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NOTE

The Calculation of Cubic Harmonics[1]

1 It is often necessary to use linear combinations

$$| \gamma i\rangle = \sum_{m=-l}^{l} a^{l\gamma i}m Y^l m(\theta\phi) \tag{1.1}$$

of spherical harmonics $Y^l m(\theta\phi)$ which transform according to an irreducible representation γ of a finite subgroup of $R3$ (e.g., the cubic group) [1] in molecular and solid-state calculations.

The classical methods for obtaining the coefficients $a^{l\gamma i}m$ are clumsy and inconvenient [2], [3], particularly for large l values. Recent work by Mueller and others [4], [5] has made it desirable to calculate these coefficients for l values up to at least 100 in the case of the cubic group.

In this paper we discuss a group theoretical extension of the familiar recursion formula for associated Legendre Polynomials [6] to cubic harmonics.

2. Although the recursion relation [6] for the $P_n{}^m$ is usually obtained by the methods of classical analysis, it is simply an expression of the reduction of the Kronecker product of two irreducible representations of the rotation group

$$\mathscr{D}_{l-1} \times \mathscr{D}_1 = \mathscr{D}_l + \mathscr{D}_{l-1} + \mathscr{D}_{l-2}\,,$$

or in terms of basis functions

$$| l, m\rangle = \sum_{m'm''} | l-1, m'\rangle \, | 1, m''\rangle\langle l-1, m'; 1, m'' \mid lm\rangle, \tag{2.1}$$

and this relation may be used to calculate $Y^l m(\theta\phi)$ from $Y^{l-1}m'(\theta\phi)$ and $Y^1 m''(\theta\phi)$.

An analogous device may be used to calculate polynomials of degree n in (x, y, z) from polynomials of degree $n-1$ in (x, y, z) and (x, y, z) for irreducible representations of the cubic group

$$| n\gamma i\rangle = \sum_{i'i''} | n-1; \gamma' i'\rangle \, | 1, \gamma'' i''\rangle\langle \gamma' i'; \gamma'' i'' \mid \gamma i\rangle \tag{2.2}$$

[1] Work performed under the auspices of the U.S. Atomic Energy Commission.

since (x, y, z) span the representation Γ_4 of the cubic group, and the cubic Wigner coefficients $\langle \gamma' i'; \gamma'' i'' \mid \gamma i \rangle$ are tabulated [7]. Although (2.2) can be used to generate sets of homogeneous polynomials of degree n in (x, y, z) which span the space of all homogeneous polynomials of degree n in (x, y, z) and transform according to irreducible representations of the cubic group, they are not all spherical harmonics of order n (e.g., $(x^2 + y^2 + z^2)^2$ is homogeneous of degree 4 but is $r^4 Po$).

However, to select out the spherical harmonics of order n, it is necessary only to apply the projection operator

$$I(n) = \sum_{m=-n}^{n} \mid nm \rangle \langle nm \mid . \tag{2.3}$$

3. Let $\mid np\alpha i \rangle$ be the ith vector of the pth occurrence of the representation Γ^{α}, and let $\mid nm \rangle$ be the mth vector of the representation Dn of the full rotation group so that

$$\mid np\alpha i \rangle = \sum_{m=-n}^{n} \mid nm \rangle \langle nm \mid np\alpha i \rangle \tag{3.1}$$

we require the coefficients $\langle nm \mid np\alpha i \rangle$.

For the Fermi-surface determination of Mueller [4], [5] we need only even n values. The coefficients $\langle 2m \mid 2\gamma k \rangle$ are tabulated by Koster *et al.* [7].

We will show how to obtain the coefficients $\langle nm \mid np\alpha i \rangle$ from the coefficients $\langle n-2, m' \mid n-2, q\beta j \rangle$

$$\mid n - 2q\beta j \rangle = \sum_{m'} \mid n - 2m' \rangle \langle n - 2m' \mid n - 2q\beta j \rangle, \tag{3.2}$$

$$\mid p\alpha i \rangle = \sum_{j,k} \mid 2\gamma k \rangle \mid n - 2q\beta j \rangle \langle \gamma k; \beta j \mid p\alpha i \rangle, \tag{3.3}$$

$$= \sum_{m'm''jk} \mid 2m'' \rangle \mid n - 2m' \rangle \langle 2m'' \mid 2\gamma k \rangle \langle n - 2m' \mid q\beta j \rangle \langle \gamma k; \beta j \mid \alpha i \rangle. \tag{3.4}$$

But

$$\mid 2m'' \rangle \mid n - 2m' \rangle = \sum_{NM} \mid NM \rangle \langle NM \mid 2m''; n - 2m' \rangle \tag{3.5}$$

so that

$$\mid p\alpha i \rangle = \sum_{NMm''m'jk} \mid NM \rangle \langle 2m'' \mid 2\gamma k \rangle \langle n - 2m' \mid q\beta j \rangle \langle \gamma k; \beta j \mid \alpha i \rangle. \tag{3.6}$$

Terms with the same N in (3.6) transform among themselves under the cubic group since the $\mid NM \rangle$, $M = -N$ to N afford a representation of the full rotation group. Therefore, the terms with $N = n$ in (3.6) are $\mid np\alpha i \rangle$; i.e.,

$$\langle nm \mid np\alpha i \rangle = \sum_{m''m'jk} \langle 2m'' \mid 2\gamma k \rangle \langle n - 2m' \mid q\beta j \rangle \langle \gamma k; \beta j \mid \alpha i \rangle \langle nm \mid 2m''; n - 2m' \rangle. \tag{3.7}$$

Equation (3.7) is deceptively simple. There are two pitfalls to beware of. One is the labeling by the variable p. It does not appear in the Wigner coefficients $\langle \beta j\, \gamma k \mid \alpha i \rangle$, and yet it springs from nowhere on the left-hand side (3.6) and (3.7). If there is only one occurrence of Γ^{α} in $\Gamma^{\beta} \times \Gamma^{\alpha}$, then p is simply a label that reflects the fact that a given representation may be accessible in more than one way and may occur more than once. When the task of programming is commenced and all the representations that belong with a given n and α are written as a sequential data set, p merely becomes the sequence number of the representation in that data set.

A related problem is that not all the representations obtained by use of (3.7) are necessarily linearly independent. Thus when a new representation $\mid p\alpha i \rangle$ $i = 1 \cdots n\alpha$ has been obtained, it must be checked for linear independence from all those already in the data set before p is incremented by one and it is added to the set.

4. A prototype program has been written in PL/1 and run on an IBM O/S 360 Model 50, making extensive use of 2311 disk and stream I/O for intermediate storage. It took about 27 minutes to reach $n = 24$.

The program is now being rewritten to run under ASP on a 360 75/50 configuration, using record I/O and extensive I/O overlap with CPU processing. It is expected that this program will reach $M = 100$ before rounding errors become significant or CPU time becomes embarrassingly long.

When this new program is running and debugged, we will be willing to distribute tapes carrying the coefficients $\langle nm \mid np\alpha i \rangle$ to interested parties. Inquiries should be addressed to the author of this paper.

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