COMPATIBILITY RELATIONS FOR FACTOR SYSTEMS AND SPACE GROUP REPRESENTATIONS

R. Dirl

1.Inst. f. theor. Physik, TU Wien; A-1040 Wien, Karlsplatz 13, Austria

I. SPACE GROUP REPRESENTATIONS

The (vector) unirreps of a non-symmorphic space group G can be written in the form [1,2]

$$D^{(\kappa,\vec{q})\uparrow G}_{\underline{\sigma},\underline{\sigma}'}(\beta|\vec{\tau}(\beta)+\vec{t}) = \Delta^{\vec{q}}(\underline{\sigma},\beta\underline{\sigma}')\, e^{-iD(\underline{\sigma})\vec{q}.(\vec{t}+\vec{t}(\beta,\underline{\sigma}')+\vec{t}(\underline{\sigma},\underline{\sigma}^{-1}\beta\underline{\sigma}'))}\,\mathbf{D}^{\kappa}(\underline{\sigma}^{-1}\beta\underline{\sigma}')$$

$$\vec{t}(\gamma,\gamma') = \vec{\tau}(\gamma)+D(\gamma)\vec{\tau}(\gamma')-\vec{\tau}(\gamma\gamma');\ \gamma,\gamma'\in P \simeq G/T$$

$$G^{\vec{q}} = \{(\alpha|\vec{\tau}(\alpha)+\vec{t}):\ D(\alpha)\vec{q} = \vec{q}+\vec{Q}\{\vec{q}(\alpha)\};\vec{t}\in T,\alpha\in P\}$$

$$\Delta^{\vec{q}}(\gamma,\gamma') = \delta_{\gamma P^{\vec{q}},\gamma' P^{\vec{q}}}\ ;\ \gamma,\gamma'\in P \supseteq P^{\vec{q}} \simeq G^{\vec{q}}/T$$

Thereby $\mathbf{D}^{\kappa}$ denotes n_{κ}-dimensional projective unirreps of the factor group $P^{\vec{q}} \simeq G^{\vec{q}}/T$ belonging to the factor system

$$R^{\vec{q}}(\alpha,\alpha') = e^{-i\vec{q}.\vec{t}(\alpha,\alpha')} \qquad \text{for all } \alpha,\alpha'\in P^{\vec{q}};$$

$D(\alpha)$ orthogonal matrices representing the point group elements; $\vec{\tau}(\alpha)$ non-primitive lattice translations; $\underline{\sigma},\underline{\sigma}'$ ($\in G{:}G^{\vec{q}}$) left coset representatives; and $\vec{Q}\{\vec{q}(\alpha)\}$ reciprocal lattice vectors.

II. FACTOR SYSTEMS

In order to simplify the following considerations we change every factor system $R^{\vec{q}}$ by means of $\mathbf{D}^{\kappa}(\alpha) = e^{-i\vec{q}.\vec{\tau}(\alpha)}\mathbf{R}^{\kappa}(\alpha)$ $(\alpha\in P^{\vec{q}})$ to

$$S^{\vec{q}}(\alpha,\beta) = e^{-i\vec{q}.(D(\alpha)-\mathbb{1})\vec{\tau}(\beta)} = e^{i\vec{Q}\{\vec{q}(\alpha)\}.(\vec{\tau}(\alpha\beta)-\vec{\tau}(\alpha))} \quad \text{for all } \alpha,\beta\in P^{\vec{q}},$$

which implies that the projective unirreps $\mathbf{R}^{\kappa}$ belong to the new factor system $S^{\vec{q}}$. Thereby we realize that $S^{\vec{q}}$ depends on $\vec{q}$ in such a way, that $S^{\vec{q}}$ does not alter, if $\vec{q}$ varies along lines or planes of the same symmetry of the fundamental domain of the Brillouin zone.

III. COMPATIBILITY RELATIONS FOR THE FACTOR SYSTEMS

Because of the special structure of the factor systems $S^{\vec{q}}$ we obtain

$$S^{\vec{q}}(\alpha,\beta) = S^{\vec{q}'}(\alpha,\beta) \quad \text{for all } \alpha,\beta \in P^{\vec{q}} \cap P^{\vec{q}'}$$

which is called hereafter compatiblity relations for the factor systems. These relations guarantee that for $\vec{q}$'s of the same symmetry the corresponding factor systems are identical, and that in case the subgroup relation $P^{\vec{q}'} \subset P^{\vec{q}}$ holds, the factor systems coincide on the common domain of definition $P^{\vec{q}'} \times P^{\vec{q}'}$.

IV. COMPATIBILITY RELATIONS FOR SPACE GROUP REPRESENTATIONS

When investigating compatibility relations for space group representations[3,1,4] it suffices to consider the (vector) unirreps of $G^{\vec{q}}$.

$$D^{\kappa,\vec{q}}(\alpha|\vec{\tau}(\alpha)+\vec{t}) = e^{-i\vec{q}.(\vec{\tau}(\alpha)+\vec{t})}\mathbb{R}^{\kappa}(\alpha) \qquad \text{for all } \vec{t} \in T \text{ and } \alpha \in P^{\vec{q}}$$

Presupposed $G^{\vec{q}'} \subseteq G^{\vec{q}}$ holds (which implies $P^{\vec{q}'} \subseteq P^{\vec{q}}$) we obtain as consequence of the compatibility relations for the factor systems compatibility relations for the space group representations as

$$D^{\kappa,\vec{q}} \downarrow G^{\vec{q}'} \simeq e^{-i\vec{q}.(\vec{\tau}(\alpha')+\vec{t})} \sum_{\kappa'} \oplus\, m_{\kappa,\kappa'}\, \mathbb{R}^{\kappa'}(\alpha') \qquad \text{for all } \alpha' \in P^{\vec{q}'}$$

where $\mathbb{R}^{\kappa'}$ denotes the projective unirreps of $P^{\vec{q}'}$ and $m_{\kappa,\kappa'}$ the multiplicity with which $\mathbb{R}^{\kappa'}$ occurs in $\mathbb{R}^{\kappa} \downarrow P^{\vec{q}'}$.

V. PROJECTIVE UNIRREPS OF $P^{\vec{q}}$

According to the formula for the space group unirreps the main problem consists in the determination of the projective unirreps of $P^{\vec{q}}$ when calculating space group unirreps. Now the compatibility relations for the factor systems allow to determine quite generally complete sets of projective unirreps of $P^{\vec{q}}$ by means of induction [2] out of projective unirreps of $P^{\vec{q}'}$ $(\subset P^{\vec{q}})$, presupposed the chain of normalizers of $P^{\vec{q}'}$ is ending in $P^{\vec{q}}$.

In the following we summarize the results of the induction procedure on hand of the example Pn3n for the point M of the fundamental domain of the Brillouin zone. We choose two different chains of groups in order to calculate complete sets of projective unirreps of P^{M}. For definitions and notations see Ref.5 and for non-primitive lattice translations, respectively factor systems see Eqs. (5.1,2,6,7,9,10) of Ref.2.

$$\text{chain 1:} \quad P^{Plane} = P \to N(P) \to N(N(P)) = P^{T} \to N(P^{T}) = P^{M}$$

$$\text{chain 2:} \quad P^{Plane} = P \to N(P) = P^{Z} \to N(P^{Z}) \to N(N(P^{Z})) = P^{M}$$

$$\begin{aligned} P &= \{E,\sigma_y\} \\ N(P) &= \{E,\sigma_x\}\times P \\ P^{T} &= \{E,\sigma_{db}\} \circledS N(P) \\ P^{M} &= \{E,I\}\times P^{T} \end{aligned} \qquad\qquad \begin{aligned} P &= \{E,\sigma_y\} \\ P^{Z} &= \{E,\sigma_z\}\times P \\ N(P^{Z}) &= \{E,I\}\times P^{Z} \\ P^{M} &= \{E,\sigma_{db}\} \circledS N(P^{Z}) \end{aligned}$$

Using Eqs.(3.20,22,36,61,62,66) of Ref.2 we obtain after simple calculations the following two sets of projective unirreps of P^{M} which are equivalent to those given by Eqs.(5.42) of Ref.2 and are written down for generating elements.

$$\begin{aligned}
\sigma_y &\to \begin{vmatrix} i & 0 \\ 0 & -i \end{vmatrix} \begin{vmatrix} i & 0 \\ 0 & -i \end{vmatrix} \begin{vmatrix} i & 0 \\ 0 & -i \end{vmatrix} \begin{vmatrix} i & 0 \\ 0 & -i \end{vmatrix} \qquad & \begin{vmatrix} i & 0 \\ 0 & -i \end{vmatrix} \begin{vmatrix} i & 0 \\ 0 & -i \end{vmatrix} \begin{vmatrix} i & 0 \\ 0 & -i \end{vmatrix} \begin{vmatrix} i & 0 \\ 0 & -i \end{vmatrix} &\leftarrow \sigma_y \\
\sigma_x &\to \begin{vmatrix} -i & 0 \\ 0 & i \end{vmatrix} \begin{vmatrix} -i & 0 \\ 0 & i \end{vmatrix} \begin{vmatrix} i & 0 \\ 0 & -i \end{vmatrix} \begin{vmatrix} i & 0 \\ 0 & -i \end{vmatrix} \qquad & \begin{vmatrix} 0 & 1 \\ 1 & 0 \end{vmatrix} \begin{vmatrix} 0 & 1 \\ 1 & 0 \end{vmatrix} \begin{vmatrix} 0 & 1 \\ 1 & 0 \end{vmatrix} \begin{vmatrix} 0 & 1 \\ 1 & 0 \end{vmatrix} &\leftarrow \sigma_z \\
\sigma_{db} &\to \begin{vmatrix} 1 & 0 \\ 0 & 1 \end{vmatrix} \begin{vmatrix} -1 & 0 \\ 0 & -1 \end{vmatrix} \begin{vmatrix} 0 & 1 \\ 1 & 0 \end{vmatrix} \begin{vmatrix} 0 & 1 \\ 1 & 0 \end{vmatrix} \qquad & \begin{vmatrix} 0 & -1 \\ -1 & 0 \end{vmatrix} \begin{vmatrix} 0 & -1 \\ -1 & 0 \end{vmatrix} \begin{vmatrix} 0 & 1 \\ 1 & 0 \end{vmatrix} \begin{vmatrix} 0 & 1 \\ 1 & 0 \end{vmatrix} &\leftarrow I \\
I &\to \begin{vmatrix} 0 & 1 \\ 1 & 0 \end{vmatrix} \begin{vmatrix} 0 & 1 \\ 1 & 0 \end{vmatrix} \begin{vmatrix} 0 & 1 \\ 1 & 0 \end{vmatrix} \begin{vmatrix} 0 & -1 \\ -1 & 0 \end{vmatrix} \qquad & \begin{vmatrix} 1 & 0 \\ 0 & 1 \end{vmatrix} \begin{vmatrix} -1 & 0 \\ 0 & -1 \end{vmatrix} \begin{vmatrix} 0 & 1 \\ 1 & 0 \end{vmatrix} \begin{vmatrix} 0 & -1 \\ -1 & 0 \end{vmatrix} &\leftarrow \sigma_{db}
\end{aligned}$$

A simple calculation (where $\sigma_x = \sigma_y\sigma_z I$ has to be taken into account) shows that apart from the third projective unirrep of P^{M} (third column) the other three representations are only equivalent, which can be linked by the same unitary matrix.

$$W = \begin{vmatrix} 1 & 0 \\ 0 & -1 \end{vmatrix}$$

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