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Comments on the decomposition of the regular representation of crystallographic space groups into band representations*

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Abstract. We discuss the decomposition of the regular representation of crystallographic space groups into elementary band representations. It is shown that the decomposition is in general not unique. In particular, we discuss some orthorhombic space groups in detail.

1. Introduction

It is well known that, under certain circumstances, any finite-dimensional representation of a group can be decomposed into its irreducible components. For instance, this is the case if the group is finite or, more generally, compact. The representation may then be written as a direct sum of its irreducible components. This decomposition is unique and there is a simple way (namely via the characters) to compute how many times an irreducible representation is contained in a given representation. Thus the irreducible representations can be seen as building blocks of any representation of the group in question. In particular, each irreducible representation λ is contained in the regular representation. In fact, it is contained exactly n_λ times in the regular representation, where n_λ is the dimension of the irreducible representation λ.

For infinite groups the situation is in general more difficult. Nevertheless, a representation may be completely decomposable. However, if one deals with infinite representations, the decomposition of a representation need not be a direct sum of its irreducible representations but may be a direct integral [1]. For instance, in the case of space groups, the representations induced from a finite representation of a finite subgroup of the space group in question can be written as the direct integral of its irreducible representations.

In the theory of energy bands the so-called band representations, which are certain representations of the crystallographic space groups, are of great importance, since they allow one to consider an energy band as a whole entity. In this context the elementary band representations play a fundamental role. Recall that a band representation is called elementary if it cannot be decomposed into two or more band representations. Although the elementary band representations are highly reducible, they can be seen as the building blocks of non-elementary band representations and hence they are somehow the analogue of the irreducible representations.

* Dedicated to Professor Louis Michel who died on 30 December 1999.

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In this paper we want to discuss the decomposition of the regular representation into elementary band representations. The regular representation can be written as a finite direct sum of elementary band representations. Note, however, that this does not mean that the regular representation is finite dimensional. In fact, both the regular representation and the band representations are infinite dimensional. Only the number of elementary band representations involved is finite. It turns out that the decomposition is in general not unique, but the number of different decompositions is at least the number of different Wyckoff positions of the space group in question. Moreover, each elementary band representation is contained in at least one of the possible decompositions, but none of the decompositions contains all elementary band representations (except in those cases where there is only one Wyckoff position with maximal site symmetry group). In addition, we show that the decompositions do not necessarily consist of elementary band representations corresponding to the same Wyckoff position but there are decompositions which are a sum of band representations corresponding to different Wyckoff positions.

The physics behind these considerations is the following. Consider a periodic solid. The corresponding energy eigenfunctions are Bloch functions which are labelled by a wavevector and a band index. The symmetry of these Bloch functions can be described by unitary irreducible representations of the underlying space group. However, Bloch functions are extended functions and one sometimes prefers to deal with localized functions. Such localized orbitals are not eigenfunctions of the Hamiltonian and do not correspond to a single energy but contain information about the energy band as a whole [2–7]. In order to fully exploit the symmetry of the solid one uses not arbitrary localized orbitals but certain symmetry-adapted orbitals that are localized at the symmetry centres of the solid in question. In a loose way of speaking, such a symmetry-adapted localized orbital induces a band representation. In fact, due to the lattice periodicity to each Wyckoff position there corresponds a lattice of equivalent positions, and hence to each position there exists a localized orbital. Accordingly, such a set of localized orbitals, which correspond to a lattice of symmetry centres, forms the basis for a band representation [2–7].

Let us compare this situation with the case of an atom or molecule. There the symmetry group is often a finite or compact continuous group of rotations. In this case we have only one symmetry centre in contrast to the lattice of symmetry centres in the case of a periodic solid. Consequently, the symmetry-adapted localized orbitals correspond to irreducible representations of the corresponding rotation group in the case of atoms or molecules, whereas the corresponding symmetry-adapted localized orbitals of a periodic solid correspond to a band representation that, due to its definition, is not irreducible but infinite dimensional.

The crucial point for fully exploiting the symmetry of a physical system is to use appropriate symmetry-adapted orbitals. In practical applications, however, one often starts with some localized orbital that is not symmetry adapted and applies later on some symmetrization procedure onto this orbital, which leads to several symmetry-adapted localized orbitals, each of which transforms according to a certain irreducible representation of the symmetry group in question. The group-theoretical background of this symmetrization procedure is the following. The original orbital induces a representation of the symmetry group in question. If the original orbital is general enough, the resulting representation is the regular representation. The decomposition of this representation into its irreducible constituents then leads to the symmetry-adapted localized orbitals. Since the decomposition is unique in these cases, the resulting symmetry-adapted orbitals are unique (up to certain unitary transformations). In fact, not the orbitals themselves but their symmetry character is unique.

In the case of periodic solids, whose symmetry is described by space groups, the situation is more involved. Applying the standard group-theoretical symmetrization procedure onto a localized orbital leads to Bloch functions, which are of course not localized but extended functions. In order to obtain symmetry-adapted localized functions one has to proceed differently. Instead of decomposing the induced representation into irreducible representations we decompose it into elementary band representations. The corresponding basis functions are then, in fact, symmetry-adapted localized functions. However, the decomposition into elementary band representations is not unique, as we show for the case of the regular representation. Thus there are several different possibilities to decompose infinite-dimensional representations of space groups, which gives rise to different symmetrization schemes, which is in contrast to the case of atoms or molecules.

The motivation for this paper may be summarized as follows. Apart from the mathematical problem of decomposing the regular representation of a given space group into band representations which is a problem in its own right, its application to band structure calculation might be of importance. For if one starts with the simplest case of perturbation theory with one localized test function whose stabilizer group (i.e. a subgroup of the space group that leaves the function invariant up to a phase factor) is trivial, then the localized test function usually induces the regular representation of the space group in question, and the complete set of alternative decompositions of the regular representation into band representations allows one to predict the band structure as regards their symmetry properties, if in addition the type of admissible Wyckoff positions for the localized functions describing the crystal constituents can be prefixed from the outset.

2. Band representations

2.1. Wyckoff positions

Let $\boldsymbol{w}$ denote a (representative of a) Wyckoff position. Of course one should distinguish between a Wyckoff position, which is a certain equivalence class of points of $\mathbb{R}^3$, and a representative of a Wyckoff position, which is a point of $\mathbb{R}^3$, but for the sake of simplicity we will not make a difference between these two concepts. It should always be clear from the context which notion is meant. For example, if we talk about the site symmetry group $\mathcal{G}_{\boldsymbol{w}}$ of a Wyckoff position $\boldsymbol{w}$ we mean, of course, the site symmetry group $\mathcal{G}_{\boldsymbol{w}}$ of the representative $\boldsymbol{w}$ of the Wyckoff position represented by $\boldsymbol{w}$, which in turn can be seen as a representative of the conjugacy class of site symmetry groups corresponding to the Wyckoff position represented by $\boldsymbol{w}$. Nevertheless, to avoid any misunderstandings, we mention that different representatives of the same Wyckoff position give rise to equivalent band representations and thus one may speak of band representations corresponding to a Wyckoff position, although the explicit matrices of course depend on the representative chosen.

2.2. Band representations: general remarks

Let us briefly review the concept of band representations [2–7]. A band representation $\mathbb{D}^{(\boldsymbol{w},\lambda)}$ is a representation of a space group $\mathcal{G}$ that is induced from a representation D^λ of a site symmetry group $\mathcal{G}_{\boldsymbol{w}} \subset \mathcal{G}$, in symbols $\mathbb{D}^{(\boldsymbol{w},\lambda)} = D^{\lambda,\mathcal{G}_{\boldsymbol{w}}\uparrow\mathcal{G}}$. For the sake of simplicity let us assume that D^λ is unitary. The band representation can be constructed in the following way. We consider the general case here. However, to understand the main part of the paper and the examples it is sufficient to be familiar with the special case of simple band representations, which shall be discussed further below. For a first reading one may skip the section below.

Take a representation D^λ of a site symmetry group $\mathcal{G}_{\boldsymbol{w}}$ and choose a basis for this representation, i.e. choose a set of functions $\varphi_j^\lambda(\boldsymbol{x})$, $j = 1, \ldots, n = \dim D^\lambda$ which are assumed to be localized functions and that transform according to the representation D^λ:

$$U_{(R|s(R))}\varphi_j^\lambda(x) = \varphi_j^\lambda(R^{-1}(x - s(R))) = \sum_{\ell=1}^{n} D_{\ell j}^\lambda(R)\varphi_\ell^\lambda(x) \tag{1}$$

for all $(R|s(R)) \in \mathcal{G}_w$. Note that $s(R) = w - Rw$ may be a non-primitive translation (if $\mathcal{G}$ is non-symmorphic). However, recall that there is the following coset decomposition of $\mathcal{G}$ with respect to the symmorphic subgroup $\mathcal{G}_w \circledS \mathcal{T}$, which is generated by $\mathcal{G}_w$ and $\mathcal{T}$, respectively,

$$\mathcal{G} = \sum_{\ell=1}^{|\mathcal{P}|/|\mathcal{G}_w|} (R_\ell|n(R_\ell))\mathcal{G}_w \circledS \mathcal{T} \tag{2}$$

where $n(R_\ell)$ are, in general, non-primitive translations. In addition, we have employed the definition $R_1 = E$ and $n(E) = \mathbf{0}$. Recall, by definition that the semidirect product of $\mathcal{G}_w$ and $\mathcal{T}$ is a symmorphic space group. The fact that there may be space group elements with non-primitive translations may seem strange. However, note that the translational part of the group elements depends on the choice of the origin. Usually one chooses the origin for a symmorphic space group such that the translational part of any space group element is a lattice translation, however, this choice although appropriate is not necessary. If we consider a symmorphic subgroup of a non-symmorphic space group, the choice of origin is fixed by the non-symmorphic supergroup and we cannot assume that the origin is chosen such that none of the elements of the subgroup has a non-primitive translation. Nevertheless, an appropriate choice of the origin would lead to vanishing non-primitive translations for all elements of the symmorphic subgroup, but of course not for all elements of the non-symmorphic supergroup. In our case such a choice of the origin would be w.

In the case where $\mathcal{G}_w$ is not isomorphic to the point group $\mathcal{P}$, i.e. isomorphic to a proper subgroup of $\mathcal{P}$, then $s := |\mathcal{P}|/|\mathcal{G}_w| > 1$. If $\mathcal{G}_w$ is isomorphic to the point group $\mathcal{P}$, then $s = 1$ and the coset decomposition reduces to $\mathcal{G} = \mathcal{G}_w \circledS \mathcal{T}$. We now apply all the elements $(R_\ell|n(R_\ell) + t)$, $\ell = 1, \ldots, s$, $t \in \mathcal{T}$ onto the functions $\varphi_j^\lambda(x)$ and define

$$\varphi_{j,(R_\ell|n(R_\ell)+t)}^\lambda(x) := U_{(R_\ell|n(R_\ell)+t)}\varphi_j^\lambda(x) = \varphi_j^\lambda(R_\ell^{-1}(x - n(R_\ell) - t)). \tag{3}$$

These localized functions form a basis for the band representation $\mathbb{D}^{(w,\lambda)}$. Note that this representation is infinite dimensional since the translation group $\mathcal{T}$ is infinite. The band representation is given explicitly by

$$U_{(R|n(R)+t)}\varphi_{j,(R_\ell|n(R_\ell)+v)}^\lambda(x)$$

$$= \sum_{j'=1}^{n}\sum_{\ell'=1}^{s} D_{j'j}^\lambda(R_{\ell'}^{-1}RR_\ell)\Delta(RR_\ell, R_{\ell'})\varphi_{j',(R_{\ell'}|n(R)+t+Rn(R_\ell)+Rv-R_{\ell'}s(R_{\ell'}^{-1}RR_\ell))}^\lambda(x) \tag{4}$$

$$= \sum_{j'=1}^{n}\sum_{\ell'=1}^{s}\sum_{v'\in\mathcal{T}} \mathbb{D}_{j',(R_{\ell'}|n(R_{\ell'})+v');\,j,(R_\ell|n(R_\ell)+v)}^{(w,\lambda)}((R|n(R)+t))\varphi_{j',(R_{\ell'}|n(R_{\ell'})+v')}^\lambda(x) \tag{5}$$

where we have employed the definitions

$$\mathbb{D}_{j',(R_{\ell'}|n(R_{\ell'})+v');\,j,(R_\ell|n(R_\ell)+v)}^{(w,\lambda)} = D_{j'j}^\lambda(R_{\ell'}^{-1}RR_\ell)\Delta(RR_\ell, R_{\ell'})\delta_{v',n(R)+t+Rw_\ell+Rv-w_{\ell'}} \tag{6}$$

$$w_\ell := R_\ell w + n(R_\ell) = (R|n(R_\ell))w \tag{7}$$

$$\Delta(RR_\ell, R_{\ell'}) := \begin{cases} 1 & \text{if } RR_\ell\mathcal{P}_w = R_{\ell'}\mathcal{P}_w \\ 0 & \text{otherwise.} \end{cases} \tag{8}$$

Note that (6) gives an explicit expression for the matrix representing $\mathbb{D}^{(\boldsymbol{w},\lambda)}$ as an infinite array whose rows and columns are indexed by pairs j, $(R_\ell|\boldsymbol{n}(R_\ell)+\boldsymbol{v})$, respectively. Alternatively, one can also be interested in the Bloch functions and their transformation properties. Instead of the (localized) functions $\varphi^\lambda_{j,(R_\ell|\boldsymbol{n}(R_\ell)+\boldsymbol{t})}(\boldsymbol{x})$, which give rise to infinite-dimensional band representations we choose alternatively the following Bloch functions by adopting the conventions

$$\psi^{(\boldsymbol{w},\lambda)}_{j,\ell}(\boldsymbol{k},\boldsymbol{x}) := |B(\mathcal{T}^*)|^{-1/2}\sum_{\boldsymbol{t}\in\mathcal{T}} \mathrm{e}^{\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{t}}\varphi^\lambda_{j,(R_\ell|\boldsymbol{n}(R_\ell)+\boldsymbol{t})}(\boldsymbol{x}) \tag{9}$$

as basis functions for the band representation $\mathbb{D}^{(\boldsymbol{w},\lambda)}$. Here $|B(\mathcal{T}^*)|$ is the volume of the Brillouin zone $B(\mathcal{T}^*)$. Equivalently, one can define these Bloch functions by

$$\psi^{(\boldsymbol{w},\lambda)}_{j}(\boldsymbol{k},\boldsymbol{x}) := |B(\mathcal{T}^*)|^{-1/2}\sum_{\boldsymbol{t}\in\mathcal{T}} \mathrm{e}^{\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{t}}\varphi^\lambda_{j}(\boldsymbol{x}-\boldsymbol{t}) \tag{10}$$

$$\psi^{(\boldsymbol{w},\lambda)}_{j,\ell}(\boldsymbol{k},\boldsymbol{x}) := U_{(R_\ell|\boldsymbol{n}(R_\ell))}\psi^{(\boldsymbol{w},\lambda)}_{j}(R_\ell^{-1}\boldsymbol{k},\boldsymbol{x}). \tag{11}$$

One can easily prove that these Bloch functions transform according to (see [3, 5, 6])

$$\begin{aligned} U_{(R|\boldsymbol{n}(R)+\boldsymbol{t})}\psi^{(\boldsymbol{w},\lambda)}_{j;\ell}(\boldsymbol{k},\boldsymbol{x}) &= \mathrm{e}^{-\mathrm{i}R\boldsymbol{k}\cdot\boldsymbol{t}}\sum_{j'=1}^{n}\sum_{\ell'=1}^{|\mathcal{P}|/|\mathcal{G}_{\boldsymbol{w}}|}\mathrm{e}^{-\mathrm{i}R\boldsymbol{k}\cdot(\boldsymbol{n}(R)+R\boldsymbol{n}(R_\ell)-\boldsymbol{n}(R_{\ell'})-R_{\ell'}\boldsymbol{s}(R_{\ell'}^{-1}RR_\ell))} \\ &\quad\times\Delta(RR_\ell,R_{\ell'})D^\lambda_{j'j}(R_{\ell'}^{-1}RR_\ell)\psi^{(\boldsymbol{w},\lambda)}_{j';\ell'}(R\boldsymbol{k},\boldsymbol{x}) \qquad (12)\\ &= \mathrm{e}^{-\mathrm{i}R\boldsymbol{k}\cdot(\boldsymbol{n}(R)+\boldsymbol{t})}\sum_{j'=1}^{n}\sum_{\ell'=1}^{|\mathcal{P}|/|\mathcal{G}_{\boldsymbol{w}}|}\mathrm{e}^{-\mathrm{i}R\boldsymbol{k}\cdot(R\boldsymbol{w}_\ell-\boldsymbol{w}_{\ell'})} \\ &\quad\times\Delta(RR_\ell,R_{\ell'})D^\lambda_{j'j}(R_{\ell'}^{-1}RR_\ell)\psi^{(\boldsymbol{w},\lambda)}_{j';\ell'}(R\boldsymbol{k},\boldsymbol{x}) \qquad (13)\\ &= \sum_{j'=1}^{n}\sum_{\ell'=1}^{|\mathcal{P}|/|\mathcal{G}_{\boldsymbol{w}}|}\mathbb{D}^{(\boldsymbol{w},\lambda)}_{j'\ell';j\ell}(\boldsymbol{k},(R|\boldsymbol{n}(R)+\boldsymbol{t}))\psi^{(\boldsymbol{w},\lambda)}_{j';\ell'}(R\boldsymbol{k},\boldsymbol{x}). \qquad (14) \end{aligned}$$

Note that the matrices

$$\mathbb{D}^{(\boldsymbol{w},\lambda)}_{j'\ell';j\ell}(\boldsymbol{k},(R|\boldsymbol{n}(R)+\boldsymbol{t})) = \mathrm{e}^{-\mathrm{i}R\boldsymbol{k}\cdot(\boldsymbol{n}(R)+\boldsymbol{t})}\mathrm{e}^{-\mathrm{i}R\boldsymbol{k}\cdot(R\boldsymbol{w}_\ell-\boldsymbol{w}_{\ell'})}\Delta(RR_\ell,R_{\ell'})D^\lambda_{j'j}(R_{\ell'}^{-1}RR_\ell) \tag{15}$$

are finite dimensional. However, this is no contradiction of the fact that the band representation $\mathbb{D}^{(\boldsymbol{w},\lambda)}$ is infinite dimensional, since the matrices $\mathbb{D}^{(\boldsymbol{w},\lambda)}(\boldsymbol{k},(R|\boldsymbol{n}(R)+\boldsymbol{t}))$ depend on the wavevector $\boldsymbol{k}\in B(\mathcal{T}^*)$, and the band representation $\mathbb{D}^{(\boldsymbol{w},\lambda)}$ consists of (non-countably) infinitely many matrices $\mathbb{D}^{(\boldsymbol{w},\lambda)}(\boldsymbol{k},(R|\boldsymbol{n}(R)+\boldsymbol{t}))$.

2.3. Simple band representations

Let us consider the special case of simple band representations now. A simple band representation is only possible if the space group in question is symmorphic, since only in this case can site symmetry groups $\mathcal{G}_{\boldsymbol{w}}$ that are isomorphic to the point group $\mathcal{P}$ exist. A simple band representation is a band representation induced from a one-dimensional representation of a site symmetry group $\mathcal{G}_{\boldsymbol{w}}$ isomorphic to the point group $\mathcal{P}$. It can be constructed as follows.

Take a one-dimensional representation D^λ of a site symmetry group $\mathcal{G}_{\boldsymbol{w}}\sim\mathcal{P}$ and choose a localized function $\varphi^\lambda(\boldsymbol{x})$ which transforms according to the representation D^λ:

$$U_{(R|\boldsymbol{s}(R))}\varphi^\lambda(\boldsymbol{x}) = \varphi^\lambda(R^{-1}(\boldsymbol{x}-\boldsymbol{s}(R))) = D^\lambda(R)\varphi^\lambda(\boldsymbol{x}) \tag{16}$$

for all $(R|\boldsymbol{s}(R))\in\mathcal{G}_{\boldsymbol{w}}$. Note that $\boldsymbol{s}(R)=\boldsymbol{w}-R\boldsymbol{w}$ is a lattice vector.

We now apply all the elements $(E|\boldsymbol{t})$, $\boldsymbol{t} \in \mathcal{T}$ onto the functions $\varphi^{\lambda}(\boldsymbol{x})$ and define

$$\varphi^{\lambda}_{\boldsymbol{t}}(\boldsymbol{x}) := U_{(E|\boldsymbol{t})}\varphi^{\lambda}(\boldsymbol{x}) = \varphi^{\lambda}(\boldsymbol{x} - \boldsymbol{t}). \tag{17}$$

These localized functions form a basis for the band representation $\mathbb{D}^{(\boldsymbol{w},\lambda)}$. Note that this representation is infinite dimensional since the translation group $\mathcal{T}$ is infinite. The band representation is given explicitly by

$$U_{(R|\boldsymbol{t})}\varphi^{\lambda}_{\boldsymbol{v}}(\boldsymbol{x}) = D^{\lambda}(R)\varphi^{\lambda}_{\boldsymbol{t}+R\boldsymbol{v}-\boldsymbol{s}(R)}(\boldsymbol{x}) = \sum_{\boldsymbol{v}'\in\mathcal{T}} \mathbb{D}^{(\boldsymbol{w},\lambda)}_{\boldsymbol{v}';\boldsymbol{v}}(R|\boldsymbol{t})\varphi^{\lambda}_{\boldsymbol{v}'}(\boldsymbol{x}) \tag{18}$$

where we have employed the definitions

$$\mathbb{D}^{(\boldsymbol{w},\lambda)}_{\boldsymbol{v}'\boldsymbol{v}} = D^{\lambda}(R)\delta_{\boldsymbol{v}',\boldsymbol{t}+R\boldsymbol{v}+R\boldsymbol{w}-\boldsymbol{w}}. \tag{19}$$

Note that (19) gives an explicit expression for the matrix representing $\mathbb{D}^{(\boldsymbol{w},\lambda)}$ Alternatively, one can also be interested in the Bloch functions and their transformation properties. Instead of the (localized) functions $\varphi^{\lambda}_{\boldsymbol{t}}(\boldsymbol{x})$, which give rise to infinite-dimensional matrix representations we choose alternatively the following Bloch function by adopting the conventions

$$\psi^{(\boldsymbol{w},\lambda)}(\boldsymbol{k}, \boldsymbol{x}) := |B(\mathcal{T}^*)|^{-1/2} \sum_{\boldsymbol{t}\in\mathcal{T}} \mathrm{e}^{\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{t}}\varphi^{\lambda}_{\boldsymbol{t}}(\boldsymbol{x}) \tag{20}$$

as basis functions for the band representation $\mathbb{D}^{(\boldsymbol{w},\lambda)}$. Here $|B(\mathcal{T}^*)|$ is the volume of the Brillouin zone $B(\mathcal{T}^*)$.

One can easily prove that these Bloch functions transform according to (see [3, 5, 6])

$$U_{(R|\boldsymbol{t})}\psi^{(\boldsymbol{w},\lambda)}(\boldsymbol{k}, \boldsymbol{x}) = \mathrm{e}^{-\mathrm{i}R\boldsymbol{k}\cdot\boldsymbol{t}}\mathrm{e}^{-\mathrm{i}R\boldsymbol{k}\cdot(R\boldsymbol{w}-\boldsymbol{w})}D^{\lambda}(R)\psi^{(\boldsymbol{w},\lambda)}(R\boldsymbol{k}, \boldsymbol{x}) \tag{21}$$

$$= \mathbb{D}^{(\boldsymbol{w},\lambda)}(\boldsymbol{k}, (R|\boldsymbol{t}))\psi^{(\boldsymbol{w},\lambda)}(R\boldsymbol{k}, \boldsymbol{x}) \tag{22}$$

where

$$\mathbb{D}^{(\boldsymbol{w},\lambda)}(\boldsymbol{k}, (R|\boldsymbol{t})) = \mathrm{e}^{-\mathrm{i}R\boldsymbol{k}\cdot\boldsymbol{t}}\mathrm{e}^{-\mathrm{i}R\boldsymbol{k}\cdot(R\boldsymbol{w}-\boldsymbol{w})}D^{\lambda}(R). \tag{23}$$

2.4. *Equivalence of band representations*

An essential concept is the notion of the equivalence of band representations. In the case of band representations there are several notions of equivalence that we briefly recall here. We call two band representations $\mathbb{D}_1$ and $\mathbb{D}_2$ weakly equivalent if and only if there exists a unitary matrix S such that

$$\mathbb{D}_1(g)S = S\mathbb{D}_2(g) \tag{24}$$

for all $g \in \mathcal{G}$. This condition may be equivalently formulated in terms of the finite dimensional but $\boldsymbol{k}$-dependent matrices $\mathbb{D}_i(\boldsymbol{k}, g)$. The band representations $\mathbb{D}_1$ and $\mathbb{D}_2$ are weakly equivalent if there exists a (finite-dimensional) unitary matrix $S(\boldsymbol{k})$ for almost every $\boldsymbol{k}$ in the Brillouin zone $B(\mathcal{T}^*)$, such that

$$\mathbb{D}_1(\boldsymbol{k}, (R|\boldsymbol{n}(R) + \boldsymbol{t}))S(\boldsymbol{k}) = S(R\boldsymbol{k})\mathbb{D}_2(\boldsymbol{k}, (R|\boldsymbol{n}(R) + \boldsymbol{t})) \tag{25}$$

holds true. In the case where the band representation is simple, $S(\boldsymbol{k})$ reduces to a unimodular function of $\boldsymbol{k}$. This is a rather coarse equivalence criterion, since the set of all special points of the Brillouin zone is of measure zero [8]. A finer classification of band representations is obtained if one requires that $S(\boldsymbol{k})$ is unitary and satisfies (25) for all $\boldsymbol{k} \in B(\mathcal{T}^*)$. If this condition is satisfied we call the two band representations equivalent. A list of all equivalent band representations can be found in [9]. This equivalence criterion is not enough for physics [10]. Here it is required in addition that $S(\boldsymbol{k})$ be continuous. In this case we call the two band representations strongly equivalent. Another notion of equivalence, the so-called physical equivalence [10], is based on the Berry phase [11, 12]. In the case of simple bands, i.e. if $\dim D^{\lambda} = 1$ and $\mathcal{G}_{\boldsymbol{w}} \simeq \mathcal{P}$, the notion of strong equivalence and physical equivalence coincide.

3. Decomposition of the regular representation—general considerations

Let us now turn to the problem of the decomposition of the regular representation into an elementary band representation. Recall that a necessary condition for a band representation to be elementary is that it corresponds to a Wyckoff position whose site symmetry group is maximal, see, e.g., [9]. Hence in the following $\boldsymbol{w}$ always denotes a Wyckoff position such that the corresponding site symmetry group $\mathcal{G}_{\boldsymbol{w}}$ is maximal. Note that $\mathcal{G}_{\boldsymbol{w}} \sim \mathcal{P}$ is possible if and only if $\mathcal{G}$ is symmorphic.

For decomposing the regular representation into an elementary band representation it is worth recalling the fact that both the regular representation and the elementary band representations can be seen as induced representations. The regular representation is the representation induced from the trivial subgroup consisting of the unit element only, whereas the band representations are induced from representations of the site symmetry group $\mathcal{G}_{\boldsymbol{w}} \subset \mathcal{G}$. Now we make use of the fact that induction is transitive and we can thus perform the induction process in two steps. In fact, we use the induction chain $\{(E|\boldsymbol{0})\} \to \mathcal{G}_{\boldsymbol{w}} \to \mathcal{G}$. Thus we obtain in the first step the regular representation of the finite subgroup $\mathcal{G}_{\boldsymbol{w}}$, and then we have to construct the representation of $\mathcal{G}$ induced from the regular representation of $\mathcal{G}_{\boldsymbol{w}}$. Thus the regular representation $\mathbb{D}^{\mathrm{reg}}$ of the space group $\mathcal{G}$ can be obtained by induction from the regular representation $D^{\boldsymbol{w},\mathrm{reg}}$ of the site symmetry group $\mathcal{G}_{\boldsymbol{w}}$, i.e. $\mathbb{D}^{\mathrm{reg}} = D^{\boldsymbol{w},\mathrm{reg}\uparrow\mathcal{G}}$. Similarly, the elementary band representations $\mathbb{D}^{(\boldsymbol{w},\lambda)}$ are defined as representations induced from the irreducible representations D^{λ} of the site symmetry group $\mathcal{G}_{\boldsymbol{w}}$. Thus we obtain a decomposition of the regular representation of $\mathcal{G}$ into elementary band representations by decomposing the regular representation of $\mathcal{G}_{\boldsymbol{w}}$ into the irreducible representations of $\mathcal{G}_{\boldsymbol{w}}$. From the decomposition $D^{\boldsymbol{w},\mathrm{reg}} = \bigoplus_{\lambda} n_{\lambda} D^{\lambda}$ we infer a decomposition of the regular representation of $\mathcal{G}$:

$$\mathbb{D}^{\mathrm{reg}} = \bigoplus_{\lambda} n_{\lambda} \mathbb{D}^{(\boldsymbol{w},\lambda)}. \tag{26}$$

Since there are, in general, several Wyckoff positions $\boldsymbol{w}$ whose site symmetry groups are maximal, the decomposition of the regular representation is not unique, in particular, if $\boldsymbol{w}$ and $\boldsymbol{w}'$ are two different Wyckoff positions with maximal site symmetry group, we have

$$\mathbb{D}^{\mathrm{reg}} = \bigoplus_{\lambda} n_{\lambda} \mathbb{D}^{(\boldsymbol{w},\lambda)} = \bigoplus_{\lambda'} n'_{\lambda'} \mathbb{D}^{(\boldsymbol{w}',\lambda')}. \tag{27}$$

These decompositions are in general not equivalent. In fact, they can be equivalent if and only if the sets of elementary band representations corresponding to the Wyckoff positions $\boldsymbol{w}$ and $\boldsymbol{w}'$ are equivalent, i.e. if each of the elementary band representations corresponding to the Wyckoff position $\boldsymbol{w}$ is equivalent to an elementary band representation corresponding to $\boldsymbol{w}'$. Thus in order to decide whether two decompositions are inequivalent or not we must know whether two elementary band representations corresponding to different Wyckoff positions are equivalent or not. The problem of (mathematical) equivalence of band representation has already been solved by Bacry *et al* [9] and they have listed all (mathematically) equivalent band representations. For our purpose only their tables 4 and 5 are important, where they list all pairs of Wyckoff positions which give rise to (mathematically) equivalent sets of band representations. Thus, except for the space groups listed in the tables 4 and 5 of [9], decompositions of the regular representation corresponding to different Wyckoff positions are (mathematically) inequivalent, and hence there are at least as many inequivalent decompositions of the regular representation as there are Wyckoff positions (with maximal site symmetry group).

However, for physics a stronger type of equivalence is necessary, namely the so-called physical equivalence [9, 10]. It turns out that in the case of symmorphic space groups all band representations corresponding to different Wyckoff positions are physically inequivalent [10]. Only in the case of non-symmorphic space groups might there be physically equivalent elementary space groups corresponding to different Wyckoff positions. In order for elementary band representations to be physically equivalent it is necessary but not sufficient that they are mathematically equivalent. The question of physical equivalence for non-symmorphic space groups has not been solved completely yet, however, some of the elementary band representations of non-symmorphic space groups which are mathematically equivalent are not physically equivalent [15, 16]. Hence we may state that there are at least as many physically inequivalent decompositions as there are Wyckoff positions (whose site symmetry group is maximal), except possibly for some of the non-symmorphic space groups listed in tables 4 and 5 of [9].

Let us call two (maximal) Wyckoff positions $\boldsymbol{w}$ and $\boldsymbol{w}'$ (mathematically, physically) b-equivalent if they give rise to a (mathematically, physically) equivalent set of band representations, i.e. if each of the elementary band representations corresponding to $\boldsymbol{w}$ is (mathematically, physically) equivalent to an elementary band representation corresponding to $\boldsymbol{w}'$ and vice versa. Then we may summarize the considerations above as follows: there are at least as many (mathematically/physically) inequivalent decompositions as there are (mathematically/physically) b-inequivalent Wyckoff positions whose site symmetry group is maximal. Except for the space groups listed in the tables 4 and 5 of [9], this number is equal to the number of different Wyckoff positions with maximal site symmetry group. In particular, for symmorphic space groups there are at least as many physically inequivalent decompositions as there are different Wyckoff positions with maximal site symmetry group.

Looking at equation (26), we see at once that each elementary band representation $(\boldsymbol{w}, \lambda)$ is contained in some decomposition of the regular representation. This is due to the fact that each of these decompositions contains all elementary band representations $(\boldsymbol{w}, \lambda)$ for fixed $\boldsymbol{w}$, and to each Wyckoff position $\boldsymbol{w}$ there corresponds a decomposition. However, note that in general a given decomposition does not contain all elementary band representations, which is in contrast to the decomposition of the regular representation into irreducible representations.

Up to know we have considered only decompositions of the regular representation which are of the form (26). However, there is no need for all decompositions to be of the form (26), and in fact, there are alternative decompositions. In the next section we will show by means of certain examples that there are decompositions of the regular representation that involve elementary band representations corresponding to different Wyckoff positions. However, a general scheme for finding all decompositions of the regular representation has not yet been found and requires further investigation.

4. Example P222

Let us consider the symmorphic orthorhombic space group P222 $=$ #16 as an example. Its point group $\mathcal{P} = \{E, C_{2x}, C_{2y}, C_{2z}\}$ is Abelian and hence all band representations are simple. A basis of the lattice is given by $\boldsymbol{a}_1 = a\boldsymbol{e}_x$, $\boldsymbol{a}_2 = b\boldsymbol{e}_y$, $\boldsymbol{a}_3 = c\boldsymbol{e}_z$, where a, b and c are the lattice constants. We have eight different Wyckoff positions whose site symmetry groups are isomorphic to the point group $\mathcal{P}$, namely $\boldsymbol{w} = \frac{1}{2}\sum_{i=1}^{3} n_i \boldsymbol{a}_i$, where $n_i \in \{0, 1\}$, respectively. The corresponding site symmetry groups read

$$\mathcal{G}_{\boldsymbol{w}} = \{(E|\boldsymbol{0}), (C_{2x}|2\boldsymbol{w} - n_1\boldsymbol{a}_x), (C_{2y}|2\boldsymbol{w} - n_2\boldsymbol{a}_y), (C_{2z}|2\boldsymbol{w} - n_3\boldsymbol{a}_z)\} \tag{28}$$

where the special translations $\boldsymbol{w} - C_{2i}\boldsymbol{w}$ with $i = x, y, z$ are represented as written above.

4.1. Elementary band representations

Let $A^{(\boldsymbol{w},\lambda)}(\boldsymbol{x})$ be a localized function transforming according to the representation λ under the action of the site symmetry group $\mathcal{G}_{\boldsymbol{w}}$ and define $A_{\boldsymbol{t}}^{(\boldsymbol{w},\lambda)}(\boldsymbol{x}) := A^{(\boldsymbol{w},\lambda)}(\boldsymbol{x} - \boldsymbol{t})$. Then these functions transform according to the band representation $(\boldsymbol{w}, \lambda)$. The transformation law reads as follows:

$$U_{(E|\boldsymbol{t})} A_{\boldsymbol{v}}^{(\boldsymbol{w},\lambda)}(\boldsymbol{x}) = A_{\boldsymbol{v}+\boldsymbol{t}}^{(\boldsymbol{w},\lambda)}(\boldsymbol{x}) = \sum_{\boldsymbol{u}\in\mathcal{T}} \mathbb{D}_{\boldsymbol{u}\boldsymbol{v}}^{(\boldsymbol{w},\lambda)}((E|\boldsymbol{t})) A_{\boldsymbol{u}}^{(\boldsymbol{w},\lambda)}(\boldsymbol{x}) \tag{29}$$

$$U_{(C_{2j}|\boldsymbol{t})} A_{\boldsymbol{v}}^{(\boldsymbol{w},\lambda)}(\boldsymbol{x}) = D^{\lambda}(C_{2j}) A_{C_{2j}\boldsymbol{v}+\boldsymbol{t}-2\boldsymbol{w}+n_j\boldsymbol{a}_j}^{(\boldsymbol{w},\lambda)}(\boldsymbol{x}) = \sum_{\boldsymbol{u}\in\mathcal{T}} \mathbb{D}_{\boldsymbol{u}\boldsymbol{v}}^{(\boldsymbol{w},\lambda)}((C_{2j}|\boldsymbol{t})) A_{\boldsymbol{u}}^{(\boldsymbol{w},\lambda)}(\boldsymbol{x}) \tag{30}$$

$$\mathbb{D}_{\boldsymbol{u}\boldsymbol{v}}^{(\boldsymbol{w},\lambda)}((E|\boldsymbol{t})) = \delta_{\boldsymbol{u},\boldsymbol{t}+\boldsymbol{v}} \tag{31}$$

$$\mathbb{D}_{\boldsymbol{u}\boldsymbol{v}}^{(\boldsymbol{w},\lambda)}((C_{2j}|\boldsymbol{t})) = D^{\lambda}(C_{2j}) \delta_{\boldsymbol{u},\boldsymbol{t}+C_{2j}\boldsymbol{v}-2\boldsymbol{w}+n_j\boldsymbol{a}_j}. \tag{32}$$

With respect to the corresponding Bloch functions

$$\phi^{(\boldsymbol{w},\lambda)}(\boldsymbol{k}, \boldsymbol{x}) = N^{(\boldsymbol{w},\lambda)} \sum_{\boldsymbol{t}\in\mathcal{T}} \mathrm{e}^{\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{t}} A_{\boldsymbol{t}}^{(\boldsymbol{w},\lambda)}(\boldsymbol{x}) \tag{33}$$

the band representation $(\boldsymbol{w}, \lambda)$ reads

$$U_{(E|\boldsymbol{t})} \phi^{(\boldsymbol{w},\lambda)}(\boldsymbol{k}, \boldsymbol{x}) = \mathrm{e}^{-\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{t}} \phi^{(\boldsymbol{w},\lambda)}(\boldsymbol{k}, \boldsymbol{x}) = D^{(\boldsymbol{w},\lambda)}(\boldsymbol{k}, (E|\boldsymbol{t})) \phi^{(\boldsymbol{w},\lambda)}(\boldsymbol{k}, \boldsymbol{x}) \tag{34}$$

$$U_{(C_{2j}|\boldsymbol{t})} \phi^{(\boldsymbol{w},\lambda)}(\boldsymbol{k}, \boldsymbol{x}) = D^{\lambda}(C_{2j}) \mathrm{e}^{-\mathrm{i}C_{2j}\boldsymbol{k}\cdot(\boldsymbol{t}-2\boldsymbol{w}+n_j\boldsymbol{a}_j)} \phi^{(\boldsymbol{w},\lambda)}(C_{2j}\boldsymbol{k}, \boldsymbol{x}) \tag{35}$$

$$= D^{(\boldsymbol{w},\lambda)}(\boldsymbol{k}, (C_{2j}|\boldsymbol{t})) \phi^{(\boldsymbol{w},\lambda)}(C_{2j}\boldsymbol{k}, \boldsymbol{x}) \tag{36}$$

$$D^{(\boldsymbol{w},\lambda)}(\boldsymbol{k}, (E|\boldsymbol{t})) = \mathrm{e}^{-\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{t}} \tag{37}$$

$$D^{(\boldsymbol{w},\lambda)}(\boldsymbol{k}, (C_{2j}|\boldsymbol{t})) = D^{\lambda}(C_{2j}) \mathrm{e}^{-\mathrm{i}C_{2j}\boldsymbol{k}\cdot(\boldsymbol{t}-2\boldsymbol{w}+n_j\boldsymbol{a}_j)}. \tag{38}$$

4.2. Regular representation

The regular representation $\mathbb{D}^{\mathrm{reg}}$ reads explicitly

$$\mathbb{D}_{(R''|\boldsymbol{t}''),(R'|\boldsymbol{t}')}^{\mathrm{reg}}((R|\boldsymbol{t})) = \delta_{(R''|\boldsymbol{t}''),(R|\boldsymbol{t})(R'|\boldsymbol{t}')} \tag{39}$$

or alternatively

$$D_{R'',R'}^{\mathrm{reg}}(\boldsymbol{k}, (E|\boldsymbol{t})) = \mathrm{e}^{-\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{t}} \delta_{R'',R'} \tag{40}$$

$$D_{R'',R'}^{\mathrm{reg}}(\boldsymbol{k}, (C_{2j}|\boldsymbol{t})) = \mathrm{e}^{-\mathrm{i}C_{2j}\boldsymbol{k}\cdot\boldsymbol{t}} \delta_{R'',C_{2j}R'}. \tag{41}$$

4.3. Decomposition of the regular representation

As mentioned above, decompositions of the regular representation can be obtained by decomposing the regular representation of the maximal site symmetry groups. In our case we have to decompose the regular representation of the point group $\mathcal{P}$. This decomposition reads

$$D^{\mathrm{reg}} = D^1 \oplus D^2 \oplus D^3 \oplus D^4 \tag{42}$$

where D^1 is the trivial representation and

$$D^2(C_{2x}) = -1 \qquad D^2(C_{2y}) = -1 \qquad D^2(C_{2z}) = +1 \tag{43}$$

$$D^3(C_{2x}) = +1 \qquad D^3(C_{2y}) = -1 \qquad D^3(C_{2z}) = -1 \tag{44}$$

$$D^4(C_{2x}) = -1 \qquad D^4(C_{2y}) = +1 \qquad D^4(C_{2z}) = -1. \tag{45}$$

Thus we have the following eight decompositions (one for each Wyckoff position $\boldsymbol{w}$) of the regular representation of $\mathcal{G}$:

$$\mathbb{D}^{\text{reg}} = \mathbb{D}^{(\boldsymbol{w},1)} \oplus \mathbb{D}^{(\boldsymbol{w},2)} \oplus \mathbb{D}^{(\boldsymbol{w},3)} \oplus \mathbb{D}^{(\boldsymbol{w},4)}. \tag{46}$$

4.4. Explicit decomposition

We can write down explicitly the matrices $S(\boldsymbol{k})$ which decompose the regular representation. Let $D^{(\boldsymbol{w},\text{reg})}(\boldsymbol{k}, g)$ be the matrices corresponding to the decomposition of the regular representation into elementary band representations corresponding to $\boldsymbol{w}$, i.e. $D^{(\boldsymbol{w},\text{reg})}_{\mu\lambda}(\boldsymbol{k}, g) = \delta_{\mu,\lambda} D^{(\boldsymbol{w},\lambda)}(\boldsymbol{k}, g)$. Then we have to find unitary matrices $S(\boldsymbol{k})$ such that the conditions

$$D^{(\boldsymbol{w},\text{reg})}(\boldsymbol{k}, (R|\boldsymbol{t}))S(\boldsymbol{k}) = S(R\boldsymbol{k})D^{\text{reg}}(\boldsymbol{k}, (R|\boldsymbol{t})) \tag{47}$$

hold true. These equations read explicitly

$$D^{(\boldsymbol{w},\lambda)}(\boldsymbol{k}, (R|\boldsymbol{t}))S_{\lambda,R'}(\boldsymbol{k}) = S_{\lambda,RR'}(R\boldsymbol{k})\mathrm{e}^{-\mathrm{i}R\boldsymbol{k}\cdot\boldsymbol{t}} \tag{48}$$

or equivalently

$$D^{\lambda}(R)\mathrm{e}^{\mathrm{i}R\boldsymbol{k}\cdot(\boldsymbol{w}-R\boldsymbol{w})}S_{\lambda,R'}(\boldsymbol{k}) = S_{\lambda,RR'}(R\boldsymbol{k}). \tag{49}$$

Note that the intertwining matrices $S(\boldsymbol{k})$ have two different indices: $\lambda = 1, \ldots, 4$, which labels the different unitary irreducible representations of the point group $\mathcal{P}$, and the index R where $R \in \mathcal{P}$. The reason for this indexing of the matrix elements is that we have to use different indices for the representations $D^{(\boldsymbol{w},\text{reg})}(\boldsymbol{k}, g)$ and $D^{\text{reg}}(\boldsymbol{k}, g)$, respectively. It is natural to use the group elements for labelling the matrix elements of the regular representation, whereas in the case of the decomposed representation it is most appropriate and sufficient to use the irrep labels as indices, since the irreps of the Abelian point group $\mathcal{P} = 222$ are all one dimensional.

Equation (49) is valid for $R = E$, whereas for $R = C_{2j}$ these equations are only satisfied if we set

$$S_{\lambda,C_{2j}}(\boldsymbol{k}) = D^{\lambda}(C_{2j})\mathrm{e}^{\mathrm{i}\boldsymbol{k}\cdot(\boldsymbol{w}-C_{2j}\boldsymbol{w})}S_{\lambda,E}(C_{2j}\boldsymbol{k}) = D^{\lambda}(C_{2j})\mathrm{e}^{\mathrm{i}\boldsymbol{k}\cdot(2\boldsymbol{w}-n_j\boldsymbol{a}_j)}S_{\lambda,E}(C_{2j}\boldsymbol{k}). \tag{50}$$

Here the elements $S_{\lambda,E}(\boldsymbol{k})$, $\lambda = 1, \ldots, 4$ are still arbitrary. To guarantee unitarity we choose

$$S_{\lambda,E}(\boldsymbol{k}) = \tfrac{1}{2} \tag{51}$$

and hence

$$S_{\lambda,C_{2j}}(\boldsymbol{k}) = \tfrac{1}{2}D^{\lambda}(C_{2j})\mathrm{e}^{\mathrm{i}\boldsymbol{k}\cdot(2\boldsymbol{w}-n_j\boldsymbol{a}_j)}. \tag{52}$$

Thus we have found unitary matrices $S(\boldsymbol{k})$ that decompose the regular representation into the elementary band reps $(\boldsymbol{w}, \lambda)$ for each fixed Wyckoff position $\boldsymbol{w}$, respectively.

4.5. Alternative decompositions

It is natural to ask whether there are still more decompositions of the regular representation, i.e. whether we can find decompositions of the form

$$\mathbb{D}^{\mathrm{reg}} = \mathbb{D}^{(\boldsymbol{w}_1,\lambda_1)} \oplus \mathbb{D}^{(\boldsymbol{w}_2,\lambda_2)} \oplus \mathbb{D}^{(\boldsymbol{w}_3,\lambda_3)} \oplus \mathbb{D}^{(\boldsymbol{w}_4,\lambda_4)} \tag{53}$$

such that not all $\boldsymbol{w}_j$ are the same Wyckoff positions. In fact, it turns out that such decompositions exist. Let $D(\boldsymbol{k}, g)$ be the matrices corresponding to the decomposition mentioned above, i.e. $D_{j\ell}(\boldsymbol{k}, g) = \delta_{j,\ell} D^{(\boldsymbol{w}_\ell,\lambda_\ell)}(\boldsymbol{k}, g)$. Again the problem is to find unitary matrices $S(\boldsymbol{k})$ such that

$$D(\boldsymbol{k}, (R|\boldsymbol{t}))S(\boldsymbol{k}) = S(R\boldsymbol{k})D^{\mathrm{reg}}(\boldsymbol{k}, (R|\boldsymbol{t})) \tag{54}$$

is satisfied for all group elements $(R|\boldsymbol{t})$, respectively. Again these equations are trivial for $R = E$, whereas for $R = C_{2j}$ we obtain

$$D^{\lambda_\ell}(C_{2j})\mathrm{e}^{\mathrm{i}C_{2j}\boldsymbol{k}\cdot(\boldsymbol{w}_\ell - C_{2j}\boldsymbol{w}_\ell)} S_{\ell,R'}(\boldsymbol{k}) = S_{\ell,C_{2j}R'}(C_{2j}\boldsymbol{k}). \tag{55}$$

In fact, a solution of these equations is given by

$$S_{\ell,C_{2j}}(\boldsymbol{k}) = D^{\lambda_\ell}(C_{2j})\mathrm{e}^{\mathrm{i}\boldsymbol{k}\cdot(\boldsymbol{w}_\ell - C_{2j}\boldsymbol{w}_\ell)} S_{\ell,E}(C_{2j}\boldsymbol{k}). \tag{56}$$

The only problem that remains is to find periodic† functions $S_{\ell,E}(\boldsymbol{k})$, $\ell = 1, \ldots, 4$ such that the matrices $S(\boldsymbol{k})$ are unitary for all $\boldsymbol{k}$, i.e. such that

$$\begin{aligned} S_{\ell,E}(\boldsymbol{k})S_{\ell',E}(\boldsymbol{k})^* + \sum_{j=1}^{3} D^{\lambda_\ell}(C_{2j})D^{\lambda_{\ell'}}(C_{2j})\mathrm{e}^{\mathrm{i}\boldsymbol{k}\cdot(\boldsymbol{w}_\ell - C_{2j}\boldsymbol{w}_\ell - \boldsymbol{w}_{\ell'} + C_{2j}\boldsymbol{w}_{\ell'})} \\ \times S_{\ell,E}(C_{2j}\boldsymbol{k})S_{\ell',E}(C_{2j}\boldsymbol{k})^* = \delta_{\ell,\ell'} \end{aligned} \tag{57}$$

is satisfied for all $\boldsymbol{k}$. For $\boldsymbol{k} = \boldsymbol{0}$ these equations reduce to

$$S_{\ell,E}(\boldsymbol{0})S_{\ell',E}(\boldsymbol{0})^* \left(1 + \sum_{j=1}^{3} D^{\lambda_\ell}(C_{2j})D^{\lambda_{\ell'}}(C_{2j})\right) = \delta_{\ell,\ell'} \tag{58}$$

which imply that all λ_ℓ have to be different. Of course, this also follows from the decomposition of the regular representation $D^{\mathrm{reg}}(\boldsymbol{k}, (R|\boldsymbol{t}))$ for $\boldsymbol{k} = \boldsymbol{0}$ into irreducible representations of P222. Without any loss of generality we may assume that $\lambda_\ell = \ell$. For all $\boldsymbol{k}$ with $\mathcal{P}(\boldsymbol{k}) = \mathcal{P}$, i.e. $k_j = m_j(\pi/a_j)$, $m_j \in \{0, 1\}$, we obtain similar equations:

$$S_{\ell,E}(\boldsymbol{k})S_{\ell',E}(\boldsymbol{k})^* \left(1 + \sum_{j=1}^{3} D^{\ell}(C_{2j})D^{\ell'}(C_{2j})\mathrm{e}^{\mathrm{i}\boldsymbol{k}\cdot(\boldsymbol{w}_\ell - C_{2j}\boldsymbol{w}_\ell - \boldsymbol{w}_{\ell'} + C_{2j}\boldsymbol{w}_{\ell'})}\right) = \delta_{\ell,\ell'}. \tag{59}$$

Without any loss of generality we may assume that $\boldsymbol{w}_1 = \boldsymbol{0}$, since we can replace $\boldsymbol{w}_j$ by $\boldsymbol{w}_j - \boldsymbol{w}_1$. Then these equations can be satisfied if only if the representations

$$D^{(\ell,\boldsymbol{k})}(C_{2j}) := D^{\ell}(C_{2j})\mathrm{e}^{\mathrm{i}\boldsymbol{k}\cdot(\boldsymbol{w}_\ell - C_{2j}\boldsymbol{w}_\ell)} \tag{60}$$

for $\ell = 2, 3, 4$ are a permutation of the representations $D^{\ell}(C_{2j})$, $\ell = 2, 3, 4$ for all $\boldsymbol{k}$ with $\mathcal{P}(\boldsymbol{k}) = \mathcal{P}$. This implies some restrictions on the possible Wyckoff positions $\boldsymbol{w}_j$. Let us discuss the case $\ell = 2$ in detail. Recall $D^2(C_{2z}) = 1$ and $D^2(C_{2x}) = D^2(C_{2y}) = -1$. Thus $D^{(2,\boldsymbol{k})} = D^2$ must hold true if $\mathrm{e}^{\mathrm{i}\boldsymbol{k}\cdot(\boldsymbol{w}_2 - C_{2z}\boldsymbol{w}_2)} = 1$, which implies that

$$\mathrm{e}^{\mathrm{i}\boldsymbol{k}\cdot(\boldsymbol{w}_2 - C_{2x}\boldsymbol{w}_2)} = \mathrm{e}^{\mathrm{i}\boldsymbol{k}\cdot(\boldsymbol{w}_2 - C_{2y}\boldsymbol{w}_2)} = 1 \qquad \text{if} \quad \mathrm{e}^{\mathrm{i}\boldsymbol{k}\cdot(\boldsymbol{w}_2 - C_{2z}\boldsymbol{w}_2)} = 1 \tag{61}$$

† Periodicity is essential. Note that the choice $S_{\ell,E}(\boldsymbol{k}) = \mathrm{e}^{\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{w}_\ell}$ leads to a unitary matrix $S(\boldsymbol{k})$, which is in general not periodic with respect to $\mathcal{T}^*$, and thus not continuous on the Brillouin zone.

has to be satisfied. Now we insert the special vectors $\boldsymbol{k} = (\pi/c)\boldsymbol{e}_z$ and $\boldsymbol{k} = (\pi/a)\boldsymbol{e}_x + (\pi/b)\boldsymbol{e}_y$ into this condition. Thus (61) reduces for $\boldsymbol{k} = (\pi/c)\boldsymbol{e}_z$ to

$$\frac{w_{2z}}{c} = 0 \tag{62}$$

and for $\boldsymbol{k} = (\pi/a)\boldsymbol{e}_x + (\pi/b)\boldsymbol{e}_y$ the condition (61) is equivalent to

$$\frac{w_{2x}}{a} + \frac{w_{2y}}{b} = 0 \quad \Longrightarrow \quad \frac{w_{2x}}{a} = \frac{w_{2y}}{b} = 0 \tag{63}$$

where all equations have to be understood mod$\mathbb{Z}$. Similarly, we infer for $\ell = 3, 4$ the following restrictions for $\boldsymbol{w}_3$, $\boldsymbol{w}_4$, respectively:

$$\frac{w_{3x}}{a} = 0 \tag{64}$$

$$\frac{w_{3y}}{b} + \frac{w_{3z}}{c} = 0 \quad \Longrightarrow \quad \frac{w_{3y}}{b} = \frac{w_{3z}}{c} = 0 \tag{65}$$

$$\frac{w_{4y}}{b} = 0 \tag{66}$$

$$\frac{w_{4x}}{a} + \frac{w_{4z}}{c} = 0 \quad \Longrightarrow \quad \frac{w_{4x}}{a} = \frac{w_{4z}}{c} = 0. \tag{67}$$

In addition, $D^{(2,\boldsymbol{k})}D^{(3,\boldsymbol{k})} = D^{(4,\boldsymbol{k})}$ from which we infer $\boldsymbol{w}_4 = \boldsymbol{w}_2 + \boldsymbol{w}_3 \bmod \mathcal{T}$. Hence we have the following restrictions for the vectors $\boldsymbol{w}_j$:

$$\frac{w_{2z}}{c} = 0 \qquad \frac{w_{3x}}{a} = 0 \qquad \frac{w_{2y}}{b} + \frac{w_{3y}}{b} = 0 \tag{68}$$

$$\frac{w_{2x}}{a} + \frac{w_{2y}}{b} = 0 \quad \Longrightarrow \quad \frac{w_{2x}}{a} = \frac{w_{2y}}{b} = 0 \tag{69}$$

$$\frac{w_{3y}}{b} + \frac{w_{3z}}{c} = 0 \quad \Longrightarrow \quad \frac{w_{3y}}{b} = \frac{w_{3z}}{c} = 0 \tag{70}$$

$$\frac{w_{2x}}{a} + \frac{w_{3z}}{c} = 0 \quad \Longrightarrow \quad \frac{w_{2x}}{a} = \frac{w_{3z}}{c} = 0 \tag{71}$$

which have the following three non-trivial solutions:

$$\boldsymbol{w}_2 = \boldsymbol{0} \qquad \boldsymbol{w}_3 = \boldsymbol{w}_4 = \tfrac{1}{2}c\boldsymbol{e}_z \tag{72}$$

$$\boldsymbol{w}_3 = \boldsymbol{0} \qquad \boldsymbol{w}_2 = \boldsymbol{w}_4 = \tfrac{1}{2}a\boldsymbol{e}_x \tag{73}$$

$$\boldsymbol{w}_4 = \boldsymbol{0} \qquad \boldsymbol{w}_2 = \boldsymbol{w}_3 = \tfrac{1}{2}b\boldsymbol{e}_y. \tag{74}$$

Apart from the obvious decompositions (46), these solutions give rise to the following additional decompositions of the regular representation:

$$\mathbb{D}^{\mathrm{reg}} = \mathbb{D}^{(\boldsymbol{w},1)} \oplus \mathbb{D}^{(\boldsymbol{w},2)} \oplus \mathbb{D}^{(\boldsymbol{w}+\frac{1}{2}\boldsymbol{a}_3,3)} \oplus \mathbb{D}^{(\boldsymbol{w}+\frac{1}{2}\boldsymbol{a}_3,4)} \tag{75}$$

$$\mathbb{D}^{\mathrm{reg}} = \mathbb{D}^{(\boldsymbol{w},1)} \oplus \mathbb{D}^{(\boldsymbol{w}+\frac{1}{2}\boldsymbol{a}_1,2)} \oplus \mathbb{D}^{(\boldsymbol{w},3)} \oplus \mathbb{D}^{(\boldsymbol{w}+\frac{1}{2}\boldsymbol{a}_1,4)} \tag{76}$$

$$\mathbb{D}^{\mathrm{reg}} = \mathbb{D}^{(\boldsymbol{w},1)} \oplus \mathbb{D}^{(\boldsymbol{w}+\frac{1}{2}\boldsymbol{a}_2,2)} \oplus \mathbb{D}^{(\boldsymbol{w}+\frac{1}{2}\boldsymbol{a}_2,3)} \oplus \mathbb{D}^{(\boldsymbol{w},4)} \tag{77}$$

where we have returned to the general case $\boldsymbol{w}_1 =: \boldsymbol{w}$. In fact, we can explicitly state the intertwining matrices for these cases. As an example we choose $\boldsymbol{w}_1 = \boldsymbol{w}_2 = \boldsymbol{w}$, $\boldsymbol{w}_3 = \boldsymbol{w}_4 = (c/2)\boldsymbol{e}_z$. Then $S(\boldsymbol{k})$ reads

$$S_{\ell,E}(\boldsymbol{k}) = \tfrac{1}{2} \qquad \ell = 1, \ldots, 4 \tag{78}$$

$$S_{\ell,C_{2j}}(\boldsymbol{k}) = \tfrac{1}{2}D^{\ell}(C_{2j})\mathrm{e}^{\mathrm{i}\boldsymbol{k}\cdot(\boldsymbol{w}-C_{2j}\boldsymbol{w})} \qquad \ell = 1, 2 \tag{79}$$

$$S_{\ell,C_{2j}}(\boldsymbol{k}) = \tfrac{1}{2}D^{\ell}(C_{2j})\mathrm{e}^{\mathrm{i}\boldsymbol{k}\cdot((\boldsymbol{w}+\frac{1}{2}\boldsymbol{a}_3)-C_{2j}(\boldsymbol{w}+\frac{1}{2}\boldsymbol{a}_3))} \qquad \ell = 3, 4 \tag{80}$$

and explicitly

$$S(\boldsymbol{k}) = \frac{1}{2}\begin{pmatrix} 1 & \mathrm{e}^{\mathrm{i}\boldsymbol{k}\cdot(\boldsymbol{w}-C_{2x}\boldsymbol{w})} & \mathrm{e}^{\mathrm{i}\boldsymbol{k}\cdot(\boldsymbol{w}-C_{2y}\boldsymbol{w})} & \mathrm{e}^{\mathrm{i}\boldsymbol{k}\cdot(\boldsymbol{w}-C_{2z}\boldsymbol{w})} \\ 1 & -\mathrm{e}^{\mathrm{i}\boldsymbol{k}\cdot(\boldsymbol{w}-C_{2x}\boldsymbol{w})} & -\mathrm{e}^{\mathrm{i}\boldsymbol{k}\cdot(\boldsymbol{w}-C_{2y}\boldsymbol{w})} & \mathrm{e}^{\mathrm{i}\boldsymbol{k}\cdot(\boldsymbol{w}-C_{2z}\boldsymbol{w})} \\ 1 & \mathrm{e}^{\mathrm{i}\boldsymbol{k}\cdot(\boldsymbol{w}-C_{2x}\boldsymbol{w}+\boldsymbol{a}_3)} & -\mathrm{e}^{\mathrm{i}\boldsymbol{k}\cdot(\boldsymbol{w}-C_{2y}\boldsymbol{w}+\boldsymbol{a}_3)} & -\mathrm{e}^{\mathrm{i}\boldsymbol{k}\cdot(\boldsymbol{w}-C_{2z}\boldsymbol{w})} \\ 1 & -\mathrm{e}^{\mathrm{i}\boldsymbol{k}\cdot(\boldsymbol{w}-C_{2x}\boldsymbol{w}+\boldsymbol{a}_3)} & \mathrm{e}^{\mathrm{i}\boldsymbol{k}\cdot(\boldsymbol{w}-C_{2y}\boldsymbol{w}+\boldsymbol{a}_3)} & -\mathrm{e}^{\mathrm{i}\boldsymbol{k}\cdot(\boldsymbol{w}-C_{2z}\boldsymbol{w})} \end{pmatrix}. \tag{81}$$

The analyticity and periodicity of $S(\boldsymbol{k})$ are obvious, which implies that the corresponding representations are also topologically equivalent.

4.6. Conclusions for P222

The decomposition of the regular representation into elementary band representations is not unique. There are 32 different decompositions of the regular representation, and thus in fact the number of different decompositions exceeds the number of different Wyckoff positions. These 32 decompositions read explicitly

$$\mathbb{D}^{\mathrm{reg}} = \mathbb{D}^{(\boldsymbol{w},1)} \oplus \mathbb{D}^{(\boldsymbol{w},2)} \oplus \mathbb{D}^{(\boldsymbol{w},3)} \oplus \mathbb{D}^{(\boldsymbol{w},4)} \tag{82}$$

$$\mathbb{D}^{\mathrm{reg}} = \mathbb{D}^{(\boldsymbol{w},1)} \oplus \mathbb{D}^{(\boldsymbol{w},2)} \oplus \mathbb{D}^{(\boldsymbol{w}+\frac{1}{2}\boldsymbol{a}_3,3)} \oplus \mathbb{D}^{(\boldsymbol{w}+\frac{1}{2}\boldsymbol{a}_3,4)} \tag{83}$$

$$\mathbb{D}^{\mathrm{reg}} = \mathbb{D}^{(\boldsymbol{w},1)} \oplus \mathbb{D}^{(\boldsymbol{w}+\frac{1}{2}\boldsymbol{a}_1,2)} \oplus \mathbb{D}^{(\boldsymbol{w},3)} \oplus \mathbb{D}^{(\boldsymbol{w}+\frac{1}{2}\boldsymbol{a}_1,4)} \tag{84}$$

$$\mathbb{D}^{\mathrm{reg}} = \mathbb{D}^{(\boldsymbol{w},1)} \oplus \mathbb{D}^{(\boldsymbol{w}+\frac{1}{2}\boldsymbol{a}_2,2)} \oplus \mathbb{D}^{(\boldsymbol{w}+\frac{1}{2}\boldsymbol{a}_2,3)} \oplus \mathbb{D}^{(\boldsymbol{w},4)}. \tag{85}$$

Note that all decompositions are of the form

$$\mathbb{D}^{\mathrm{reg}} = \mathbb{D}^{(\boldsymbol{w}_1,1)} \oplus \mathbb{D}^{(\boldsymbol{w}_2,2)} \oplus \mathbb{D}^{(\boldsymbol{w}_3,3)} \oplus \mathbb{D}^{(\boldsymbol{w}_4,4)} \tag{86}$$

where $\boldsymbol{w}_1+\boldsymbol{w}_2+\boldsymbol{w}_3+\boldsymbol{w}_4 \in \mathcal{T}$. This fact can be easily explained with the help of the generalized Berry phases $a(\boldsymbol{K})$ (for a definition of the Berry phases see [11–15]). Since the generalized Berry phases for the regular representation vanish, i.e. $a(\boldsymbol{K}) = 0$, the generalized Berry phases for the decompositions have to satisfy $a(\boldsymbol{K}) = \sum_{j=1}^{4} \boldsymbol{K}\cdot\boldsymbol{w}_j = 0 \pmod{2\pi}$, which implies that $\sum_{j=1}^{4} \boldsymbol{w}_j \in \mathcal{T}$. Note that the criterion $\sum_{j=1}^{4} \boldsymbol{w}_j \in \mathcal{T}$ is necessary but not sufficient for a sum of representations of the form (86) to be a decomposition of the regular representation.

5. Some remarks on F222

The face-centred orthorhombic space group F222 $=$ #22 has four different Wyckoff positions with maximal site symmetry group $\mathcal{G}_{\boldsymbol{w}}$, namely $\boldsymbol{w}_a = (0, 0, 0)$, $\boldsymbol{w}_b = (0, 0, \frac{1}{2})$, $\boldsymbol{w}_c = (\frac{1}{4}, \frac{1}{4}, \frac{1}{4})$, $\boldsymbol{w}_d = (\frac{1}{4}, \frac{1}{4}, \frac{3}{4})$, where the pairs $\boldsymbol{w}_a$, $\boldsymbol{w}_b$ and $\boldsymbol{w}_c$, $\boldsymbol{w}_d$ induce equivalent band representations [9, 10]. However, these equivalent band representations are not physically equivalent, since they give rise to different Berry phases [9, 10], i.e. they are topologically inequivalent. Consequently, these band representations cannot be connected by a continuous $\boldsymbol{k}$-dependent phase factor. Thus we have to distinguish carefully between these two notions of equivalence.

If we use the first notion of equivalence, which is based on symmetry, then we obtain two different decompositions of the regular representation, namely

$$\mathbb{D}^{\mathrm{reg}} = \mathbb{D}^{(\boldsymbol{w},1)} \oplus \mathbb{D}^{(\boldsymbol{w},2)} \oplus \mathbb{D}^{(\boldsymbol{w},3)} \oplus \mathbb{D}^{(\boldsymbol{w},4)} \tag{87}$$

where $\boldsymbol{w} = (0, 0, 0)$, $(\frac{1}{4}, \frac{1}{4}, \frac{1}{4})$. Equivalently, one could choose $\boldsymbol{w} = (0, 0, \frac{1}{2})$, $(\frac{1}{4}, \frac{1}{4}, \frac{3}{4})$, respectively.

Now let us turn to the other notion of equivalence, namely physical equivalence, which is the more interesting one. Since the band representations corresponding to the four Wyckoff positions $\boldsymbol{w}_j$, $j = a, \ldots, d$ are all physically inequivalent, we have the following four different decompositions:

$$\mathbb{D}^{\mathrm{reg}} = \mathbb{D}^{(\boldsymbol{w},1)} \oplus \mathbb{D}^{(\boldsymbol{w},2)} \oplus \mathbb{D}^{(\boldsymbol{w},3)} \oplus \mathbb{D}^{(\boldsymbol{w},4)} \tag{88}$$

where $\boldsymbol{w} = \boldsymbol{w}_j$, $j = a, \ldots, d$. In addition, we have the following four decompositions:

$$\mathbb{D}^{\mathrm{reg}} = \mathbb{D}^{(\boldsymbol{w},1)} \oplus \mathbb{D}^{(\boldsymbol{w},2)} \oplus \mathbb{D}^{(\boldsymbol{w}+\frac{1}{2}\boldsymbol{a}_3,3)} \oplus \mathbb{D}^{(\boldsymbol{w}+\frac{1}{2}\boldsymbol{a}_3,4)}. \tag{89}$$

Here we have employed again the definitions $\boldsymbol{a}_1 = a\boldsymbol{e}_x$, $\boldsymbol{a}_2 = b\boldsymbol{e}_y$, $\boldsymbol{a}_3 = c\boldsymbol{e}_z$. Note that these vectors are still lattice vectors, but they do not form a basis of the face-centred lattice. The intertwining matrices $S(\boldsymbol{k})$ are again given by (81). Thus we have eight different decompositions of the regular representation.

In addition, we can infer from the last decomposition the following interesting fact. The sum of the two elementary band representations $\mathbb{D}^{(\boldsymbol{w}_a,3)} \oplus \mathbb{D}^{(\boldsymbol{w}_a,4)}$ is physically equivalent to $\mathbb{D}^{(\boldsymbol{w}_b,3)} \oplus \mathbb{D}^{(\boldsymbol{w}_b,4)}$, whereas the components $\mathbb{D}^{(\boldsymbol{w}_a,3)}$ and $\mathbb{D}^{(\boldsymbol{w}_a,4)}$ are equivalent, but not physically equivalent to the band representations $\mathbb{D}^{(\boldsymbol{w}_b,3)}$ and $\mathbb{D}^{(\boldsymbol{w}_b,4)}$, respectively. Thus there does not exist a continuous phase connecting the equivalent band representations $\mathbb{D}^{(\boldsymbol{w}_a,\lambda)}$ and $\mathbb{D}^{(\boldsymbol{w}_b,\lambda)}$, but there exists a continuous and even analytic intertwining matrix for the sums $\mathbb{D}^{(\boldsymbol{w}_a,3)} \oplus \mathbb{D}^{(\boldsymbol{w}_a,4)}$ and $\mathbb{D}^{(\boldsymbol{w}_b,3)} \oplus \mathbb{D}^{(\boldsymbol{w}_b,4)}$. An equivalent statement is valid for $\boldsymbol{w}_c$ and $\boldsymbol{w}_d$.

In the case of the space group P222 we have a decomposition of the form (89), too, and thus $\mathbb{D}^{(\boldsymbol{w},3)} \oplus \mathbb{D}^{(\boldsymbol{w},4)} \sim \mathbb{D}^{(\boldsymbol{w}+\frac{1}{2}\boldsymbol{a}_3,3)} \oplus \mathbb{D}^{(\boldsymbol{w}+\frac{1}{2}\boldsymbol{a}_3,4)}$ is also valid for the space group P222. However, note the following subtle difference: in the case of the space group P222 the band representations $\mathbb{D}^{(\boldsymbol{w},\lambda)}$ and $\mathbb{D}^{(\boldsymbol{w}+\frac{1}{2}\boldsymbol{a}_3,\lambda)}$ are inequivalent, whereas in the case of F222 they are equivalent but not physically equivalent.

6. Some remarks on I222

We consider the orthorhombic space group I222 = #23, too. There are again four Wyckoff positions that have a maximal site symmetry group, namely $\boldsymbol{w}_a = \boldsymbol{0}$, $\boldsymbol{w}_b = (\frac{1}{2}, 0, 0)$, $\boldsymbol{w}_c = (0, 0, \frac{1}{2})$ and $\boldsymbol{w}_d = (0, \frac{1}{2}, 0)$. Again we find the decompositions

$$\mathbb{D}^{\mathrm{reg}} = \mathbb{D}^{(\boldsymbol{w},1)} \oplus \mathbb{D}^{(\boldsymbol{w},2)} \oplus \mathbb{D}^{(\boldsymbol{w},3)} \oplus \mathbb{D}^{(\boldsymbol{w},4)} \tag{90}$$

$$\mathbb{D}^{\mathrm{reg}} = \mathbb{D}^{(\boldsymbol{w},1)} \oplus \mathbb{D}^{(\boldsymbol{w},2)} \oplus \mathbb{D}^{(\boldsymbol{w}+\frac{1}{2}\boldsymbol{a}_3,3)} \oplus \mathbb{D}^{(\boldsymbol{w}+\frac{1}{2}\boldsymbol{a}_3,4)} \tag{91}$$

$$\mathbb{D}^{\mathrm{reg}} = \mathbb{D}^{(\boldsymbol{w},1)} \oplus \mathbb{D}^{(\boldsymbol{w}+\frac{1}{2}\boldsymbol{a}_1,2)} \oplus \mathbb{D}^{(\boldsymbol{w},3)} \oplus \mathbb{D}^{(\boldsymbol{w}+\frac{1}{2}\boldsymbol{a}_1,4)} \tag{92}$$

$$\mathbb{D}^{\mathrm{reg}} = \mathbb{D}^{(\boldsymbol{w},1)} \oplus \mathbb{D}^{(\boldsymbol{w}+\frac{1}{2}\boldsymbol{a}_2,2)} \oplus \mathbb{D}^{(\boldsymbol{w}+\frac{1}{2}\boldsymbol{a}_2,3)} \oplus \mathbb{D}^{(\boldsymbol{w},4)}. \tag{93}$$

Apart from the obvious decompositions (90), all the other decompositions so far have one feature in common. Two elementary band representations correspond to one Wyckoff position and the other two correspond to a second Wyckoff position. For I222, however, there exist decompositions such that each band representation corresponds to a different Wyckoff position. We find

$$\mathbb{D}^{\mathrm{reg}} = \mathbb{D}^{(\boldsymbol{w},1)} \oplus \mathbb{D}^{(\boldsymbol{w}+\boldsymbol{a}_1,2)} \oplus \mathbb{D}^{(\boldsymbol{w}+\boldsymbol{a}_2,3)} \oplus \mathbb{D}^{(\boldsymbol{w}+\boldsymbol{a}_3,4)} \tag{94}$$

$$\mathbb{D}^{\mathrm{reg}} = \mathbb{D}^{(\boldsymbol{w},1)} \oplus \mathbb{D}^{(\boldsymbol{w}+\boldsymbol{a}_2,2)} \oplus \mathbb{D}^{(\boldsymbol{w}+\boldsymbol{a}_3,3)} \oplus \mathbb{D}^{(\boldsymbol{w}+\boldsymbol{a}_1,4)}. \tag{95}$$

Also for these cases appropriate intertwining matrices $S(\boldsymbol{k})$ can be constructed, however, they have no simple structure. In total one has 24 different decompositions.

7. Conclusions

The decomposition of the regular representation of a space group into elementary band representations is, in general, not unique. The number of different decompositions is at least the number of non-equivalent Wyckoff positions with maximal site symmetry group, and it may be larger. For example, the space group P222 has eight Wyckoff positions but 32 different decompositions of the regular representation. In particular, there are decompositions which consist of elementary band representations corresponding to different Wyckoff positions.

To recapitulate, the important result of this paper is that the decomposition of the regular representation of any crystallographic space group into a band representation is, in general, *not* unique, since one may find different decompositions of the regular representation into distinct band representations. In other words, one has more than one possibility for the decomposition of the regular representation, which conversely allows one to predict the corresponding band structure by pure group-theoretical arguments, if the type of Wyckoff position and the transformation properties of the wavefunctions with respect to the corresponding site groups are fixed. To be more strict, when starting from a given localized function (test function), whose stabilizer group (which is a finite subgroup of the space group that leaves the given localized function up to a phase factor invariant) is trivial, i.e. consists of the identity only, then the space group elements applied to the localized function usually induce the regular representation of the space group in question. Once this situation is realized, one can predict the global band structure as regards their symmetry properties of any model Hamiltonian with respect to this type of test function space by symmetry arguments only, if in addition admissible Wyckoff positions, as possible candidates for the positions of the crystal constituents, can be prefixed by the considered physical problem. The generalization of this statement is obvious. For if n localized test functions are given which cannot be mutually interrelated by space group elements and whose stabilizer groups are trivial, one induces the n-fold direct sum of the regular representation. Similar conclusions can be made as regards the symmetry properties of the global band structure of any Hamiltonian, if in addition admissible Wyckoff positions can be prefixed by the considered physical problem. However, it should be noted that an increasing number of possible decompositions of the n-fold direct sum of the regular representation is possible which is due to the n-fold appearance of the regular representation and hence increasing number of possible combinations of different Wyckoff positions.

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