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## Abstract

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# ALGEBRA OF IRREDUCIBLE CUBIC TENSORS

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For solving problems in which the angular momentum is a conserved quantity, a powerful mathematical apparatus has been created in quantum mechanics, the development of which is due mainly to E. Wigner (1) and G. Racah (2). This apparatus includes the theory of $3j$, $6j$, $9j, \dots, 3nj$-symbols (1–3), the theory of genealogical coefficients (2), and the algebra of tensor operators (2,3). It has found wide application in the theory of atomic and nuclear spectra; with its aid various calculations connected with the use of eigenfunctions of angular momentum, or basis functions of irreducible representations of the group of three-dimensional rotations $R_3$, are substantially simplified.

If a problem possesses not spherical symmetry but some other symmetry characterized by a group $G$, then it becomes necessary to generalize this technique to groups different from $R_3$. Wigner showed that the theory of $3j, 6j, \dots, 3nj$-symbols for the so-called simply reducible groups can be constructed in complete analogy with the corresponding theory for $R_3$. The simply reducible groups include a number of point groups (the cubic $3/4\,T_d$, $3/4 = O$, $\bar{6}/4 = O_h$; the group $3 \cdot m = C_{3v}$, etc.), the permutation groups $S_3$ and $S_4$, and others. The Wigner–Eckart theorem, the fundamental theorem of the algebra of tensor operators (4), was extended to all groups. In recent years, a similar mathematical apparatus has been intensively developed for cubic groups, since in practice one very often has to deal with problems possessing cubic symmetry. These are, first of all, the problem of the spectrum of an ion in a strong crystalline field (5). We encounter problems possessing cubic symmetry in the consideration of many molecules. The same problems also arise in the $\alpha$-particle model of the nucleus (6). The properties of $3j$, $6j$, and $9j$-symbols for cubic groups were studied in works (5,7–10), where tables of numerical values of these quantities were compiled. One-particle genealogical coefficients for these groups were considered and calculated (7,11).

At present, the technique of $3nj$-symbols and genealogical coefficients is widely used in ligand-field theory for studying the spectra of impurity ions in crystals and the spectra of complex ions (5,7). It seems expedient to supplement this apparatus with the algebra of cubic tensors, which is a generalization of the algebra of tensor operators for the group $R_3$. The need for this generalization arises in considering electromagnetic transitions for ions in a crystal. This technique will also be useful in the case when, along with cubic fields, fields of lower symmetries must also be taken into account. Moreover, it can be used to analyze the coupling of vibrations with rotations in molecular spectra ([12]), etc.

Let there be a set of orthonormal functions $\psi_{j\mu}(\mathbf{r})$ forming a basis of an irreducible representation $j$ of some cubic group (for definiteness we shall have in mind the tetrahedral group 3/4). The index $\mu$ indicates the row of the representation matrix according to which transforms

The function $\psi_{j\mu}$; $\mu$ takes as many different values as the dimension of the irreducible representation $j$, which we shall denote by the symbol $[j]$.

When the operation $R$ of the given cubic group is performed, the basis functions $\psi_{j\mu}$ of the irreducible representation $j$ are transformed by means of the matrix of this representation $\Delta^j_{\mu\mu'}(R)$:

$$R\psi_{j\mu'} = \sum_{\mu} \psi_{j\mu}\Delta^j_{\mu\mu'}(R). \tag{1}$$

When the same operation $R$ is performed, the operator $U$, acting on the basis functions $\psi_{j\mu}$, is transformed according to the law

$$U' = RUR^{-1}. \tag{2}$$

An irreducible cubic tensor of type $k$ is defined as a set $[k]$ of operators $U^k_q$, which under the operations of the given cubic group are transformed in the same way as the functions $\psi_{kq}$ forming a basis of the irreducible representation $k$ of this group, i.e.,

$$Ru^{kR^{-1}}_{q'} = \sum_{q} u^k_q \Delta^k_{qq'}(R). \tag{3}$$

Most operators used in quantum-mechanical calculations either are themselves irreducible cubic tensors or can be represented in the form of a certain combination of them. Thus, the coordinate and momentum operators of a particle are tensors of type $T_2$ (the group $3/\bar{4}$ is meant), the operators of orbital angular momentum, spin, and magnetic moment are tensors of type $T_1$, the operator of an electric dipole transition transforms according to the representation $T_2$, the 5 components of the electric quadrupole-moment operator decompose into 2 cubic tensors of types $E$ and $T_2$, etc. Cubic tensors occur in molecular theory, in the $\alpha$-particle model of the nucleus, in crystal-field theory, and so on. In particular, for molecules possessing symmetries $3/\bar{4}$, 3/4, etc., the coordinate operators of normal vibrations $Q_{kq}$, or the corresponding operators of creation and absorption of vibrational quanta, are components of a cubic tensor of type

$k$. In crystal-field theory, along with the principal field possessing cubic symmetry, the influence of fields of lower symmetry (trigonal, tetragonal) is taken into account. The potentials describing fields of lower symmetry also constitute a set of cubic tensors.

For irreducible cubic tensors, as for spherical tensors, the Wigner—Eckart theorem is valid ⁽⁵⁾:

$$\langle \gamma' j' m' \mid U_q^k \mid \gamma j m \rangle = \frac{\langle jmkq \mid j'm' \rangle}{[j']^{1/2}} \langle \gamma' j' \| U^k \| \gamma j \rangle = \left\langle \begin{matrix} jkj' \\ mqm' \end{matrix} \right\rangle \langle \gamma' j' \| U^k \| \gamma j \rangle. \tag{4}$$

This equality is not only an expression of the Wigner—Eckart theorem, but also a definition of the reduced matrix element $\langle \gamma' j' \| U^k \| \gamma j \rangle$. Here $j, k, j'$ are symbols of irreducible representations of the cubic group; $\gamma, \gamma'$ are other quantum numbers characterizing the wave function (for example, the magnitude of the angular-momentum quantum number $l$ in a cubic harmonic, etc.).

In order to calculate the reduced matrix element, one must calculate the full matrix element for a concrete set of values $m, q, m'$ and then divide it by the values of the $3j$-symbol (tables of $3j$-symbols or equivalent quantities may be found in works ⁽⁶, ⁸⁻¹¹⁾).

The basic propositions and relations of the algebra of spherical tensors ⁽¹⁻³⁾ are directly generalized to cubic groups.

The tensor product of two cubic tensors $T_{q_1}^{k_1}$ and $U_{q_2}^{k_2}$ is defined as follows:

$$[T_{q_1}^{k_1} \times U_{q_2}^{k_2}]_q^k = \sum_{q_1 q_2} T_{q_1}^{k_1} U_{q_2}^{k_2} [k]^{1/2} \left\langle \begin{matrix} k_1 k_2 k \\ q_1 q_2 q \end{matrix} \right\rangle . \tag{5}$$

If, from the functions $\psi_{j_1\mu_1}(x_1)$, $\psi_{j_2\mu_2}(x_2)$, a total function $|j_1 j_2 j \mu\rangle$ has been constructed, transforming according to the representation $j$ of the given cubic group, and the operator $T$ acts only on the variables $x_1$, while the operator $U$ acts only on $x_2$, then the reduced matrix element of the tensor product (5) has the form

$$\langle \gamma j_1 j_2 : j \| [T^{k_1} \times U^{k_2}]^k \| \gamma' j_1' j_2' : j' \rangle =$$

$$= [j]^{1/2} [j']^{1/2} [k]^{1/2} \begin{bmatrix} k & j & j' \\ k_1 & j_1 & j_1' \\ k_2 & j_2 & j_2' \end{bmatrix} \sum_{\gamma''} \langle \gamma j_1 \| T^{k_1} \| \gamma'' j_1' \rangle \langle \gamma'' j_2 \| U^{k_2} \| \gamma' j_2' \rangle. \tag{6}$$

The properties of the 9-$j$ symbols for cubic groups entering this formula have been investigated in paper (⁷); the numerical values of these coefficients are also given there (see also (⁸)).

If one of the representations $j$, $k$, $j'$ is the totally symmetric one ($A_1$), then formula (6) is simplified. For example, for $k = A_1$ ($k = 0$) we have*

$$\langle \gamma j_1 j_2 : j\mu \| [T^{k_1} \times U^{k_1}]^0 \| \gamma' j_1' j_2' : j'\mu' \rangle =$$

$$= \delta_{jj'} \delta_{\mu\mu'} (-1)^{j_2+j_2+j+k_1} \begin{bmatrix} j_1 & j_2 & j \\ j_2' & j_1' & k_2 \end{bmatrix} [k_1]^{-1/2} \sum_{\gamma''} \langle \gamma' j_1 \| T^{k_1} \| \gamma'' j_2' \rangle \langle \gamma'' j_2' \| U^{k_1} \| \gamma j_2' \rangle. \tag{7}$$

If the operator $U^{k_2}_{q_2} = 1$, then

$$\langle \gamma j_1 j_2 : j \| T^{k_1} \| \gamma' j_1' j_2' : j' \rangle =$$

$$= \delta_{j_2 j_2'} (-1)^{j_1+j_2+j'+k_1} [j]^{1/2} [j']^{1/2} \begin{bmatrix} j_1 & j_2 & j \\ j' & k_1 & j_1' \end{bmatrix} \langle \gamma j_1 \| U^{k_1} \| \gamma' j_1' \rangle. \tag{8}$$

The formula for the matrix element of the tensor product of two operators acting on one and the same variable has the form

$$\langle \gamma' j' \| [T^{k_1} \times U^{k_2}]^k \| \gamma j \rangle =$$

$$= (-1)^{j+j'+k} [k]^{1/2} \sum_{\gamma'' j''} \langle \gamma' j' \| T^{k_1} \| \gamma'' j'' \rangle \langle \gamma'' j'' \| U^{k_2} \| \gamma j \rangle \begin{bmatrix} k_1 k_2 k & & \\ j & j' & j'' \end{bmatrix}. \tag{9}$$

In contrast to paper ($^{13}$), where, in the mean crystal-field approximation, $j$-symbols and genealogical coefficients for the group $R_3$ are used and where the energy of an ion in a crystal field is expanded in spherical harmonics, in the strong crystal-field approximation it is expanded in crystal harmonics

$$V_{\text{cr}}(\mathbf{r}_1, \dots, \mathbf{r}_N) = \sum_{l\gamma j\mu} \sum_{i=1}^{N} B^{l\pi}_{\gamma j\mu} t^{l\pi}_{\gamma j\mu}(\mathbf{r}_i), \tag{10}$$

where

$$t^{l\pi}_{\gamma j\mu}(\mathbf{r}) = V_l(r) \, |(l^\pi)\gamma j\mu\rangle. \tag{11}$$

*

In formula (7) and in what follows the expression $(-1)^j$ may be understood literally if the irreducible representations of the cubic groups $A_1, E, T_2$ are numbered by even integers $j$, and the representations $A_2$ and $T_1$ by odd integers. For example, one may, as is done in paper ($^{10}$) for the tetrahedron group, assign $j = 0, 1, 2, 3, 4$ to the representations $A_1, A_2, E, T_1, T_2$, respectively.

The formula for the reduced matrix element has the form

$$\left\langle (l_2^{\tau_2})\gamma_2 j_2 \left\| t_{\gamma\mu}^{l\pi} \right\| (l_1^{\pi_1})\gamma_1 j_1 \right\rangle = \sum_{\substack{lmm_1m_2\\ \mu\mu_1\mu_2}} \left\langle \begin{matrix} j_1 j j_2 \\ \mu_1 \mu \mu_2 \end{matrix} \right\rangle \left( \alpha_{\gamma_2 j_2 \mu_2}^{l_2^{\pi_2} m_2} \right)^* \cdot \alpha_{\gamma j \mu}^{l\pi m} \alpha_{\gamma_1 j_1 \mu_1}^{l_1 \pi_1 m_1} \left\langle \psi_{\gamma_2 j_2}(\mathbf{r}) \left| V_l(\mathbf{r}) \right| \psi_{\gamma_1 j_1}(\mathbf{r}) \right\rangle (l_1 m_1 l m \mid l_2 m_2)(l_2 \| l \| l_1), \tag{12}$$

where the reduced matrix element for spherical harmonics is calculated from the formula

$$(l_2 \| l \| l_1) = \sqrt{\frac{(2l+1)(2l_1+1)}{4\pi(2l_2+1)}}\,(l_1 0 l 0 \mid l_2 0). \tag{13}$$

The combined use of the formulas and relations given in the present article and of the ordinary algebra of spherical tensors makes it possible to calculate, in a uniform way, matrix elements encountered in practice, into which enter irreducible representations both of the rotation group and of point groups.

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*Note: Figure translations are in progress. See original paper for figures.*

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