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1977 J. Phys. A: Math. Gen. 10 2041

(http://iopscience.iop.org/0305-4470/10/12/013)

J. Phys. A: Math. Gen., Vol. 10, No. 12, 1977. Printed in Great Britain. © 1977

On the recoupling coefficients and isoscalar factors of a chain of groups

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Received 16 May 1977, in final form 14 July 1977

Abstract. Recoupling coefficients and isoscalar factors of a chain of compact topological groups (finite or continuous) are discussed in terms of character formulae. Special emphasis is put on the chain $SU_2 \supset G$, where G is isomorphic with the spinor group of a point symmetry group.

1. Introduction

The theory of invariants is of intrinsic importance in mathematics (Weyl 1939) and plays an essential role in the applications of group theory to (atomic and molecular) physics (Wigner 1941, published in Biedenharn and van Dam 1965, pp 87–133, Racah 1942, 1949). The various mathematical invariants (e.g. invariant functions, Casimir operators, characters, isoscalar factors, recoupling coefficients, reduced matrix elements) associated with a group J or a chain $J \supset G$ of groups arise in numerous areas of mathematics and mathematical physics. They also supply basic quantities for specifying the physical properties of a (quantum) system which is invariant with respect to J or G.

From a conceptual point of view, characters belong to the simplest family of mathematical invariants. It thus appears legitimate to try to relate mathematical and physical invariants to characters.

Weyl (1931) obtained formulae connecting energy levels for an N-equivalent-particle system to the characters of S_N, the symmetric group on N objects. Wigner (1941) derived formulae involving 6-j symbols and irreducible characters of a simply reducible finite or compact group. Following Wigner's pioneer work, Sharp (1960) proved character formulae for 6-j and 9-j symbols of a quasi-simply reducible finite or (locally) compact group. Derome and Sharp (1965) extended some of the latter character formulae to the case of an arbitrary finite or compact group. (At this point, it is perhaps interesting to note that the papers by Wigner (1941), Sharp (1960), and Derome and Sharp (1965) are of central importance for the Wigner–Racah algebra of a chain of groups, a fact that is now only being fully recognised by molecular physicists.) More recently, Fieck (1977) rederived character formulae for 6-j symbols, expressed in the W notation of Griffith (1962), of a simply reducible finite group having integer representations only. In addition, he developed some new character formulae for symmetrised isoscalar factors of a multiplicity-free chain of simply reducible finite groups with integer representations.

There are numerous points that warrant further development of the above mentioned character formulae. As a matter of fact, the chains we deal with in physics are far from being all multiplicity-free chains of simply reducible finite (or compact continuous) groups having integer representations only. In atomic and molecular physics we are generally concerned with multiplicity-non-free chains of compact or locally compact topological groups. Such chains present fundamental interest both from a mathematical standpoint (classification, selection rules, calculation of matrix elements, etc) and a physical standpoint (state and operator labelling problem, descent in symmetry or symmetry breaking, perturbation theory, etc). On the other hand, the Clebsch–Gordan coefficient and the isoscalar factor enter into the physical applications in a more natural way than the symmetrised Clebsch–Gordan coefficient (or 3-jm symbol) and the symmetrised isoscalar factor (or 3-$ja\Gamma$ symbol), respectively. Similarly, the recoupling coefficient relative to the coupling, via inner Kronecker product, of $n>2$ classes of irreducible representations appears to be more fundamental, on physical grounds, than its symmetrised version, i.e. the $3(n-1)$-j symbol. (Observe that the 3-jm, 6-j, and 9-j symbols correspond respectively to the V, W, and X symbols introduced by Griffith (1962) in molecular physics.) Furthermore, the interest in character formulae involving recoupling coefficients and isoscalar factors is threefold: (i) they provide, in a few cases, formulae for checking or computing recoupling coefficients and isoscalar factors, or formulae for computing integrals over special functions; (ii) they elucidate the symmetries of the recoupling coefficients and isoscalar factors; and (iii) they constitute a starting point for a further geometrical investigation, besides the standard diagram techniques (Yutsis *et al* 1962, Agrawala and Belinfante 1968, El Baz and Castel 1972, Stedman 1975, 1976, Lulek 1975, Guichon 1975), of the recoupling coefficients and isoscalar factors.

It is the aim of this work to report character formulae for recoupling coefficients and isoscalar factors of an arbitrary chain $J \supset G$ of compact topological groups. In § 2 we deal with recoupling coefficients for irreducible representations classes of J while we devote § 3 to isoscalar factors of $J \supset G$. As a molecular example, the chain $SU_2 \supset G$ is considered in § 4.

For the purpose of comparison, the relation analogous, if any, to (a) of Fieck (1977) shall be quoted as (Fa).

2. Recoupling coefficients for an isolated group

We adopt the following notation for our group J: j stands for a class of irreducible representations of J, D^j for the unitary matrix representation associated with j, and $[j]$ for the dimension of D^j; the elements of J are denoted as $R, S, T, \ldots$; the matrix $D^j(R)$, whose elements are $D^j(R)_{mm'}$, is the representative of R in D^j; $\chi^j(R)$ denotes the character of R in j; lastly, $\langle j_1 j_2 m_1 m_2 | bjm\rangle$ stands for a Clebsch–Gordan coefficient of J with b being an inner multiplicity label necessary when the inner Kronecker product $j_1 \otimes j_2$ contains j more than once. (Note that the notation just described follows closely the standard notation for the group SU_2 or rather the chain $SU_2 \supset U_1$.)

Our basic relation reads

$$\sum_b \langle j_1 j_2 m_1 m_2 | bjm\rangle \langle j_1 j_2 m_1' m_2' | bjm'\rangle^* = [j]|\hat{J}|^{-1} \int_J D^{j_1}(R)_{m_1 m_1'} D^{j_2}(R)_{m_2 m_2'} D^j(R)^*_{mm'}\, dR, \tag{F2}$$

where the (Stieltjes) integral $\int_{\hat{J}} \ldots \mathrm{d}R$ is to be taken over the (topological) space $\hat{J}$ of the compact (topological) group J and $|\hat{J}| \equiv \int_{\hat{J}} \mathrm{d}R$ is the volume of $\hat{J}$. When J is finite, $\int_{\hat{J}} \ldots \mathrm{d}R$ and $|\hat{J}|$ reduce to $\Sigma_{R\in J} \ldots$ and to the order of J, respectively. Following Sharp (1960), we shall refer to (F2) as Gaunt's formula. ((F2) is of importance in the theory of special functions. In the $J \equiv \mathrm{SU}_2$ case, the left-hand side of (F2) may be specialised to an integral over the product of three Legendre functions. Gaunt (1929) directly worked out such an integral in his work on the triplets of He.)

We start from the definition (cf Kibler 1970)

$$\langle j_1(j_2j_3)b_{23}j_{23}b'j'm'|(j_1j_2)b_{12}j_{12}j_3bjm\rangle = \sum_{\substack{m_1m_2m_3\\ m_{12}m_{23}}} \langle j_1j_2m_1m_2|b_{12}j_{12}m_{12}\rangle\langle j_{12}j_3m_{12}m_3|bjm\rangle \times \langle j_2j_3m_2m_3|b_{23}j_{23}m_{23}\rangle^*\langle j_1j_{23}m_1m_{23}|b'j'm'\rangle^*. \tag{F1}$$

As a consequence of Schur's lemma, we have the property

$$\langle j_1(j_2j_3)b_{23}j_{23}b'j'm'|(j_1j_2)b_{12}j_{12}j_3bjm\rangle = \delta(j'j)\delta(m'm)\langle j_1(j_2j_3)b_{23}j_{23}b'j|(j_1j_2)b_{12}j_{12}j_3bj\rangle,$$

where

$$\langle j_1(j_2j_3)b_{23}j_{23}b'j|(j_1j_2)b_{12}j_{12}j_3bj\rangle \equiv [j]^{-1}\sum_m \langle j_1(j_2j_3)b_{23}j_{23}b'jm|(j_1j_2)b_{12}j_{12}j_3bjm\rangle$$

is independent of the generalised magnetic quantum number m. Clearly, $\langle j_1(j_2j_3)b_{23}j_{23}b'j|(j_1j_2)b_{12}j_{12}j_3bj\rangle$ is a recoupling coefficient for the $n=3$ classes of irreducible representations j_1, j_2, and j_3 which makes it possible to pass from the coupling scheme $(((j_1\otimes j_2)b_{12}j_{12})\otimes j_3)bj$ to the coupling scheme $(j_1\otimes((j_2\otimes j_3)b_{23}j_{23}))b'j$.

Character formulae involving recoupling coefficients for $n=3$ classes of irreducible representations are easily obtainable from repeated applications of (F1) and (F2). As an example, we get the symmetric form

$$\sum_{b_{12}bb_{23}b'} |\langle j_1(j_2j_3)b_{23}j_{23}b'j|(j_1j_2)b_{12}j_{12}j_3bj\rangle|^2 = [j_{12}][j_{23}]|\hat{J}|^{-4}\int_{\hat{J}\otimes 4} \chi^{j_1}(RU)\chi^{j_2}(RT)\chi^{j_3}(ST)\chi^{j_{12}}(R^{-1}S)\chi^{j_{23}}(T^{-1}U) \times\chi^{j}(S^{-1}U^{-1})\,\mathrm{d}R\,\mathrm{d}S\,\mathrm{d}T\,\mathrm{d}U, \tag*{(F4)$'$}$$

where we have used the abbreviation $\int_{\hat{J}\otimes P}$ for $\int_{\hat{J}}\int_{\hat{J}}\ldots\int_{\hat{J}}$ (P times). It should be mentioned that the latter formula remains valid when substituting $[j]^2D^j(S^{-1})_{mm'}D^j(U^{-1})_{m'm}$ in place of $\chi^j(S^{-1}U^{-1})$. Further integration leads to the asymmetric form

$$\sum_{b_{12}bb_{23}b'} |\langle j_1(j_2j_3)b_{23}j_{23}b'j|(j_1j_2)b_{12}j_{12}j_3bj\rangle|^2 = [j_{12}][j_{23}]|\hat{J}|^{-3}\int_{\hat{J}\otimes 3} \chi^{j_1}(R_1)\chi^{j_2}(R_2)\chi^{j_{12}}(R_3^{-1})\chi^{j_3}(R_3^{-1}R_2)\chi^{j_{23}}(R_2^{-1}R_1) \times\chi^{j}(R_1^{-1}R_3)\,\mathrm{d}R_1\,\mathrm{d}R_2\,\mathrm{d}R_3. \tag{F4}$$

Relations (F4)′ and (F4) were first derived by Wigner (1941) in the simply reducible case. In addition, (F4) is nothing but the transcription of relation (ii) of Derome and Sharp (1965) in terms of recoupling coefficients.

In a similar way, we can obtain character formulae involving recoupling coefficients for $n=4$ classes of irreducible representations. The relation (cf Kibler 1970)

$$\begin{aligned}\langle(j_1j_3)b_{13}j_{13}(j_2j_4)b_{24}j_{24}b'j'm'|(j_1j_2)b_{12}j_{12}(j_3j_4)b_{34}j_{34}bjm\rangle \\ = \sum_{\substack{m_1m_2m_3m_4\\ m_{12}m_{34}m_{13}m_{24}}} \langle j_1j_2m_1m_2|b_{12}j_{12}m_{12}\rangle\langle j_3j_4m_3m_4|b_{34}j_{34}m_{34}\rangle \\ \times\langle j_{12}j_{34}m_{12}m_{34}|bjm\rangle\langle j_1j_3m_1m_3|b_{13}j_{13}m_{13}\rangle^*\langle j_2j_4m_2m_4|b_{24}j_{24}m_{24}\rangle^* \\ \times\langle j_{13}j_{24}m_{13}m_{24}|b'j'm'\rangle^*\end{aligned}$$

defines the recoupling coefficient

$$\begin{aligned}\langle(j_1j_3)b_{13}j_{13}(j_2j_4)b_{24}j_{24}b'j|(j_1j_2)b_{12}j_{12}(j_3j_4)b_{34}j_{34}bj\rangle \\ = [j]^{-1}\sum_m \langle(j_1j_3)b_{13}j_{13}(j_2j_4)b_{24}j_{24}b'jm|(j_1j_2)b_{12}j_{12}(j_3j_4)b_{34}j_{34}bjm\rangle\end{aligned}$$

useful for passing from the coupling $(((j_1\otimes j_2)b_{12}j_{12})\otimes((j_3\otimes j_4)b_{34}j_{34}))bj$ to the coupling $(((j_1\otimes j_3)b_{13}j_{13})\otimes((j_2\otimes j_4)b_{24}j_{24}))b'j$. By using the property

$$\begin{aligned}\langle(j_1j_3)b_{13}j_{13}(j_2j_4)b_{24}j_{24}b'j'm'|(j_1j_2)b_{12}j_{12}(j_3j_4)b_{34}j_{34}bjm\rangle \\ = \delta(j'j)\delta(m'm)\langle(j_1j_3)b_{13}j_{13}(j_2j_4)b_{24}j_{24}b'j|(j_1j_2)b_{12}j_{12}(j_3j_4)b_{34}j_{34}bj\rangle\end{aligned}$$

conjointly with Gaunt's formula, we obtain the highly symmetric form

$$\begin{aligned}\sum_{b_{12}b_{34}bb_{13}b_{24}b'} |\langle(j_1j_3)b_{13}j_{13}(j_2j_4)b_{24}j_{24}b'j|(j_1j_2)b_{12}j_{12}(j_3j_4)b_{34}j_{34}bj\rangle|^2 \\ = [j_{12}][j_{34}][j_{13}][j_{24}]|\hat{J}|^{-6}\int_{\hat{J}\otimes 6}\chi^{j_1}(RU)\chi^{j_2}(RV)\chi^{j_{12}}(R^{-1}T) \\ \times\chi^{j_3}(SU)\chi^{j_4}(SV)\chi^{j_{34}}(S^{-1}T)\chi^{j_{13}}(WU^{-1})\chi^{j_{24}}(WV^{-1}) \\ \times\chi^{j}(W^{-1}T^{-1})\,\mathrm{d}R\,\mathrm{d}S\,\mathrm{d}T\,\mathrm{d}U\,\mathrm{d}V\,\mathrm{d}W\end{aligned}$$

which also holds if $\chi^j(W^{-1}T^{-1})$ is replaced by $[j]^2D^j(T^{-1})_{mm'}D^j(W^{-1})_{m'm}$. A convenient manipulation would allow the latter sixfold symmetric integral to be transformed into a fivefold asymmetric one.

Before leaving § 2 let us offer a remark (inspired by the work of Sharp 1960) concerning the preceding character formulae. For both the $n=3$ and $n=4$ cases, we have emphasised two forms for the character formulae: (i) a symmetric form which shows how to define, up to a phase, the 6-j and 9-j symbols respectively from the recoupling coefficients for $n=3$ and $n=4$ classes of irreducible representations and (ii) an asymmetric form (after the redundant integrations have been performed) which seems to be more practical as far as computational purposes are concerned. We should like to point out that the symmetric forms can be written down immediately without detailed algebra by applying the following (heuristic) rules.

Rule 1. Write $\Pi_j\chi^j(\ )$ where the product is to be extended over all the distinct j's ($j\equiv j_1, j_2, \ldots, j_{12}, \ldots$) appearing on the left-hand side. In $\Pi_j\chi^j(\ )$ consider the subproduct $\chi^{j_1}(\ )\chi^{j_2}(\ )\chi^{j_{12}}(\ )$ for which the frequency $\sigma(j_{12}|j_1\otimes j_2)$ of j_{12} in $j_1\otimes j_2$ is different from zero (that is to say for which j_1, j_2, and j_3 form an (ordered) triad). Then write $|\hat{J}|^{-1}\int_{\hat{J}}\chi^{j_1}(R\ldots)\chi^{j_2}(R\ldots)\chi^{j_{12}}(R^{-1}\ldots)\,dR$, a way of depicting the coupling $(j_1\otimes j_2)b_{12}j_{12}$ without complex conjugation. Such an expression involves one integration variable R or S or $T\ldots$ for each triad in $\Pi_j\chi^j(\ )$. Once all the triads (or couplings) have been exhibited, we have the number P of integration variables.

Rule 2. The desired quantity is thus simply

$$[j_{12}][\ ]\ldots|\hat{J}|^{-P}\int_{\hat{J}\otimes P}\chi^{j_1}(R\ldots)\chi^{j_2}(R\ldots)\chi^{j_{12}}(R^{-1}\ldots)\ldots dR\ldots,$$

where we (only) include the intermediate classes of irreducible representations $j_{12}\ldots$ inside the $[\ ]$'s.

Rules 1 and 2 can be applied to higher recoupling coefficients. By way of illustration let us consider

$$Q_{12}=\sum_{\substack{b_{23}b_{123}b_{45}b\\ b_{24}b_{124}b_{35}b'}} |\langle\{[j_1(j_2j_4)b_{24}j_{24}]b_{124}j_{124}(j_3j_5)b_{35}j_{35}\}b'j|\{[j_1(j_2j_3)b_{23}j_{23}]b_{123}j_{123}(j_4j_5)b_{45}j_{45}\}bj\rangle|^2,$$

where the recoupling coefficient $\langle\ |\ \rangle$ is defined by

$$\begin{aligned}
&\delta(j'j)\delta(m'm)\\
&\quad\times\langle\{[j_1(j_2j_4)b_{24}j_{24}]b_{124}j_{124}(j_3j_5)b_{35}j_{35}\}b'j|\{[j_1(j_2j_3)b_{23}j_{23}]b_{123}j_{123}(j_4j_5)b_{45}j_{45}\}bj\rangle\\
&\qquad=\sum_{\substack{m_1m_2m_3m_4m_5\\ m_{23}m_{123}m_{45}\\ m_{24}m_{124}m_{35}}}\langle j_2j_3m_2m_3|b_{23}j_{23}m_{23}\rangle\langle j_1j_{23}m_1m_{23}|b_{123}j_{123}m_{123}\rangle\\
&\qquad\quad\times\langle j_4j_5m_4m_5|b_{45}j_{45}m_{45}\rangle\langle j_{123}j_{45}m_{123}m_{45}|bjm\rangle\\
&\qquad\quad\times\langle j_2j_4m_2m_4|b_{24}j_{24}m_{24}\rangle^*\langle j_1j_{24}m_1m_{24}|b_{124}j_{124}m_{124}\rangle^*\\
&\qquad\quad\times\langle j_3j_5m_3m_5|b_{35}j_{35}m_{35}\rangle^*\langle j_{124}j_{35}m_{124}m_{35}|b'j'm'\rangle^*,
\end{aligned}$$

a relation occurring in the coupling of $n=5$ classes of irreducible representations. (When applied to SU_2, the latter recoupling coefficient turns out to be proportional to the Jahn 12-j symbol (Jahn and Hope 1954), to be distinguished from the Elliott–Flowers 12-j symbol (Elliott and Flowers 1955).) From rule 1, the product $\Pi_j\chi^j(\ )$ to be considered is clearly

$$\chi^{j_1}(\ )\chi^{j_2}(\ )\chi^{j_3}(\ )\chi^{j_4}(\ )\chi^{j_5}(\ )\chi^{j_{23}}(\ )\chi^{j_{123}}(\ )\chi^{j_{45}}(\ )\chi^{j_{24}}(\ )\chi^{j_{124}}(\ )\chi^{j_{35}}(\ )\chi^{j}(\ ).$$

Further, the parentheses in $\Pi_j\chi^j(\ )$ are easily completed by the $P=8$ integration variables R, S, T, U, V, W, X, and Y corresponding to the triads $(j_2j_3)b_{23}j_{23}$, $(j_1j_{23})b_{123}j_{123}$, $(j_4j_5)b_{45}j_{45}$, $(j_{123}j_{45})bj$, $(j_2j_4)b_{24}j_{24}$, $(j_1j_{24})b_{124}j_{124}$, $(j_3j_5)b_{35}j_{35}$, and $(j_{124}j_{35})b'j$, respectively. From rule 2, the dimensionality factor $[j_{12}][\ ]\ldots$ is simply

$$[j_{23}][j_{123}][j_{45}][j_{24}][j_{124}][j_{35}].$$

As a final result we obtain the symmetric form

$$Q_{12} = [j_{23}][j_{123}][j_{45}][j_{24}][j_{124}][j_{35}]|\hat{J}|^{-8}$$
$$\times \int_{\hat{J}\otimes 8} \chi^{j_1}(SW)\chi^{j_2}(RV)\chi^{j_3}(RX)\chi^{j_4}(TV)\chi^{j_5}(TX)\chi^{j_{23}}(R^{-1}S)$$
$$\times \chi^{j_{123}}(S^{-1}U)\chi^{j_{45}}(T^{-1}U)\chi^{j_{24}}(V^{-1}W)\chi^{j_{124}}(W^{-1}Y)\chi^{j_{35}}(X^{-1}Y)$$
$$\times \chi^{j}(U^{-1}Y^{-1})\, dR\, dS\, dT\, dU\, dV\, dW\, dX\, dY,$$

in agreement with a direct but long calculation†.

3. Isoscalar factors of a chain of groups

Let us now turn our attention to the chain $J \supset G$. We take for the subgroup G of the group J the notation deduced from that of J through the correspondence: $j \to \Gamma$; $R, S, T, \ldots \to r, s, t, \ldots$; $m \to \gamma$; $b \to \beta$. In addition Γ_0 denotes the identity irreducible representation class of G.

The reduction of the matrix representation D^j of G into the direct sum $\oplus_\Gamma \sigma(\Gamma|j)D^\Gamma$, where $\sigma(\Gamma|j)$ stands for the frequency of Γ in j, may be achieved by means of a unitary transformation of which $\langle jm|ja\Gamma\gamma\rangle$ denotes the m-$a\Gamma\gamma$ matrix element. For fixed j and Γ, the outer or branching multiplicity label a classifies the various D^Γ-subspaces contained in the D^j-space and thus takes on $\sigma(\Gamma|j)$ values. Such a label may be either: (i) a simple numeral; or (ii) characterised, at least partially, by the classes of irreducible representations of a chain of groups between J and G; or (iii) an eigenvalue λ of a labelling operator invariant under G (Patera and Winternitz 1976, Bickerstaff and Wybourne 1976, Kibler 1977). The $\langle jm|ja\Gamma\gamma\rangle$'s obey (Koster 1958, Kibler 1969)

$$\sum_a \langle jm|ja\Gamma\gamma\rangle\langle jm'|ja\Gamma\gamma'\rangle^* = [\Gamma]|\hat{G}|^{-1} \int_{\hat{G}} D^j(r)_{mm'} D^\Gamma(r)^*_{\gamma\gamma'}\, dr, \tag{F10}$$

a relation which proves useful for determining the $\langle jm|ja\Gamma\gamma\rangle$ matrix elements. (Note that a dimension factor is missing in (10) of Fieck (1977).)

When going from the isolated group J to the chain $J \supset G$, the J Clebsch–Gordan coefficients $\langle j_1j_2m_1m_2|bjm\rangle$ combine to produce

$$\langle j_1j_2a_1\Gamma_1\gamma_1a_2\Gamma_2\gamma_2|bja\Gamma\gamma\rangle$$
$$= \sum_{m_1m_2m} \langle j_1m_1|j_1a_1\Gamma_1\gamma_1\rangle^*\langle j_2m_2|j_2a_2\Gamma_2\gamma_2\rangle^*\langle j_1j_2m_1m_2|bjm\rangle\langle jm|ja\Gamma\gamma\rangle, \tag{F7}$$

which is a J Clebsch–Gordan coefficient adapted to G or a $J \supset G$ symmetry-adapted Clebsch–Gordan coefficient. (In the case where $a \equiv \lambda$, we refer to $\langle j_1j_2\lambda_1\Gamma_1\gamma_1\lambda_2\Gamma_2\gamma_2|bj\lambda\Gamma\gamma\rangle$ as a $J \supset G$ supersymmetry-adapted Clebsch–Gordan coefficient (Kibler 1977).) In physical applications it appears worthwhile, on computational grounds, to introduce the f symbol defined via

$$f\begin{pmatrix} bj_1 & j_2 & j \\ a_1\Gamma_1\gamma_1 & a_2\Gamma_2\gamma_2 & a\Gamma\gamma \end{pmatrix} = [j_1]^{-1/2}\langle j_2ja_2\Gamma_2\gamma_2a\Gamma\gamma|bj_1a_1\Gamma_1\gamma_1\rangle^*$$

† For $J \equiv SU_2$, the relation so obtained provides a character formula for the twisted 12-j symbol of Jahn. In a similar way, we could obtain a character formula for the untwisted 12-j symbol of Elliott and Flowers.

up to a phase factor $\exp(i\phi(bj_1j_2j))$. In this respect, the Wigner–Eckart theorem for a compact continuous group (Wigner 1941, Racah 1942, 1949, Stone 1961), or a finite group (Koster 1958), or a locally compact group (Hillion 1966, Klimyk 1975) assumes a particularly simple form when using f symbols. We shall go back to the f's in § 4.

The J Clebsch–Gordan coefficients adapted to G are connected to the G Clebsch–Gordan coefficients $\langle\Gamma_1\Gamma_2\gamma_1\gamma_2|\beta\Gamma\gamma\rangle$ and the $J\supset G$ isoscalar factors $\langle j_1a_1\Gamma_1j_2a_2\Gamma_2|bja\beta\Gamma\rangle$ through

$$\sum_{\gamma_1\gamma_2}\langle j_1j_2a_1\Gamma_1\gamma_1a_2\Gamma_2\gamma_2|bja\Gamma\gamma\rangle\langle\Gamma_1\Gamma_2\gamma_1\gamma_2|\beta\Gamma'\gamma'\rangle^* = \delta(\Gamma'\Gamma)\delta(\gamma'\gamma)\langle j_1a_1\Gamma_1j_2a_2\Gamma_2|bja\beta\Gamma\rangle, \tag{F9}$$

a relation that easily follows from Schur's lemma. Inversion of (F9) leads to the lemma of Racah (1949):

$$\langle j_1j_2a_1\Gamma_1\gamma_1a_2\Gamma_2\gamma_2|bja\Gamma\gamma\rangle=\sum_{\beta}\langle\Gamma_1\Gamma_2\gamma_1\gamma_2|\beta\Gamma\gamma\rangle\langle j_1a_1\Gamma_1j_2a_2\Gamma_2|bja\beta\Gamma\rangle \tag{F8}$$

of great importance in calculating Clebsch–Gordan coefficients as well as coefficients of fractional parentage.

By combining (F9), (F7), (F2) for J, (F2) for G, and (F10) three times, we obtain the symmetric character formula

$$\sum_{\substack{a_1a_2a\\ b\beta}}|\langle j_1a_1\Gamma_1j_2a_2\Gamma_2|bja\beta\Gamma\rangle|^2 = [j][\Gamma_1][\Gamma_2]|\hat{J}|^{-1}|\hat{G}|^{-4}\int_{\hat{J}}\int_{\hat{G}\otimes 4}\chi^{j_1}(Rs)\chi^{j_2}(Rt)\chi^{j}(R^{-1}u)\chi^{\Gamma_1}(rs^{-1}) \times\chi^{\Gamma_2}(rt^{-1})\chi^{\Gamma}(r^{-1}u^{-1})\,dR\,dr\,ds\,dt\,du, \tag{F11$'$}$$

which may be rewritten as:

$$\sum_{\substack{a_1a_2a\\ b\beta}}|\langle j_1a_1\Gamma_1j_2a_2\Gamma_2|bja\beta\Gamma\rangle|^2 = [j][\Gamma_1][\Gamma_2]|\hat{J}|^{-1}|\hat{G}|^{-3}\int_{\hat{J}}\int_{\hat{G}\otimes 3}\chi^{j_1}(Rs)\chi^{j_2}(Rt)\chi^{j}(R^{-1}u)\chi^{\Gamma_1}(s^{-1}) \times\chi^{\Gamma_2}(t^{-1})\chi^{\Gamma}(u^{-1})\,dR\,ds\,dt\,du. \tag{F11}$$

(F11) may be particularised to the case $\Gamma\equiv\Gamma_0$. Thus we get

$$\sum_{\substack{a_2a_0a_1\\ b}}|\langle j_2a_2\Gamma_2ja_0\Gamma_0|bj_1a_1\Gamma_1\rangle|^2 = \delta(\Gamma_2\Gamma_1)[j_1]|\hat{J}|^{-1}|\hat{G}|^{-2}\int_{\hat{J}}\int_{\hat{G}\otimes 2}\chi^{j_2}(Rs)\chi^{j}(R)\chi^{j_1}(R^{-1}t) \times\chi^{\Gamma_1}(s^{-1}t^{-1})\,dR\,ds\,dt. \tag{F12$'$}$$

Further specialisation yields

$$\sum_{\substack{a_2a_0a_1\\ b}}|\langle j_1a_2\Gamma_1ja_0\Gamma_0|bj_1a_1\Gamma_1\rangle|^2 = [j_1]|\hat{J}|^{-1}|\hat{G}|^{-2}\int_{\hat{J}}\int_{\hat{G}\otimes 2}\chi^{j_1}(R^{-1}s)\chi^{j_1}(Rt)\chi^{j}(R)\chi^{\Gamma_1}(s^{-1}t^{-1})\,dR\,ds\,dt. \tag{F12}$$

It should be noted that the form for (F12) differs from the one for (12) of Fieck (1977). A more similar form would be obtained if

$$\int_J \int_{\hat{G}\otimes 2} \chi^{j_1}(R^{-1}s)\chi^{j_1}(Rt)\chi^{j}(R)\chi^{\Gamma_1}(s^{-1}t^{-1})\,\mathrm{d}R\ \mathrm{d}s\ \mathrm{d}t$$

$$= \int_J \int_{\hat{G}\otimes 2} \chi^{j_1}(R^{-1}s\,Rt)\chi^{j}(R)\chi^{\Gamma_1}(s^{-1})\chi^{\Gamma_1}(t^{-1})\,\mathrm{d}R\ \mathrm{d}s\ \mathrm{d}t,$$

an identity that holds when the reduction $j_1 \downarrow \Gamma_1$ is multiplicity free, i.e. when $\sigma(\Gamma_1|j_1)=1$.

Finally, when using eigenvalues of a normal (for example Hermitian) tensor operator $T^{j}_{a_0\Gamma_0\gamma_0}$ for describing outer multiplicity labels, relations (F12)′ and (F12) can be modified according to

$$\langle j_1 j\lambda_1\Gamma_1\gamma_1 a_0\Gamma_0\gamma_0|bj_1\lambda'_1\Gamma'_1\gamma'_1\rangle = \delta(\lambda'_1\lambda_1)\delta(\Gamma'_1\Gamma_1)\delta(\gamma'_1\gamma_1)\lambda_1(j_1 j a_0\Gamma_1),$$

where the eigenvalue $\lambda_1(j_1 j a_0\Gamma_1)$ of $T^{j}_{a_0\Gamma_0\gamma_0}$ depends on j_1, j, a_0, and Γ_1.

To close § 3 let us note that, when transcribed in terms of f symbols, the integrals reported here can be written down in symmetric form by applying rule 1 for the triads of J and G in conjunction with the following rule.

Rule 3. The reduction $j \downarrow \Gamma$ is depicted by

$$[\Gamma]|\hat{G}|^{-1} \int_{\hat{G}} \chi^{j}(\ldots r)\chi^{\Gamma}(\ldots r^{-1})\,\mathrm{d}r.$$

By way of illustration let us consider

$$Q_{13} = \sum_{\substack{ba_1a_2a\\ \gamma_1\gamma_2\gamma}} \left| f\begin{pmatrix} bj_1 & j_2 & j \\ a_1\Gamma_1\gamma_1 & a_2\Gamma_2\gamma_2 & a\Gamma\gamma \end{pmatrix}\right|^2.$$

The couplings for J and G introduce the factors

$$|\hat{J}|^{-1} \int_J \chi^{j_2}(R\ldots)\chi^{j}(R\ldots)\chi^{j_1}(R^{-1}\ldots)\,\mathrm{d}R$$

and

$$|\hat{G}|^{-1} \int_{\hat{G}} \chi^{\Gamma_2}(r\ldots)\chi^{\Gamma}(r\ldots)\chi^{\Gamma_1}(r^{-1}\ldots)\,\mathrm{d}r,$$

respectively, while the reductions $j_2 \downarrow \Gamma_2$, $j \downarrow \Gamma$, and $j_1 \downarrow \Gamma_1$ are depicted by

$$[\Gamma_2]|\hat{G}|^{-1} \int_{\hat{G}} \chi^{j_2}(\ldots s)\chi^{\Gamma_2}(\ldots s^{-1})\,\mathrm{d}s,$$

$$[\Gamma]|\hat{G}|^{-1} \int_{\hat{G}} \chi^{j}(\ldots t)\chi^{\Gamma}(\ldots t^{-1})\,\mathrm{d}t,$$

and

$$[\Gamma_1]|\hat{G}|^{-1}\int_{\hat{G}}\chi^{j_1}(\ldots u)\chi^{\Gamma_1}(\ldots u^{-1})\,\mathrm{d}u,$$

respectively. As a final result we obtain

$$Q_{13}=[\Gamma_2][\Gamma][\Gamma_1]|\hat{J}|^{-1}|\hat{G}|^{-4}\int_{\hat{J}}\int_{\hat{G}\otimes 4}\chi^{j_2}(Rs)\chi^{j}(Rt)$$
$$\times\chi^{j_1}(R^{-1}u)\chi^{\Gamma_2}(rs^{-1})\chi^{\Gamma}(rt^{-1})\chi^{\Gamma_1}(r^{-1}u^{-1})\,\mathrm{d}R\,\mathrm{d}r\,\mathrm{d}s\,\mathrm{d}t\,\mathrm{d}u,$$

which may also be deduced from (F11)′ through some algebraic manipulations.

Rules 1, 2, and 3 might be generalised for writing down any product of recoupling coefficients for $n=3, 4, \ldots$ classes of irreducible representations of J and G and isoscalar factors of $J\supset G$ (modulo summation over all relevant inner and outer multiplicity labels), that is, any product such that a given triad for J or G appears as many times in covariant form as in contravariant form. These and related matters will be the subject of future investigations. In particular, we (Kibler and Elbaz 1977, to be submitted for publication) hope to establish a further connection, based on the diagrammatic equivalent of the characters, between plane geometry and theory of invariants.

4. The chain $SU_2\supset G$

We now go to the chain $SU_2\supset G$. The group G may be realised as the double group of a (finite) subgroup of the proper rotation group in three dimensions so that the chain $SU_2\supset G$ finds uses in molecular and solid state physics. For the $J\equiv SU_2$ case, we have $j\equiv 0, \frac{1}{2}, 1, \ldots$ and $[j]\equiv 2j+1$. Further, there is no need for the inner multiplicity label b. Finally, the transformation $\langle jm|ja\Gamma\gamma\rangle$ allows one to pass from the axial chain $SU_2\supset U_1$, a multiplicity-free chain associated with the $\{J^2, J_z\}$ scheme, to the molecular chain $SU_2\supset G$, a generally multiplicity-non-free chain associated with the $\{J^2, P_\gamma^\Gamma\}$ scheme, where P_γ^Γ is a $\Gamma\gamma$-projection operator for G.

In the situation where $J\equiv SU_2$, it is convenient to define the f symbol outlined in § 3 by (Kibler 1968)

$$f\begin{pmatrix} j_1 & j_2 & j \\ a_1\Gamma_1\gamma_1 & a_2\Gamma_2\gamma_2 & a\Gamma\gamma\end{pmatrix}=(-1)^{2j}(2j_1+1)^{-1/2}\langle j_2ja_2\Gamma_2\gamma_2a\Gamma\gamma|j_1a_1\Gamma_1\gamma_1\rangle^*.$$

Alternatively we have

$$f\begin{pmatrix} j_1 & j_2 & j \\ a_1\Gamma_1\gamma_1 & a_2\Gamma_2\gamma_2 & a\Gamma\gamma\end{pmatrix}$$
$$=\sum_{m_1m_2m}(-1)^{j_1+m_1}\langle j_1-m_1|j_1a_1\Gamma_1\gamma_1\rangle^*$$
$$\times\langle j_2m_2|j_2a_2\Gamma_2\gamma_2\rangle\langle jm|ja\Gamma\gamma\rangle\bar{V}\begin{pmatrix} j_1 & j_2 & j \\ m_1 & m_2 & m\end{pmatrix}$$

in terms of the $\bar{V}$ symbol of Fano and Racah (1959). Note that the f parallels to some extent the $\bar{V}$ while the $\bar{f}$ symbol defined by (Kibler 1968)

$$\bar{f}\begin{pmatrix} j_1 & j_2 & j_3 \\ a_1\Gamma_1\gamma_1 & a_2\Gamma_2\gamma_2 & a_3\Gamma_3\gamma_3 \end{pmatrix}$$

$$= (2j_3+1)^{1/2} \sum_{a_3'\Gamma_3'\gamma_3'} f\begin{pmatrix} 0 & j_3 & j_3 \\ \Gamma_0 & a_3\Gamma_3\gamma_3 & a_3'\Gamma_3'\gamma_3' \end{pmatrix}^*$$

$$\times f\begin{pmatrix} j_3 & j_2 & j_1 \\ a_3'\Gamma_3'\gamma_3' & a_2\Gamma_2\gamma_2 & a_1\Gamma_1\gamma_1 \end{pmatrix}^*$$

fully parallels the 3-*jm* symbol of Wigner. The f and $\bar{f}$ symbols turn out to be of great importance in molecular physics and more specifically in electronic and vibrational–rotational spectroscopy of molecular aggregates. In particular, the interest of the f symbols for ligand field theory and related phenomena has been discussed by Kibler (1968, 1969). As a result, they prove to be very useful in determining optical and magnetic properties of d^N and f^N systems in molecular or solid state environments. The case $\Gamma \equiv \Gamma_0$ is of special importance for the applications. From Racah's lemma it can be shown that

$$f\begin{pmatrix} j_1 & j_2 & j \\ a_1\Gamma\gamma & a_2\Gamma'\gamma' & a_0\Gamma_0\gamma_0 \end{pmatrix} = \delta(\Gamma'\Gamma)\delta(\gamma'\gamma) f\begin{pmatrix} j_1 & j_2 & j \\ a_1\Gamma & a_2\Gamma & a_0\Gamma_0 \end{pmatrix},$$

where

$$f\begin{pmatrix} j_1 & j_2 & j \\ a_1\Gamma & a_2\Gamma & a_0\Gamma_0 \end{pmatrix} \equiv [\Gamma]^{-1} \sum_\gamma f\begin{pmatrix} j_1 & j_2 & j \\ a_1\Gamma\gamma & a_2\Gamma\gamma & a_0\Gamma_0\gamma_0 \end{pmatrix}.$$

The coefficient $f\begin{pmatrix} j_1 & j_2 & j \\ a_1\Gamma & a_2\Gamma & a_0\Gamma_0 \end{pmatrix}$ is particularly appropriate for calculating matrix elements of an SU_2 irreducible tensor operator invariant under G. It generalises the f coefficient used by Schönfeld, Flato, and Rosengarten (cf Low and Rosengarten 1964, Flato 1965) in the study of energy levels for transition-metal ions in cubical, tetragonal or trigonal crystalline fields. The f coefficients for numerous chains $SU_2 \supset G_1 \supset G_2 \supset \ldots$ of physical and chemical interest are presently under study in connection with molecular structure calculations on molecular and solid state aggregates. As a preliminary result, extensive tables of f coefficients for the chain $SU_2 \supset O^* \supset D_4^* \supset D_2^*$, i.e. working for cubical, tetragonal, and orthorhombic symmetries, have been the subject of an unpublished report by Kibler and Guichon (1975) which is obtainable from the present author. The f's we deal with in this paper are useful for computing matrix elements, between state vectors of total angular momenta $j_1, j_2 = 0, \frac{1}{2}, \ldots, 6$, of operators transforming as

$$\Phi^4_{\text{cub}} \equiv Y^4_{A_1A_1A} = (7/12)^{1/2} Y^4_0 + (5/24)^{1/2}(Y^4_{-4} + Y^4_4),$$

$$\Phi^6_{\text{cub}} \equiv Y^6_{A_1A_1A} = (1/8)^{1/2} Y^6_0 - (7/16)^{1/2}(Y^6_{-4} + Y^6_4),$$

$$\Phi^2_{\text{tet}} \equiv Y^2_{EA_1A} = Y^2_0,$$

$$\Phi^4_{\text{tet}} \equiv Y^4_{EA_1A} = -(5/12)^{1/2} Y^4_0 + (7/24)^{1/2}(Y^4_{-4} + Y^4_4),$$

$$\Phi^6_{\text{tet}} \equiv Y^6_{EA_1A} = (7/8)^{1/2} Y^6_0 + (1/16)^{1/2}(Y^6_{-4} + Y^6_4),$$

$$\Phi^2_{\text{ort}} \equiv Y^2_{EB_1A} = (1/2)^{1/2}(Y^2_{-2} + Y^2_2),$$

$$\Phi^4_{\text{ort}} \equiv Y^4_{EB_1A} = (1/2)^{1/2}(Y^4_{-2} + Y^4_2),$$

$$\Phi^6_{\text{ort},1} \equiv Y^6_{A_2B_1A} = (11/32)^{1/2}(Y^6_{-2} + Y^6_2) - (5/32)^{1/2}(Y^6_{-6} + Y^6_6),$$

and

$$\Phi^{6}_{\mathrm{ort},2} \equiv Y^{6}_{EB_1A} = (5/32)^{1/2}(Y^{6}_{-2} + Y^{6}_{2}) + (11/32)^{1/2}(Y^{6}_{-6} + Y^{6}_{6}),$$

where Y^k_q denotes the qth spherical harmonic of order k. The basis $\{|ja\Gamma(\mathrm{O}^*)\Gamma(\mathrm{D}_4^*)\Gamma(\mathrm{D}_2^*)\gamma\rangle : j = 0, \frac{1}{2}, \ldots, 6$ and $a\Gamma\gamma$ ranging$\}$ has been chosen in order to get real coefficients in the form $\pm\sqrt{(p/q)}$ $(p, q \in \mathbb{N})$ with simple symmetry properties.

Relation (F11) may be transcribed to $\mathrm{SU}_2 \supset G$ in terms of f symbols as

$$\sum_{\substack{a_1a_2a\\ \gamma_1\gamma_2\gamma}} \left| f\begin{pmatrix} j_1 & j_2 & j \\ a_1\Gamma_1\gamma_1 & a_2\Gamma_2\gamma_2 & a\Gamma\gamma \end{pmatrix} \right|^2$$

$$= [\Gamma_2][\Gamma][\Gamma_1]|\widehat{\mathrm{SU}}_2|^{-1}|\hat{G}|^{-3} \int_{\widehat{\mathrm{SU}}_2} \int_{\hat{G}\otimes 3} \chi^{j_2}(Rs)\chi^{j}(Rt)\chi^{j_1}(R^{-1}u)\chi^{\Gamma_2}(s^{-1})$$

$$\times \chi^{\Gamma}(t^{-1})\chi^{\Gamma_1}(u^{-1})\,\mathrm{d}R\,\mathrm{d}s\,\mathrm{d}t\,\mathrm{d}u.$$

As a special case, we get finally

$$\sum_{a_1a_2a_0} \left| f\begin{pmatrix} j_1 & j_2 & j \\ a_1\Gamma & a_2\Gamma & a_0\Gamma_0 \end{pmatrix} \right|^2$$

$$= |\widehat{\mathrm{SU}}_2|^{-1}|\hat{G}|^{-2} \int_{\widehat{\mathrm{SU}}_2} \int_{\hat{G}\otimes 2} \chi^{j_2}(Rs)\chi^{j}(R)\chi^{j_1}(R^{-1}t)\chi^{\Gamma}(s^{-1}t^{-1})\,\mathrm{d}R\,\mathrm{d}s\,\mathrm{d}t.$$

Acknowledgments

The author's subconscious is indebted to Professor M Flato for pertinent remarks about the theory of invariants ten years ago. Thanks are due to the referees for constructive criticism of the manuscript.

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