R}) \right\} \\
\varepsilon &= (R_\omega|\mathbf{t}) \\
R_\omega &= (R_\phi, J^\sigma) \in \mathbf{SO}(3,\mathbb{R}) \times \mathbf{S}_2 \\
& \quad \sigma = 0, 1 \qquad J^0 = E, J^1 = J
\end{aligned}
$$

$$
\begin{aligned}
\mathbb{D}^{aug}(R_\omega|\mathbf{t}) &= \begin{bmatrix} \mathbb{D}(R_\omega) & \underline{t} \\ 0\,0\,0 & 1 \end{bmatrix} \\
\mathcal{R}_\omega \, \mathbf{e}_j &= \sum_{k=1}^{3} \mathbb{D}_{kj}(R_\omega)\, \mathbf{e}_k \\
\mathbb{D}(R_\omega) &\in \mathbb{O}(3,\mathbb{R}) \\
\mathbb{D}(R_\omega) &= \mathbb{D}(R_\phi)\, \mathbb{D}(J^\sigma) \\
\mathbb{D}(R_\phi) &= \mathbb{D}(\alpha)\, \mathbb{D}(\beta)\, \mathbb{D}(\gamma) \\
\mathbb{D}(\alpha) &= \begin{bmatrix} \cos\alpha & \sin\alpha & 0 \\ -\sin\alpha & \cos\alpha & 0 \\ 0 & 0 & 1 \end{bmatrix} \\
\mathbb{D}(\beta) &= \begin{bmatrix} \cos\beta & 0 & \sin\beta \\ 0 & 1 & 0 \\ -\sin\beta & 0 & \cos\beta \end{bmatrix} \\
\mathbb{D}(\gamma) &= \begin{bmatrix} \cos\gamma & \sin\gamma & 0 \\ -\sin\gamma & \cos\gamma & 0 \\ 0 & 0 & 1 \end{bmatrix}
\end{aligned}
$$

6. EUCLIDEAN GROUP (cont'd)

Transformation Group of Space $\mathbb{R}^3$:

$$
\begin{aligned}
\mathcal{M}(\mathsf{E}(3,\mathbb{R})) &= \left\{\mathcal{M}(\varepsilon)\,\middle|\,\varepsilon \in \mathsf{E}(3,\mathbb{R})\right\} \\
\mathcal{M}(\varepsilon) &: \mathbb{R}^3 \longrightarrow \mathbb{R}^3 \\
\mathcal{M}(\varepsilon)\,\mathbf{x} &= \mathbf{x}_\varepsilon = \mathcal{R}_\omega\,\mathbf{x} + \mathbf{t} = \vec{\mathbf{e}} \cdot \underline{x}_\varepsilon \\
\mathcal{M}(R_\omega|\mathbf{0})\,\mathbf{e}_j &= \mathcal{R}_\omega\,\mathbf{e}_j = \sum_{k=1}^{3} \mathbb{D}_{kj}(R_\omega)\,\mathbf{e}_k \\
\underline{x}_\varepsilon &= \mathbb{D}(R_\omega)\,\underline{x} + \underline{t} = \underline{x}_{(R_\omega|\mathbf{t})}
\end{aligned}
$$

Note: The transformations $\mathcal{M}(R_\omega|\mathbf{t})$ are non-linear transformations iff $\mathbf{t} \neq \mathbf{0}$ is valid, whereas all $\mathcal{M}(R_\omega|\mathbf{0})$ represent linear transformations.

$$
\begin{aligned}
\mathbf{x}_{(R_\omega|\mathbf{0})} \cdot \mathbf{x}'_{(R_\omega|\mathbf{0})} &= \mathcal{R}_\omega\,\mathbf{x} \cdot \mathcal{R}_\omega\,\mathbf{x}' = \mathbf{x} \cdot \mathbf{x}' \\
d(\mathbf{x}_\varepsilon, \mathbf{x}'_\varepsilon) &= \|\mathcal{R}_\omega\,\mathbf{x} - \mathcal{R}_\omega\,\mathbf{x}'\| = d(\mathbf{x}, \mathbf{x}') \\
\|\mathbf{x}_{(R_\omega|\mathbf{0})}\| &= \sqrt{\mathcal{R}_\omega\,\mathbf{x} \cdot \mathcal{R}_\omega\,\mathbf{x}} = \|\mathbf{x}\|
\end{aligned}
$$

Transformation Groups of (finite or infinite) Sets: Stabilizers, Orbits, Strata

$$\mathcal{M}(\mathbf{G}) \;=\; \left\{\mathcal{M}(g)\,\middle|\, g\in\mathbf{G}\right\} \;\ldots$$

Transformation Group

$$\mathcal{S} \;=\; \left\{x\,\middle|\, x\in \mathsf{S}\right\} \;\ldots$$

(finite of infinite) Set

$$\mathcal{M}(g)\,x \;=\; g\circ x = x' \in \mathcal{S} \;\ldots$$

Group action on Set $\mathcal{S}$

$$\mathbf{Stab}(x,\mathbf{G}) \;=\; \left\{g\in\mathbf{G}\,\middle|\, g\circ x = x\right\} = \mathbf{S}_{(x,G)}$$

Stabilizer of $x\in\mathcal{S}$ w.r.t. $\mathbf{G}$

$$\mathbf{Orb}(x,\mathbf{G}) \;=\; [x]_G = \left\{x'\,\middle|\, x' = g\circ x\,,\; g\in\mathbf{G}\right\}$$

Orbit of $x\in\mathcal{S}$ w.r.t. $\mathbf{G}$

$$[x]_G \;\sim\; [\tilde{x}]_G \Longleftrightarrow \mathbf{S}_{(\tilde{x},G)} = g\,\mathbf{S}_{(x,G)}\,g^{-1}$$

Equivalence Relation

$$\mathbf{Strat}(x,\mathbf{G}) \;=\; \left\{\bigcup_{x\in\mathcal{S}} [x]_G \subseteq \mathcal{S}\,\middle|\, [x]_G \sim [\tilde{x}]_G\right\}$$

Stratum of $x\in\mathcal{S}$ w.r.t. $\mathbf{G}$

Transformation Groups (cont'd):

Consequence: Subdivision of Set $\mathcal{S}$ into mutually disjoint Subsets

Example A: 1-dimensional Lattice

Group: $\mathbf{G} = \mathbb{Z}$
Set: $\mathcal{S} = \mathbb{R}$

Mapping: $\mathcal{M}(z)\,x = x + z \qquad x \in \mathbb{R}, z \in \mathbb{Z}$

Stabilizer: $\mathbf{Stab}(x, \mathbb{Z}) = \{0\}$

Orbit: $\mathbf{Orb}(x, \mathbb{Z}) = \{x + z | z \in \mathbb{Z}\}$ ...
1-dimensional Lattice
for fixed element $x \in \mathbb{R}$
Consequence: $x \in [0, 1)$

Stratum: $\mathbf{Strat}(x, \mathbb{Z}) = \mathbb{R}$

Example B: Wyckoff Positions

Group: $\mathbf{G} =$ Space Group
Set: $\mathcal{S} = \mathbb{R}^3$ ... Euclidean Space

Euclidean Group as Transformation Group:

Euclidean Group: $\mathsf{E}(3,\mathbb{R}) = \mathsf{T}(3,\mathbb{R}) \circledS \mathsf{O}(3,\mathbb{R})$

Seitz Symbol: $\varepsilon = (R_\omega|\mathbf{v}) \in \mathsf{E}(3,\mathbb{R})$

Transformation: $\mathcal{M}(\varepsilon) : \mathbb{R}^3 \longrightarrow \mathbb{R}^3$

$$\mathcal{M}(\varepsilon)\,\mathbf{x} = \mathbf{x}_\varepsilon$$

$$\mathbf{x}_\varepsilon = \mathcal{R}_\omega\,\mathbf{x} + \mathbf{v}$$

$$\mathbf{x} = \vec{\mathbf{e}} \cdot \underline{x}$$

$$\mathbf{v} = \vec{\mathbf{e}} \cdot \underline{v}$$

$$\mathbf{x}_\varepsilon = \vec{\mathbf{e}} \cdot \underline{x}_\varepsilon$$

$$\underline{x}_\varepsilon = \mathbb{D}(R_\omega)\,\underline{x} + \underline{v}$$

Augmentation: $\mathbb{D}^{aug}(R_\omega|\mathbf{v}) = \begin{bmatrix} \mathbb{D}(R_\omega) & \underline{v} \\ 0\,0\,0 & 1 \end{bmatrix}$

Note that $\mathcal{M}(\varepsilon)$ represent non-linear transformations of the space $\mathbb{R}^3 \longrightarrow \mathbb{R}^3$ for all non-zero translations $\mathbf{v} \in \mathsf{T}(3,\mathbb{R})$, whereas the elements $(R_\omega|\mathbf{0})$ represent linear transformations.

$$\mathsf{E}(3,\mathbb{R}) \;\subset\; \mathsf{A}(3,\mathbb{R})$$

Embedding of Space Groups as countable **Subgroups** of the Euclidean Group:

Step 1: **Bravais Lattice**

$$\mathsf{T} = \left\{ \mathrm{t} = \vec{\mathrm{t}} \cdot \underline{n} \,\middle|\, \underline{n} \in \mathbb{Z}^3 \right\}$$

$$\vec{\mathrm{t}} = (\mathrm{t}_1, \mathrm{t}_2, \mathrm{t}_3) = \vec{\mathrm{e}}\, \mathbb{D}(L)$$

$$\mathrm{t}_j = \sum_{k=1}^{3} \mathbb{D}_{kj}(L)\, \mathrm{e}_k$$

$$\mathbb{D}(L) \in \mathbb{SL}(3, \mathbb{R}) \iff \mathtt{Det}\, \mathbb{D}(L) > 0$$

$\{\vec{\mathrm{t}}\} \ldots$ **Primitive Basis of** T

(defines **Primitive Cell**)

$$\mathtt{Vol}\,(\mathbf{E}(\mathsf{T})) = \mathtt{Det}\,\{\vec{\mathrm{t}}\} = \mathtt{Det}\,\mathbb{D}(L)$$

$$\vec{\mathrm{t}}(z) = \vec{\mathrm{t}}\, \mathbb{M}(z)$$

$$\mathrm{t}_j(z) = \sum_{k=1}^{3} \mathbb{M}_{kj}(z)\, \mathrm{t}_k$$

$$\mathbb{M}(z) \in \mathbb{SL}(3, \mathbb{Z}) \iff \mathtt{Det}\, \mathbb{M}(z) = 1$$

$\{\vec{\mathrm{t}}(z)\} \ldots$ Equivalent Basis of T

($\Rightarrow$ $\mathbb{SL}(3, \mathbb{Z})$–ambiguity)

Embedding of Space Groups (cont'd):

Step 2: **Holohedral Point Group**

of **Bravais Lattice T**

$$\mathbf{P}_{max}(L) = \mathbf{P}(L)$$

$$\mathbf{P}(L) = \left\{ R_\omega \in \mathbf{O}(3,\mathbb{R}) \,\middle|\, \mathcal{R}_\omega \mathbf{T} = \mathbf{T} \right\}$$

$$\mathcal{R}_\omega \mathbf{T} = \mathbf{T} \Longleftrightarrow \begin{cases} \mathcal{R}_\omega \vec{\mathfrak{t}} = \vec{\mathfrak{t}}\, \mathbb{D}(R_\omega) \\ \mathbb{D}(R_\omega) \in \mathbb{GL}(3,\mathbb{Z}) \end{cases}$$

Step 3: **Space Groups**

$$\mathbf{G} = \left\{ \mathbf{T}, \mathbf{P} | \mathcal{O}, \mathbf{w}_{\mathbf{P}} \right\}$$

$$\mathbf{P}_{min}(L) \subseteq \mathbf{P} \subseteq \mathbf{P}_{max}(L)$$

$\mathcal{O}$ ... `Origin`

$$\mathbf{w}_{\mathbf{P}} = \left\{ \mathbf{w}_R = \mathbf{n}(R) \,\middle|\, R \in \mathbf{P} \right\} \ \ldots$$

`Set of Fractional Translations`

`(Non-primitive Translations)`

$$\mathbf{T} \triangleleft \mathbf{G} \Rightarrow \mathbf{G}/\mathbf{T} \sim \mathbf{P} \Longleftrightarrow$$

$$h : \mathbf{G} \longrightarrow \mathbf{T} \Longleftrightarrow \mathrm{ker}_h = \mathbf{T}$$

Details of Space Groups:

Space Group Types: **230 (219)**

Space Group Elements:

$g = (R|\mathbf{w}_R + \mathbf{t})$

$\mathbf{w}_{\mathsf{P}} = \left\{ \mathbf{w}_R \middle| R \in \mathsf{P} \right\}$

$R \in \mathsf{P}$

$\mathbf{w}_R = \vec{\mathsf{t}} \cdot \underline{w}_R \,, \ \underline{w}_R \in \mathbb{Q}^3$

$\mathbf{t} = \vec{\mathsf{t}} \cdot \underline{n} \,, \ \underline{n} \in \mathbb{Z}^3$

Factorization:

$(R|\mathbf{w}_R + \mathbf{t}) =$
$(E|\mathbf{t}) * (R|\mathbf{w}_R)$

1. Symmorphic Space Groups:

$$\mathsf{G} \ = \ \mathsf{T} \circledS \mathsf{P} \quad \Longleftrightarrow \quad \mathbf{w}_{\mathsf{P}} \sim \{0\}$$

2. Non-Symmorphic Space Groups:

$$\mathsf{G} \ \neq \ \mathsf{T} \circledS \mathsf{P} \quad \Longleftrightarrow \quad \mathbf{w}_{\mathsf{P}} \nsim \{0\}$$

Space Groups: Symmorphic

$$
\begin{aligned}
\mathsf{G} &= \mathsf{T} \circledS \mathsf{P} \\
(R|\mathbf{t})(S|\mathbf{u}) &= (RS|\mathbf{t} + \mathcal{R}\mathbf{u})
\end{aligned}
$$

Shift of Origin: $\mathbf{v} = \vec{\mathbf{e}} \cdot \underline{v}, \ \underline{v} \in \mathbb{R}^3$

$$
\begin{aligned}
\mathsf{G}^{(E|\mathbf{v})} &= (E|\mathbf{v}) * \mathsf{G} * (E|\mathbf{v})^{-1} \\
(E|\mathbf{v})(R|\mathbf{t})(E|\mathbf{v})^{-1} &= (R|\mathbf{v}_R + \mathbf{t}) \\
\mathbf{v}_R &= \mathbf{v} - \mathcal{R}\mathbf{v} \\
(R|\mathbf{v}_R)(S|\mathbf{v}_S) &= (RS|\mathbf{v}_{RS})
\end{aligned}
$$

Space Groups: Non-Symmorphic

$$
\begin{aligned}
\mathsf{G} &= \{\mathsf{T}, \mathsf{P}|\mathcal{O}, \mathbf{w}_{\mathsf{P}}\} \\
& \quad (R|\mathbf{w}_R + \mathbf{t})(S|\mathbf{w}_S + \mathbf{u}) = \\
& \quad (RS|\mathbf{w}_{RS} + \mathbf{t}(R,S) + \mathbf{t} + \mathcal{R}\,\mathbf{u}) \\
\mathbf{t}(R,S) &= \mathbf{w}_R + \mathcal{R}\,\mathbf{w}_S - \mathbf{w}_{RS} \in \mathsf{T}
\end{aligned}
$$

Note: Iff some $\mathbf{t}(R,S) \neq \mathbf{0}$, then the space group G is non-symmorphic.

`Equivalence Relation:` Arithmetic Classes

$$
\begin{aligned}
\mathsf{G} &= \{\mathsf{T}, \mathsf{P} | \mathcal{O}, \mathbf{w}_{\mathsf{P}}\} \\
g &= (R | \mathbf{w}_R + \mathbf{t}) \\
\vec{\mathrm{t}} &= \vec{\mathrm{e}} \cdot \mathbb{D}(L) \Longleftrightarrow \mathbb{D}(L) \in \mathbb{SL}(3, \mathbb{R}) \\
\mathrm{t} &= \vec{\mathrm{t}} \cdot \underline{n} \Longleftrightarrow \underline{n} \in \mathbb{Z}^3 \\
\mathbf{w}_R &= \vec{\mathrm{t}} \cdot \underline{w}_R \Longleftrightarrow \underline{w}_R \in \mathbb{Q}^3 \\
\mathcal{R}\,\vec{\mathrm{t}} &= \vec{\mathrm{t}}\, \mathbb{D}(R) \Longleftrightarrow \mathbb{D}(R) \in \mathbb{GL}(3, \mathbb{Z}) \\
\mathbb{D}^{aug}(g) &= \begin{bmatrix} \mathbb{D}(R) & \underline{w}_R + \underline{n} \\ 0\,0\,0 & 1 \end{bmatrix}
\end{aligned}
$$

$$
\begin{aligned}
\mathsf{G}' &= \left\{\mathsf{T}', \mathsf{P}' | \mathcal{O}', \mathbf{w}'_{\mathsf{P}'}\right\} \\
g' &= (R' | \mathbf{w}'_{R'} + \mathbf{t}') \\
\vec{\mathrm{t}}' &= \vec{\mathrm{e}} \cdot \mathbb{D}(L') \Longleftrightarrow \mathbb{D}(L') \in \mathbb{SL}(3, \mathbb{R}) \\
\mathrm{t}' &= \vec{\mathrm{t}}' \cdot \underline{n}' \Longleftrightarrow \underline{n}' \in \mathbb{Z}^3 \\
\mathbf{w}'_{R'} &= \vec{\mathrm{t}}' \cdot \underline{w}'_{R'} \Longleftrightarrow \underline{w}'_{R'} \in \mathbb{Q}^3 \\
\mathcal{R}'\,\vec{\mathrm{t}}' &= \vec{\mathrm{t}}'\, \mathbb{D}(R') \Longleftrightarrow \mathbb{D}(R') \in \mathbb{GL}(3, \mathbb{Z}) \\
\mathbb{D}^{aug}(g') &= \begin{bmatrix} \mathbb{D}(R') & \underline{w}'_{R'} + \underline{n}' \\ 0\,0\,0 & 1 \end{bmatrix}
\end{aligned}
$$

$$
\begin{aligned}
\left\{\mathbb{D}(\mathsf{P}')\right\} &= \left\{\mathbb{W}\, \mathbb{D}(\mathsf{P})\, \mathbb{W}^{-1}\right\} \Longleftrightarrow \mathbb{W} \in \mathbb{SL}(3, \mathbb{Z}) \\
\left|\mathcal{A}(\mathsf{G})\right| &= \mathbf{73} \;\ldots\; \texttt{Arithmetic Classes}
\end{aligned}
$$

■ Born von Karman Bravais Lattices

$$\begin{aligned}
\vec{t}(\underline{N}) &= \vec{t}\,\mathbb{M}(\underline{N}) = \left(N_1\mathbf{t}_1, N_2\mathbf{t}_2, N_3\mathbf{t}_3\right) \\
\mathbb{M}(\underline{N}) &= \begin{bmatrix} N_1 & 0 & 0 \\ 0 & N_2 & 0 \\ 0 & 0 & N_3 \end{bmatrix} \\
\underline{N} &= (N_1, N_2, N_3)^{\mathrm{T}} \\
\mathbf{T}(\underline{N}) &= \left\{\vec{\mathrm{T}} = \vec{t}(\underline{N})\cdot\underline{m}\,\middle|\,\underline{m}\in\mathbb{Z}^3\right\} \subset \mathbf{T} \\
\mathbf{T}_{\underline{N}} &\sim \mathbf{T}/\mathbf{T}(\underline{N}) \sim \mathbf{C}_{\underline{N}} \\
\mathbf{C}_{\underline{N}} &= \mathbf{C}_{N_1}\otimes\mathbf{C}_{N_2}\otimes\mathbf{C}_{N_3}
\end{aligned}$$

Cubic:
Trigonal: $\underline{N} = (N_1, N_1, N_1)$

Hexagonal:
Tetragonal: $\underline{N} = (N_1, N_1, N_3)$

Orthorhombic:
Monoclinic:
Triclinic: $\underline{N} = (N_1, N_2, N_3)$

■ Born von Karman Space Groups

$$\begin{aligned}
\mathbf{G}(\underline{N}) &\sim \mathbf{G}/\mathbf{T}(\underline{N}) \Rightarrow |\mathbf{G}(\underline{N})| = |\mathbf{P}|\cdot N^3 \\
N &= \text{multiple of } 24 \quad \texttt{(conjectured)}
\end{aligned}$$

Remarks on Bravais Lattices

$$\begin{array}{ccc}
\text{Bravais System} & \longleftrightarrow & \text{Crystal System} \\
\texttt{Point Group:} & \ldots & \mathbf{P}_{max}(L) \\
 & \Rightarrow & \mathbf{7}\ \text{Crystal Systems}
\end{array}$$

$$\begin{array}{rcl}
\vec{\mathfrak{t}} & = & (\mathfrak{t}_1, \mathfrak{t}_2, \mathfrak{t}_3) = \vec{\mathfrak{e}}\,\mathbb{D}(L) \\
\mathbb{D}(L) & = & \mathbb{D}(R_\phi)\,\mathbb{C}(L)\,\mathbb{M}(q)\,\mathbb{M}(z) \\
\mathbb{D}(R_\phi) & \in & \mathbb{SO}(3,\mathbb{R}) \\
\mathbb{M}(z) & \in & \mathbb{SL}(3,\mathbb{Z}) \\
\mathbb{C}(L) & = & \mathbb{T}(\alpha,\beta,\gamma)\,\mathbb{D}(a,b,c)\ \ \ldots \\
 & & \texttt{Conventional Basis of Bravais Lattice} \\
\mathbb{T}(\alpha,\beta,\gamma) & = & \begin{bmatrix} 1 & v & x \\ 0 & w & y \\ 0 & 0 & z \end{bmatrix} \\
\mathbb{D}(a,b,c) & = & \begin{bmatrix} a & 0 & 0 \\ 0 & b & 0 \\ 0 & 0 & c \end{bmatrix} \\
\mathbb{M}(q) & \ldots & \texttt{Centring Matrices} \\
v & = & \cos\gamma \\
w & = & \sin\gamma \\
x & = & \cos\beta \\
y & = & (\cos\alpha - \cos\beta\cos\gamma)/\sin\gamma \\
z & = & \dfrac{\sqrt{1-\cos^2\alpha-\cos^2\beta-\cos^2\gamma+2\cos\alpha\cos\beta\cos\gamma}}{\sin\gamma}
\end{array}$$

Remarks on Bravais Lattices (cont'd)

Triclinic:	$a \neq b$ $b \neq c$ $c \neq a$ $\alpha \neq \beta$ $\beta \neq \gamma$ $\gamma \neq \alpha$
Monoclinic:	$a \neq b$ $b \neq c$ $c \neq a$ $\alpha = \gamma = \pi/2 \neq \beta$
Orthorhombic:	$a \neq b$ $b \neq c$ $c \neq a$ $\alpha = \beta = \gamma = \pi/2$
Tetragonal:	$a = b$ $b \neq c$ $c \neq a$ $\alpha = \beta = \gamma = \pi/2$
Hexagonal:	$a = b$ $b \neq c$ $c \neq a$ $\alpha = \beta = \pi/2$ $\gamma = 2\pi/3$
Trigonal:	$a = b$ $b = c$ $c = a$ $\alpha = \beta = \gamma \neq 2\pi/3, \pi/2, \pi/3$
Cubic:	$a = b$ $b = c$ $c = a$ $\alpha = \beta = \gamma = \pi/2$

Triclinic:	$\bar{1}$	$\mathbf{S}_2 = \{E, I\}$
Monoclinic:	$2/m$	$\mathbf{C}_{2h} = \mathbf{C}_2 \otimes \mathbf{S}_2$
Orthorhombic:	mmm	$\mathbf{D}_{2h} = \mathbf{D}_2 \otimes \mathbf{S}_2$
Tetragonal:	$4/mmm$	$\mathbf{D}_{4h} = \mathbf{D}_4 \otimes \mathbf{S}_2$
Hexagonal:	$6/mmm$	$\mathbf{D}_{6h} = \mathbf{D}_6 \otimes \mathbf{S}_2$
Trigonal:	$\bar{3}m$	$\mathbf{D}_{3d} = \mathbf{D}_3 \otimes \mathbf{S}_2$
Cubic:	$m\bar{3}m$	$\mathbf{O}_h = \mathbf{O} \otimes \mathbf{S}_2$

Remarks on Bravais Lattices (cont'd)

$$\text{Bravais Class} \longleftrightarrow \text{Crystal Class}$$

Lattices: ... various centrings

$\Rightarrow$ **14** Crystal Classes

Triclinic:	$\longmapsto$	$\{P\}$
Monoclinic:	$\longmapsto$	$\{P, B\}$
Orthorhombic:	$\longmapsto$	$\{P, B, I, F\}$
Tetragonal:	$\longmapsto$	$\{P, I\}$
Hexagonal:	$\longmapsto$	$\{P\}$
Trigonal:	$\longmapsto$	$\{P\}$
Cubic:	$\longmapsto$	$\{P, I, F\}$

P ... Primitive

B ... Base centred

I ... Body centred

F ... Face centred

Remarks on Bravais Lattices (cont'd)

Triclinic:	$\mathbb{C}(L) = \mathbb{SL}(3,\mathbb{R})$–Matrix
Monoclinic:	$\begin{bmatrix} a & b\cos\gamma & 0 \\ 0 & b\sin\gamma & 0 \\ 0 & 0 & c \end{bmatrix}$
Orthorhombic:	$\begin{bmatrix} a & 0 & 0 \\ 0 & b & 0 \\ 0 & 0 & c \end{bmatrix}$
Tetragonal:	$\begin{bmatrix} a & 0 & 0 \\ 0 & a & 0 \\ 0 & 0 & c \end{bmatrix}$
Hexagonal:	$\begin{bmatrix} a & -a/2 & 0 \\ 0 & a\sqrt{3}/2 & 0 \\ 0 & 0 & c \end{bmatrix}$
Trigonal:	$\begin{bmatrix} a & -a/2 & -a/2 \\ 0 & a\sqrt{3}/2 & -a\sqrt{3}/2 \\ c & c & c \end{bmatrix}$
Cubic:	$\begin{bmatrix} a & 0 & 0 \\ 0 & a & 0 \\ 0 & 0 & a \end{bmatrix}$

$$\begin{aligned} \mathbb{M}(q) &= \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix} \quad \texttt{... primitive (P)} \\ &= \tfrac{1}{2}\begin{bmatrix} 1 & 1 & 0 \\ -1 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix} \quad \texttt{... base (B)} \\ &= \tfrac{1}{2}\begin{bmatrix} -1 & 1 & 1 \\ 1 & -1 & 1 \\ 1 & 1 & -1 \end{bmatrix} \quad \texttt{... body (I)} \\ &= \tfrac{1}{2}\begin{bmatrix} 0 & 1 & 1 \\ 1 & 0 & 1 \\ 1 & 1 & 0 \end{bmatrix} \quad \texttt{... face (F)} \end{aligned}$$

Problems: Bravais Lattices

[1] Identification of Bravais Lattices:

$$\mathbb{D}(L) = \mathbb{D}(R_\phi)\,\mathbb{C}(L)\,\mathbb{M}(q)\,\mathbb{M}(z)$$

$$\begin{aligned}
\mathbb{S}(L) &= \mathbb{C}(L)\,\mathbb{M}(q) \\
\mathbb{D}(R_\phi) &\in \mathbb{SO}(3,\mathbb{R}) \\
\mathbb{C}(L) &\in \mathbb{SL}(3,\mathbb{R}) \\
\mathbb{M}(z) &\in \mathbb{SL}(3,\mathbb{Z}) \\
\vec{\mathbf{c}} &= (\mathbf{c}_1, \mathbf{c}_2, \mathbf{c}_3) \\
&= \vec{\mathbf{e}}\,\mathbb{C}(L)
\end{aligned}$$

[2] Deformation of Bravais Lattices:
Continuous change of lattice parameters

[3] Distortion of Bravais Lattices:

$$\mathbb{D}(L(\delta)) = \mathbb{D}(L)\,\mathbb{D}(\delta)$$

$$\mathbb{D}(\delta) = \begin{bmatrix} 1+\delta_{11} & \delta_{12} & \delta_{13} \\ \delta_{21} & 1+\delta_{22} & \delta_{23} \\ \delta_{31} & \delta_{32} & 1+\delta_{33} \end{bmatrix}$$

[4] Periodic (**BvK**) Boundary Conditions:
Appropriate choice of the boundary integer N, such that space group properties of the finite images are not violated and that group-subgroup relations are not distroyed.

Details on Wyckoff Positions

$$
\begin{aligned}
\mathsf{G} &= \{\mathsf{T},\mathsf{P}|\mathcal{O},\mathbf{w}_{\mathsf{P}}\} \\
g &= (R|\mathbf{w}_R+\mathbf{t}) \in \mathsf{G} \\
\mathbf{w}_R &= \vec{\mathrm{t}}\cdot \underline{w}_R \;\Rightarrow\; \underline{w}_R \in \mathbb{Q}^3 \\
\mathbf{t} &= \vec{\mathrm{t}}\cdot \underline{n} \;\Rightarrow\; \underline{n} \in \mathbb{Z}^3 \\
\mathcal{R}\vec{\mathrm{t}} &= \vec{\mathrm{t}}\,\mathbb{D}(R) \;\Rightarrow\; \mathbb{D}(R) \in \mathbb{SL}(3,\mathbb{Z}) \\
\mathcal{M}(g) &: \mathbb{R}^3 \longrightarrow \mathbb{R}^3 \\
\mathbf{x} &= \vec{\mathrm{e}}\cdot \underline{x} = \vec{\mathrm{t}}\cdot \underline{x}^* \Rightarrow \underline{x} = \mathbb{D}(L)\,\underline{x}^* \\
\mathbf{x}_g &= \mathcal{M}(g)\,\mathbf{x} = \mathcal{R}\,\mathbf{x} + \mathbf{w}_R + \mathbf{t} = \vec{\mathrm{t}}\cdot \underline{x}_g^* \\
\underline{x}_g^* &= \mathbb{D}(R)\,\underline{x}^* + \underline{w}_R + \underline{n}
\end{aligned}
$$

$$
\begin{aligned}
\mathsf{Stab}(\mathbf{x},\mathsf{G}) &= \mathsf{S}_{(\mathbf{x},G)} \;\ldots\; \texttt{Site Group} \subset \mathsf{G} \\
\mathsf{Orb}(\mathbf{x},\mathsf{G}) &= \left\{\mathcal{M}(g)\,\mathbf{x} \,\middle|\, g \in \mathsf{G}\right\} \cap \mathsf{E}(\mathsf{T}) \\
\mathsf{Strat}(\mathbf{x},\mathsf{G}) &= \texttt{Union of Set of Orbits} \\
&\quad \texttt{that satisfy equivalence rel's} \\
&\quad \mathsf{S}_{(\mathbf{x}',G)} = g * \mathsf{S}_{(\mathbf{x},G)} * g^{-1}
\end{aligned}
$$

Note: This leads to a subdivision of the primitive cell into mutually disjoint subsets that are periodically repeated because of the Bravais lattice.

[2] Group Representations

$$\textbf{Rep}(\mathbf{G}) \quad \ldots \quad \texttt{Homomorphism:} \quad h(\mathbf{G}) = \mathcal{M}(\mathbf{G})$$

$$\mathcal{M}(\mathbf{G}) \quad \ldots \quad \texttt{Non-singular Transformation Group of Vector Space } \mathbf{V}_{\mathbb{K}}$$

$$\begin{aligned} \mathcal{M}(\mathbf{G}) &= \left\{ \mathcal{M}(e), \mathcal{M}(g_2), \mathcal{M}(g_3), \ldots \right\} \\ & \quad \mathcal{M}(g) : \mathbf{V}_{\mathbb{K}} \longrightarrow \mathbf{V}_{\mathbb{K}} \end{aligned}$$

$$\begin{array}{ll} [1] & \mathcal{M}(g)\,\mathbf{v} = \mathbf{v}_g = \mathbf{w} \in \mathbf{V}_{\mathbb{K}} \\ [2] & \mathcal{M}(g)\left[\mathcal{M}(g')\right]\,\mathbf{v} = \left[\mathcal{M}(gg')\right]\,\mathbf{v} \\ [3] & \mathcal{M}(e)\,\mathbf{v} = \mathbf{v} \\ [4] & \mathcal{M}(g)^{-1}\,\mathbf{v} = \mathcal{M}(g^{-1})\,\mathbf{v} \\ & \forall \mathbf{v}, \mathbf{w} \in \mathbf{V}_{\mathbb{K}} \quad \& \quad \forall g, g' \in \mathbf{G} \end{array}$$

Example: Euclidean Group $\mathbf{E}(3,\mathbb{R})$ as Transformation Group of the Euclidean Vector Space $\mathbb{R}^3$

$$\begin{aligned} g &= (R_\omega|\mathbf{v}) \in \mathbf{E}(3,\mathbb{R}) \\ \mathcal{M}(g)\,\mathbf{x} &= \mathcal{R}_\omega\,\mathbf{x} + \mathbf{v} \\ \mathcal{M}(R_\omega|\mathbf{v})\,\mathcal{M}(R'_\omega|\mathbf{v}') &= \mathcal{M}(R_\omega R'_\omega|\mathbf{v} + \mathcal{R}_\omega\,\mathbf{v}') \\ \mathcal{M}(g)\,(a\mathbf{x}) &\neq a\mathcal{M}(g)\,\mathbf{x} \quad \texttt{unless} \quad \mathbf{v} = \mathbf{0} \end{aligned}$$

- **Linear Operator Representation**

$$
\begin{array}{rcl}
h(\mathbf{G}) & = & \mathcal{L}(\mathbf{G}) \\
\mathcal{L}(g)\,(a\mathbf{v} + b\mathbf{w}) & = & a\mathcal{L}(g)\,\mathbf{v} + b\mathcal{L}(g)\,\mathbf{w} \\
\texttt{Basis of } \mathbf{V}_{\mathbb{K}} : & & \{\mathbf{v}_\ell\} = \left\{\mathbf{v}_1, \mathbf{v}_2, \mathbf{v}_3, \ldots \mathbf{v}_n\right\} \\
 & & \texttt{dim } \mathbf{V}_{\mathbb{K}} = n \\
\texttt{Matrix } \mathbf{D}(\mathbf{G}) : & & \mathcal{L}(g)\,\mathbf{v}_j = \sum_{k=1}^{n} \mathbf{D}_{kj}^{[v]}(g)\,\mathbf{v}_k \\
\mathcal{L}(g)\mathcal{L}(g') & & \mathbf{D}^{[v]}(g)\mathbf{D}^{[v]}(g') \\
= \mathcal{L}(gg') & \Longleftrightarrow & = \mathbf{D}^{[v]}(gg') \\
\texttt{Change of Basis} : & & \{\mathbf{v}_\ell\} \longrightarrow \{\mathbf{w}_\ell\} \\
 & & \mathbf{w}_k = \sum_{j=1}^{n} \mathsf{W}_{jk}\mathbf{v}_j \\
 & & \left\{\mathbf{D}^{[v]}(g)\right\} \longrightarrow \left\{\mathbf{D}^{[w]}(g)\right\} \\
 & & \mathbf{D}^{[w]}(g) = \mathsf{W}^{-1}\mathbf{D}^{[v]}(g)\mathsf{W}
\end{array}
$$

Note: The set $\{\mathcal{L}(g)\}$ is called linear operator representation of the group $\mathbf{G}$ with $\mathbf{V}_{\mathbb{K}}$ as its carrier space. The set $\{\mathbf{D}^{[v]}(g)\}$ is called matrix representation of $\mathbf{G}$ and $\{\mathbf{D}^{[v]}(g)\} \longleftrightarrow \{\mathbf{D}^{[w]}(g)\}$ equivalent matrix representations of the group $\mathbf{G}$.

★ Anti-Linear Operator Representation

$$
\begin{aligned}
h(\mathbf{G}) &= \mathcal{A}(\mathbf{M}) \\
\mathbf{M} &= \mathbf{G} \cup \{a\} * \mathbf{G} \\
aa &= a^2 = g_o \in \mathbf{G} \\
\mathcal{A}(g)\,(\alpha\mathbf{v} + \beta\mathbf{w}) &= \alpha\mathcal{A}(g)\,\mathbf{v} + \beta\mathcal{A}(g)\,\mathbf{w} \\
\mathcal{A}(a)\,(\alpha\mathbf{v} + \beta\mathbf{w}) &= \alpha^*\mathcal{A}(a)\,\mathbf{v} + \beta^*\mathcal{A}(a)\,\mathbf{w}
\end{aligned}
$$

Example: $\mathcal{A}(a)\ \ldots$

`Time Reversal Operator`

`Basis` $\{\mathbf{v}_\ell\}$: $\Rightarrow$ `Co-Matrix Representation`

$$
\begin{aligned}
\mathcal{A}(m)\,\mathbf{v}_\ell &= \textstyle\sum_{k=1}^{n} \mathbf{D}_{k\ell}(m)\,\mathbf{v}_k \\
\mathbf{D}(g)\,\mathbf{D}(g') &= \mathbf{D}(gg') \\
\mathbf{D}(g)\,\mathbf{D}(a) &= \mathbf{D}(ga) \\
\mathbf{D}(a)\,\mathbf{D}^*(g) &= \mathbf{D}(ag) \\
\mathbf{D}(a)\,\mathbf{D}^*(a) &= \mathbf{D}(a^2) = \mathbf{D}(g_o)
\end{aligned}
$$

Remarks: The generalisation of space groups to magnetic space groups are called after Shubnikov, where in total 1651 Shubnikov space group types exist.

▲ Unitary Operator Representation

$$
\begin{array}{rcl}
h(\mathbf{G}) & = & \mathsf{U}(\mathbf{G}) = \{\mathsf{U}(g) | g \in \mathbf{G}\} \\
\mathsf{U}(g) & \ldots & \texttt{linear \& unitary operators} \\
\left\langle \phi \,, \psi \right\rangle & = & \left\langle \mathsf{U}(g)\phi \,, \mathsf{U}(g)\psi \right\rangle
\end{array}
$$

Unitary **Matrix Representation**

$$
\mathsf{U}(g) \longmapsto \mathbf{D}^w(g) \Longleftrightarrow \mathbf{D}^w(g^{-1}) = \mathbf{D}^w(g)^\dagger
$$

ONB:

$$
\{\mathbf{w}_i\} = \left\{\mathbf{w}_1, \mathbf{w}_2, \ldots \mathbf{w}_s\right\}
$$

$$
\left\langle \mathbf{w}_i \,, \mathbf{w}_j \right\rangle = \delta_{ij}
$$

$$
\mathsf{U}(g)\,\mathbf{w}_i = \textstyle\sum_{j=1}^{s} \mathbf{D}^w_{ji}(g)\,\mathbf{w}_j
$$

$$
\mathbf{D}^w_{ji}(g) = \left\langle \mathbf{w}_j \,, \mathsf{U}(g)\mathbf{w}_i \right\rangle
$$

Remarks: The matrix representation $\{\mathbf{D}^w(g)\}$ assigned to the unitary operator representation $\{\mathsf{U}(g)\}$ need not be unitary if the basis $\{\mathbf{w}_i\}$ does not form an orthonormal basis (**ONB**).

Example: Unitary Operator Representation of Space Group $\mathbf{G}$ with $\mathsf{L}^2(\mathbb{R}^3)$ as Carrier Space

$$
\begin{aligned}
\mathbf{G} &= \left\{\mathbf{T}, \mathbf{P} | \mathcal{O}, \mathbf{w}_{\mathsf{P}}\right\} \\
g &= (R|\mathbf{w}_R + \mathbf{t}) \in \mathbf{G} \\
g &\longmapsto \mathcal{M}(g) \longmapsto \mathsf{U}(g) \\
[\mathsf{U}(g)\phi]\,(\mathbf{x}) &= \phi(\mathcal{M}(g)^{-1}\mathbf{x}) \\
\mathsf{U}(g)\,\mathsf{U}(g') &= \mathsf{U}(gg') \\
\left\langle \phi \,\mathbf{,}\, \psi \right\rangle &= \left\langle \mathsf{U}(g)\phi \,\mathbf{,}\, \mathsf{U}(g)\psi \right\rangle
\end{aligned}
$$

$\mathbf{G}$ – Invariant Subspace $\mathbf{W}_{\mathbb{K}} \subset \mathbf{V}_{\mathbb{K}}$

$\mathbf{G}$ – `Invariance` $\quad \mathcal{L}(g)\mathbf{w} = \mathbf{w}_g \in \mathbf{W}_{\mathbb{K}}$

$\forall \mathbf{w} \in \mathbf{W}_{\mathbb{K}}$ and $\forall g \in \mathbf{G}$

`Basis of` $\mathbf{W}_{\mathbb{K}}$ $\quad \{\mathbf{w}_s\} = \left\{\mathbf{w}_1, \mathbf{w}_2, \ldots \mathbf{w}_m\right\}$

$\mathtt{dim}\ \mathbf{W}_{\mathbb{K}} = m < \mathtt{dim}\ \mathbf{V}_{\mathbb{K}} = n$

`Matrix` $\mathbf{D}^w(\mathbf{G})$ $\quad \mathcal{L}(g)\,\mathbf{w}_s = \sum_{r=1}^{m} \mathbf{D}^w_{rs}(g)\,\mathbf{w}_r$

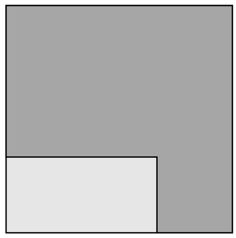
$\mathcal{L}(g)\mathcal{L}(g') = \mathcal{L}(gg') \Longleftrightarrow$

$\mathbf{D}^w(g)\mathbf{D}^w(g') = \mathbf{D}^w(gg')$

■ Reducible and Irreducible Representations:

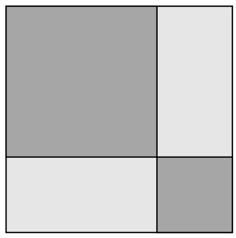
Reducible
Representation

$\mathbf{D}^{v}(\mathbf{G}) =$



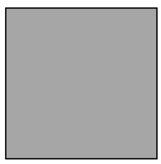
Completely
Reducible
Representation

$\mathbf{D}^{w}(\mathbf{G}) =$



Irreducible
Representation

$\mathbf{D}^{z}(\mathbf{G}) =$



Criterion for the Irreducibility of Matrix Representations:

Notations and Definitions:

$$
\begin{array}{rcl}
\textbf{UIR} & \ldots & \texttt{Unitary Irreducible Representation} \\
\mathbf{D}^{\alpha}(\mathbf{G}) & = & \left\{ \mathbf{D}^{\alpha}(g) \,\middle|\, g \in \mathbf{G} \right\} \ \ldots\ \textbf{UIR} \\
\chi^{\alpha}(g) & = & \texttt{trace}\ \mathbf{D}^{\alpha}(g) \ \ldots\ \text{Character} \\
\bar{\chi}^{\alpha}(g) & = & \texttt{trace}\ (\mathbf{W}^{-1}\,\mathbf{D}^{\alpha}(g)\,\mathbf{W}) = \chi^{\alpha}(g) \\
\alpha & \in & A(\mathbf{G}) \ \ldots\ \texttt{Set of Labels of UIR's} \\
n(\alpha) & = & \texttt{dim}\ \mathbf{D}^{\alpha}(\mathbf{G}) \\
\mathbf{D}^{\alpha}_{jk}(g) & \ldots & \texttt{Matrix Elements} \\
 & & j,k = 1,2,\ldots n(\alpha)
\end{array}
$$

- **Representation Property:**

$$
\mathbf{D}^{\alpha}(g)\,\mathbf{D}^{\alpha}(g') \;=\; \mathbf{D}^{\alpha}(gg') \qquad \forall g, g' \in \mathbf{G}
$$

- **Irreducibility Criterion:**

$$
|\mathbf{G}|^{-1} \sum_{g \in \mathbf{G}} |\chi^{\alpha}(g)|^{2} \;=\; 1
$$

⋆ Properties of UIR's:

- **Representation Property**

$$\mathbf{D}^{\alpha}(g)\,\mathbf{D}^{\alpha}(g') \;=\; \mathbf{D}^{\alpha}(gg')$$

- **Unitarity Property**

$$\mathbf{D}^{\alpha}_{jk}(g^{-1}) \;=\; \mathbf{D}^{\alpha}_{jk}(g)^{\dagger} = \mathbf{D}^{\alpha}_{kj}(g)^{*}$$

- **Orthogonality Relations**

$$\sum_{g\in\mathbf{G}} \mathbf{D}^{\alpha}_{jk}(g)^{*}\,\mathbf{D}^{\beta}_{st}(g) \;=\; \frac{|\mathbf{G}|}{n(\alpha)}\delta_{\alpha\beta}\delta_{js}\delta_{kt}$$

- **Completeness Relations**

$$\sum_{\alpha jk} n(\alpha)\,\mathbf{D}^{\alpha}_{jk}(g)^{*}\,\mathbf{D}^{\alpha}_{jk}(g') \;=\; |\mathbf{G}|\delta_{gg'}$$

`Characters:` $$|\mathbf{G}|\sum_{g\in\mathbf{G}} \chi^{\alpha}(g)^{*}\,\chi^{\alpha}(g) = \delta_{\alpha\beta}$$

`Burnside:` $$\sum_{\alpha\in A(\mathbf{G})} n(\alpha)^{2} = |\mathbf{G}|$$

Schur's Lemma:

$$\mathbf{D}^{\alpha}(g)\,\mathbf{S} \;=\; \mathbf{S}\,\mathbf{D}^{\beta}(g) \qquad \forall g \in \mathbf{G}$$

Question: `Form of Intertwining Matrix` $\mathbf{S}$ **?**

Case A: $\alpha = \beta \;\Rightarrow\; \mathbf{S} = a\,\mathbf{E}^{\alpha}$

$$\mathbf{E}^{\alpha} = \begin{bmatrix} 1 & 0 & \cdots & 0 \\ 0 & 1 & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & 1 \end{bmatrix} = \mathbf{D}^{\alpha}(e)$$

Case B: $\alpha \neq \beta \;\Rightarrow\; \mathbf{S} = \mathbf{0}$

Special Situations:

[1] $\mathbf{D}(g) = \mathbf{D}^{\alpha}(g) \oplus \mathbf{D}^{\beta}(g) \Longleftrightarrow$

$$\mathbf{S} = a\,\mathbf{E}^{\alpha} \oplus b\,\mathbf{E}^{\beta}$$

[2] $\mathbf{D}(g) = \mathbf{D}^{\alpha}(g) \oplus \mathbf{D}^{\alpha}(g) \Longleftrightarrow$

$$\mathbf{S} = \begin{bmatrix} a & 0 & \cdots & 0 & b & 0 & \cdots & 0 \\ 0 & a & \cdots & 0 & 0 & b & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & a & 0 & 0 & \cdots & b \\ c & 0 & \cdots & 0 & d & 0 & \cdots & 0 \\ 0 & c & \cdots & 0 & 0 & d & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & c & 0 & 0 & \cdots & d \end{bmatrix}$$

Remarks on Finite Groups:

$$
\begin{aligned}
\mathbf{G} &= \{e, g_2, g_3, \ldots g_n\} \Rightarrow |\mathbf{G}| = n \\
\mathcal{K}(\mathbf{G}) &= \{\mathcal{K}(e), \mathcal{K}(g_i), \ldots \mathcal{K}(g_s)\} \Rightarrow s \leq n \\
\mathcal{K}(g_i) &= \{\hat{g} = g g_i g^{-1} | g \in \mathbf{G}\} \subset \mathbf{G} \quad \ldots \\
& \quad \texttt{Class of Conjugate Elements} \\
A(G) &= \{\alpha\} = \{\alpha_1, \alpha_2, \ldots \alpha_s\} \quad \ldots \\
& \quad \texttt{Set of IRREP Labels}
\end{aligned}
$$

- **Theorem**: $|\mathcal{K}(\mathbf{G})| = s = |A(\mathbf{G})|$

Examples of Group–UIR's:

[1] Cyclic Group: $\mathbf{C}^{\mathsf{N}}$
[2] Group of Integers: $\mathbb{Z}$
[3] Unitary Group: $\mathbf{U}(1)$
[4] Permutation Group: $\mathbf{S}_3$
[5] Rotation Group: $\mathbf{SO}(3, \mathbb{R})$
[6] Special Unitary Group: $\mathbf{SU}(2)$

[1] Cyclic Group: $\mathbf{C}^{\mathsf{N}}$

$$
\begin{aligned}
\mathbf{G} &= \mathbf{C}^{\mathsf{N}} \sim \mathbb{Z}\big/(\mathsf{N} * \mathbb{Z}) \\
c^m * c^{m'} &= c^{m+m'} \quad \mathtt{mod}\ \mathsf{N} \\
\mathcal{K}(c^m) &= \{c^m\} \\
|\mathcal{K}(\mathbf{C}^{\mathsf{N}})| &= \mathsf{N} = |A(\mathbf{C}^{\mathsf{N}})| \\
\alpha &\longleftrightarrow k \in \frac{2\pi}{\mathsf{N}} * \{0, 1, \ldots \mathsf{N}-1\} \quad \ldots
\end{aligned}
$$

Finite Brillouin Zone

$$
\begin{aligned}
\mathrm{D}^k(c^m) &= e^{-ikm} \\
\mathtt{dim}\ \mathrm{D}^k &= n(k) = 1 \\
\mathsf{N} &= \textstyle\sum_k n(k)^2
\end{aligned}
$$

[2] Group of Integers: $\mathbb{Z} = \mathtt{dual}\ \mathbf{U}(1)$

$$
\begin{aligned}
\mathbf{G} &= \mathbb{Z} \\
\mathrm{D}^k(z) &= e^{-ikz} \qquad z \in \mathbb{Z} \\
k &\in [0, 2\pi) \quad \ldots
\end{aligned}
$$

Brillouin Zone

[3] Unitary Group: $\mathbf{U}(1) = \mathtt{dual}\ \mathbb{Z}$

$$
\begin{aligned}
\mathbf{G} &= \mathbf{U}(1) \\
\mathrm{D}^m(\phi) &= e^{-im\phi} \qquad \phi \in [0, 2\pi) \\
m &\in \mathbb{Z} \quad \ldots
\end{aligned}
$$

Group of Integers

[4] Permutation Group: $\mathbf{S}_3$

$$\mathbf{G} = \{e, g_2, g_3, g_4, g_5, g_6\}$$

$$\begin{array}{rcl}
e & : & (1,2,3) \longmapsto (1,2,3) \\
g_2 & : & (1,2,3) \longmapsto (2,3,1) \\
g_3 & : & (1,2,3) \longmapsto (3,1,2) \\
g_4 & : & (1,2,3) \longmapsto (2,1,3) \\
g_5 & : & (1,2,3) \longmapsto (3,2,1) \\
g_6 & : & (1,2,3) \longmapsto (1,3,2)
\end{array}$$

$$\begin{array}{rcl}
\mathcal{K}(e) & = & \{e\} \\
\mathcal{K}(g_2) & = & \{g_2, g_3\} \\
\mathcal{K}(g_4) & = & \{g_4, g_5, g_6\}
\end{array}$$

$$\mathcal{K}(\mathbf{S}_3) = 3 = |A(\mathbf{S}_3)|$$

Partition:

$$\begin{array}{l}
3 = 3+0+0 \\
3 = 1+1+1 \\
3 = 2+1+0
\end{array}$$

$$\begin{array}{rcl}
\alpha & = & 1 = [3] \\
\alpha & = & 2 = [1,1,1] \\
\alpha & = & 3 = [2,1]
\end{array}$$

$$\alpha = 1 \longleftrightarrow \begin{array}{|c|c|c|}\hline 1 & 2 & 3 \\ \hline\end{array}$$

$$\alpha = 2 \longleftrightarrow \begin{array}{|c|}\hline 1 \\ \hline 2 \\ \hline 3 \\ \hline\end{array}$$

$$\alpha = 3 \longleftrightarrow \begin{array}{|c|c|}\hline 1 & 2 \\ \hline 3 & \multicolumn{1}{c}{} \\ \cline{1-1}\end{array} \qquad \begin{array}{|c|c|}\hline 1 & 3 \\ \hline 2 & \multicolumn{1}{c}{} \\ \cline{1-1}\end{array}$$

Burnside: $|\mathbf{S}_3| = 1^2 + 1^2 + 2^2$

Characters:

	$\mathcal{K}(e)$	$\mathcal{K}(g_2)$	$\mathcal{K}(g_4)$
$\alpha = 1$	1	1	1
$\alpha = 2$	1	1	-1
$\alpha = 3$	2	-1	0

UIR: $\alpha = 1$ $\quad \mathbf{D}^\alpha(g) = +1 \qquad g \in \mathbf{S}_3$

UIR: $\alpha = 2$ $\quad \mathbf{D}^\alpha(g) = +1 \qquad g \in \{e, g_2, g_3\}$

$$\mathbf{D}^\alpha(g) = -1 \qquad g \in \{g_4, g_5, g_6\}$$

UIR: $\alpha = 3$ $\quad \mathbf{D}^\alpha(g_1) = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}$

$$\mathbf{D}^\alpha(g_2) = \begin{bmatrix} -\frac{1}{2} & \frac{\sqrt{3}}{2} \\ -\frac{\sqrt{3}}{2} & -\frac{1}{2} \end{bmatrix}$$

$$\mathbf{D}^\alpha(g_3) = \begin{bmatrix} -\frac{1}{2} & -\frac{\sqrt{3}}{2} \\ \frac{\sqrt{3}}{2} & -\frac{1}{2} \end{bmatrix}$$

$$\mathbf{D}^\alpha(g_4) = \begin{bmatrix} -\frac{1}{2} & \frac{\sqrt{3}}{2} \\ \frac{\sqrt{3}}{2} & \frac{1}{2} \end{bmatrix}$$

$$\mathbf{D}^\alpha(g_5) = \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}$$

$$\mathbf{D}^\alpha(g_6) = \begin{bmatrix} -\frac{1}{2} & -\frac{\sqrt{3}}{2} \\ -\frac{\sqrt{3}}{2} & \frac{1}{2} \end{bmatrix}$$

D.E. Rutherford: `Substitutional Analysis`
(Edinburgh at the University Press, 1948)

[5] Rotation Group: $\mathbf{SO}(3,\mathbb{R})$

$$
\begin{aligned}
\mathbf{G} &= \mathbf{SO}(3,\mathbb{R}) \\
g &= \tilde{\omega} = (\alpha,\beta,\gamma) \quad \ldots \quad \texttt{Eulerian Angles} \\
& \quad\ \alpha{\in}[0,2\pi) \qquad \beta{\in}[0,\pi) \qquad \gamma{\in}[0,2\pi) \\
\tilde{\omega} * \tilde{\omega}' &= \tilde{\omega}'' = (\alpha'',\beta'',\gamma'') \\
\alpha &= \ell \in A(\mathbf{SO}(3,\mathbb{R})) = \mathbb{Z}_0^+ \\
\mathbf{D}^{\ell}(\tilde{\omega}) &= (2\ell{+}1)\times(2\ell{+}1) - \texttt{Matrices} \\
2\ell{+}1 &= \texttt{dim}\ \mathbf{D}^{\ell}(\tilde{\omega})
\end{aligned}
$$

$$
\begin{aligned}
\mathbf{D}^{\ell}_{mn}(\tilde{\omega}) &= e^{-im\alpha}\, \mathbf{d}^{\ell}_{mn}(\beta)\, e^{-in\gamma} \\
& \quad -\ell \le m, n \le +\ell
\end{aligned}
$$

$$
\begin{aligned}
\mathbf{d}^{\ell}_{mn}(\beta) &= \sum_s A^{\ell}{}_{mn}(s)\, \mathsf{c}^{2\ell+n-m-2s}\, (-\mathsf{s})^{m-n+2s} \\
& \qquad \mathsf{c} = \cos\tfrac{\beta}{2} \qquad \mathsf{s} = \sin\tfrac{\beta}{2}
\end{aligned}
$$

$$
A^{\ell}{}_{mn}(s) = \frac{(-1)^s[(\ell{+}n)!(\ell{-}n)!(\ell{+}m)!(\ell{-}m)!]^{1/2}}{s!(\ell{-}s{-}m)!(\ell{+}n{-}s)!(m{+}s{-}n)!}
$$

$\mathbf{d}^{\ell}_{mn}(\beta)$ ... **Wigner Formula**

[6] Special Unitary Group: $\mathbf{SU}(2)$

$$\begin{aligned}
\mathbf{G} &= \mathbf{SU}(2) \\
g &= \tilde{\omega} = (\alpha, \beta, \gamma) \longleftrightarrow \mathbf{u} = \begin{bmatrix} a & b \\ -b^* & a^* \end{bmatrix} \\
& \quad \mathtt{det}\ \mathbf{u} = |a|^2 + |b|^2 = 1 \\
& \quad \alpha\in[0,2\pi) \qquad \beta\in[0,\pi) \qquad \gamma\in[0,4\pi)
\end{aligned}$$

$$\begin{aligned}
\phi(\mathbf{SU}(2)) &= \mathbf{SO}(3,\mathbb{R}) \sim \mathbf{SU}(2)/\mathbf{ker}_\phi \\
\mathbf{ker}_\phi &= \mathbf{Z}(\mathbf{SU}(2)) = \left\{ \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}, \begin{bmatrix} -1 & 0 \\ 0 & -1 \end{bmatrix} \right\}
\end{aligned}$$

$$\begin{aligned}
\alpha &= j \in A(\mathbf{SU}(2)) \\
&= \mathbb{Z}_0^+ \cup \left\{ \frac{2z+1}{2} \,\middle|\, z \in \mathbb{Z}_0^+ \right\}
\end{aligned}$$

$$\begin{aligned}
\mathbf{D}^j(\tilde{\omega}) &= (2j+1)\times(2j+1) - \mathtt{Matrices} \\
2j+1 &= \mathtt{dim}\ \mathbf{D}^j(\tilde{\omega})
\end{aligned}$$

$$\begin{aligned}
\mathbf{D}^j_{mn}(\tilde{\omega}) &= e^{-im\alpha}\, \mathbf{d}^j_{mn}(\beta)\, e^{-in\gamma} \\
& \quad -j \le m, n \le +j
\end{aligned}$$

$$\mathbf{D}^{\frac{1}{2}}(\tilde{\omega}) = \begin{bmatrix} e^{-i\frac{\alpha}{2}} & 0 \\ 0 & e^{i\frac{\alpha}{2}} \end{bmatrix} \begin{bmatrix} \cos\frac{\beta}{2} & -\sin\frac{\beta}{2} \\ \sin\frac{\beta}{2} & \cos\frac{\beta}{2} \end{bmatrix} \begin{bmatrix} e^{-i\frac{\gamma}{2}} & 0 \\ 0 & e^{i\frac{\gamma}{2}} \end{bmatrix}$$

★ Decomposition of Unitary Reducible Matrix Representations into direct Sums of their Unitary Irreducible Constituents

Matrix Rep: $\mathbf{D}(\mathbf{G}) = \{\mathbf{D}(g) | g \in \mathbf{G}\}$

Character: $\chi^{\mathbf{D}}(g) = \text{trace } \mathbf{D}(g)$

Character Test: $\frac{1}{|\mathbf{G}|} \sum_{g \in \mathbf{G}} |\chi^{\mathbf{D}}(g)|^2 > 1 \quad \Rightarrow$

Reducible Matrix Representation

$$\mathbf{D}(g) \sim \sum_{\alpha \in A(\mathbf{G})} \oplus\, m(\mathbf{D}|\alpha)\, \mathbf{D}^{\alpha}(g)$$

$$m(\mathbf{D}|\alpha) = \sum_{g \in \mathbf{G}} \chi^{\alpha}(g)^* \chi^{\mathbf{D}}(g) \in \mathbb{Z}_0^+$$

$m(\mathbf{D}|\alpha)$ ... **Multiplicity of $\mathbf{D}^{\alpha}$ in $\mathbf{D}$**

Dimension Test: $\dim \mathbf{D} = N = \sum_{\alpha} m(\mathbf{D}|\alpha)\, n(\alpha)$

Similarity Matrix: $\mathbf{W}$

$$\boxed{\mathbf{W}^{\dagger}\, \mathbf{D}(g)\, \mathbf{W} = \sum_{\alpha} \oplus\, m(\mathbf{D}|\alpha)\, \mathbf{D}^{\alpha}(g)}$$

Matrix Elements: $\mathbf{W}_{j;\alpha v a}$

Row Index: $\{j\}$ $\quad j=1,2,3,\ldots N$

Column Index: $\{(\alpha,v,a)\}$ $\quad \alpha \in A(\mathbf{G})$
$v=1,2,\ldots m(\mathbf{D}|\alpha)$
$a=1,2,\ldots n(\alpha)$

[3] App's: Quantum Theory

Aim: Simplification of the eigenvalue problem, if the Hamiltonian **H** has a symmetry group.

Carrier Space	Hilbert Space: $\mathcal{H}$ dim $\mathcal{H} = N$
Hamiltonian	$\mathbf{H} = \mathbf{T} + \mathbf{V}$
Group	$\mathbf{G} = \{e, g_2, g_3, \ldots\}$
Unitary Operators	$\mathsf{U}(\mathbf{G}) = \{\mathsf{U}(g) \vert g \in \mathbf{G}\}$
Symmetry Group	$[\mathbf{H}, \mathsf{U}(g)] = 0 \qquad \forall g \in \mathbf{G}$
Eigenvalue Equ's	$\mathbf{H}\,\Phi_s^\lambda = \lambda\,\Phi_s^\lambda$ λ ... Eigenvalue $s = 1,2,3,\ldots \deg \lambda$
Consequence:	$\mathbf{H}\,\Phi_s^\lambda = \lambda\,\Phi_s^\lambda \quad \Rightarrow$ $\mathbf{H}\,(\mathsf{U}(g)\,\Phi_s^\lambda) = \lambda\,(\mathsf{U}(g)\,\Phi_s^\lambda)$

Remarks: Accordingly, if $\{\Phi_s^\lambda\}$ are eigenvectors to the eigenvalue λ of the Hamiltonian **H**, then also the set of vectors $\{\mathsf{U}(g)\,\Phi_s^\lambda \,|\, g \in \mathbf{G}\}$ have to be eigenvectors of the Hamiltonian to the same eigenvalue.

■ G–adapted Basis:

Carrier Space ... Hilbert Space $\mathcal{H}$

$$\dim \mathcal{H} = N = \textstyle\sum_\alpha m(\alpha)\, n(\alpha)$$

$$\left\{\Psi_a^{\alpha v}\right\} = \left\{\Psi_a^{\alpha v} \,\middle|\, \begin{array}{l} \alpha \in A(\mathbf{G}) \\ v=1,2,\ldots m(\alpha) \\ a=1,2,\ldots n(\alpha) \end{array}\right\}$$

■ $\left\langle \Psi_a^{\alpha v}, \Psi_{a'}^{\alpha' v'} \right\rangle = \delta_{\alpha\alpha'}\, \delta_{vv'}\, \delta_{aa'}$

■ $\mathsf{U}(g)\, \Psi_a^{\alpha v} = \sum_{b=1}^{n(\alpha)} \mathbf{D}_{ba}^{\alpha}(g)\, \Psi_b^{\alpha v}$

■ Matrix Representation of Hamiltonian H w.r.t. $\left\{\Psi_a^{\alpha v}\right\} \Longleftrightarrow$ Schur's Lemma:

$$\boxed{\left\langle \Psi_a^{\alpha v}, \mathsf{H}\, \Psi_{a'}^{\alpha' v'} \right\rangle = \mathsf{H}_{vv'}^{\alpha}\, \delta_{\alpha\alpha'}\, \delta_{aa'}}$$

Note: This is a special case of Wigner Eckart's Theorem, since H is invariant w.r.t. **G**, i.e. possesses this group as symmetry group.

Construction of G–adapted Bases of $\mathcal{H}$ by means of the Projection Method (Several refined methods exist: eg. Chen et al (2001))

$$\mathbf{E}^{\alpha}_{ab} = \frac{n(\alpha)}{|\mathbf{G}|} \sum_{g\in\mathbf{G}} \mathbf{D}^{\alpha}_{ab}(g)^{*}\, \mathsf{U}(g)$$

Properties of Units:

$$\begin{array}{lrcl}
[1] & (\mathbf{E}^{\alpha}_{ab})^{\dagger} & = & \mathbf{E}^{\alpha}_{ba} \\
[2] & \mathbf{E}^{\alpha}_{ab}\, \mathbf{E}^{\alpha'}_{st} & = & \delta_{\alpha\alpha'}\, \delta_{bs}\, \mathbf{E}^{\alpha}_{at} \\
[3] & \mathsf{U}(g)\, \mathbf{E}^{\alpha}_{ab} & = & \sum_{c=1}^{n(\alpha)} \mathbf{D}^{\alpha}_{ca}(g)\, \mathbf{E}^{\alpha}_{cb} \\
[4] & \mathbf{1} & = & \sum_{\alpha\in A(\mathbf{G})} \mathbf{E}^{\alpha}_{aa}
\end{array}$$

Subdivision of Units:

$$\left\{ \mathbf{E}^{\alpha}_{aa} \;\middle|\; \begin{matrix} \alpha\in A(\mathbf{G}) \\ a = b \end{matrix} \right\} \quad \ldots \quad \text{Projection Operators}$$

$$\left\{ \mathbf{E}^{\alpha}_{ab} \;\middle|\; \begin{matrix} \alpha\in A(\mathbf{G}) \\ a \neq b \end{matrix} \right\} \quad \ldots \quad \text{Shift Operators}$$

Details of Projection Method:

[1] **ONB** of Hilbertspace $\mathcal{H}$

$$\{\phi_j\} = \left\{\phi_j \,\middle|\, j = 1, 2, 3, \ldots N\right\}$$

[2] Matrix Rep of Symmetry Group $\mathbf{G} \longrightarrow \mathsf{U}(\mathbf{G})$

$$\mathsf{U}(g)\,\phi_j = \sum_{k=1}^{N} \mathbf{D}_{kj}(g)\,\phi_k$$

$$\chi(g) = \mathtt{trace}\,\mathbf{D}(g)$$

[3] Determination of the Multiplicity $m(\alpha)$

$$m(\alpha) = \frac{1}{|\mathbf{G}|} \sum_{g \in \mathbf{G}} \chi^{\alpha}(g)^{*}\,\chi(g)$$

[4] Dimension Check: $N = \sum_{\alpha} m(\alpha) n(\alpha)$

[5] Projection into Subspace $\mathcal{H}_a^{\alpha}$
($\alpha \longleftrightarrow m(\alpha)>0$ & $a = \mathtt{fixed}$)

$$\mathcal{H}_a^{\alpha} = \mathbf{E}_{aa}^{\alpha}\,\mathcal{H} \quad \Longleftrightarrow \quad \dim \mathcal{H}_a^{\alpha} = m(\alpha)$$

[6] Construction of **ONB** of Subspace $\mathcal{H}_a^{\alpha}$
(eg. Gram-Schmidt Procedure)

$$\left\{\mathbf{E}_{aa}^{\alpha}\,\phi_j\right\} \longrightarrow \left\{\Psi_a^{\alpha v} \,\middle|\, v = 1,2,\ldots m(\alpha)\right\}$$

$$\left\langle \Psi_a^{\alpha v}, \Psi_a^{\alpha v'} \right\rangle = \delta_{vv'}$$

Note: Usually, this cannot be done by means of group-theoretical methods

Details of Projection Method: (cont'd)

[7] Projection onto Partnerspaces $\mathcal{H}_b^{\alpha}$

$\mathcal{H}_b^{\alpha} = \mathbf{E}_{ba}^{\alpha}\, \mathcal{H}_a^{\alpha} \quad \Longleftrightarrow$

dim $\mathcal{H}_b^{\alpha} = m(\alpha) \qquad b = 1,2,\ldots n(\alpha)$

[8] Construction of **Partnerfunctions**

$$\boxed{\Psi_b^{\alpha v} = \mathbf{E}_{ba}^{\alpha}\, \Psi_a^{\alpha v} \qquad \begin{cases} v = 1,2,\ldots m(\alpha) \\ b = 1,2,\ldots n(\alpha) \end{cases}}$$

$$\left\langle \Psi_a^{\alpha v}\, ,\, \Psi_{a'}^{\alpha' v'} \right\rangle = \delta_{\alpha\alpha'}\, \delta_{vv'}\, \delta_{aa'}$$

$$\mathsf{U}(g)\, \Psi_a^{\alpha v} = \sum_{b=1}^{n(\alpha)} \mathbf{D}_{ba}^{\alpha}(g)\, \Psi_b^{\alpha v}$$

[9] Repetition of Step **[5]** till Step **[8]**
for all β $(\neq\alpha)$ with $m(\beta)>0$

Result: **G**-adapted Basis of $\mathcal{H}$

$$\Psi_a^{\alpha v} = \sum_{j=1}^{N} \mathbf{X}_{j;\alpha v a}\, \phi_j$$

Relation between: $\{\Phi_s^{\lambda}\} \longleftrightarrow \{\Psi_a^{\alpha v}\}$

$$\begin{array}{lrcl}
\star & \mathsf{U}(g)\,\Phi_s^{\lambda} & = & \sum_{s'=1}^{\deg\lambda} \mathbf{D}^{\lambda}_{s's}(g)\,\Phi_{s'}^{\lambda} \\
 & \dim \mathbf{D}(g) & = & \deg\lambda \\
 & \mathbf{E}^{\lambda} & = & \sum_{s=1}^{\deg\lambda} |\lambda s><\lambda s| \\
 & \mathcal{H}^{\lambda} & = & \mathbf{E}^{\lambda}\mathcal{H} \\
 & \Phi_s^{\lambda} & = & \sum_{j=1}^{N} \mathbf{V}_{j;\lambda s}\,\phi_j
\end{array}$$

$$\begin{array}{lrcl}
\star & \mathbf{D}^{\lambda}(g) & \sim & \sum_{\alpha} \oplus\, m(\lambda|\alpha)\,\mathbf{D}^{\alpha}(g) \\
 & m(\lambda|\alpha) & = & \frac{1}{|\mathbf{G}|}\sum_g \chi^{\lambda}(g)\,\chi^{\alpha}(g)^* \\
 & \mathbf{W}^{\lambda\dagger}\mathbf{D}^{\lambda}(g)\,\mathbf{W}^{\lambda} & = & \sum_{\alpha} \oplus\, m(\lambda|\alpha)\,\mathbf{D}^{\alpha}(g)
\end{array}$$

$$\begin{array}{lrcl}
\star & \Psi_a^{\lambda\alpha w} & = & \sum_{s=1}^{\deg\lambda} \mathbf{W}^{\lambda}_{s;\alpha wa}\,\Phi_s^{\lambda} \\
 & m(\alpha) & = & \sum_{\lambda} m(\lambda|\alpha)
\end{array}$$

Matrix Elements:	$\mathbf{W}^{\lambda}_{s;\alpha wa}$
Row Index: $\{s\}$	$s=1,2,3,\ldots\deg\lambda$
Column Index: $\{(\alpha,w,a)\}$	$\alpha\in A(\mathbf{G})$ $w=1,2,\ldots m(\lambda\|\alpha)$ $a=1,2,\ldots n(\alpha)$

Relation: $\{\Phi_s^{\lambda}\} \longleftrightarrow \{\Psi_a^{\alpha v}\}$ (cont'd)

$$
\begin{aligned}
\Psi_a^{\alpha v} &= \textstyle\sum_{j=1}^{N} \mathbf{X}_{j;\alpha v a}\, \phi_j \\
\phi_j &= \textstyle\sum_{\alpha v a} \mathbf{X}^{*}_{j;\alpha v a}\, \Psi_a^{\alpha v}
\end{aligned}
$$

$$
\begin{aligned}
\Psi_a^{\lambda\alpha w} &= \textstyle\sum_{s=1}^{\deg\lambda} \mathbf{W}^{\lambda}_{s;\alpha w a}\, \Phi_s^{\lambda} \\
\Phi_s^{\lambda} &= \textstyle\sum_{j=1}^{N} \mathbf{V}_{j;\lambda s}\, \phi_j
\end{aligned}
$$

$$
\begin{aligned}
\Psi_a^{\lambda\alpha w} &= \textstyle\sum_{js} \mathbf{V}_{j;\lambda s}\, \mathbf{W}^{\lambda}_{s;\alpha w a}\, \phi_j \\
&= \textstyle\sum_{js;\alpha' v a'} \mathbf{X}^{\dagger}_{\alpha' v a';j}\, \mathbf{V}_{j;\lambda s}\, \mathbf{W}^{\lambda}_{s;\alpha w a}\, \Psi_{a'}^{\alpha' v} \\
&= \textstyle\sum_{js;v} \mathbf{X}^{\dagger}_{\alpha v a;j}\, \mathbf{V}_{j;\lambda s}\, \mathbf{W}^{\lambda}_{s;\alpha w a}\, \Psi_a^{\alpha v} \\
&= \textstyle\sum_{vs} \{\mathbf{X}^{\dagger}\mathbf{V}\}_{\alpha v a;\lambda s}\, \mathbf{W}^{\lambda}_{s;\alpha w a}\, \Psi_a^{\alpha v}
\end{aligned}
$$

$$
\begin{aligned}
\Phi_s^{\lambda} &= \textstyle\sum_{\alpha v a;j} \mathbf{X}^{\dagger}_{\alpha v a;j}\, \mathbf{V}_{j;\lambda s}\, \Psi_a^{\alpha v} \\
&= \textstyle\sum_{\alpha v a} \{\mathbf{X}^{\dagger}\mathbf{V}\}_{\alpha v a;\lambda s}\, \Psi_a^{\alpha v}
\end{aligned}
$$

Note: $m(\alpha) = 1 \;\Rightarrow\; \alpha \longleftrightarrow \lambda \iff \Psi_a^{\alpha} \sim \Phi_s^{\lambda}$

$m(\lambda|\alpha) = 1 \;\Rightarrow\; \lambda \longmapsto \alpha \;\Rightarrow\; \Phi_s^{\lambda} \sim \Psi_a^{\lambda\alpha}$

$m(\lambda|\alpha) > 1$ and/or $\sum_{\alpha} m(\lambda|\alpha) > 1 \;\Rightarrow$

Accidental Degeneracy

⋆ Wigner-Eckart Theorem:

[1] Hilbert Space $\mathcal{H}$

[2a] Unitary Operator Representation of Group $\mathbf{G}$

$$\mathsf{U}(\mathbf{G}) = \{\mathsf{U}(e), \mathsf{U}(g_2), \mathsf{U}(g_3), \ldots\}$$

$$\mathsf{U}(g)\,\mathsf{U}(g') = \mathsf{U}(gg')$$

$$\Big\langle \mathsf{U}(g)\,\psi\,,\,\mathsf{U}(g)\,\phi \Big\rangle = \Big\langle \psi\,,\,\phi \Big\rangle$$

[2b] Unirreps of Group $\mathbf{G}$

$$\mathbf{D}^{\xi}(\mathbf{G}) = \Big\{ \mathbf{D}^{\xi}(g) \,\Big|\, g \in \mathbf{G} \Big\}$$

[2c] Symmetry adapted **ONB**-Basis

$$\left\{ \Psi_k^{\beta v} \right\} = \left\{ \Psi_k^{\beta v} \,\middle|\, \begin{array}{l} \beta \in A(\mathbf{G}) \\ v = 1,2,\ldots m(\beta) \\ k = 1,2,\ldots n(\beta) \end{array} \right\}$$

$$\mathsf{U}(g)\,\Psi_k^{\beta v} = \sum_{k'=1}^{n(\beta)} \mathbf{D}^{\beta}_{k'k}(g)\,\Psi_{k'}^{\beta v}$$

[3] **Irreducible Tensor Operator**

$$\mathsf{T}^{\alpha} = \Big\{ \mathsf{T}_a^{\alpha} \,\Big|\, a = 1, 2, 3, \ldots n(\alpha) \Big\}$$

$$\mathsf{U}(g)\,\mathsf{T}_a^{\alpha}\,\mathsf{U}(g)^{\dagger} = \sum_{a'=1}^{n(\alpha)} \mathbf{D}^{\beta}_{a'a}(g)\,\mathsf{T}_{a'}^{\alpha}$$

★ Wigner-Eckart Theorem: (cont'd)

$$\left\langle \Psi^{\gamma}_{j}\,,\, \mathbf{T}^{\alpha}_{a}\, \Psi^{\beta}_{k} \right\rangle = \sum_{w=1}^{m(\alpha\beta|\gamma)} \left(\begin{array}{cc|c} \alpha & \beta & \gamma w \\ a & k & j \end{array} \right)^{*} \left\langle \gamma \| \mathbf{T}^{\alpha} \| \beta \right\rangle_{w}$$

$\left(\begin{array}{cc|c} \alpha & \beta & \gamma w \\ a & k & j \end{array} \right)$ ... Clebsch Gordan Coefficients

$\left\langle \gamma \| \mathbf{T}^{\alpha} \| \beta \right\rangle_{w}$ ... Reduced Matrix Elements

■ Clebsch Gordan Series (Kronecker Products)

$$\mathbf{D}^{\alpha\boxtimes\beta}(g) = \mathbf{D}^{\alpha}(g) \otimes \mathbf{D}^{\beta}(g)$$

$$\mathbf{D}^{\alpha\boxtimes\beta}(g) \sim \sum_{\gamma\in A(\mathbf{G})} \oplus\, m(\alpha\beta|\gamma)\, \mathbf{D}^{\gamma}(g)$$

Example: **Rotation Group** $\mathbf{SO}(3,\mathbb{R})$

$$\mathbf{D}^{j}(\omega) \otimes \mathbf{D}^{j'}(\omega) \;\sim\; \sum_{J\,=\,|j-j'|}^{|j+j'|} \oplus\, \mathbf{D}^{J}(\omega)$$

$$0 \le m(j,j'|J) \le 1$$

★ **Clebsch-Gordan Matrices**:

$$\mathbf{C}^{\alpha\beta\dagger}\,\mathbf{D}^{\alpha\boxtimes\beta}(g)\,\mathbf{C}^{\alpha\beta} = \sum_{\gamma\in A(\mathbf{G})} \oplus\, m(\alpha\beta|\gamma)\,\mathbf{D}^{\gamma}(g)$$

$\mathbf{C}^{\alpha\beta}$ ... `Clebsch-Gordan Matrices`

$n(\alpha)n(\beta)$ — `dim. unitary Matrices`

$$\begin{aligned} \mathbf{C}^{\alpha\beta}_{\alpha a,\beta k;\gamma w j} &= \{\mathbf{C}^{\alpha\beta}\}_{\alpha a,\beta k;\gamma w j} = \\ &= \left(\begin{array}{cc|c} \alpha & \beta & \gamma w \\ a & k & j \end{array}\right) = \\ &= \left\langle \alpha a, \beta k | \gamma w j \right\rangle \end{aligned}$$

... `Clebsch-Gordan Coefficients`

App's: Clebsch-Gordan Coefficients

[1] Coupling of Product Bases

`Product Space:` $\mathcal{H}_{1,2} = \mathcal{H}_1 \otimes \mathcal{H}_2$

`Product Group:` $\mathbf{G}^2 = \mathbf{G} \times \mathbf{G} = \{(g, g') | g, g' \in \mathbf{G}\}$

$(g, g') \longmapsto \mathsf{U}(g, g') = \mathsf{U}(g) \otimes \mathsf{U}(g')$

$\mathbf{G}^2$ — `Basis:` $\phi^{\alpha\alpha'}_{aa'} = \phi^{\alpha}_{a} \otimes \phi^{\alpha'}_{a'}$

$\longleftrightarrow \mathbf{D}^{\alpha}(g) \otimes \mathbf{D}^{\alpha'}(g')$

$\mathsf{U}(g, g')\, \phi^{\alpha\alpha'}_{aa'} =$

$\sum_{bb'} \mathbf{D}^{\alpha}_{ba}(g)\, \mathbf{D}^{\alpha'}_{b'a'}(g')\, \phi^{\alpha\alpha'}_{bb'}$

$\mathbf{G}^{\boxtimes 2}$ — `Basis:` $\mathbf{G} \boxtimes \mathbf{G} = \{(g, g) | g \in \mathbf{G}\} \sim \mathbf{G}$

$\left\{\phi^{\alpha\alpha'}_{aa'}\right\} \longrightarrow \left\{\phi^{(\alpha\alpha')\gamma w}_{c}\right\}$

$$\phi^{(\alpha\alpha')\gamma w}_{c} = \sum_{aa'} \left(\begin{array}{cc|c} \alpha & \beta & \gamma w \\ a & k & j \end{array} \right) \phi^{\alpha\alpha'}_{aa'}$$

$\mathsf{U}(g, g)\, \phi^{(\alpha\alpha')\gamma w}_{c} =$

$\sum_{c'} \mathbf{D}^{\gamma}_{c'c}(g)\, \phi^{(\alpha\alpha')\gamma w}_{c'}$

[2] Wigner Eckart Theorem for $\mathsf{SU}(2)$

$\mathsf{SU}(2)$ – IT's: $\quad \mathsf{T}^J = \{\mathsf{T}^J_M | -J \leq M \leq +J\}$

global: $\quad \mathsf{U}(\omega)\, \mathsf{T}^J_M\, \mathsf{U}(\omega)^\dagger = \sum_{M'=-J}^{+J} \mathbf{D}^J_{M'M}(\omega)\, \mathsf{T}^J_{M'}$

local: $\quad \left[\mathbf{J}_\pm , \mathsf{T}^J_M\right] = \sqrt{(J \mp M)(J \pm M + 1)}\, \mathsf{T}^J_{M\pm 1}$

$$\left[\mathbf{J}_3 , \mathsf{T}^J_M\right] = M\, \mathsf{T}^J_M$$

WE-Theorem: $\quad \left\langle \Phi^{j'}_{m'} , \mathsf{T}^J_M\, \Phi^j_m \right\rangle = \left(\begin{array}{cc|c} J & j & j' \\ M & m & m' \end{array} \right) < j' \| \mathsf{T}^J \| j >$

Selection Rules: $\quad |j - J| \leq j' \leq |j + J|$

$$M + m = m'$$

★ Construction of Space Group-Unirreps by Induction

[1] Reciprocal Lattice

$\vec{\mathrm{K}} = \vec{\mathrm{e}}\, \mathbb{D}(L^\star)$

$\mathbb{D}(L^\star) = 2\pi\, \mathbb{D}(L^{-1})^{\mathtt{T}}$

$\vec{\mathrm{t}} = \vec{\mathrm{e}}\, \mathbb{D}(L)$

$\mathrm{t}_j \cdot \mathrm{K}_\ell = 2\pi\, \delta_{j\ell}$

$\mathrm{k} = x\mathrm{K}_1 + y\mathrm{K}_2 + z\mathrm{K}_3 \in \mathsf{E}(\mathsf{T}^\star)$

$0 \le x, y, z \le 1$

$\mathsf{E}(\mathsf{T}^\star)$ ... Unit Cell of $\mathsf{T}^\star$

$\mathsf{E}(\mathsf{T}^\star) \longrightarrow \mathsf{B}(\mathsf{T}^\star)$

$\mathsf{B}(\mathsf{T}^\star)$ ... Brillouin Zone

[2] $\mathsf{G} = \left\{ \mathsf{T}, \mathsf{P} | \mathcal{O}, \mathbf{w}_{\mathsf{P}} \right\}$

$g = (R|\mathrm{t}) \in \mathsf{G}_{\mathtt{sym}}$

$g = (R|\mathbf{w}_R + \mathrm{t}) \in \mathsf{G}_{\mathtt{non-sym}}$

$\mathsf{T} \triangleleft \mathsf{G}(\mathrm{k}) \subseteq \mathsf{G}$

Induction Procedure (cont'd)

[3] `Right Coset Decomposition of` G `w.r.t.` T

[a] `Symmorphic Space Groups`

$$\mathsf{G} = \bigcup_{R \in \mathsf{P}} \mathsf{T} * (R|\mathbf{0})$$

$$(R|\mathbf{0})\,(S|\mathbf{0}) = (RS|\mathbf{0})$$

[b] `Non-Symmorphic Space Groups`

$$\mathsf{G} = \bigcup_{R \in \mathsf{P}} \mathsf{T} * (R|\mathbf{w}_R)$$

$$(R|\mathbf{w}_R)\,(S|\mathbf{w}_S) = (RS|\mathbf{w}_{RS} + \mathbf{t}(R,S))$$

[4] T – **UIR's**

$$\mathrm{D}^{\mathbf{k}}(E|\mathbf{t}) = e^{-i\mathbf{k}\cdot\mathbf{t}}$$

$$\mathbf{k} \in \mathsf{B}(\mathsf{T}^{\star}) \qquad \mathbf{t} \in \mathsf{T}$$

[5] `Little Group` $\mathsf{G}(\mathbf{k}) \longrightarrow$ `Little Co-Group` $\mathsf{P}(\mathbf{k})$

$$\mathsf{P}(\mathbf{k}) \sim \mathsf{G}(\mathbf{k})/\mathsf{T}$$

$$\mathsf{G}(\mathbf{k}) = \left\{ g \in \mathsf{G} \,\middle|\, \mathrm{D}^{\mathbf{k}}(g^{-1}(E|\mathbf{t})g) = \mathrm{D}^{\mathbf{k}}(E|\mathbf{t}) \right\}$$

$$g^{-1}(E|\mathbf{t})g = (E|\mathcal{R}^{-1}\,\mathbf{t}) \Longleftrightarrow$$

$$\mathrm{D}^{\mathbf{k}}(g^{-1}(E|\mathbf{t})g) = \mathrm{D}^{\mathbf{k}}(E|\mathcal{R}^{-1}\,\mathbf{t}) = \mathrm{D}^{\mathcal{R}\,\mathbf{k}}(E|\mathbf{t})$$

$$\mathsf{P}(\mathbf{k}) = \left\{ R \in \mathsf{P} \,\middle|\, \mathcal{R}\,\mathbf{k} = \mathbf{k} + \mathbf{K} \right\} \ \ldots$$

Group of $\mathbf{k}$ **– Vector**

Induction Procedure (cont'd)

[6] Coset Decomposition of $\mathbf{P}$ w.r.t. $\mathbf{P}(\mathrm{k})$

$$\mathbf{P} = \mathbf{P}(\mathrm{k}) \cup \underline{R}_2 * \mathbf{P}(\mathrm{k}) \cup \ldots \cup \underline{R}_m * \mathbf{P}(\mathrm{k})$$

$$m = |\mathbf{P}|:|\mathbf{P}(\mathrm{k})|$$

[7] Coset Decomposition of $\mathbf{G}$ w.r.t. $\mathbf{G}(\mathrm{k})$

[7a] Symmorphic Space Group $\mathbf{G}$

$$\mathbf{G} = \bigcup_{\underline{R}_m} (\underline{R}_m|\mathbf{0}) * \mathbf{G}(\mathrm{k})$$

[7b] Non-Symmorphic Space Group $\mathbf{G}$

$$\mathbf{G} = \bigcup_{\underline{R}_m} (\underline{R}_m|\mathbf{w}_{\underline{R}_m}) * \mathbf{G}(\mathrm{k})$$

[8] **Star of k – Vector**

$$\mathrm{k}^\star(\mathbf{P}) = \{\mathrm{k}_j = \underline{R}_j\,\mathrm{k}\,|\,j = 1,2,\ldots m\}$$

[8] **Fundamental Domain $\Delta\mathbf{B}(\mathbf{T}^\star|\mathbf{P})$**

$\Delta\mathbf{B}(\mathbf{T}^\star|\mathbf{P})$ ... Set (connected) of all k – Vectors, such that from each star $\mathrm{k}^\star(\mathbf{P})$ exactly **one** element (arm) is taken.

Induction Procedure (cont'd)

[10] Projective $\mathbf{P}(\mathrm{k})$ – UIR's

$$\mathbf{D}^{\xi}(\mathbf{P}(\mathrm{k})) = \left\{ \mathbf{D}^{\xi}(R) \,\middle|\, R \in \mathbf{P}(\mathrm{k}) \right\}$$

$$\mathbf{D}^{\xi}(R)\mathbf{D}^{\xi}(S) = e^{-i\mathrm{k}\cdot\mathrm{t}(R,S)}\,\mathbf{D}^{\xi}(RS)$$

Note: $\mathrm{t}(R,S) = \mathbf{0} \quad \forall R,S \in \mathbf{P}$ iff $\mathbf{G}$ forms a symmorphic Space Group, otherwise **NOT**. Hence if $\mathbf{G}$ is symmorphic, then $\mathbf{D}^{\xi}(\mathbf{P}(\mathrm{k}))$ form ordinary vector **UIR's** of $\mathbf{P}(\mathrm{k})$, otherwise, they are projective **UIR's**.

[11] Induction: $\mathbf{T} \uparrow \mathbf{G}(\mathrm{k}) \;\Rightarrow\; \mathbf{G}(\mathrm{k})$ – UIR's

$$\mathbf{D}^{\mathrm{k},\xi}(R|\mathrm{w}_R{+}\mathrm{t}) = e^{-i\mathrm{k}\cdot\mathrm{t}}\,\mathbf{D}^{\xi}(R)$$

$$g = (R|\mathrm{w}_R{+}\mathrm{t}) \in \mathbf{G}(\mathrm{k})$$

$$\mathbf{D}^{\mathrm{k},\xi}(R|\mathrm{w}_R{+}\mathrm{t})\;\mathbf{D}^{\mathrm{k},\xi}(R'|\mathrm{w}_{R'}{+}\mathrm{t}') =$$
$$\mathbf{D}^{\mathrm{k},\xi}(RR'|\mathrm{w}_{RR'}{+}\mathrm{t}(R,R'){+}\mathrm{t}{+}\mathcal{R}\,\mathrm{t}')$$
$$g, g', g'' \in \mathbf{G}(\mathrm{k})$$

Induction Procedure (cont'd)

[12] Induction: $\mathbf{G}(\mathbf{k}) \uparrow \mathbf{G} \;\Rightarrow\; \mathbf{G}$ – **UIR's**

[12a] Symmorphic Space Groups

$$\boxed{\begin{array}{c} \mathbf{D}^{[\mathbf{k},\xi]\uparrow\mathbf{G}}_{\underline{R}a;\underline{S}b}(R|\mathbf{t}) = \\ \Delta^{\mathbf{k}}(\underline{R},R\underline{S})\, e^{-i\mathcal{R}\mathbf{k}\cdot\mathbf{t}}\, \mathbf{D}^{\xi}_{ab}(\underline{R}^{-1}R\underline{S}) \end{array}}$$

$$\mathbf{D}^{\xi}(R)\mathbf{D}^{\xi}(S) = \mathbf{D}^{\xi}(RS)$$

[12b] Non-Symmorphic Space Groups

$$\boxed{\begin{array}{c} \mathbf{D}^{[\mathbf{k},\xi]\uparrow\mathbf{G}}_{\underline{R}a;\underline{S}b}(R|\mathbf{w}_R+\mathbf{t}) = \\ \Delta^{\mathbf{k}}(\underline{R},R\underline{S})\, e^{-i\mathcal{R}\mathbf{k}\cdot\mathbf{t}}\, \Phi^{\mathbf{k}}_{\underline{R},\underline{S}}(R)\, \mathbf{D}^{\xi}_{ab}(\underline{R}^{-1}R\underline{S}) \end{array}}$$

$$\mathbf{D}^{\xi}(R)\mathbf{D}^{\xi}(S) = e^{-i\mathbf{k}\cdot\mathbf{t}(R,S)}\, \mathbf{D}^{\xi}(RS)$$

$$\Phi^{\mathbf{k}}_{\underline{R},\underline{S}}(R) = e^{-i\mathbf{k}\cdot\mathbf{t}_{\underline{R},\underline{S}}(R)}$$

$$\mathbf{t}_{\underline{R},\underline{S}}(R) = \mathbf{t}(\underline{R}^{-1},R) + \mathbf{t}(\underline{R}^{-1}R,\underline{S}) - \underline{R}^{-1}\mathbf{t}(\underline{R},\underline{R}^{-1})$$

$$\Delta^{\mathbf{k}}(\underline{R},R\underline{S}) = \begin{cases} 1 & \Longleftrightarrow \quad \underline{R}^{-1}R\underline{S} \in \mathbf{P}(\mathbf{k}) \\ 0 & \Longleftrightarrow \quad \texttt{otherwise} \end{cases}$$

$$\texttt{dim}\; \mathbf{D}^{[\mathbf{k},\xi]\uparrow\mathbf{G}} = |\mathbf{P}:\mathbf{P}(\mathbf{k})|\, n(\xi)$$

Induction Procedure (Summary)

$\mathbf{T}$ – UIR's: $\quad D^{\mathbf{k}}(E|\mathbf{t}) = e^{-i\mathbf{k}\cdot\mathbf{t}}$

Induction: $\quad D^{\mathbf{k}} \uparrow \mathbf{G}(\mathbf{k}) = \mathbf{B}^{\mathbf{k}\uparrow\mathbf{G}}$

$$\dim \mathbf{B}^{\mathbf{k}\uparrow\mathbf{G}} = n(\xi)$$

$$\mathbf{B}^{\mathbf{k}\uparrow\mathbf{G}}_{RS}(g) = \mathbf{B}^{\mathbf{k}\uparrow\mathbf{G}}_{RS}(Q|\mathbf{w}_Q+\mathbf{t}) =$$

$$e^{-i\mathbf{k}\cdot\mathbf{t}}\, e^{-i\mathbf{k}\cdot\mathbf{t}(R,S)}\, \delta_{R,QS}$$

$$\mathbf{B}^{\mathbf{k}\uparrow\mathbf{G}}(g) \sim \sum_{\xi} \oplus\; m(\mathbf{k}|\xi)\, \mathbf{D}^{\mathbf{k},\xi}(g)$$

$\mathbf{G}(\mathbf{k})$ – UIR's: $\quad \mathbf{D}^{\mathbf{k},\xi}(R|\mathbf{w}_R+\mathbf{t}) = e^{-i\mathbf{k}\cdot\mathbf{t}}\, \mathbf{D}^{\xi}(R)$

Induction: $\quad \mathbf{D}^{\mathbf{k},\xi} \uparrow \mathbf{G} = \mathbf{D}^{[\mathbf{k},\xi]\uparrow\mathbf{G}}$

$\mathbf{G}$ – UIR's: $\quad \mathbf{D}^{[\mathbf{k},\xi]\uparrow\mathbf{G}}_{\underline{R}a;\underline{S}b}(g) =$

$$\Delta^{\mathbf{k}}(\underline{R},R\underline{S})\, e^{-i\underline{\mathcal{R}}\mathbf{k}\cdot\mathbf{t}} \times$$

$$\Phi^{\mathbf{k}}_{\underline{R},\underline{S}}(R)\, \mathbf{D}^{\xi}_{ab}(\underline{R}^{-1}R\underline{S})$$

Induction Procedure (Summary (cont'd))

$$
\begin{array}{ccccc}
\{E\} & \longrightarrow & \mathbf{P}(\mathbf{k}) & \longrightarrow & \mathbf{P} \\
\uparrow & & \uparrow & & \uparrow \\
\mathbf{T} & \longrightarrow & \mathbf{G}(\mathbf{k}) & \longrightarrow & \mathbf{G} \\
\updownarrow & & \updownarrow & & \updownarrow \\
\mathrm{D}^{\mathbf{k}} & \longrightarrow & \mathbf{D}^{\mathbf{k},\xi} & \longrightarrow & \mathbf{D}^{[\mathbf{k},\xi]\uparrow \mathbf{G}}
\end{array}
$$

Examples:

[1] $\mathbf{G} = \#221$

$\mathbf{k}_{\mathsf{R}} = \frac{1}{2}(\mathbf{K}_1 + \mathbf{K}_2 + \mathbf{K}_3)$

$A_{221}(\mathbf{k}_{\mathsf{R}}) = \{\Gamma_1^{\pm}, \Gamma_2^{\pm}, \Gamma_3^{\pm}, \Gamma_4^{\pm}, \Gamma_5^{\pm}\}$

$\Gamma_j^{\pm}$ ... `Ordinary Vector UIR's of` $\mathbf{O}_h$

[2] $\mathbf{G} = \#222$

$A_{222}(\mathbf{k}_{\mathsf{R}}) = \{\Gamma_7, \Gamma_8, \Gamma_9, \Gamma_{14}\}$

$\mathrm{dim}\,\Gamma_7 = \mathrm{dim}\,\Gamma_8 = \mathrm{dim}\,\Gamma_9 = 2, \mathrm{dim}\,\Gamma_{14} = 6$

Γ_j ... `Projective UIR's of` $\mathbf{O}_h$

[4] App's: Solid State

Aim: To explain Bloch's Theorem, to discuss the spectral properties of periodic Hamiltonians H, to discuss the spectral properties of space group-invariant Hamiltonians, to explain compatibility relations (BSW) of energy bands, to discuss the relationship of Bloch- and Wannier-functions, and finally to explain how to identify the symmetry porperties of Bloch states, with and without imposing periodic boundary conditions (BvK).

[A] Periodic Hamiltonians

[1] `Hilbert space:` $\mathcal{H}$

$\mathcal{H} = \mathsf{L}^2(\mathbb{R}^3)$ or if imposing **BvK**-conditions

$\mathcal{H} = \mathsf{L}^2([\mathbf{0},\mathbf{N}\mathbf{t}_1]\times[\mathbf{0},\mathbf{N}\mathbf{t}_2]\times[\mathbf{0},\mathbf{N}\mathbf{t}_3])$

[2] `Hamiltonian:` H

$$\mathsf{H} = \frac{\mathbf{P}^2}{2m} + \mathsf{V}(\mathbf{X})$$

[3] `Symmetry Group:` G

$$\mathsf{G} = \left\{\mathsf{T}, \mathsf{P}|\mathcal{O}, \mathbf{w}_{\mathsf{P}}\right\}$$

$$[\mathsf{U}(g)\,\phi]\,(\mathbf{x}) = \phi(\mathcal{M}(g^{-1})\,\mathbf{x})$$

[a] Bloch Functions

[a1] $\mathcal{H} = \mathsf{L}^2(\mathbb{R}^3) \quad \Longleftrightarrow$

$\mathbf{k} = x\mathbf{K}_1 + y\mathbf{K}_2 + z\mathbf{K}_3 \in \mathsf{B}(\mathsf{T}^\star)$

x,y,z ... `continuous parameters`

[a2] $\mathcal{H} = \mathsf{L}^2([\mathbf{0},\mathtt{N}\mathbf{t}_1]\times[\mathbf{0},\mathtt{N}\mathbf{t}_2]\times[\mathbf{0},\mathtt{N}\mathbf{t}_3]) \quad \Longleftrightarrow$

$\mathbf{k} = \frac{1}{\mathtt{N}}\sum_{j=1}^{3} m_j\,\mathbf{K}_j \in \mathsf{B}_{\mathtt{N}}(\mathsf{T}^\star)$

$m_j = \{0,1,2,3,\ldots\mathtt{N}-2,\mathtt{N}-1\}$

★ Since the potential $\mathsf{V}(\mathbf{X})$ is periodic, ie.

$[\mathsf{U}(E|\mathbf{t})\,,\mathsf{V}(\mathbf{X})] = 0 \quad \forall\ \mathbf{t} \in \mathsf{T}$,

the Hamiltonian H and all $\{\mathsf{U}(E|\mathbf{t})\}$

can be dialgonalized simultaneously.

Simultaneous Eigenfunctions of $\{\mathsf{U}(E|\mathbf{t})\}$

$\Longleftrightarrow$ **Bloch Functions**

$$\begin{array}{rcl} \Phi^{\mathbf{k}}(\mathbf{x}) & = & e^{i\mathbf{k}\cdot\mathbf{x}}\,w(\mathbf{x}) \\ w(\mathbf{x}) & = & w(\mathbf{x}+\mathbf{t}) \end{array}$$

[b] Bloch Theorem

Separation ansatz with Bloch functions for the eigenvalue equation leads, depending on $L^2(\mathbb{R}^3)$ or $L^2([\mathbf{0},N\mathbf{t}_1]\times[\mathbf{0},N\mathbf{t}_2]\times[\mathbf{0},N\mathbf{t}_3])$, to a continuous or finite set of **decoupled** eigenvalue equations: $w(\mathbf{x}) \longrightarrow w(\mathbf{k},\mathbf{x})$

$$\mathsf{H}\,\Phi^{\mathbf{k}} = E(\mathbf{k})\,\Phi^{\mathbf{k}} \qquad \Rightarrow$$

$$\left[\frac{1}{2m}\left(\mathbf{Q}^2 + 2\mathbf{k}\cdot\mathbf{Q}\right) + \mathsf{V}(\mathbf{X})\right] w_n(\mathbf{k},\mathbf{x}) = \left(E_n(\mathbf{k}) - \frac{\mathbf{k}^2}{2m}\right) w_n(\mathbf{k},\mathbf{x})$$

$[\mathbf{Q}\,\psi]\,(\mathbf{x}) = \; - i\hbar\nabla\,\psi(\mathbf{x})$ together with the boundary condition: $\psi(\mathbf{x}) = \psi(\mathbf{x}+\mathbf{t})$

[c] Energy Bands

[c1] $E_n(\mathbf{k}) \leq E_{n+1}(\mathbf{k})$

[c2] $E_n(\mathbf{k})$ ... `continuous in` $\mathbf{k} \in \mathsf{B}(\mathsf{T}^\star)$

$$\begin{array}{lllll} E_n & : & \mathsf{B}(\mathsf{T}^\star) & \longrightarrow & \mathbb{R} & \texttt{(continuous)} \\ E_n & : & \mathsf{B}_{\mathrm{N}}(\mathsf{T}^\star) & \longrightarrow & \mathbb{R} & \texttt{(discrete)} \end{array}$$

[d] Symmetrized Bloch Functions

$$\mathsf{H}\,\Psi^{[\mathbf{k}\xi|n]}_{\underline{R}a} = E^{\xi}_{n}(\mathbf{k})\,\Psi^{[\mathbf{k}\xi|n]}_{\underline{R}a}$$

$\mathbf{k} \in \Delta\mathsf{B}(\mathsf{T}^{\star}|\mathsf{P})$
$\xi \in A(\mathsf{P}(\mathbf{k}))$
n `... Band index`

$\underline{R} \in \mathsf{P}:\mathsf{P}(\mathbf{k})$
$a = 1, 2, \ldots n(\xi)$

$$\mathsf{U}(R|\mathbf{w}_R{+}\mathbf{t})\,\Psi^{[\mathbf{k}\xi|n]}_{\underline{R}a} =$$
$$\sum_{\underline{S}b} \mathsf{D}^{[\mathbf{k},\xi]\uparrow\mathsf{G}}_{\underline{S}b;\underline{R}a}(R|\mathbf{w}_R{+}\mathbf{t})\,\Psi^{[\mathbf{k}\xi|n]}_{\underline{S}b}$$

$$\boxed{E^{\xi}_{n}(\mathbf{k}) = E^{\xi}_{n}(\underline{\mathcal{R}}\,\mathbf{k})}$$

$$\mathtt{deg}\ E^{\xi}_{n}(\mathbf{k}^{\star}) = \mathtt{dim}\ \mathsf{D}^{[\mathbf{k},\xi]\uparrow\mathsf{G}} = |\mathbf{k}^{\star}(\mathsf{P})|\,n(\xi)$$

$$\begin{aligned}\Psi^{[\mathbf{k}\xi|n]}_{\underline{R}a} &= \mathsf{U}(\underline{R}|\mathbf{w}_{\underline{R}})\,\Phi^{\mathbf{k}\xi,n}_{a}\\ \Phi^{\mathbf{k}\xi,n}_{a}(\mathbf{x}) &= e^{i\mathbf{k}\cdot\mathbf{x}}\,w^{\xi}_{n,a}(\mathbf{k},\mathbf{x})\end{aligned}$$

Symmetries of Energy Bands (Summary)

$$
\begin{array}{ccccc}
\mathbf{T} & \longrightarrow & \mathbf{G}(\mathbf{k}) & \longrightarrow & \mathbf{G} \\
\downarrow & & \downarrow & & \downarrow \\
\mathrm{D}^{\mathbf{k}} & \longrightarrow & \mathbf{D}^{\mathbf{k},\xi} & \longrightarrow & \mathbf{D}^{[\mathbf{k},\xi]\uparrow \mathbf{G}} \\
\updownarrow & & \updownarrow & & \updownarrow \\
\mathbf{k} & \longrightarrow & \mathbf{k},\xi & \longrightarrow & [\mathbf{k},\xi]\uparrow \mathbf{G} \\
\downarrow & & \downarrow & & \downarrow \\
E_n(\mathbf{k}) & \longrightarrow & E_n^{\xi}(\mathbf{k}) & \longrightarrow & \boxed{\begin{array}{l} E_n^{\xi}(\mathbf{k}) = \\ E_n^{\xi}(\underline{\mathcal{R}}\,\mathbf{k}) \end{array}} \\
\updownarrow & & \updownarrow & & \updownarrow \\
\Phi^{\mathbf{k},n} & \longrightarrow & \Phi_a^{\mathbf{k}\xi,n} & \longrightarrow & \Psi_{\underline{R}a}^{[\mathbf{k}\xi|n]}
\end{array}
$$

$\mathbf{G}_{\mathtt{sym}}$: $\mathbf{D}^{\xi}$ = Ordinary Vector UIR's of $\mathbf{P}(\mathbf{k})$

$\mathbf{G}_{\mathtt{non-sym}}$: $\mathbf{D}^{\xi}$ = Projective UIR's of $\mathbf{P}(\mathbf{k})$

[e] Compatibility Relations (BSW)

BSW-Rule: The energy eigenvalues $E_n(\mathrm{k})$ of neighboring k-vectors are related by symmetry arguments, ie. relation between $E_n(\mathrm{k})$ and $E_n(\mathrm{k}')$ where $|\mathrm{k}-\mathrm{k}'|<\varepsilon$ and $\mathrm{k},\mathrm{k}'\in\triangle\mathbf{B}(\mathbf{T}^\star|\mathbf{P})$.

L.P. Bouckaert, R. Smoluchowski, E.P. Wigner: Phys.Rev. **50** (1936) 58 - 67

[e1] $\mathbf{P}(\mathrm{k}') = \mathbf{P}(\mathrm{k}) \quad \Rightarrow$ **NO** splitting of the eigenvalue $E_n(\mathrm{k})$ when passing over continuously from $\mathrm{k} \longmapsto \mathrm{k}'$, since $\mathbf{D}^\xi \downarrow \mathbf{P}(\mathrm{k}')$ must remain **irreducible**.

[e2] $\mathbf{P}(\mathrm{k}') \subset \mathbf{P}(\mathrm{k}) \quad \Rightarrow$ **NO** splitting of the eigenvalue $E_n(\mathrm{k})$ when passing over continuously from $\mathrm{k} \longmapsto \mathrm{k}'$, iff $\mathbf{D}^\xi \downarrow \mathbf{P}(\mathrm{k}')$ remains **irreducible**.

[e3] $\mathbf{P}(\mathrm{k}') \subset \mathbf{P}(\mathrm{k}) \quad \Rightarrow$ **Splitting** of the eigenvalue $E_n(\mathrm{k})$ when passing over continuously from $\mathrm{k} \longmapsto \mathrm{k}'$, iff $\mathbf{D}^\xi \downarrow \mathbf{P}(\mathrm{k}')$ turns out to be **reducible**.

$$\mathbf{D}^\xi \downarrow \mathbf{P}(\mathrm{k}') \;\sim\; \sum_{\xi' \in A(\mathbf{P}(\mathrm{k}'))} \oplus\, m(\xi|\xi')\, \mathbf{D}^{\xi'}$$

$$\deg E^\xi(\mathrm{k}) \;=\; \sum_{\xi'} m(\xi|\xi') \deg E^{\xi'}(\mathrm{k}')$$

[f] Symmetry analysis of Bloch States

$$\left[\frac{1}{2m}\left(\mathbf{Q}^2+2\mathbf{k}\cdot\mathbf{Q}\right)+\mathsf{V}(\mathbf{X})\right] w_{n,s}(\mathbf{k},\mathbf{x}) =$$
$$\left(E_n(\mathbf{k})-\frac{\mathbf{k}^2}{2m}\right) w_{n,s}(\mathbf{k},\mathbf{x}) \qquad s = 1,2,3,\ldots \deg E_n(\mathbf{k})$$

$$\boxed{\Phi_s^{\mathbf{k},n}(\mathbf{x}) = e^{i\mathbf{k}\cdot\mathbf{x}}\, w_{n,s}(\mathbf{k},\mathbf{x})} \qquad \forall s$$

$$g = (R|\mathbf{w}_R+\mathbf{t}) \in \mathbf{G}(\mathbf{k})$$
$$\mathsf{U}(g)\,\Phi_s^{\mathbf{k},n} = \sum_r \mathbf{D}_{rs}^{\mathbf{k},n}(g)\,\Phi_r^{\mathbf{k},n}$$

$$\boxed{\mathbf{D}_{rs}^{\mathbf{k},n}(R|\mathbf{w}_R+\mathbf{t}) = e^{-i\mathbf{k}\cdot\mathbf{t}}\,\mathbf{D}_{rs}^{n}(R)}$$

$$\mathbf{D}^n(R)\,\mathbf{D}^n(S) = e^{-i\mathbf{k}\cdot\mathbf{t}(R,S)}\,\mathbf{D}^n(RS)$$

$$\boxed{\begin{aligned} \mathbf{D}^n(R) &\sim \sum_{\xi\in A(\mathbf{P}(\mathbf{k}))} \oplus\, m(n|\xi)\,\mathbf{D}^{\xi}(R) \\ \chi^n(R) &= \sum_{\xi\in A(\mathbf{P}(\mathbf{k}))} m(n|\xi)\,\chi^{\xi}(R) \end{aligned}}$$

$$\sum_\xi m(n|\xi) = 1 \iff n \longleftrightarrow \xi_o$$

Generic Degeneracy

$$\sum_\xi m(n|\xi) > 1 \iff n \longleftrightarrow \{\xi_1,\xi_2,\ldots\}$$

Accidental Degeneracy

[g] Symmetry analysis of Bloch Factors

$$\Psi^{[\mathbf{k}\xi|n]}_{\underline{R}a}(\mathbf{x}) = e^{i\underline{\mathcal{R}}\mathbf{k}.\mathbf{x}}\, w^{\xi,n}_{a}(\underline{\mathcal{R}}\mathbf{k},\mathbf{x})$$

$$\Psi^{[\mathbf{k}\xi|n]}_{\underline{E}a}(\mathbf{x}) = e^{i\mathbf{k}.\mathbf{x}}\, w^{\xi,n}_{a}(\mathbf{k},\mathbf{x})$$

$\underline{(R|\mathbf{w}_R) \in \mathbf{G}(\mathbf{k})\text{:}}$

$$\mathsf{U}(R|\mathbf{w}_R)\,\Psi^{[\mathbf{k}\xi|n]}_{\underline{E}a} = \sum_{b=1}^{n(\xi)} \mathbf{D}^{\mathbf{k},\xi}_{ba}(R)\,\Psi^{[\mathbf{k}\xi|n]}_{\underline{E}b}$$

Isometrical Mappings:

$$\left[\mathsf{U}(R|\mathbf{w}_R)\,\Psi^{[\mathbf{k}\xi|n]}_{\underline{E}a}\right](\mathbf{x}) =$$

$$\Psi^{[\mathbf{k}\xi|n]}_{\underline{E}b}(\mathcal{M}(R|\mathbf{w}_R)^{-1}\mathbf{x}) =$$

$$e^{i\mathbf{k}.\mathbf{x}}\left[\mathsf{V}^{\mathbf{k}}(R,\mathbf{w}_R)\,w^{\xi,n}_{a}(\mathbf{k})\right](\mathbf{x})$$

Note: Operator $\mathsf{V}^{\mathbf{k}}(R,\mathbf{w}_R)$ are mapping $\mathcal{L}^2(\mathbf{E}(\mathbf{T})) \longrightarrow \mathcal{L}^2(\mathbf{E}(\mathbf{T}))$

$$\boxed{\begin{gathered}\left[\mathsf{V}^{\mathbf{k}}(R,\mathbf{w}_R)\,w_s(\mathbf{k})\right](\mathbf{x}) = \\ e^{-iR\mathbf{k}.\mathbf{w}_R}\, e^{i\mathbf{K}(\mathbf{k},R).\mathbf{x}}\, w_s(\mathbf{k}, R^{-1}(\mathbf{x}-\mathbf{w}_R))\end{gathered}}$$

[g'] Projective Multiplier Reps

$$\mathsf{V}^{\mathbf{k}}(R, \mathbf{w}_R)\,\mathsf{V}^{\mathbf{k}}(S, \mathbf{w}_S) \;=\; e^{-i\mathbf{k}.\mathbf{t}(R,S)}\,\mathsf{V}^{\mathbf{k}}(RS, \mathbf{w}_{RS})$$

[g''] Symmetrized Plane Waves

$$\Phi^{\mathbf{K}}(\mathbf{x}) = \frac{1}{\sqrt{|\mathbf{E}(\mathbf{T}^\star)|}}\, e^{i\mathbf{K}.\mathbf{x}} \qquad \mathbf{K} \in \mathbf{T}^\star$$

$$\mathsf{V}^{\mathbf{k}}(R, \mathbf{w}_R)\,\Phi^{\mathbf{K}} = e^{-iR(\mathbf{k}+\mathbf{K}).\mathbf{w}_R}\,\Phi^{\mathbf{K}+\mathbf{K}(\mathbf{k},R)}$$

$$R \in \mathbf{P}(\mathbf{k}) \Longleftrightarrow \mathcal{R}\,\mathbf{k} = \mathbf{k} + \mathbf{K}(\mathbf{k}, R)$$

Closure Relations: $\forall\, R, S \in \mathbf{P}(\mathbf{k})$

$$\mathbf{K}(\mathbf{k}, RS) = \mathbf{K}(\mathbf{k}, R) + \mathcal{R}\,\mathbf{K}(\mathbf{k}, S)$$

[g] Band representations

Aim: Band representations are specific representations of crystallographic space groups, which are of great importance, since they allow one to consider an energy band as a whole entity.

Site groups: Every **finite** subgroup $\mathbf{G}_{\mathrm{w}}$ of an **infinite** space group $\mathbf{G}$ can be interpreted as **site** group that has to be isomorphic to the point group $\mathbf{P}$ or any of its subgroups.

$$\begin{aligned}
\mathbf{G}_{\mathrm{w}} &= \{g \in \mathbf{G} \,|\, \mathcal{M}(g)\,\mathbf{w} = \mathbf{w}\} \\
\mathcal{M}(g)\,\mathbf{x} &= R\,\mathbf{x} + \mathbf{w}_R + \mathbf{t} \\
g &= (R|\mathbf{s}(R)) \\
\mathbf{s}(R) &= \mathbf{w} - \mathcal{R}\,\mathbf{w} = \mathbf{w}_R + \mathbf{t}(R) \\
& \quad R \in \mathbf{P} \quad \& \quad \mathbf{t}(R) \in \mathbf{T}
\end{aligned}$$

$$\begin{aligned}
\mathbf{G}_{\mathrm{w}} &\sim \mathbf{P}_{\mathrm{w}} \subseteq \mathbf{P} \\
\mathbf{G}_{\mathrm{w}} &= \{(R|\mathbf{s}(R)) \,|\, R \in \mathbf{P}_{\mathrm{w}}\}
\end{aligned}$$

$$\begin{aligned}
(RS|\mathbf{s}(RS)) &= (R|\mathbf{s}(R)) * (S|\mathbf{s}(S)) \\
\mathbf{t}(R,S) &= \mathbf{t}(RS) - \mathbf{t}(R) - \mathcal{R}\,\mathbf{t}(S)
\end{aligned}$$

Band representation: Let

$$\mathbf{D}^{\lambda} = \{\mathbf{D}^{\lambda}(g) \,|\, g \in \mathbf{G}_{\mathrm{w}}\}$$

be a given unitary matrix representation of the site group $\mathbf{G}_{\mathrm{w}}$ which need not be irreducible. Then the following induced matrix representation defines a band representation of $\mathbf{G}$.

$$\mathbb{D}^{(\mathrm{w},\lambda)\uparrow\mathbf{G}} = \{\mathbf{D}^{\lambda} \uparrow \mathbf{G}\}$$

Note in particular that any type of band representations is **infinite**-dimensional.

Elementary band representation: A band representation is called **elementary** if it cannot be decomposed into a direct sum of two or more band representations.

A necessary condition for a band representation to be **elementary** is that it corresponds to a Wyckoff position whose **site** symmetry group is **maximal**, which means $\mathbf{P}_{\mathrm{w}} = \mathbf{P}$ and that the $\mathbf{G}_{\mathrm{w}}$-representation $\mathbf{D}^{\lambda}$ is **irreducible**.

Simple band representation: An **elementary** band representation is called **simple** if, apart from $\mathbf{P}_{w} = \mathbf{P}$, it is assumed that the $\mathbf{P}$-irrep $\mathbf{D}^{\lambda}$ is **one**-dimensional. Thus

$$\mathbb{D}^{(w,\lambda)\uparrow\mathbf{G}} = \{\mathbf{D}^{\lambda} \uparrow \mathbf{G}\}$$

and the graph for the corresponding energy band contains only a single branch.

Composite band representation: Any band representation is called **composite** if it can be decomposed into a direct sum of two or more **elementary** band representations. Since

$$\mathbf{D}^{reg}(\mathbf{G}) = \mathbb{D}^{(w_o,\lambda_o)\uparrow\mathbf{G}} = \{\mathbf{D}^{\lambda_o} \uparrow \mathbf{G}\}$$

where $\mathbf{P}_{w_o} = \{g_o\} \subseteq \mathbf{P}$ with $g_o = (E|\mathbf{0})$ is the trivial point group and $\mathbf{D}^{\lambda_o}(g_o) = 1$ the trivial irrep, the **regular** representation of $\mathbf{G}$ forms, apart from the trivial space group $\mathbf{G} = \#\mathbf{1}$, a **composite** band representation.

★ **Band Representations:** (Final remarks)

- **Mathematical facts:** A special and important example of a band representation is the regular representation of a crystallographic space group. It turns out that the regular representation can be decomposed into elementary band representations, in particular, it can be written as a finite direct sum of elementary band representations. However, such decompositions are not unique **!!!**

- **Physical implications:** Prediction of the admissible band structures based on pure group-theoretical arguments.

- **Open questions:** Lack of general formula, like Burnside theorem, for the decomposition of regular representations into **elementary** band representations.

[B] Bloch and Wannier States

[1] Localized atomic wave functions

$\Phi_o(\mathrm{x}) \in \mathsf{L}^2(\mathbb{R}^3)$

If imposing periodic boundary conditions:

$\Phi_o(\mathrm{x}) \longmapsto \phi_o(\mathrm{x}) = \phi_o(\mathrm{x}+\mathbf{T}) \qquad \forall \mathbf{T} \in \mathsf{T}_{\underline{\mathtt{N}}}$

Normalization condition: $\|\phi_o\|^2 = 1$

$\mathsf{U}(E|\mathbf{t})\,\phi_o = \phi_{\mathbf{t}} \iff \|\phi_{\mathbf{t}}\|^2 = 1 \quad \forall \mathbf{t} \in \mathsf{T}_{\underline{\mathtt{N}}}$

Overlap integrals:

$\left\langle \phi_{\mathbf{t}}\,,\phi_{\mathbf{t}'} \right\rangle = \mathcal{O}(\mathbf{t},\mathbf{t}') \neq \delta_{\mathbf{t},\mathbf{t}'}$ (in general)

[2] Bloch functions

$\psi_{\mathbf{k}} = \sum_{\mathbf{t}} e^{+i\mathbf{k}\cdot\mathbf{t}}\,\phi_{\mathbf{t}}$

Normalization condition: $\psi_{\mathbf{k}} \longmapsto \Psi_{\mathbf{k}}$

$\left\langle \Psi_{\mathbf{k}}\,,\Psi_{\mathbf{k}'} \right\rangle = \delta_{\mathbf{k},\mathbf{k}'}$

[3] Wannier functions

$w_{\mathbf{t}} = \frac{1}{\sqrt{\mathtt{N}^3}} \sum_{\mathbf{k}} e^{-i\mathbf{k}\cdot\mathbf{t}}\,\Psi_{\mathbf{k}}$

$w_{\mathbf{t}}(\mathrm{x})$ ... localized functions

$\left\langle w_{\mathbf{t}}, w_{\mathbf{t}'} \right\rangle = \delta_{\mathbf{t},\mathbf{t}'}$

$w_{\mathbf{t}}(\mathrm{x}) \neq \phi_{\mathbf{t}}(\mathrm{x}) \iff \mathcal{O}(\mathbf{t},\mathbf{t}') \neq \delta_{\mathbf{t},\mathbf{t}'}$

[C] Selection Rules

[1] Space group symmetry adapted states
[2] Space group symmetry adapted operators
[3] Space groups: Wigner-Eckart Theorem
[4] Space groups: Selection rules