Products of generalized equivalent operators in angular momentum theory[1]

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Generalized operator equivalents to the (bipolar) spherical harmonics $T^{(l_1l_2)}_{lm}(\omega_1, \omega_2)$ are considered, viz. $P_{F_1}P_{F_2}T^{(l_1l_2)}_{lm}(\omega_1, \omega_2)\, P_{J_1}P_{J_2}$, where the P_J are projection operators on the manifolds of definite angular momenta. A closed formula is derived for the coefficients of the Clebsch–Gordan decomposition of products of such operators.

On considère des opérateurs généralisés équivalents aux harmoniques sphériques (bipolaires) $T^{(l_1l_2)}_{lm}(\omega_1, \omega_2)$ à savoir $P_{F_1}P_{F_2}T^{(l_1l_2)}_{lm}(\omega_1, \omega_2)\, P_{J_1}P_{J_2}$, où les P_J sont des opérateurs de projection sur les ensembles de moments cinétiques à valeurs définies. On établit une expression finie pour les coefficients de la décomposition Clebsch–Gordan des produits d'opérateurs de ce type.

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1. Introduction

In various physical problems one meets irreducible tensor operators formed by restricting spherical harmonics to a finite portion of the Hilbert space, viz.

$$[1] \qquad \hat{C}_{lm}(F, J) = P_F C_{lm}(\omega) P_J / \langle F || C_l || J \rangle$$

where $C_{lm}(\omega)$ is a spherical harmonic in the notation of Brink and Satchler (1), and P_F is the projection operator on the manifold of states of angular momentum $\mathbf{J}^2 = F(F+1)$, i.e.,

$$[2] \qquad P_F = \sum_{M=-F}^{F} |FM\rangle\langle FM|$$

When $F = J$, one usually replaces the operators

$$[3] \qquad \hat{C}_{lm}(J) \equiv \hat{C}_{lm}(J, J)$$

by explicit expressions constructed out of the components of the vector operator $\mathbf{J}$. These explicit expressions, first introduced by Stevens (2), are called the equivalent operators, and their equivalence to [3] is valid only within the manifold J.

In certain problems one encounters products of equivalent operators $\hat{C}_{lm}(J)$ or the generalized equivalent operators $\hat{C}_{lm}(F, J)$. These problems arise, for example, in studying rotational correlation functions for particles confined to a given manifold (3). To calculate matrix elements of a product of equivalent operators it is convenient to expand the latter in a Clebsch–Gordan series, e.g.,

$$[4] \qquad \hat{C}_{l_1m_1}(F, J)\hat{C}_{l_2m_2}(J, F) = \sum_{lm} \alpha_{lm} C(l_1 l_2 l;\, m_1 m_2 m)\hat{C}_{lm}(F)$$

where the coefficients α_{lm} depend on F and J. One of the purposes of this work is to give a closed expression for these coefficients. It should be noted that, in general, the class of operators $\hat{C}_{lm}(F)$ which appears in the right-hand side of [4] is wider than that defined by [1] and [3], since spherical harmonics do not form a complete set of operators in F. In ref. 3, the coefficients α_{lm} were tabulated for the case $J = F = 1$ which is relevant for ortho-hydrogen molecules at low temperature.

Another example of equivalent-operator products occurs in perturbation calculations (4). In problems involving two orientations one often uses the so-called bipolar harmonics (1), which are the irreducible tensors formed by coupling two spherical harmonics with different arguments,

$$[5] \qquad T^{(l_1l_2)}_{lm}(\omega_1, \omega_2) = \sum_{m_1m_2} C(l_1 l_2 l;\, m_1 m_2 m) C_{l_1m_1}(\omega_1) C_{l_2m_2}(\omega_2)$$

These tensors can be used to expand an arbitrary anisotropic potential $V(\omega_1, \omega_2, q)$, viz.

$$[6] \qquad V(\omega_1, \omega_2, q) = \sum_{lm} \sum_{l_1l_2} V^{(l_1l_2)}_{lm}(q)^* T^{(l_1l_2)}_{lm}(\omega_1, \omega_2)$$

where q denotes the totality of variables other than ω_1 and ω_2 on which the potential may depend. Consider two particles which, in the absence of anisotropic interaction [6], are in the degenerate angular momentum manifold

$$[7] \qquad F_1 \otimes F_2 = \text{Span}\,\{|F_1M_1\rangle\, |F_2M_2\rangle\}$$

The effect of [6] on the states [7] to second order is given by the eigenvalues of an effective operator (5) which contains operator products of the form

$$[8] \qquad \hat{O}(1, 2) = P_{F_1}P_{F_2}T^{(Q_1Q_2)}_{Qq}(\omega_1, \omega_2) \times P_{J_1}P_{J_2}T^{(Q_1'Q_2')}_{Q'q'}(\omega_1, \omega_2) P_{F_1}P_{F_2}$$

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The operator $\hat{O}(1, 2)$ is not a *function* of ω_1 and ω_2 in the coordinate representation, and thus cannot be expanded in terms of the bipolar harmonics [5] even within the manifold F. Choosing a complete set $\hat{T}^{(l_1 l_2)}_{lm}$ of tensor operators in F, we can write

$$[9]\quad \hat{O}(1, 2) = \sum_{lm} \sum_{l_1 l_2} \beta^{(l_1 l_2)}_{lm} \hat{T}^{(l_1 l_2)}_{lm} C(QQ'l;\, qq'm)$$

where the coefficients β are functions of F_1, F_2, J_1, J_2 as well as of all the Q's. In the present work a closed formula for these coefficients is derived, which involves no summation over the magnetic quantum numbers. For the special case with $F_i = 1$, $J_i = 1$ or 3, a set of coefficients equivalent to $\beta^{(l_1 l_2)}_{lm}$ was tabulated in ref. 4.

2. Expressions for the Coefficients α and β

A complete set of tensor operators in the single-particle manifold F is defined by

$$[10]\quad \hat{C}_{lm}(F) = \sum_{MM'} |FM\rangle C(FlF;\, M'mM)\langle FM'|$$

These are 'unit' operators, in the sense that their reduced matrix elements in the manifold F are equal to unity. It is easy to prove that the tensors [10] transform irreducibly under rotations. As pointed out by Biedenharn and Van Dam (ref. 6, p. 8), the assertion of completeness of such a set of operators is, in essence, the content of the Wigner–Eckart theorem. For even values of l the operators $\hat{C}_{lm}(F)$ coincide with those given by [1] and [3], whereas for odd l explicit expressions for $\hat{C}_{lm}(F)$ can be constructed out of components of the angular momentum operator J, e.g.,

$$[11]\quad \hat{C}_1(F) = P_F\, J\, P_F/[F(F+1)]^{1/2}$$

(cf. the operator harmonics of Schwinger, ref. 6, p. 226).

To derive an expression for the coefficients α_{lm} in [4], we invert [4] by using the orthogonality of the Clebsch–Gordan coefficients, and then take matrix elements on both sides of the operator equation, viz.

$$[12]\quad \alpha_{lm}\langle FM|\hat{C}_{lm}|FM'\rangle = \sum_{n} \sum_{m_1 m_2} C(l_1 l_2 l;\, m_1 m_2 m)\langle FM|\hat{C}_{l_1 m_1}|Jn\rangle\langle Jn|\hat{C}_{l_2 m_2}|FM'\rangle$$

Multiplying [12] by $C(FlF;\, M'mM)$ and summing over M, M', we get

$$[13]\quad \frac{2F+1}{2l+1}\alpha_{lm} = \sum C(FlF;\, M'mM)C(l_1 l_2 l;\, m_1 m_2 m)C(Jl_1F_1;\, \mu m_1 M)C(Fl_2J;\, M'm_2\mu)$$

where the summation is over all the magnetic numbers but m. Contraction of the Clebsch–Gordan coefficient gives, finally,

$$[14]\quad \alpha_{lm} = (-)^l \Pi(lJ)\begin{Bmatrix} l_1 l_2 l \\ FFJ \end{Bmatrix}$$

independent of m. Here and in what follows we use the notation

$$[15]\quad \Pi(ab\ldots) \equiv [(2a+1)(2b+1)\ldots]^{1/2}$$

As an example of the application of this formula, we shall evaluate the commutator of two equivalent operators,

$$[16]\quad [\hat{C}_{l_1 m_1}(F), \hat{C}_{l_2 m_2}(F)] = \sum_{lm} 2\gamma_l C(l_1 l_2 l;\, m_1 m_2 m)\hat{C}_{lm}(F)$$

The coefficients γ_l in [16] vanish for even values of $l_1 + l_2 + l$ and are given by

$$[17]\quad \gamma_l = (-)^l \Pi(lF)\begin{Bmatrix} l_1 l_2 l \\ FFF \end{Bmatrix}$$

for odd $l_1 + l_2 + l$. This result agrees with that derived by Nakamura (7) for the special case $F = 1$.

Next, we derive an expression for the β-coefficients, eq. [9]. As a complete set of two-body operators in the manifold $F_1 \otimes F_2$ we take the following tensors

$$[18]\quad \hat{T}^{(l_1 l_2)}_{lm} = \sum \hat{C}_{l_1 m_1}(F_1)\hat{C}_{l_2 m_2}(F_2)C(l_1 l_2 l;\, m_1 m_2 m)$$

The reduced matrix elements of these operators are given in terms of a single $9j$ symbol (ref. 1, p. 152).

The operator $\hat{O}(1, 2)$ in [8] can be rewritten in the form

$$[19] \quad \Delta^{-1}\hat{O}(1,2) = \sum \hat{C}_{Q_1q_1}(F_1, J_1)\hat{C}_{Q_1'q_1'}(J_1, F_1)\hat{C}_{Q_2q_2}(F_2, J_2)\hat{C}_{Q_2'q_2'}(J_2, F_2)C(Q_1Q_2Q; q_1q_2q) \times C(Q_1'Q_2'Q'; q_1'q_2'q')$$

where

$$[20] \quad \Delta = C(J_1Q_1F_1; 00)C(J_2Q_2F_2; 00)C(F_1Q_1'J_1; 00)C(F_2Q_2'J_2; 00)$$

is the factor containing the product of the reduced matrix elements of the spherical harmonics $C_{lm}(\omega)$. Evaluating the one-body operator products with the help of [4] and [14], and using [18] we get

$$[21] \quad \Delta^{-1}\hat{O}(1,2) = \sum_{lm}\sum_{l_1l_2} \hat{T}_{lm}^{(l_1l_2)}\begin{Bmatrix} Q_1Q_1'l_1 \\ F_1F_1J_1 \end{Bmatrix}\begin{Bmatrix} Q_2Q_2'l_2 \\ F_2F_2J_2 \end{Bmatrix}\Pi(l_1l_2J_1J_2)(-)^{l_1+l_2}$$
$$\times \sum C(l_1l_2l; m_1m_2m)C(Q_1Q_1'l_1; q_1q_1'm_1)C(Q_2Q_2'l_2; q_2q_2'm_2)C(Q_1Q_2Q; q_1q_2q)C(Q_1'Q_2'Q'; q_1'q_2'q')$$

In the bottom line of [21] the summation extends over all the magnetic quantum numbers, except q, q', and m. The sum contracts to

$$[22] \quad \Pi(l_1l_2QQ')\begin{Bmatrix} Q & Q' & l \\ Q_1 & Q_1' & l_1 \\ Q_2 & Q_2' & l_2 \end{Bmatrix} C(QQ'l; qq'm)$$

whence we find that the β-coefficients are also independent of m and are given by

$$[23] \quad \Delta^{-1}\beta_{lm} = (-)^{l_1+l_2}(2l_1+1)(2l_2+1)\Pi(J_1J_2QQ')\begin{Bmatrix} Q_1Q_1'l_1 \\ F_1F_1J_1 \end{Bmatrix}\begin{Bmatrix} Q_2Q_2'l_2 \\ F_2F_2J_2 \end{Bmatrix}\begin{Bmatrix} Q & Q' & l \\ Q_1 & Q_1' & l_1 \\ Q_2 & Q_2' & l_2 \end{Bmatrix}$$

A number of examples of the use of this formula are given in an accompanying paper (8).

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