# Comment on Takagi's method for the construction of unitary representations of space groups

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Recently Takagi has given a method for the construction of unitary representations of space groups which differs from the usual method. In this paper we compare both methods.

## I. INTRODUCTION

Let $G$ be a space group, $H$ its subgroup of translations, and $K$ the point group $G/H$. Usually the unitary irreducible representations of $G$ are obtained with the induction procedure from the unitary irreducible representations of $H$ and are given by a couple $(\vec{k},D)$ where $\vec{k}$ is a vector from the fundamental domain of the Brillouin zone and $D$ is an irreducible unitary projective representation of the group $K^{\vec{k}}$, which consists of those elements of $K$ which leave $\vec{k}$ invariant modulo a reciprocal-lattice vector.

Recently Takagi[1] has given a method for the construction of unitary representations of $G$ for which he did not need the projective representations of $K^{\vec{k}}$. His representations are given by a couple $(\vec{k},D)_T$, where $\vec{k}$ is again a vector from the fundamental domain of the Brillouin zone and $D$ is an irreducible unitary representation of $K$. (The subscript $T$ stands for Takagi.)

Let $\overline{K}^{\vec{k}}$ be the subgroup of $K^{\vec{k}}$ which consists of those elements of $K^{\vec{k}}$ which leave $\vec{k}$ invariant. The factor system $\omega$ of $K^{\vec{k}}$ which has to be considered can be chosen from its equivalence class such that it is trivial on $\overline{K}^{\vec{k}}$. In this paper we will show that $(\vec{k},D)_T$, being reducible in general, can be decomposed in irreducible components according to

$$(\vec{k},D)_T \sim \sum_{\oplus i} (\vec{k},\Delta_i)\,, \tag{1.1}$$

where $\sum_{\oplus i}$ indicates a direct sum and

$$\sum_{\oplus i} \Delta_i \sim (D\downarrow\overline{K}^{\vec{k}})\uparrow K^{\vec{k}}\,. \tag{1.2}$$

Here $\uparrow$ is a symbol for the induction of projective representations (see for instance Shaw and Lever[2] and van den Broek[3]).

In Sec. II A we describe briefly the usual way of constructing irreducible unitary representations of $G$. For details see for instance the book by Bradley and Cracknell.[4] In Sec. II B we give the method used by Takagi, and in Sec. III the relation between the two methods is investigated. A discussion is given in Sec. IV, where we also reexamine the examples of Takagi's paper.

## II. SPACE-GROUP REPRESENTATIONS

### A. Usual method

Elements of $G$ will be denoted by $(\vec{t},R)$, where $\vec{t}\in H$ and $R\in K$. We define $(\vec{t},R)$ by

$$(\vec{t},R)\vec{x} = R\vec{x}+\vec{t}+\vec{t}_R\,, \tag{2.1}$$

where $\vec{t}_R$ is a fixed nonprimitive translation associated with $R$. The identities of $H$ and $K$ will be denoted by $\vec{e}$ and $E$, respectively. The multiplication of elements of $G$ is given by

$$(\vec{t},R)(\vec{t}\,',R') = (\vec{t}+R\vec{t}\,'+\vec{m}(R,R'),RR')\,, \tag{2.2}$$

where the mapping $\vec{m}: K\times K\to H$ is given by

$$\vec{m}(R,R') = \vec{t}_R + R\vec{t}_{R'} - \vec{t}_{RR'}\,. \tag{2.3}$$

For each $\vec{k}$ from the fundamental domain of the Brillouin zone the little cogroup $K^{\vec{k}}$ is defined by

$$K^{\vec{k}} = \{R\in K\,|\,R\vec{k}\approx\vec{k}\}\,, \tag{2.4}$$

where $\approx$ means "equal modulo a reciprocal lattice vector." The little group $G^{\vec{k}}$ is defined by

$$G^{\vec{k}} = \{(\vec{t},R)\,|\,\vec{t}\in H;\ R\in K^{\vec{k}}\}\,. \tag{2.5}$$

The allowable representations of $G^{\vec{k}}$ are given by

$$\mathfrak{D}^{\vec{k},\mu}(\vec{t},R) = e^{i\vec{k}\cdot\vec{t}}E^{\mu}(R)\,,\quad \forall(\vec{t},R)\in G^{\vec{k}}\,, \tag{2.6}$$

where $E^{\mu}$ runs through the irreducible unitary projective representations of $K^{\vec{k}}$ with the factor system

$$\sigma(R,R') = \exp[i\vec{k}\cdot\vec{m}(R,R')]\,. \tag{2.7}$$

All irreducible unitary representations of $G$ are obtained if for each $\vec{k}$ from the fundamental domain of the Brillouin zone each allowable representation $\mathfrak{D}^{\vec{k},\mu}$ of $G^{\vec{k}}$ is induced to $G$. The definition of the induced representation $(\mathfrak{D}^{\vec{k},\mu}\uparrow G)$ is

$$(\mathfrak{D}^{\vec{k},\mu}\uparrow G)(\vec{t},R)_{jt,ks} = \mathfrak{D}^{\vec{k},\mu}_{ts}((\vec{e},R_j)^{-1}(\vec{t},R)(\vec{e},R_k))\,\delta(R_j^{-1}RR_k,K^{\vec{k}})\,, \tag{2.8}$$

where $R_i$ are fixed chosen left coset representatives of $K$ with respect to $K^{\vec{k}}$:

$$K = \sum_i R_i K^{\vec{k}} \tag{2.9}$$

 

and $\delta$ is given by

$$\delta(R,K^{\vec{k}})=\begin{cases}1 & \text{if } R\in K^{\vec{k}}\\ 0 & \text{if } R\notin K^{\vec{k}}\end{cases}. \tag{2.10}$$

Using Eqs. (2.2) and (2.6), we can write Eq. (2.8) as

$$(\mathfrak{D}^{\vec{k},\mu}\uparrow G)(\vec{t},R)_{jt,ks} = \exp\{i\vec{k}\cdot[R_j^{-1}\vec{t}+R_j^{-1}\vec{m}(R,R_k) - R_j^{-1}\vec{m}(R_j,R_j^{-1}RR_k)]\} \times E^{\mu}_{ts}(R_j^{-1}RR_k)\delta(R_j^{-1}RR_k,K^{\vec{k}}). \tag{2.11}$$

The representation $\mathfrak{D}^{\vec{k},\mu}\uparrow G$ may also be denoted as $(\vec{k},E^{\mu})$, which notation was used in the introduction.

### B. Method of Takagi

Let $\bar{K}^{\vec{k}}$ be the group given by

$$\bar{K}^{\vec{k}}=\{R\in K\,|R\vec{k}=\vec{k}\}. \tag{2.12}$$

Obviously $\bar{K}^{\vec{k}}$ is a subgroup of $K^{\vec{k}}$. For each $\vec{k}$ from the fundamental domain of the Brillouin zone and each irreducible unitary representation $D^n$ of $K$, Takagi defines the representation $\Gamma^{\vec{k},n}$ of $G$ by

$$\Gamma^{\vec{k},n}(\vec{t},R)_{jt,ks} = D^n(R)_{ts}\exp[i\bar{R}_j\vec{k}\cdot(\vec{t}+\vec{t}_R)]\delta(\bar{R}_j^{-1}R\bar{R}_k,\bar{K}^{\vec{k}}), \tag{2.13}$$

where $\bar{R}_i$ are left coset representatives of $K$ with respect to $\bar{K}^{\vec{k}}$:

$$K=\sum_i \bar{R}_i\bar{K}^{\vec{k}}. \tag{2.14}$$

This representation is unitary, but not necessarily irreducible; it may also be denoted as $(\vec{k},D^n)_T$, which notation was used in the introduction.

## III. COMPARISON OF BOTH METHODS

In this section we will investigate the question which of the irreducible unitary representations $\mathfrak{D}^{\vec{k},\mu}\uparrow G$, defined by equation (2.11), occur in the unitary representation $\Gamma^{\vec{k},n}$, defined by equation (2.13). From equation (2.13) it follows that the restriction of $\Gamma^{\vec{k},n}$ to $H$ only contains irreducible components whose $\vec{k}$ vectors belong to the star of $\vec{k}$. (The star of $\vec{k}$ consists of the vectors $R\vec{k}$ with $R\in K$; the fundamental zone of the Brillouin zone consists by definition of one vector from each star.) From this it follows that $\Gamma^{\vec{k},n}$ can only contain representations $\mathfrak{D}^{\vec{k},\mu}\uparrow G$ with the same vector $\vec{k}$. Thus we may write

$$\Gamma^{\vec{k},n}\sim\sum_{\mu}c(\mu)(\mathfrak{D}^{\vec{k},\mu}\uparrow G) \tag{3.1}$$

or

$$(\vec{k},D^n)_T\sim\sum_{\mu}c(\mu)(\vec{k},E^{\mu}). \tag{3.2}$$

Our aim is to determine the coefficients $c(\mu)$. For this purpose it is sufficient to consider only the characters of the representations. Let us denote the characters of $\Gamma^{\vec{k},n}$, $D^n$, $(\mathfrak{D}^{\vec{k},\mu}\uparrow G)$, and $E^{\mu}$ by $\chi^{\vec{k},n}$, $\chi^n$, $\chi^{\vec{k},\mu}$, and $\chi^{\mu}$, respectively. From (2.13) it then follows that

$$\chi^{\vec{k},n}(\vec{t},R)=\chi^n(R)\sum_j\exp[i\bar{R}_j\vec{k}\cdot(\vec{t}+\vec{t}_R)]\delta(\bar{R}_j^{-1}R\bar{R}_j,\bar{K}^{\vec{k}}) \tag{3.3}$$

and from (2.11) it follows that

$$\chi^{\vec{k},\mu}(\vec{t},R)=\sum_j\exp\{i\vec{k}\cdot[R_j^{-1}\vec{t}+R_j^{-1}\vec{m}(R,R_j) - R_j^{-1}\vec{m}(R_j,R_j^{-1}RR_j)]\} \times\chi^{\mu}(R_j^{-1}RR_j)\delta(R_j^{-1}RR_j,K^{\vec{k}}). \tag{3.4}$$

Let us define

$$\tilde{E}^{\mu}(R)=e^{-i\vec{k}\cdot\vec{t}_R}E^{\mu}(R),\quad \forall R\in K^{\vec{k}}, \tag{3.5}$$

where $\tilde{E}^{\mu}$ is an irreducible unitary projective representation with factor system

$$\omega(R,R')=e^{i\vec{k}\cdot(R\vec{t}_{R'}-\vec{t}_{R'})},\quad \forall R,R'\in K^{\vec{k}}. \tag{3.6}$$

The advantage of this factor system $\omega$ above the factor system $\sigma$ of equation (2.7) is that $\omega$ is equal to 1 on $\bar{K}^{\vec{k}}\times\bar{K}^{\vec{k}}$. If the character of $\tilde{E}^{\mu}$ is denoted by $\tilde{\chi}^{\mu}$, Eq. (3.4) becomes

$$\chi^{\vec{k},\mu}(\vec{t},R)=\sum_j\exp[i\vec{k}\cdot(R_j^{-1}\vec{t}+R_j^{-1}\vec{t}_R + R_j^{-1}R\vec{t}_{R_j}-R_j^{-1}\vec{t}_{R_j})] \times\tilde{\chi}^{\mu}(R_j^{-1}RR_j)\delta(R_j^{-1}RR_j,K^{\vec{k}}). \tag{3.7}$$

Let $S_i$ be left coset representatives of $K^{\vec{k}}$ with respect to $\bar{K}^{\vec{k}}$:

$$K^{\vec{k}}=\sum_i S_i\bar{K}^{\vec{k}}. \tag{3.8}$$

Then,

$$K=\sum_j R_jK^{\vec{k}}=\sum_j\sum_i R_jS_i\bar{K}^{\vec{k}}. \tag{3.9}$$

So the left coset representatives $\bar{R}_j$ of $K$ with respect to $\bar{K}^{\vec{k}}$ [Eq. (2.14)] can be chosen to be $R_jS_i$. With this choice Eq. (3.3) becomes

$$\chi^{\vec{k},n}(\vec{t},R)=\chi^n(R)\sum_{i,j}\exp[iR_jS_i\vec{k}\cdot(\vec{t}+\vec{t}_R)] \times\delta(S_i^{-1}R_j^{-1}RR_jS_i,\bar{K}^{\vec{k}}). \tag{3.10}$$

From Eq. (3.1) it follows that

$$\chi^{\vec{k},n}(\vec{t},R)=\sum_{\mu} c(\mu)\chi^{\vec{k},\mu}(\vec{t},R). \qquad (3.11)$$

Combining the Eqs. (3.7), (3.10), and (3.11) gives

$$\chi^n(R)\sum_i e^{iR_jS_i\vec{k}\cdot\vec{t}_R}\delta(S_i^{-1}R_j^{-1}RR_jS_i,\bar{K}^{\vec{k}})$$

$$=\sum_{\mu} c(\mu)\exp[i\vec{k}\cdot(R_j^{-1}\vec{t}_R+R_j^{-1}R\vec{t}_{R_j}-R_j^{-1}\vec{t}_{R_j})]$$

$$\times\tilde{\chi}^{\mu}(R_j^{-1}RR_j)\delta(R_j^{-1}RR_j,K^{\vec{k}}), \qquad (3.12)$$

where we used the fact that the irreducible representations of $H$ are linearly independent. This equation can be written as

$$\sum_{\mu} c(\mu)\tilde{\chi}^{\mu}(R)$$

$$=\exp[-i\vec{k}\cdot(R_j^{-1}\vec{t}_{R_jRR_j^{-1}}+RR_j^{-1}\vec{t}_{R_j}-R_j^{-1}\vec{t}_{R_j})]$$

$$\times\chi^n(R_jRR_j^{-1})\sum_i e^{i\vec{k}\cdot S_i^{-1}R_j^{-1}\vec{t}_{R_jRR_j^{-1}}}$$

$$\times\delta(S_i^{-1}RS_i,\bar{K}^{\vec{k}}),\quad \forall R\in K^{\vec{k}}. \qquad (3.13)$$

Since the right-hand side of this equation does not depend on $j$, we may take $R_j=E$ to obtain

$$\sum_{\mu} c(\mu)\tilde{\chi}^{\mu}(R)=\sum_i e^{i\vec{k}\cdot(S_i^{-1}\vec{t}_R-\vec{t}_R)}$$

$$\times\chi^n(R)\delta(S_i^{-1}RS_i,\bar{K}^{\vec{k}}),\quad \forall R\in K^{\vec{k}}. \qquad (3.14)$$

The right-hand side of this equation is a character of a projective representation of $K^{\vec{k}}$ with the factor system $\omega$ of Eq. (3.6). We will show that this projective representation is $(\chi^n\downarrow\bar{K}^{\vec{k}})\uparrow K^{\vec{k}}$, where the symbol $\uparrow$ means induction with respect to the factor system $\omega$. Since $\chi^n\downarrow\bar{K}^{\vec{k}}$ is a vector representation of $\bar{K}^{\vec{k}}$, induction to $K^{\vec{k}}$ is only possible for a factor system which is equal to 1 on $\bar{K}^{\vec{k}}\times\bar{K}^{\vec{k}}$. This was exactly the reason we made the transformation of Eq. (3.5) that changed the factor system $\sigma$ of Eq. (2.7) to the factor system $\omega$ of Eq. (3.6), which indeed is equal to 1 on $\bar{K}^{\vec{k}}\times\bar{K}^{\vec{k}}$.

By definition the character $\psi$ of the representation $(\chi^n\downarrow\bar{K}^{\vec{k}})\uparrow K^{\vec{k}}$ is given by[2,3]

$$\psi(R)=\sum_i\frac{\omega(R,S_i)}{\omega(S_i,S_i^{-1}RS_i)}\chi^n(S_i^{-1}RS_i)\delta(S_i^{-1}RS_i,\bar{K}^{\vec{k}}). \qquad (3.15)$$

Since $D^n$ is a representation of $K$, we have $\chi^n(R)=\chi^n(S_i^{-1}RS_i)$. Therefore the right-hand sides of Eqs. (3.14) and (3.15) are proved to be equal if we show that

$$e^{i\vec{k}\cdot(S_i^{-1}\vec{t}_R-\vec{t}_R)}=\omega(R,S_i)\omega^*(S_i,S_i^{-1}RS_i) \qquad (3.16)$$

for each $R\in K^{\vec{k}}$ and each $S_i$ such that $S_i^{-1}RS_i\in\bar{K}^{\vec{k}}$. Equation (3.16) can be proved with a tedious but straightforward calculation, using Eqs. (3.6) and (2.3) and the following equation, which is a trivial consequence of Eq. (2.2):

$$\vec{m}(R,R')+\vec{m}(RR',R'')=\vec{m}(R,R'R'')+R\vec{m}(R',R''),$$

$$\forall R,\ R',\ R''\in K. \qquad (3.17)$$

So the result of this section is that $\Gamma^{\vec{k},n}$ contains $\mathfrak{D}^{\vec{k},\mu}\uparrow G$ as irreducible component as often as $(D^n\downarrow\bar{K}^{\vec{k}})\uparrow K^{\vec{k}}$ contains $\tilde{E}^{\mu}$ as irreducible component.

## IV. DISCUSSION

From the results of the previous section it follows immediately that the representations $\Gamma^{\vec{k},n}$ of Takagi are not in general irreducible. For instance a necessary (but not sufficient) condition for $\Gamma^{\vec{k},n}$ to be irreducible is that $D^n\downarrow\bar{K}^{\vec{k}}$ is irreducible. It may happen that $\Gamma^{\vec{k},n}$ contains the same irreducible component more than once. This happens in particular if $D^n\downarrow\bar{K}^{\vec{k}}$ contains the same irreducible component more than once. It is also possible that $\Gamma^{\vec{k},n_1}$ and $\Gamma^{\vec{k},n_2}$ have an irreducible component in common, which will occur for instance if $D^{n_1}\downarrow\bar{K}^{\vec{k}}$ and $D^{n_2}\downarrow\bar{K}^{\vec{k}}$ have an irreducible component in common. It is however easy to see from the definition of induced representation that each irreducible representation of $G$ is contained in at least one of the representations $\Gamma^{\vec{k},n}$.

The results of Sec. III considerably simplify for vectors $\vec{k}$ which belong to the interior of the Brillouin zone. For these $\vec{k}$ we have $\bar{K}^{\vec{k}}=K^{\vec{k}}$, and therefore Eq. (1.2) reduces to

$$\sum_{\oplus i}\Delta_i\sim D\downarrow K^{\vec{k}}. \qquad (4.1)$$

Let us finally consider the example of the space group $P2_12_12_1$ which Takagi considered. The point group $K$ is $D_2$ and has four one-dimensional irreducible representations: $D^1$, $D^2$, $D^3$, and $D^4$. For a general $\vec{k}$ one has $\bar{K}^{\vec{k}}=K^{\vec{k}}=C_1$ and with the method of Takagi one thus obtains four four-dimensional representations. Since $D^i\downarrow K^{\vec{k}}$ $(i=1,2,3,4)$ is the trivial representation of the trivial group these four representations are irreducible and equivalent. Note that the irreducibility comes from the fact that $D_2$ has only one-dimensional irreducible representations. For a vector $\vec{k}$ on one of the rotation axes but not on the boundary of the Brillouin zone, one has $\bar{K}^{\vec{k}}=K^{\vec{k}}=C_2$. Then the set of representations $D^i\downarrow K^{\vec{k}}$ $(i=1,2,3,4)$ consists of two times the trivial representation of $C_2$ and two times the irreducible nontrivial representation of $C_2$. Therefore the four two-dimensional representations found with Takagi's method are irreducible, and among them there are two inequivalent representations, each occurring twice. In Takagi's paper these results could only be found by writing down the representation matrices and examining their traces.

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