Clebsch-Gordan coefficients for nonunitary groups

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It is shown that calculating Clebsch–Gordan coefficients of a nonunitary group can be reduced to formulas containing only representations of the unitary subgroup and additional conditions due to the antiunitary symmetry. This is another example demonstrating that, in applications involving corepresentations of nonunitary groups, the analysis can be made mainly in terms of representations of its unitary part.

I. INTRODUCTION

Nonunitary groups and their corepresentations are of great importance in magnetic materials. In such material an antiunitary element is a product of time reversal and an element of a space group. In nonmagnetic materials time reversal is itself a symmetry element. In every case where an antiunitary element is added to the ordinary space group there is a need to deal with corepresentations. The theory of nonunitary groups and their corepresentations was founded by Wigner,[1] developed by Dimmock and Wheeler,[2–4] Dimmock,[5] and has been reviewed by Bradley and Davis.[6]

The problem often arises of decomposing a reducible corepresentation of a nonunitary group into a sum of irreducible parts. An example of this is in determining selection rules governing transitions in magnetic crystals, where the reducible corepresentation is a direct product of two irreducible corepresentations. Sometimes more detailed information is required, and one must calculate the matrix which transforms the corepresentation into a reduced form. The elements of this matrix are called the Clebsch–Gordan coefficients. Such information is needed, for example, in the Eckart–Wigner theorem.[1,7]

The Eckart–Wigner theorem was originally applied to calculate matrix elements of operators in physical systems of spherical symmetry, and found widespread use in such varied fields as atomic spectra, NMR, and elementary particles. Koster[8] generalized this theorem to make it applicable to other unitary groups, and this generalization takes the form

$$(\psi_\alpha^i | P_\sigma^k | \psi_\beta^j) = a_1 U_{\sigma,(\alpha\beta)} + a_2 U_{\sigma+n_k,(\alpha\beta)} + \cdots,$$

where $i, j,$ and k denote irreducible representations of a unitary group G; $a_1, a_2, \cdots$ are constants called "reduced matrix elements" and U is the matrix of Clebsch–Gordan coefficients.

For physical systems of spherical symmetry the Eckart–Wigner theorem takes on a simple form with only one term on the right-hand side of the above relation. In such a case knowing only the Clebsch–Gordan coefficients one is able to find selection rules and compare transition intensities. For systems of other unitary symmetry one usually needs to know more information about the physical system.

The Eckart–Wigner theorem has been generalized by Aviran and Zak[9] to nonunitary groups. It was shown that the addition of an antiunitary element leads in general to additional connections among the reduced matrix elements.

This paper deals with the problem of finding the Clebsch–Gordan coefficients for nonunitary groups. The method used is one put forward by Aviran and Zak[9,10] based on the method developed by Koster[8] for unitary groups. It is shown that the finding of Clebsch–Gordan coefficients can be reduced to formulas containing only representations of the unitary subgroup of the nonunitary group, and additional conditions due to the antiunitary symmetry.

We review in Sec. II the construction of irreducible corepresentations and the calculation of reduction coefficients for nonunitary groups. We emphasize the role played by the unitary subgroup. In Sec. III a method is derived of finding the Clebsch–Gordan coefficients for nonunitary groups. An example is given in Sec. IV.

II. COREPRESENTATIONS OF NONUNITARY GROUPS

A nonunitary group H contains elements half of which are unitary and half antiunitary. The $N/2$ unitary elements, denoted by u, form an invariant subgroup G of index two and we can write H as $H = G + Ga_0$, where a_0 is a fixed antiunitary element. The irreducible corepresentations D^k of a nonunitary group H are constructed in one of three ways depending on the following classification of the irreducible representations $\Delta^k(a_0^{-1}ua_0)^*$ of the unitary subgroup G of H[1]:

Type I: $\Delta^k(u)$ is equivalent to $\Delta^k(a_0^{-1}ua_0)^*$,

$$\Delta^k(a_0^{-1}ua_0)^* = \beta^{k^{-1}}\Delta^k(u)\beta^k \quad \text{and} \quad \beta^k\beta^{k*} = \Delta^k(a_0^2).$$

Type II: $\Delta^k(u)$ is equivalent to $\Delta^k(a_0^{-1}ua_0)^*$,

$$\Delta^k(a_0^{-1}ua_0)^* = \beta^{k^{-1}}\Delta^k(u)\beta^k \quad \text{but} \quad \beta^k\beta^{k*} = -\Delta^k(a_0^2).$$

Type III: $\Delta^k(u)$ is not equivalent to $\Delta^k(a_0^{-1}ua_0)^*$.

The three types of irreducible corepresentations of H corresponding to the above classification are[1]

Type I: $D^k(u) = \Delta^k(u), \quad D^k(ua_0) = \Delta^k(u)\beta^k.$

Type II:

$$D^k(u) = \begin{pmatrix} \Delta^k(u) & \\ & \Delta^k(u) \end{pmatrix},$$

$$D^k(ua_0) = \begin{pmatrix} & \Delta^k(u)\beta^k \\ -\Delta^k(u)\beta^k & \end{pmatrix}. \tag{1}$$

Type III:

$$D^k(u) = \begin{pmatrix} \Delta^k(u) & \\ & \Delta^k(a_0^{-1}ua)^* \end{pmatrix},$$

$$D^k(ua_0) = \begin{pmatrix} & \Delta^k(ua_0^2) \\ \Delta^k(a_0^{-1}ua_0)^* & \end{pmatrix}.$$

The number of times an irreducible corepresentation D^k is contained in a reducible corepresentation D is denoted by C^k and calculated from[11]

$$C^k = \sum_u \chi(D(u))\chi(D^k(u))^* / \sum_u \chi(D^k(u))\chi(D^k(u))^*, \tag{2}$$

where $\chi(D^k(u))$ is the character of $D^k(u)$. The sums in (2) are over the elements u of the unitary subgroup only. When the reducible corepresentation is direct product of two irreducible corepresentations, $D = D^i \times D^j$, eq. (2) takes the form[11]

$$C_{ij}^k = \sum_u \chi(D^i(u))\, \chi(D^j(u))\chi(D^k(u))^* \Big/ \sum_u \chi(D^k(u))\chi(D^k(u))^*. \tag{3}$$

By using the explicit form of the irreducible corepresentations given in (1), the coefficients C_{ij}^k can be written in terms of coefficients d_{ij}^k, the number of times the irreducible representations Δ^k of the unitary subgroup is contained in the reduced form of the direct product $\Delta^i \times \Delta^j$. The explicit form of the relation between the C_{ij}^k and the d_{ij}^k depends on the types of the irreducible corepresentations D^i, D^j, and D^k appearing in (3). The relation between C_{ij}^k and the d_{ij}^k, for all possible cases, has been given by Bradley and Davis.[6]

III. CLEBSCH–GORDAN COEFFICIENTS FOR NONUNITARY GROUPS

The matrix U, whose elements are the Clebsch–Gordan coefficients, transform a corepresentation D into reduced form in the following manner[1]:

$$UD(u)U^{-1} = D_r(u) = \begin{pmatrix} D^k(u) & & & \\ & \ddots & & \\ & & D^k(u) & \\ & & & D^m(u) \\ & & & & \ddots \end{pmatrix}, \tag{4}$$

$$UD(a)U^{-1*} = D_r(a) = \begin{pmatrix} D^k(a) & & & \\ & \ddots & & \\ & & D^k(a) & \\ & & & D^m(a) \\ & & & & \ddots \end{pmatrix}, \tag{5}$$

where u is a unitary element, a an antiunitary element, and D_r the reduced form of D.

The matrices $D(u)$, for all u, form a representation of the unitary subgroup G of H. The irreducible corepresentations appearing in $D_r(u)$, for all u, are either irreducible representations or sums of irreducible representations of the unitary group G. Consequently, to find the matrix U from (4) alone can be considered a calculation of a matrix which transforms a representation of a unitary group into reduced form. Such a calculation can be preformed using Koster's method.[8] The matrix U so found is not unique, and requiring that U also satisfies (5) imposes additional conditions on its elements.

The theory of corepresentations is such that a single method applicable simultaneously to all three types of irreducible corepresentations which may appear in D_r is unobtainable. We therefore discuss three cases corresponding to the three types of irreducible corepresentations. In each case we derive from (4), using Koster's method,[8] equations from which the elements of U are calculated, and the additional conditions on these elements imposed by (5).

A. Type I corepresentations

We assume that a Type I irreducible corepresentation D^k of dimension d appears l times in the reduced form D_r. To calculate the dl rows of U corresponding to these corepresentations, we rewrite (4) as $D(u) = U^{-1}D_r(u)U$ take the pqth element, multiply by $D^k(u)^*_{mn} = \Delta^k(u)^*_{mn}$, sum on u:

$$\frac{d}{N/2}\sum_u D(u)_{pq}\Delta^k(u)^*_{mn} = \frac{d}{N/2}\sum_{st} U^*_{sp}U_{tq}\sum_u D_r(u)_{st}\Delta^k(u)^*_{mn}.$$

Using the explicit form of $D_r(u)$ and the orthogonality relations for irreducible representations, we have

$$\frac{d}{N/2}\sum_u D(u)_{pq}\Delta^k(u)^*_{mn} = U^*_{mp}U_{nq} + U^*_{d+m,p}U_{d+n,q} + \cdots + U^*_{(l-1)d+m,p}U_{(l-1)d+n,q}. \tag{6}$$

The elements of U calculated from (6) satisfy (4),[8] but not necessarily (5). We now derive the additional conditions on the elements of U calculated from (6) imposed by (5). We rewrite (5) as $D(a) = U^{-1}D_r(a)U^*$. Every antiunitary element a can be written as $a = ua_0$ and $D(a)$ as $D(u)D(a_0)$. Taking the pqth element, multiplying by $D^k(ua_0)^*_{mn} = (\Delta^k(u)\beta^k)^*_{m,n}$, using the explicit form of $D_r(a)$, and summing over u, we have

$$\frac{d}{N/2}\sum_u (D(u)D(a_0))_{pq}(\Delta^k(u)\beta_k)^*_{m,n} = U^*_{mp}U^*_{nq} + U^*_{d+m,p}U^*_{d+n,q} + \cdots + U^*_{(l-1)d+m,p}U^*_{(l-1)d+n,q}.$$

We rearrange the left-hand side as

$$\sum_{xy} D(a_0)_{xq}\beta^{k*}_{yn}\left(\frac{d}{N/2}\sum_u D(u)_{px}\Delta^k(u)_{my}\right),$$

and, using (6), we have

$$\sum_{xy} D(a_0)_{xq}\beta^{k*}_{yn}[U^*_{mp}U_{yx} + U^*_{d+m,p}U_{d+y,x} + \cdots + U^*_{(l-1)d+m,p}U_{(l-1)d+y,x}] = U^*_{m,p}U^*_{n,q} + U^*_{d+m,p}U^*_{d+n,q} + \cdots + U^*_{(l-1)d+m,p}U^*_{(l-1)d+n,q}.$$

Multiplying by $U_{bd+m,p}$, summing on p, and using the orthogonality relations of the rows of U gives

$$U_{bd+n,q} = \sum_{xy}\beta^k_{yn}U^*_{bd+y,x}D(a_0)^*_{xq}, \tag{7}$$

where $b = 0, 1, \ldots, l-1$. Relation (7) is the additional condition imposed by (5) on the elements of the matrix U calculated from (6).

TABLE I: Corepresentations of the unitary subgroup C_{3v} and θ.

	E	C_3	C_3^2	δ_v	δ_v^1	δ_v^{11}	θ
D^1	1	1	1	1	1	1	$e^{i\varphi}$
D^2	1	1	1	-1	-1	-1	$e^{i\zeta}$
D^3	$\begin{pmatrix}1 & \\ & 1\end{pmatrix}$	$\begin{pmatrix}\epsilon & \\ & \epsilon^2\end{pmatrix}$	$\begin{pmatrix}\epsilon^2 & \\ & \epsilon\end{pmatrix}$	$\begin{pmatrix} & 1\\ 1 & \end{pmatrix}$	$\begin{pmatrix} & \epsilon^2\\ \epsilon & \end{pmatrix}$	$\begin{pmatrix} & \epsilon\\ \epsilon^2 & \end{pmatrix}$	$\begin{pmatrix} & \epsilon^{i\psi}\\ e^{i\psi} & \end{pmatrix}$
D^4	$\begin{pmatrix}1 & \\ & 1\end{pmatrix}$	$\begin{pmatrix}-\epsilon & \\ & -\epsilon^2\end{pmatrix}$	$\begin{pmatrix}\epsilon^2 & \\ & \epsilon\end{pmatrix}$	$\begin{pmatrix} & i\\ i & \end{pmatrix}$	$\begin{pmatrix} & \epsilon^2 i\\ \epsilon i & \end{pmatrix}$	$\begin{pmatrix} & \epsilon i\\ \epsilon^2 i & \end{pmatrix}$	$\begin{pmatrix} & e^{i\alpha}\\ -e^{i\alpha} & \end{pmatrix}$
D^5	$\begin{pmatrix}1 & \\ & 1\end{pmatrix}$	$\begin{pmatrix}-1 & \\ & -1\end{pmatrix}$	$\begin{pmatrix}1 & \\ & 1\end{pmatrix}$	$\begin{pmatrix}i & \\ & -i\end{pmatrix}$	$\begin{pmatrix}-i & \\ & i\end{pmatrix}$	$\begin{pmatrix}i & \\ & -i\end{pmatrix}$	$\begin{pmatrix} & -1\\ 1 & \end{pmatrix}$

$\epsilon = e^{i2\pi/3}$

B. Type II corepresentations

We assume that a Type II irreducible corepresentation D^k of dimension $2d$ appears l times in D_γ. From (4), the $2ld$ rows of U associated with these corepresentations are calculated from

$$\frac{d}{N/2}\sum_u D(u)_{pq}\Delta^k(u)^*_{mn} = U^*_{m,p}U_{n,q} + U^*_{d+m,p}U_{d+n,q} + \cdots + U^*_{(2l-1)d+m,p}U_{(2l-1)d+n,q}. \quad (8)$$

From (5) one derives the additional conditions on the elements of U calculated from (8) to be

$$U_{(b+1)d+n,q} = \sum_{xy}\beta^k_{yn}U^*_{bd+y,x}D(a_0)^*_{xq}$$

for $b = 0, 2, 4, \ldots, 2l-2$.

C. Type III corepresentations

We assume that a Type III irreducible corepresentation D^k of dimension $2d$ appears l times in D_γ. From (4), the $2ld$ rows of U associated with these corepresentations are calculated from

$$\frac{d}{N/2}\sum_u D(u)_{pq}\Delta^k(u)^*_{mn} = U^*_{m,p}U_{n,q} + U^*_{2d+m,p}U_{2d+n,q} + \cdots + U^*_{(2l-2)d+m,p}U_{(2l-2)d+n,q} \quad (9a)$$

and

$$\frac{d}{N/2}\sum_u D(u)_{pq}\Delta^k(a_0^{-1}ua_0)_{mn} = U^*_{d+m,p}U_{d+n,q} + U^*_{3d+m,p}U_{3d+n,q} + \cdots + U^*_{(2l-1)d+m,p}U_{(2l-1)d+n,q} \quad (9b)$$

From (5) one derives the additional conditions imposed on the elements of U calculated from (9a), (9b) to be

$$U_{bd+n,q} = \sum_x U^*_{(b+1)d+n,x}D(a_0)^*_{xq}, \quad (10)$$

where $b = 0, 2, 4, \ldots, 2l-2$.

IV. EXAMPLE: C_{3v} WITH TIME REVERSAL

We calculate the matrix U which transforms into reduced form the direct product $D^3 \times D^3 \times D^5$ of irreducible corepresentations of the nonunitary group $H = C_{3v} + C_{3v}\theta$, where $a_0 = \theta$, i.e., time reversal. The irreducible corepresentations of this nonunitary group are given in Table I. The corepresentations are all of Type I with the exception of D^5 which is of Type III.

Using relation (2), one finds that the reduced form contains the irreducible corepresentations D^4 and D^5 each two times, i.e., $D^3 \times D^3 \times D^5 = D^4 + D^4 + D^5 + D^5$. To calculate U, we first use (4). Specifically, to calculate the first four rows of U corresponding to the two $D^4(u)$ appearing on the right-hand side of (4), we use relation (6), and for the last four rows, corresponding to the two $D^5(u)$, we use relations (9a), (9b). The matrix U so derived is

$$\begin{pmatrix}
0 & 0 & 0 & 0 & 0 & 0 & b_{12}e^{i\Delta} & b_{11}e^{i\delta}\\
b_{12}e^{i\Delta} & -b_{11}e^{i\delta} & 0 & 0 & 0 & 0 & 0 & 0\\
0 & 0 & 0 & 0 & 0 & 0 & b_{22}e^{i\Delta} & b_{21}e^{i\delta}\\
b_{22}e^{i\Delta} & -b_{21}e^{i\delta} & 0 & 0 & 0 & 0 & 0 & 0\\
0 & 0 & (c_{11}/\sqrt{2})e^{i\tau} & (c_{12}/\sqrt{2})e^{i\Omega} & (c_{11}/\sqrt{2})e^{i\tau} & -(c_{12}/\sqrt{2})e^{i\Omega} & 0 & 0\\
0 & 0 & (d_{11}/\sqrt{2})e^{i\gamma} & (d_{12}/\sqrt{2})e^{i\nu} & -(d_{11}/\sqrt{2})e^{i\gamma} & (d_{12}/\sqrt{2})e^{i\nu} & 0 & 0\\
0 & 0 & (c_{21}/\sqrt{2})e^{i\tau} & (c_{22}/\sqrt{2})e^{i\Omega} & (c_{21}/\sqrt{2})e^{i\tau} & -(c_{22}/\sqrt{2})e^{i\Omega} & 0 & 0\\
0 & 0 & (d_{21}/\sqrt{2})e^{i\gamma} & (d_{22}/\sqrt{2})e^{i\nu} & -(d_{21}/\sqrt{2})e^{i\gamma} & (d_{22}/\sqrt{2})e^{i\nu} & 0 & 0
\end{pmatrix},$$

where $\begin{pmatrix}b_{11} & b_{12}\\ b_{21} & b_{22}\end{pmatrix}$, $\begin{pmatrix}c_{11} & c_{12}\\ c_{21} & c_{22}\end{pmatrix}$, and $\begin{pmatrix}d_{11} & d_{12}\\ d_{21} & d_{22}\end{pmatrix}$, are unitary matrices,[8] and $\Delta, \delta, \tau, \Omega, \gamma$, and ν are arbitrary phases.

The additional conditions imposed by (5) due to the antiunitary symmetry for the rows of the matrix U corresponding to the corepresentations D^4 are derived from relation (7), and for the rows corresponding to the D^5 from relation (10). From (7) we derive the additional conditions

$$b_{j2}e^{i\Delta} = b_{j1}^{*}e^{i(\alpha-2\psi-\delta)}, \qquad (11)$$

where $j = 1, 2$. From (10) we derive the additional conditions

$$c_{j1}e^{i\tau} = d_{j2}^{*}e^{-i(2\psi+\nu)},$$

$$c_{j2}e^{i\Omega} = d_{j1}^{*}e^{-i(2\psi+\gamma)}, \qquad (12)$$

where $j = 1, 2$. In addition, from the unitarity of the matrix $\begin{pmatrix} b_{11} & b_{12} \\ b_{21} & b_{22} \end{pmatrix}$ and (11), one derives that $b_{11} = 1/\sqrt{2}\, e^{i\xi}$ and $b_{12} = \pm i b_{11}$, where ξ is an arbitrary phase factor. By using conditions (11) and (12), and writing $\beta = \xi + \delta$, the matrix U takes the form

$$\frac{1}{\sqrt{2}}\begin{pmatrix} 0 & 0 & 0 & 0 & 0 & 0 & e^{i(\alpha-2\psi-\beta)} & -e^{i\beta} \\ e^{i(\alpha-2\psi-\beta)} & -e^{i\beta} & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & \mp ie^{i(\alpha-2\psi-\beta)} & \pm ie^{i\beta} \\ \mp ie^{i(\alpha-2\psi-\beta)} & \mp ie^{i\beta} & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & d_{12}^{*}e^{-i(2\psi+\nu)} & d_{11}^{*}e^{-i(2\psi+\gamma)} & d_{12}^{*}e^{-i(2\psi+\nu)} & -d_{11}^{*}e^{-i(2\psi+\gamma)} & 0 & 0 \\ 0 & 0 & d_{11}e^{i\gamma} & d_{12}e^{i\nu} & -d_{11}e^{i\gamma} & d_{12}e^{i\nu} & 0 & 0 \\ 0 & 0 & d_{22}^{*}e^{-i(2\psi+\nu)} & d_{21}^{*}e^{-i(2\psi+\gamma)} & d_{22}^{*}e^{-i(2\psi+\nu)} & -d_{21}^{*}e^{-i(2\psi+\gamma)} & 0 & 0 \\ 0 & 0 & d_{21}e^{i\gamma} & d_{22}e^{i\nu} & -d_{21}e^{i\gamma} & d_{22}e^{i\nu} & 0 & 0 \end{pmatrix},$$

where $\begin{pmatrix} d_{11} & d_{12} \\ d_{21} & d_{22} \end{pmatrix}$ is a unitary matrix and β, ν, and γ are arbitrary phases.

By using the additional conditions imposed by (5), the ambiguity of the matrix U calculated from (4) has been greatly reduced. From three two-dimensional unitary matrices and six arbitrary phases, we have now only a single unitary matrix and three arbitrary phases.

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