Equivalence of induced representations

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Equivalence of induced representations for finite groups is considered in order to determine those equivalence classes of space group representations which are linked by complex conjugation.

1. INTRODUCTION

An interesting group theoretical problem is to correlate induced representations which originate from different members of the same orbit. The reason for considering this problem arises there from that, e.g., the complex conjugation (or more general automorphisms) of representations of a given (finite) group are of interest for physical applications.^{1,2} In particular complex conjugation of representations is of importance for the problem of determining "coupling coefficients",³ whose utility in various branches of physics is well known (e.g., "equivalent operators"). So the main objective of this article is to correlate induced representations belonging to different members of an orbit, to specify the general results to space-group representations and to give rules (concerning the star and the projective representations of the corresponding little cogroup) determining those equivalence classes of space-group representations which are linked by complex conjugation. One of the reasons for discussing the last problem is to generalize the results of Ref. 2 to arbitrary space groups, since in Ref. 2 only space groups were considered which contain the inversion as point group operation.

The material is organized as follows: In Sec. 2 the usual induction procedure^{4,5,6} is briefly recalled. In the following section we discuss in general the problem of carrying out the induction procedure from different members of the same orbit. There we derive the conditions under which the corresponding representations are identical. In order to be able to apply the results to space-group representations, we recall briefly their definitions and properties in Sec. 4. Section 5 is devoted to derive representations of the little cogroups whose corresponding space-group representations are obtained by induction from different members of the considered star. These results are then used in Sec. 6 to derive the corresponding equivalence relations for complex conjugation and to verify the results of Ref. 2.

2. THE INDUCTION PROCEDURE

Let H be an invariant subgroup of a given finite group G . The elements of H are denoted by $a, b, \dots$ (identity e), the elements of the factor group $K = G/H$ by $\alpha, \beta, \dots$ (identity ϵ), and for each $\alpha \in K$, a fixed chosen right coset representative is denoted by $r(\alpha)$, where $r(\epsilon) = e$.

Let Δ be an unitary irreducible representation (unirrep) of H . For each $\alpha \in K$ we define Δ_α by

$$\Delta_\alpha(a) = \Delta(r^{-1}(\alpha)ar(\alpha)), \quad \text{for all } a \in H, \quad (2.1)$$

which admits to define the little cogroup

$$\bar{K} = \{\alpha \in K \mid \Delta_\alpha \simeq \Delta\} \subseteq K. \quad (2.2)$$

Hence the corresponding little group of Δ is given by

$$L = \{ar(\alpha) \mid a \in H, \alpha \in \bar{K}\}. \quad (2.3)$$

Since for each $\alpha \in \bar{K}$ there exists a unitary matrix $U(\alpha)$ satisfying

$$\Delta(a) = U(\alpha)\Delta(r^{-1}(\alpha)ar(\alpha))U^\dagger(\alpha), \quad \text{for all } a \in H, \quad (2.4)$$

the following matrices

$$V(ar(\alpha)) = \Delta(a)U(\alpha), \quad \text{for all } a \in H \text{ and } \alpha \in \bar{K}, \quad (2.5)$$

form a projective unirrep of L which belongs to a factor system μ_Δ of K , i.e.,

$$V(ar(\alpha))V(br(\beta)) = \mu_\Delta(\alpha, \beta)V(ar(\alpha)br(\beta)). \quad (2.6)$$

The subscript Δ occurring in the factor system μ shall indicate that the factor system depends on the given unirrep Δ . In fact only the equivalence class of μ is determined by Δ . The actual form of μ_Δ still depends on the choice of the phases of the matrices $U(\alpha)$.

Due to the known induction procedure the allowable unirreps of L are given by

$$D(ar(\alpha)) = V(ar(\alpha)) \otimes E(\alpha), \quad \text{for all } a \in H \text{ and } \alpha \in \bar{K}, \quad (2.7)$$

where E runs through a complete set of projective unirreps of $\bar{K}$ which belong to the factor system μ_Δ^* .

Summarizing the induction procedure which gives a complete set of unirreps of G , one has to proceed as follows:

(i) Take one Δ from each orbit of unirreps of H , where the orbit of Δ is defined to be the set $\{\Delta_\alpha \mid \alpha \in K\}$,

(ii) Construct for each such Δ the allowable unirreps of L by means of (2.5) and (2.7),

(iii) Induce these allowable representations to G , where the general definition of the induced representation ($\mathcal{D} \uparrow G$) of G which is induced from $\mathcal{D}$ is as follows: If a left coset decomposition of G with respect to L is given by $G = \sum_i g_i L$, then

$$(\mathcal{D} \uparrow G)_{j_l, k_s}(g) = \delta(g_j^{-1}gg_k, L)\mathcal{D}_{is}(g_j^{-1}gg_k), \quad (2.8)$$

where

$$\delta(g, L) = \begin{cases} 0, & \text{if } g \notin L, \\ 1, & \text{if } g \in L. \end{cases} \quad (2.9)$$

3. INDUCTION FROM DIFFERENT MEMBERS OF THE ORBIT

For the following considerations it is assumed that the given unirrep D of G has been obtained by inducing the allowable unirrep $\mathcal{D}$ of L to G , where $\mathcal{D}$ is given through (2.7) and (2.5) for some unirrep Δ of H and some projective unirrep E_0 of $\bar{K}$. For notational convenience we will write $\mathcal{D} = (\Delta, E_0)$.

In this section we will examine how D is obtained, if we do not start from Δ , but from a different member of the orbit of Δ . Suppose we start from Δ_γ where $\gamma \in \bar{K}$ we derive by means of

$$(\Delta_\gamma)_\alpha(a) = \Delta^+(r^{-1}(\alpha\gamma)r(\alpha)r(\gamma))\Delta(r^{-1}(\alpha\gamma)a r(\alpha\gamma)) \times \Delta(r^{-1}(\alpha\gamma)r(\alpha)r(\gamma)), \quad (3.1)$$

that the equivalence relation

$$(\Delta_\gamma)_\alpha \simeq \Delta_{\alpha\gamma} \quad (3.2)$$

holds, since $r^{-1}(\alpha\gamma)r(\alpha)r(\gamma) \in H$. Consequently

$$\bar{K}_\gamma = \gamma\bar{K}\gamma^{-1}, \quad (3.3)$$

which implies that the corresponding little cogroup L_γ is given by

$$L_\gamma = r(\gamma)Lr^{-1}(\gamma). \quad (3.4)$$

Furthermore for each $\beta \in \bar{K}_\gamma$ there exists a unitary matrix $\tilde{U}(\beta)$ such that

$$(\Delta_\gamma)_\alpha(a) = \tilde{U}(\beta)\Delta_\gamma(r^{-1}(\beta)a r(\beta))\tilde{U}^+(\beta), \quad (3.5)$$

or, with (2.1),

$$\Delta(a) = \tilde{U}(\beta)\Delta(r^{-1}(\gamma)r^{-1}(\beta)r(\gamma)a r^{-1}(\gamma)r(\beta)r(\gamma)) \times \tilde{U}^+(\beta). \quad (3.6)$$

Utilizing (2.4) we rewrite (3.6) as

$$\Delta(a) = \tilde{U}(\beta)U^+(\gamma^{-1}\beta\gamma)\Delta^+(x_\gamma(\beta))\Delta(a) \times \Delta(x_\gamma(\beta))U(\gamma^{-1}\beta\gamma)\tilde{U}^+(\beta), \quad (3.7)$$

where we have introduced the notation

$$x_\gamma(\beta) = r^{-1}(\gamma)r(\beta)r(\gamma)r^{-1}(\gamma^{-1}\beta\gamma), \quad (3.8)$$

which is an element of H . Due to Schur's lemma we may take

$$\tilde{U}(\beta) = \Delta(x_\gamma(\beta))U(\gamma^{-1}\beta\gamma), \quad \text{for all } \beta \in \bar{K}_\gamma. \quad (3.9)$$

Consequently in accordance to (2.5) we define by

$$\tilde{V}(b r(\beta)) = \Delta_\gamma(b)\tilde{U}(\beta), \quad \text{for all } b \in H \text{ and } \beta \in \bar{K}_\gamma, \quad (3.10)$$

a projective unirrep of L_γ . Its multiplication law is given by

$$\tilde{V}(b r(\beta))\tilde{V}(b' r(\beta')) = \mu_{\Delta_\gamma}(\beta, \beta')\tilde{V}(b r(\beta)b' r(\beta')), \quad (3.11)$$

where the factor system μ_{Δ_γ} of $\bar{K}_\gamma$ is correlated by a simple formula to the original factor system μ_Δ of $\bar{K}$

$$\mu_{\Delta_\gamma}(\beta, \beta') = \mu_\Delta(\gamma^{-1}\beta\gamma, \gamma^{-1}\beta'\gamma), \quad \text{for all } \beta, \beta' \in \bar{K}_\gamma. \quad (3.12)$$

In order to verify (3.12) one has to use (3.8), (3.9), and (3.11), where it suffices to set $b = b' = e$. Now it is obvious that the projective unirreps $\tilde{E}$ of $\bar{K}_\gamma$ with factor system μ_{Δ_γ} can be chosen as

$$\tilde{E}(\beta) = E(\gamma^{-1}\beta\gamma), \quad \text{for all } \beta \in \bar{K}_\gamma, \quad (3.13)$$

where E runs through all projective unirreps of $\bar{K}$, which belong to the factor system Δ_γ . Hence the corresponding allowable unirreps of L_γ are given by

$$\tilde{\mathcal{D}}(b r(\beta)) = \tilde{V}(b r(\beta)) \otimes \tilde{E}(\beta), \quad \text{for all } b \in H, \beta \in \bar{K}_\gamma, \quad (3.14)$$

and the unirreps of G can be written as

$$(\tilde{\mathcal{D}} \uparrow G)_{j,ks}(\mathbf{g}) = \delta(\tilde{g}_j^{-1} \mathbf{g} \tilde{g}_k, L_\gamma) \tilde{\mathcal{D}}_{ts}(\tilde{g}_j^{-1} \mathbf{g} \tilde{g}_k), \quad (3.15)$$

where the $\tilde{g}_j$ are left coset representatives of G with respect to L_γ . The aim of this section is to show that the equivalence relation

$$(\Delta, E_0) \uparrow G \simeq (\Delta_\gamma, \tilde{E}_0) \uparrow G, \quad (3.16)$$

holds. In order to simplify the following considerations we choose the left coset representatives $\tilde{g}_j$ as

$$\tilde{g}_j = g_j r^{-1}(\gamma). \quad (3.17)$$

With this choice (3.16) becomes an identity:

$$[(\Delta, E_0) \uparrow G](\mathbf{g}) = [(\Delta_\gamma, \tilde{E}_0) \uparrow G](\mathbf{g}) \quad \text{for all } \mathbf{g} \in G. \quad (3.18)$$

In order to prove this result we have to show that

$$\delta(\tilde{g}_j^{-1} \mathbf{g} \tilde{g}_k, L_\gamma) = \delta(g_j^{-1} \mathbf{g} g_k, L), \quad \text{for all } \mathbf{g} \in G, \quad (3.19)$$

and

$$(\Delta_\gamma, \tilde{E}_0)(\tilde{g}_j^{-1} \mathbf{g} \tilde{g}_k) = (\Delta, E_0)(g_j^{-1} \mathbf{g} g_k), \quad \text{for all } \mathbf{g} \in G, L g_k^{-1} = \tilde{g}_j L_\gamma \tilde{g}_k^{-1}. \quad (3.20)$$

The proof of (3.19) is trivial. The proof of (3.20) is less trivial, but still straightforward. If $g_j^{-1} \mathbf{g} g_k = a r(\alpha)$ with $a \in H$ and $\alpha \in \bar{K}$ then

$$(\Delta, E_0)(g_j^{-1} \mathbf{g} g_k) = V(a r(\alpha)) \otimes E_0(\alpha). \quad (3.21)$$

Now

$$\tilde{g}_j^{-1} \mathbf{g} \tilde{g}_k = r(\gamma) a r(\alpha) r^{-1}(\gamma) r^{-1}(\gamma \alpha \gamma^{-1}) r(\gamma \alpha \gamma^{-1}). \quad (3.22)$$

Since $r(\gamma) a r(\alpha) r^{-1}(\gamma) r^{-1}(\gamma \alpha \gamma^{-1}) \in H$ we have

$$(\Delta_\gamma, \tilde{E}_0)(\tilde{g}_j^{-1} \mathbf{g} \tilde{g}_k) = \tilde{V}(r(\gamma) a r(\alpha) r^{-1}(\gamma)) \otimes \tilde{E}_0(\gamma \alpha \gamma^{-1}). \quad (3.23)$$

But $E_0(\alpha) = \tilde{E}_0(\gamma \alpha \gamma^{-1})$, so (3.20) is proved if we show that

$$V(a r(\alpha)) = \tilde{V}(r(\gamma) a r(\alpha) r^{-1}(\gamma)). \quad (3.24)$$

This equation can be proved in a straightforward way, first using the definitions (2.5) and (3.10), then the definitions (2.1), (3.8), and (3.9). This completes the proof of (3.18) for the case that the leftcoset representatives satisfy (3.17); therefore for arbitrary leftcoset representatiaves (3.16) has been proved.

4. UNIRREPS OF SPACE GROUPS

In order to be able to specialize our results to space groups let us briefly recall the basic definitions and notations concerning such groups with their unirreps. Let G be a space group and $H = T$ its subgroup of translations. The elements of T are denoted by $(E | \mathbf{t})$ (or briefly $\mathbf{t} \in T$), elements of $G/H = K = P$ are denoted by R (representing either an abstract group element of the point group P or the corresponding faithful matrix representation⁶) and coset representatives are denoted by $(R | \tau(R))$ [where $\tau(R)$ represents nonprimitive lattice translations], so that a general group element takes the form $(R | \tau(R) + \mathbf{t})$. The multiplication

rule reads as

$$(R_1 | \tau(R_1) + t_1)(R_2 | \tau(R_2) + t_2) = (R_1 R_2 | \tau(R_1 R_2) + t(R_1, R_2) + t_1 + R_1 t_2), \quad (4.1)$$

where

$$t(R_1, R_2) = \tau(R_1) + R_1 \tau(R_2) - \tau(R_1 R_2). \quad (4.2)$$

Let us start from the unirrep Δ^q of H given by

$$\Delta^q(t) = e^{-iq \cdot t}, \quad q \in BZ, \quad (4.3)$$

where BZ denotes the Brillouin zone. Because of

$$\begin{aligned} \Delta_R^q(t) &= \Delta^q((R | \tau(R))^{-1}(E | t)(R | \tau(R))) \\ &= \Delta^q(R^{-1}t) = e^{-iRq \cdot t}, \end{aligned} \quad (4.4)$$

the corresponding little cogroup $\bar{K} = P^q$ is given by

$$P^q = \{R \in P | Rq = q + Q\{Rq\}\}, \quad (4.5)$$

where $Q\{Rq\}$ is a reciprocal lattice vector. Hence

$$G^q = \{(R | \tau(R) + t) | R \in P^q, t \in T\}. \quad (4.6)$$

Obviously we can choose

$$U^q(R) = 1, \quad \text{for all } R \in P^q, \quad (4.7)$$

which implies that

$$V^q(R | \tau(R) + t) = \Delta^q(t), \quad \text{for all } R \in P^q, t \in T, \quad (4.8)$$

and that the corresponding factor system is given by

$$\mu^q(R, R') = e^{iq \cdot t(R, R')}, \quad \text{for all } R, R' \in P^q. \quad (4.9)$$

Hence the allowable unirreps of G^q are given by

$$\mathcal{D}^q(R | \tau(R) + t) = e^{-iq \cdot t} B(R) \quad \text{for all } R \in P^q, t \in T, \quad (4.10)$$

where B runs through all inequivalent projective unirreps of P^q with factor system $\mu^q(R, R')^* = e^{-iq \cdot t(R, R')}$.

The corresponding induced unirreps of G can be written as

$$\begin{aligned} (\mathcal{D}^q \uparrow G)_{j,ks}(R | \tau(R) + t) &= \delta(R_j^{-1} R R_k, P^q) \mathcal{D}_{is}^q((R_j | \tau(R_j))^{-1} \\ &\quad \times (R | \tau(R) + t)(R_k | \tau(R_k))), \end{aligned} \quad (4.11)$$

where $(R_j | \tau(R_j))$ are left coset representatives of G with respect to G^q .

5. INDUCTION FROM DIFFERENT MEMBERS OF THE STAR

Let q' be a member of the star of q where

$$q' = R_0 q + Q, \quad R_0 \in P, \quad R_0 \notin P^q, \quad (5.1)$$

such that $q' \in BZ$. From the results of Sec. 3 it follows that

$$P^{q'} = R_0 P^q R_0^{-1} \quad (5.2)$$

and

$$G^{q'} = (R_0 | \tau(R_0)) G^q (R_0 | \tau(R_0))^{-1}. \quad (5.3)$$

Equation (3.9) specializes to

$$\begin{aligned} U^{q'}(R) &= \Delta^q(x_{R_0}(R)) \\ &= \exp[-iq' \cdot x_{R_0}(R)], \quad \text{for all } R \in P^{q'}, \end{aligned} \quad (5.4)$$

where the vectors $x_{R_0}(R)$ are given by

$$\begin{aligned} (E | x_{R_0}(R)) &= (R_0 | \tau(R_0))^{-1} (R | \tau(R)) \\ &\quad \times (R_0 | \tau(R_0)) (R_0^{-1} R R_0 | \tau(R_0^{-1} R R_0)). \end{aligned} \quad (5.5)$$

A simple calculation gives

$$\begin{aligned} x_{R_0}(R) &= R_0^{-1} [-\tau(R_0) + \tau(R) \\ &\quad + R \tau(R_0) - R_0 \tau(R_0^{-1} R R_0)]. \end{aligned} \quad (5.6)$$

Note that usually one would take $U^{q'}(R) = 1$. Therefore Eq. (5.4) will turn out to be the reason for the occurrence of unimodular factors.

From (3.16) it follows that the allowable unirrep $\mathcal{D}^q$ of G^q given by (4.10) corresponds to the allowable unirrep $\mathcal{D}^{q'}$ of $G^{q'}$ which is given by

$$\begin{aligned} \mathcal{D}^{q'}(R | \tau(R) + t) &= e^{-iR_0 q' \cdot t} e^{-iq' \cdot x_{R_0}(R)} B(R_0^{-1} R R_0), \\ &\quad \text{for all } R \in P^{q'} = R_0 P^q R_0^{-1}. \end{aligned} \quad (5.7)$$

Hence if coset representatives are used which are defined by (3.17), it follows from (3.18) that

$$(q, B) \uparrow G = (q', B') \uparrow G, \quad (5.8)$$

where we have introduced obvious notation with

$$\begin{aligned} B'(R) &= \exp[-iq' \cdot x_{R_0}(R)] B(R_0^{-1} R R_0), \\ &\quad \text{for all } R \in P^{q'}. \end{aligned} \quad (5.9)$$

6. COMPLEX CONJUGATION OF SPACE-GROUP REPRESENTATIONS

Now we are in the position to consider in more detail the problem of complex conjugation of space-group unirreps $(q, B) \uparrow G$, where q belongs to the so-called "representation domain" Δ BZ of BZ. From (2.8) and (4.10) it follows that

$$[(q, B) \uparrow G]^* = (-q, B^*) \uparrow G. \quad (6.1)$$

The vector $-q$ does not in general belong to Δ BZ, not even to BZ. Since it is usual to consider only vectors from Δ BZ we want to rewrite the right-hand side of (6.1) as $(q', B') \uparrow G$, where $q' \in \Delta$ BZ. Here q' is of course of the form

$$q' = -R_0 q + Q, \quad (6.2)$$

for some $R_0 \in P$ and some Q from the reciprocal lattice. Both R_0 and Q can be easily determined in practical problems.

The form of B' can now be determined at once from (5.8) and (5.9):

$$\begin{aligned} B'(R) &= \exp[iq' \cdot x_{R_0}(R)] B^*(R_0^{-1} R R_0), \\ &\quad \text{for all } R \in P^{-R_0 q} = R_0 P^{-q} R_0^{-1}. \end{aligned} \quad (6.3)$$

So our result is

$$[(q, B) \uparrow G]^* = (-R_0 q + Q, B') \uparrow G, \quad (6.4)$$

where B' is given by (6.3) and R_0 and Q are easily determined such that $-R_0 q + Q \in \Delta$ BZ. Note that the equals sign in (6.4) should be replaced by an equivalence sign if the condition (3.17) is not taken into account, which says that the left coset representatives of G with respect to G^q (respectively $G^{-R_0 q}$) should be related as follows: If $(R_j | \tau(R_j))$ is the j th left coset representative of G with respect to G^q , then $(R_j R_0 | \tau(R_j R_0))$ is the j th left coset representative of G with respect to $G^{-R_0 q}$. Also the equals sign should be replaced by an equivalence sign if B' is not taken equal to the right-hand side of (6.3) but is only equivalent with it. This may happen for instance if one determines only the characters of B' from

(6.3) and then takes the matrices of B' from some other source.

Let us consider the special case

$$I \in P \simeq G/T, \quad (6.5)$$

i.e., the inversion I belongs to the point group P . This special case was considered in detail in Ref. 2. For this case we have to distinguish two cases. Especially if for a given $\mathbf{q}$ we have $I \notin P^{\mathbf{q}}$ or $I \in P^{\mathbf{q}}$.

Case $I \notin P^{\mathbf{q}}$: Because of (6.2) it is possible to choose $R_0 = I$ what leads us to

$$B'(R) = e^{i\mathbf{q} \cdot \mathbf{x}_I(R)} B^*(R), \quad \text{for all } R \in P^{\mathbf{q}}, \quad (6.6)$$

where

$$\mathbf{x}_I(R) = \tau(I) - 2\tau(R) - R\tau(I). \quad (6.7)$$

Changing the factor system of the projective unirreps according to Eq. (1.9) of Ref. 7, i.e.,

$$B(R) = e^{-i\mathbf{q} \cdot \tau(R)} F(R), \quad (6.8)$$

$$B'(R) = e^{-i\mathbf{q} \cdot \tau(R)} F'(R), \quad (6.9)$$

we obtain

$$F'(R) = e^{i(\mathbf{q} - R^{-1}\mathbf{q}) \cdot \tau(I)} F(R)^*, \quad (6.10)$$

which coincides with Eq. (3.8) of Ref. 2, if one uses that $R\mathbf{q} = \mathbf{q} + \mathbf{Q}\{R\mathbf{q}\}$, if $R \in P^{\mathbf{q}}$. Obviously if $\mathbf{q}$ does not belong to the boundary of ΔBZ , we have $\mathbf{Q}\{R\mathbf{q}\} = \mathbf{0}$, which implies that

$$F(R)^* = F'(R), \quad \text{for all } R \in P^{\mathbf{q}}. \quad (6.11)$$

Note that we do not have $B'(R) = B^*(R)$ in this case; so the

disappearance of the unimodular factor is due to the choice of the factor system.

Case $I \in P^{\mathbf{q}}$: Since we have $-\mathbf{q} = \mathbf{q} + \mathbf{Q}$ in this case we can take R_0 equal to E in (6.2). Equation (6.4) then becomes

$$[(\mathbf{q}, B) \uparrow G]^* = (\mathbf{q}, B') \uparrow G, \quad (6.12)$$

and Eq. (6.3) becomes

$$B'(R) = B^*(R), \quad \text{for all } R \in P^{\mathbf{q}}. \quad (6.13)$$

If changing the factor system in the same way as in (6.8) and (6.9) we arrive to the equivalence relation

$$F'(R) \simeq e^{-i\mathbf{Q} \cdot \tau(R)} F^*(R). \quad (6.14)$$

Equation (6.14) is equal to Eq. (3.16) of Ref. 2. Opposite to case $I \notin P^{\mathbf{q}}$, here the change of the factor system is the reason for the occurrence of the unimodular factor in (6.14).

Concluding remarks: The aim of this paper was to compare equivalent induced representations and to derive conditions under what circumstances such representations are identical. The results obtained have been applied to space-group representations. There we succeeded in deriving a simple relation which determines those equivalence classes which are linked by complex conjugation.

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