Irreducible representations of subperiodic rod groups

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The procedure of how to take the irreducible representations of subperiodic rod groups from Tables of irreducible representations of three-periodical space groups is derived. Examples demonstrating the use of this procedure and derivation of selection rules for direct and phonon assisted electrical dipole transitions are presented.

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1. Introduction

The subperiodic rod groups R are the 75 three-dimensional groups with one-dimensional translations which turn up to be in concomitant relationships with three-dimensional space groups G [1]. Rod groups describe the symmetry of one-periodic systems and can be used for studying polymeric molecules, nanotubes and others similar objects. Besides, this geometrical symmetry appears when applying a uniform magnetic field on bulk crystals, superlattices, quantum wells [2]. Irreducible representations (IRs) of rod groups are necessary for physical applications (e. g., deriving selection rules for optical transitions).

A subperiodic rod group R can contain the following elements: translations in one direction (of a vector $\mathbf{d}$); two-, three-, four- or six-fold rotation or screw axes pointed in this direction; two-fold axes perpendicular to it; reflection planes containing $\mathbf{d}$; reflection planes perpendicular to $\mathbf{d}$. Every subperiodic rod group R is in one-to-one correspondence with some three-periodic space group G: it is a subgroup of G ($R \subset G$) and has the same point symmetry group. To obtain a rod group R, it is sufficient to keep translations only in one direction in a related space group G. These groups (R and G) have the same international notations. For example, G $143\,C_3^1\,(P3) \leftrightarrow R\,42\,(p3)$; G $173\,C_6^6\,(P6_3) \leftrightarrow R\,56\,(p6_3)$.

The IRs of rod groups R may be generated in the same way as for three-periodic space groups G. All the IRs of R are contained in the IRs of the related space group G and can be taken directly from, e. g., Tables of Ref. [3]. The procedure how to make this is given in Section 2.

2. The relation between IRs of space and subperiodic rod groups

Let $(g_i|\mathbf{v}_i + \mathbf{a}_m) \in R$ be elements of a rod group R, where g_i is a proper or improper rotation followed by improper translation $\mathbf{v}_i$ and $\mathbf{a}_m = m\mathbf{a}_3$ are lattice translations of R. Consider a group $T^{(2)}$ of two-dimensional translations $\mathbf{a}_\mathbf{n}^{(2)} = n_1\mathbf{a}_1 + n_2\mathbf{a}_2$ in the plane Σ which does not contain the vectors $\mathbf{a}_n = m\mathbf{a}_3$ (n_1, n_2, m are integers). The set of elements

$$(E|\mathbf{a}_\mathbf{n}^{(2)})(g_i|\mathbf{v}_i + \mathbf{a}_m) \qquad (1)$$

contains a group of three-dimensional translations $(E|\mathbf{a}_\mathbf{n}^{(2)} + \mathbf{a}_m) \in T$ and is some space group provided the translational symmetry (the group T) is compatible with the point symmetry F of the rod group R. This condition is fulfilled if the vector $\mathbf{a}_3$ is perpendicular to the plane Σ of the translations $\mathbf{a}_\mathbf{n}^{(2)}$. Indeed the translations $m\mathbf{a}_3$ are compatible with F as they are elements of R. The compatibility of the translations $\mathbf{a}_\mathbf{n}^{(2)} \in T^{(2)}$ with point group F follows from the fact that the rotations (proper and improper) from R transform the rod into itself and, therefore, any vector perpendicular to the rod — into the vector also perpendicular to the rod. Thus the set of elements (1) forms one of three-periodic space groups G which has the same point symmetry as the rod group R. Moreover, the translational group $T^{(2)}$ is invariant in G: along with the translation $(E|\mathbf{a}_\mathbf{n}^{(2)})$ it contains also the translation $(E|g_i\mathbf{a}_\mathbf{n}^{(2)}) = (g_i|\mathbf{v}_i + \mathbf{a}_m)(E|\mathbf{a}_\mathbf{n}^{(2)})(g_i|\mathbf{v}_i + \mathbf{a}_m)^{-1}$ for any g_i from (1). The group G may be represented as a semi-direct product of $T^{(2)}$ and R

$$G = T^{(2)} \wedge R, \quad G = \sum_i (g_i|\mathbf{v}_i + \mathbf{a}_m)T^{(2)}. \qquad (2)$$

For some rod groups ($R\,1$, $R\,2$, $R\,4$, $R\,5$) of low point symmetry, the plane Σ may be inclined with respect to the vector $\mathbf{a}_3$. In this case, the translational group $T^{(2)}$ remains invariant in G. A rod group R is a subgroup of G and isomorphous to the factor group $G/T^{(2)}$. According to the little group method ([4,5], see also Appendix) every IR of R is related to a definite IR of G of the same dimension. In these IRs of G all the elements of the coset $(g_i|\mathbf{v}_i + \mathbf{a}_m)T^{(2)}$ are mapped by the same matrix. In particular, all the translations in $T^{(2)}$ (coset $(E|\mathbf{0})T^{(2)}$) are mapped by unit matrices.

Let us choose, in the space of an IR of G, the basis which is at the same time the basis of the IRs of its invariant subgroup $T^{(2)}$. Then the translations belonging to $T^{(2)}$

are mapped by the diagonal matrices with the elements $\exp(-i\mathbf{k}^{(3)} \cdot \mathbf{a}_\mathbf{n}^{(2)})$. These matrices become the unit ones, if at any integers n_1 and n_2

$$\exp(-i\mathbf{k}^{(3)} \cdot \mathbf{a}_\mathbf{n}^{(2)}) = 1. \qquad (3)$$

This condition holds for any $\mathbf{k}^{(3)} = \alpha \mathbf{K}_3$ in the direction of the basic translation vector $\mathbf{K}_3 = \frac{2\pi}{V_\mathbf{a}} \mathbf{a}_1 \times \mathbf{a}_2$ of the three-dimensional Brillouin zone (BZ) of the space group G, which is perpendicular to the plane Σ. The only primitive translation vector $\mathbf{K} = \frac{2\pi}{|\mathbf{a}|^2}\mathbf{a}$ and all the wave vectors $\mathbf{k} = \beta\mathbf{K} (-1/2 < \beta \le 1/2)$ in the one-dimensional BZ of the rod group R are directed along the vector $\mathbf{a} = \mathbf{a}_3$. The correspondence between $\mathbf{k}^{(3)}$ and $\mathbf{k}$ is established by the transformation law of basic vectors of IRs under translation operations $\mathbf{a}_n$ of the rod group: $\exp(-i\mathbf{k}^{(3)} \cdot \mathbf{a}_3) = \exp(-i\mathbf{k} \cdot \mathbf{a})$, i.e. $\alpha = \beta$. If $\mathbf{a} \perp \Sigma$ then $\mathbf{k} = \mathbf{k}^{(3)}$, otherwise $\mathbf{k}$ is the projection of $\mathbf{k}^{(3)}$ on the direction of $\mathbf{a} = \mathbf{a}_3$.

The star of any vector $\mathbf{k}^{(3)}$ lies entirely in the direction of the primitive vector $\mathbf{K}_3$. Therefore the correspondence of IRs mentioned above takes place both for allowed IRs of little groups $G_{\mathbf{k}^{(3)}}$ (in G) and $R_\mathbf{k}$ (in R) and for the full IRs of G and R. So the subduction of any small IR of a little group $G_{\mathbf{k}^{(3)}}$ (full IR of G with wave vector star $^*\mathbf{k}^{(3)}$) on the elements of the rod group R generates some small IR of the little group $R_\mathbf{k}$ (full IR of R with the wave vector star $^*\mathbf{k}$) of the same dimension.

In Tables of IRs of space groups, one finds usually small IRs of little groups G_k (see, e.g., Ref. [3]). An IR $d^{(\mathbf{k}^{(3)},\lambda)}(g)$ of a little group $G_\mathbf{k} \subseteq G$ is at the same time an IR $d^{(\mathbf{k},\lambda)}(g)$ of a little rod group $R_\mathbf{k} \subseteq R$ with $\mathbf{k} = \mathbf{k}^{(3)}$, when $\mathbf{a} \perp \Sigma$, or $\mathbf{k}$ being projection of $\mathbf{k}^{(3)}$ on the direction of $\mathbf{a} = \mathbf{a}_3$.

The analogous procedure of IRs generation is valid for IRs of 80 three-dimensional groups with two-dimensional translations (layer) groups [5].

3. Discussion

To illustrate the proposed procedure let us consider semiconductor structures under a magnetic field. Let us consider the symmetry of bulk semiconductors with the zinc blende structure (the $T_d^{(2)}$ symmorphic space group), such as the GaAs or AlAs crystals for example, under a magnetic field $\mathbf{B}$ parallel to the symmetry axis C_3, or superlattices of the $(GaN)_m(AlN)_n$ type with an even value of $m+n$ (the C_{3v}^1 symmorphic space group), when the magnetic field B is directed along the symmetry axis C_3. These systems have the geometrical symmetry described by the rod group $R\,42\,(p3)$, whose IRs are related to those of the space group G 143 (C_3^1). In this case the plane Σ of the lattice translations $\mathbf{a}_\mathbf{n}^{(2)} = n_1\mathbf{a}_1 + n_2\mathbf{a}_2$ is perpendicular to the translation vector $\mathbf{a}$ of the rod group which coincides with lattice translation vector $\mathbf{a}_3$ of G. Thus $\mathbf{k}^{(3)} = \mathbf{k}$. One takes the IRs of R for point Γ (the center of one-dimensional BZ) and A (the edge of one-dimensional BZ) directly from Tables of Ref. [3] for $G = C_3^1$ space group. The group C_3^1 is symmorphic. The IRs with $\mathbf{k}$ on the line Γ A for the elements $(C_3|m\mathbf{a})$ differ from those for $(C_3|0)$ by the factor $\exp(-i\mathbf{k} \cdot m\mathbf{a})$ as this factor corresponds to the translation $m\mathbf{a}$. Another example is the non-symmorphic rod group $R\,56\,(p6_3)$. Its IRs are related to the IRs of the non-symmorphic space group G 173 (C_6^6). This is the geometrical symmetry of bulk materials with the wurtzite structure (e.g. bulk GaN) and the superlattices of the $(GaN)_m(AlN)_n$ type with odd values of $m+n$ (the C_{6v}^4 non-symmorphic space group), when the magnetic field $\mathbf{B}$ is directed along the symmetry axis. Since the crystal system is the same as in the first example (hexagonal lattice), one has also $\mathbf{k}^{(3)} = \mathbf{k}$ and takes the IRs of $R\,56$ for point Γ (the center of one-dimensional BZ, Table 1) and A (the edge of one-dimensional BZ, Table 2) directly from Tables of Ref. [3] for $G = C_6^6$ space group. Note that all the points in the BZ of the rod group $R\,56$ have the same point symmetry C_6. The IRs with $\mathbf{k}$ on the line ΓA for the elements $(C_6|\mathbf{a}/2 + m\mathbf{a})$ differ by the factor $\exp\big(-i\mathbf{k} \cdot (m + 1/2)\mathbf{a}\big)$ from those for element $(C_6|\mathbf{a}/2)$ at Γ $(\mathbf{k} = 0)$ as it follows from the theory of projective representations.

Table 1. Single- $(\Gamma_1{-}\Gamma_6)$ and double-valued $(\Gamma_7{-}\Gamma_{12})$ IRs of the rod group $R\,56\,(p6_3)$ at the point Γ $(k = 0)$ of the one-dimensional BZ ($\alpha = (0,\ 0,\ c/2)$, $\nu \equiv \exp(i\pi/6)$)

Element	Γ_1	Γ_2	$\Gamma_3 = \Gamma_5^*$	$\Gamma_4 = \Gamma_6^*$	$\Gamma_7 = \Gamma_{12}^*$	$\Gamma_8 = \Gamma_{11}^*$	$\Gamma_9 = \Gamma_{10}^*$
$\bar{E}$	1	1	1	1	-1	-1	-1
$(C_6\|\alpha)$	1	-1	$-i\nu^*$	$i\nu^*$	ν	$-\nu$	$-i$
$(C_3\|0)$	1	1	$i\nu$	$i\nu$	$i\nu^*$	$i\nu^*$	-1
$(C_2\|\alpha)$	1	-1	1	-1	i	$-i$	i
$(C_3^2\|0)$	1	1	$-i\nu^*$	$-i\nu^*$	$i\nu$	$i\nu$	1
$(C_6^5\|\alpha)$	1	-1	$i\nu$	$-i\nu$	$-\nu^*$	ν^*	$-i$

Table 2. Single- $(A_1{-}A_6)$ and double-valued $(A_7{-}A_{12})$ IRs of the rod group $R\,56\,(p6_3)$ at the point A $(k = \pi/c)$ of the one-dimensional BZ ($\alpha = (0,\ 0,\ c/2)$, $\nu \equiv \exp(i\pi/6)$)

Element	$A_1 = A_2^*$	$A_3 = A_6^*$	$A_4 = A_5^*$	$A_7 = A_{11}^*$	$A_8 = A_{12}^*$	A_9	A_{10}
$\bar{E}$	1	1	1	-1	-1	-1	-1
$(C_6\|\alpha)$	$-i$	$-\nu^*$	ν^*	$i\nu$	$-i\nu$	1	-1
$(C_3\|0)$	1	$i\nu$	$i\nu$	$i\nu^*$	$i\nu^*$	-1	-1
$(C_2\|\alpha)$	$-i$	$-i$	i	-1	1	-1	1
$(C_3^2\|0)$	1	$-i\nu^*$	$-i\nu^*$	$i\nu$	$i\nu$	1	1
$(C_6^5\|\alpha)$	$-i$	ν	$-\nu$	$-i\nu^*$	$i\nu^*$	1	-1

4. Selection rules for electrical dipole transitions

The stationary states of a system with the symmetry of a rod group R are classified according to the small IRs $|\mathbf{k}, \gamma\rangle$ of the little group $R_\mathbf{k} \subset R$.

Table 3. Direct (Kronecker) products ($A_i \times A_j$ and $A_j^* \times A_j$) of the single- (A_1–A_6) and double-valued (A_7–A_{12}) IRs at A-point of the BZ for rod group $R\,56\,(p6_3)$

IR		A_1	A_2	A_3	A_4	A_5	A_6	A_7	A_8	A_9	A_{10}	A_{11}	A_{12}
A_2^*	A_1	Γ_2	Γ_1	Γ_4	Γ_3	Γ_6	Γ_5	Γ_7	Γ_8	Γ_9	Γ_{10}	Γ_{11}	Γ_{12}
A_1^*	A_2	Γ_1	Γ_2	Γ_3	Γ_4	Γ_5	Γ_6	Γ_8	Γ_7	Γ_{10}	Γ_9	Γ_{12}	Γ_{11}
A_6^*	A_3	Γ_4	Γ_3	Γ_6	Γ_5	Γ_2	Γ_1	Γ_9	Γ_{10}	Γ_{11}	Γ_{12}	Γ_7	Γ_8
A_5^*	A_4	Γ_3	Γ_4	Γ_5	Γ_6	Γ_1	Γ_2	Γ_{10}	Γ_9	Γ_{12}	Γ_{11}	Γ_8	Γ_7
A_4^*	A_5	Γ_6	Γ_5	Γ_2	Γ_1	Γ_4	Γ_3	Γ_{11}	Γ_{12}	Γ_7	Γ_8	Γ_9	Γ_{10}
A_3^*	A_6	Γ_5	Γ_6	Γ_1	Γ_2	Γ_3	Γ_4	Γ_{12}	Γ_{11}	Γ_8	Γ_7	Γ_{10}	Γ_9
A_{11}^*	A_7	Γ_7	Γ_8	Γ_9	Γ_{10}	Γ_{11}	Γ_{12}	Γ_3	Γ_4	Γ_5	Γ_6	Γ_1	Γ_2
A_{12}^*	A_8	Γ_8	Γ_7	Γ_{10}	Γ_9	Γ_{12}	Γ_{11}	Γ_4	Γ_3	Γ_6	Γ_5	Γ_2	Γ_1
A_9^*	A_9	Γ_9	Γ_{10}	Γ_{11}	Γ_{12}	Γ_7	Γ_8	Γ_5	Γ_6	Γ_1	Γ_2	Γ_3	Γ_4
A_{10}^*	A_{10}	Γ_{10}	Γ_9	Γ_{12}	Γ_{11}	Γ_8	Γ_7	Γ_6	Γ_5	Γ_2	Γ_1	Γ_4	Γ_3
A_7^*	A_{11}	Γ_{11}	Γ_{12}	Γ_7	Γ_8	Γ_9	Γ_{10}	Γ_1	Γ_2	Γ_3	Γ_4	Γ_5	Γ_6
A_8^*	A_{12}	Γ_{12}	Γ_{11}	Γ_8	Γ_7	Γ_{10}	Γ_9	Γ_2	Γ_1	Γ_4	Γ_3	Γ_6	Γ_5

Note. $\Gamma_3 = \Gamma_5^*$, $\Gamma_4 = \Gamma_6^*$, $\Gamma_7 = \Gamma_{12}^*$, $\Gamma_8 = \Gamma_{11}^*$, $\Gamma_9 = \Gamma_{10}^*$.

Let us consider the selection rules [6] for transitions between stationary states of symmetry $|\mathbf{k}^{(f)}, \gamma^{(f)}\rangle$ and $|\mathbf{k}^{(i)}, \gamma^{(i)}\rangle$ caused by an operator $P(\mathbf{k}^{(p)}, \gamma^{(p)})$ transforming according to the IR $({}^*\mathbf{k}^{(p)}, \gamma^{(p)})$ of R. If the operator P transforms according some reducible rep of R, one can consider the selection rules for every of its irreducible components separately.

The transition probability is governed by the value of the matrix element

$$\langle \mathbf{k}^{(f)}, \gamma^{(f)} | P(\mathbf{k}^{(p)}, \gamma^{(p)}) | \mathbf{k}^{(i)}, \gamma^{i} \rangle. \tag{4}$$

The transition is referred to as allowed by symmetry, if the triple direct (Kronecker) product

$$(\mathbf{k}^{(f)}, \gamma^{(f)})^* \times (\mathbf{k}^{(p)}, \gamma^{(p)}) \times (\mathbf{k}^{(i)}, \gamma^{(i)}) \tag{5}$$

contains the identity IR of R, or

$$(\mathbf{k}^{(f)}, \gamma^{(f)})^* \times (\mathbf{k}^{(i)}, \gamma^{(i)}) \cap (\mathbf{k}^{(p)}, \gamma^{(p)})^* \neq 0, \tag{6}$$

i. e., it is necessary to find the direct product of two IRs of the rod group R (complex conjugate IRs are also IRs of R).

Let us take the case of GaN bulk crystal with the wurtzite structure under the magnetic field $\mathbf{B}$ directed along the symmetry axis (rod group $R\,56\,(p6_3)$). The symmetry of the electrical dipole operator in this group described by vector representation $\Gamma_v = \Gamma_1(z) + \Gamma_4(x - iy) + \Gamma_6(x + iy)$. As $\mathbf{k}^{(p)} \approx 0$, $\mathbf{k}^{(f)} \approx \mathbf{k}^{(i)}$, only the so-called direct transitions: $\Gamma \to \Gamma$, $A \to A$, etc. are allowed (wave vector selection rules). In particular, when the spin-orbit interaction is taken into account, the symmetry of allowed final stated for $A \to A$ transitions is pointed out in Table 3 by the entries of the rows containing $\Gamma_1^* = \Gamma_1$, $\Gamma_4^* = \Gamma_6$, or $\Gamma_6^* = \Gamma_4$ in the columns corresponding to the symmetry of the initial state. For example, the direct transitions are allowed from the initial state of symmetry A_8 to final states of symmetry A_8, A_9 and A_{11}.

In the case of phonon assisted electric dipole transitions, these selection rules have to be supplemented with the selection rules, where the operator P has the symmetry of phonon participating in the transition. In GaN crystal, atoms occupy the sites of b-type of symmetry C_{3v}. Under the magnetic field $\mathbf{B}$ directed along the symmetry axis, the symmetry of the system reduces down to rod group $R\,56$, and the site symmetry of atoms down to C_3. In this case the symmetries of phonons are given by representations of rod group $R\,56$ induced by the vector representation $a + e^{(1)} + e^{(2)}$ of the site symmetry group C_3. The short symbol [5] of this representation is $\Gamma\ (1, 4, 2, 5, 3, 6)$, i. e., phonons can be of any symmetry. The short symbol determines the symmetry of phonons in all the points in a one-dimensional BZ. For example, as it was established above, the electric dipole transtitions are allowed from initial electronic A_8 state to the intermediate A_8, A_9, A_{11} states. From these states, with assistance of the phonons of symmetry A_3, the transitions are allowed into the final Γ_9, Γ_8, Γ_{12} states (see Table 3). If the intermediate state is of symmetry Γ_9, the same phonon allows the transition in the finale state A_{12}.

5. Conclusion

It is not necessary to generate IRs of rod groups R. As it is demonstrated above, they can be taken directly from the existing Tables of IRs for space groups with three-dimensional translations.

Appendix

Let H be an invariant subgroup of a group G ($H \triangleleft G$, $gHg^{-1} = H$, $g \in G$) and $d^{(\gamma)}(h)$ be an IR of H. The group G can be developed in terms of left cosets with respect to H

$$G = \sum_{j=1}^{t} g_j H, \quad g_1 = E \quad \text{(identity element)}. \tag{A1}$$

The cosets g_jH compose a factor group G/H with composition law

$$g_iHg_jH = g_ig_jg_j^{-1}Hg_jH = g_ig_jHH = g_ig_jH. \qquad \text{(A2)}$$

The matrices $d^{(\mu)}(g_jhg_j^{-1})$ form an IR of H conjugate to $d^{(\mu)}(h)$ by means of g_j. The set of elements of those left cosets g_pH $(p = 1, 2, \ldots, s \le t)$ for which the IRs $d^{(\mu)}(g_phg_p^{-1})$ are equivalent to the IR $d^{(\mu)}(h)$ $(d^{(\mu)}(g_phg_p^{-1}) = Ad^{(\mu)}(h)A^{-1}$, where A is some non-singular matrix of the same order as $d^{(\mu)}(h))$, forms a group $G_\mu \subseteq G$ called the little group for the IR $d^{(\mu)}(h)$ of $H \triangleleft G$ [4,5]. If the IR of G_μ, when restricted to H, contains only the IR $d^{(\mu)}(h)$ of H, it is called allowed (small). Small IRs of the little group G_μ compose a part of all the IRs of G_μ.

According to the little group method [4,5], the little group G_1 for the identical IR $d^{(1)}(h) = 1$ $(h \in H$, all the elements are mapped by $1)$ of an invariant subgroup H coincides with the whole group G $(G_1 = G)$. Then there is a simple relation between the allowed IRs of the group $G_1 = G$ and the IRs of the factor group G/H: every IR of G/H generates some allowed IR of G, in which all the elements of the coset g_iH in the decomposition (A1) are mapped by the same matrix, namely by the matrix of the factor-group G/H IR for the coset g_iH.

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