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Dipole sum rules for products of 3-j symbols

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Abstract. New sum rules involving particular products of many 3-j symbols are established. These sum rules are useful in multiphoton calculations.

A number of new interesting identities satisfied by n-j symbols have been discovered in the course of recent work on simple many-particle systems such as the hydrogen molecular ion (Dunlap and Judd 1975) and the helium atom (Morgan 1975, 1977). In this connection we would like to call attention to a somewhat different kind of sum rule for products of many 3-j symbols, which occur naturally in a perturbation treatment of higher-order radiative transitions in one-electron atoms. To the best of our knowledge, no equivalent results have been reported before, although the sums involved present some analogy with those entering the so called contraction formulae.

The sums we were concerned with may be written as

$$S_q^{(N)} = \sum_{L,\lambda,\lambda'} [L;\lambda,\lambda'] \begin{pmatrix} L & 1 & \lambda_{N-1} \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} L & 1 & \lambda'_{N-1} \\ 0 & 0 & 0 \end{pmatrix} \cdots \begin{pmatrix} \lambda_i & 1 & \lambda_{i-1} \\ 0 & 0 & 0 \end{pmatrix}$$
$$\times \begin{pmatrix} \lambda'_i & 1 & \lambda'_{i-1} \\ 0 & 0 & 0 \end{pmatrix} \cdots \begin{pmatrix} \lambda_1 & 1 & l \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} \lambda'_1 & 1 & l \\ 0 & 0 & 0 \end{pmatrix} \sum_{M,\mu,\mu',m} \begin{pmatrix} L & 1 & \lambda_{N-1} \\ -M & q & \mu_{N-1} \end{pmatrix}$$
$$\times \begin{pmatrix} L & 1 & \lambda'_{N-1} \\ -M & q & \mu'_{N-1} \end{pmatrix} \cdots \begin{pmatrix} \lambda_i & 1 & \lambda_{i-1} \\ -\mu_i & q & \mu_{i-1} \end{pmatrix} \begin{pmatrix} \lambda'_i & 1 & \lambda'_{i-1} \\ -\mu'_i & q & \mu'_{i-1} \end{pmatrix}$$
$$\times \cdots \begin{pmatrix} \lambda_1 & 1 & l \\ -\mu_1 & q & m \end{pmatrix} \begin{pmatrix} \lambda'_1 & 1 & l \\ -\mu'_1 & q & m \end{pmatrix}, \tag{1}$$

where

$$[L;\lambda,\lambda'] = (2L+1)\prod_{i=1}^{N-1}(2\lambda_i+1)(2\lambda'_i+1) \qquad \text{and} \qquad q = 0, \pm 1.$$

For brevity in equation (1) we have used a single greek summation index to denote a whole set of the same name (e.g. λ stands for $\lambda_1, \lambda_2, \ldots, \lambda_{N-1}$), so that each term is in fact a weighted product of $4N$ 3-j symbols. In spite of its intricate appearance the summation above may be evaluated easily in closed form. The result looks surprisingly simple, and does not depend on l:

$$S_0^{(N)} = 1/(2N+1); \qquad S_{\pm 1}^{(N)} = N!/(2N+1)!!. \tag{2}$$

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In order to get a better understanding of the genesis and the significance of equation (1) it is necessary to go back to the associated physical process: ionisation of an atom initially in the state $|n, l\rangle$ through absorption of N photons of energy $\hbar\omega$ and polarisation $\boldsymbol{\epsilon}$ from a laser beam (see, for instance, Maquet 1977 and references therein). Within the framework of conventional perturbation theory the total cross section of this process in the dipole approximation is given by

$$\sigma_{nl;q}^{(N)} = (2l+1)^{-1} \sum_{m=-l}^{l} \int \mathrm{d}\Omega_{\hat{k}} |\langle \hat{k} | A_{nlm;q}^{(N)} \rangle|^2, \tag{3}$$

where $\hat{k}$ is a unit vector along the propagation direction of the outgoing photoelectron, and

$$|A_{nlm;q}^{(N)}\rangle = (4\pi/3)^{N/2} \sum_{L,M,\lambda,\mu} |LM\rangle\langle LM| Y_{1,q} |\lambda_{N-1}\mu_{N-1}\rangle \ldots \langle \lambda_1 \mu_1 | Y_{1,q} | lm \rangle T_{L,\lambda,l;n}^{(N)}(\omega) \tag{4}$$

represents the Nth-order transition amplitude. The ket $|\hat{k}\rangle$ denotes an angular state in which the polar coordinates have definite values θ, ϕ, and in particular one has $\langle \hat{k} | lm \rangle = Y_{l,m}(\theta, \phi)$. The spherical harmonic $Y_{1,q}$ stems from the electric dipole operator $\boldsymbol{\epsilon} \cdot \boldsymbol{r}$ with $q = 0$ for linear polarisation, and $q = \pm 1$ for circular polarisation. On the other hand, the quantities $T_{L,\lambda,l;n}^{(N)}(\omega)$ are essentially the radial amplitudes for the different transitions from the initial to the final state through intermediate states of angular momenta $\lambda_1, \lambda_2, \ldots, \lambda_{N-1}$, and their evaluation is in general a very difficult task. However, in view of the increasing complexity of the angular momentum algebra, much care must be exercised also to ensure that all the components are correctly taken into account (Heno *et al* 1976). In this respect the above results may provide a useful check for numerical calculations.

A simple proof of our sum rules may be given on starting from the fictitious Nth-order amplitude

$$|B_{lm;q}^{(N)}\rangle = (4\pi/3)^{N/2} \sum_{L,M,\lambda,\mu} |LM\rangle\langle LM| Y_{1,q} |\lambda_{N-1}\mu_{N-1}\rangle \ldots \langle \lambda_1 \mu_1 | Y_{1,q} | lm \rangle, \tag{5}$$

which is obtained by discarding all the radial factors in equation (4). It is then easy to see that the sum $S_q^{(N)}$ is just the pseudo-cross section corresponding to this fictitious amplitude, i.e.

$$S_q^{(N)} = (2l+1)^{-1} \sum_{m=-l}^{+l} \int \mathrm{d}\Omega_{\hat{k}} |\langle \hat{k} | B_{lm;q}^{(N)} \rangle|^2. \tag{6}$$

To this end it suffices to express the integrals as usual over a product of three spherical harmonics in terms of 3-j symbols (Edmonds 1960) and to insert equation (5) as it stands into equation (6).

The crucial point now is to notice that the absence of the radial amplitudes allows us to rewrite equation (5) in the contracted form

$$|B_{lm;q}^{(N)}\rangle = (4\pi/3)^{N/2} (Y_{1,q})^N |lm\rangle \tag{7}$$

by using the closure theorem for spherical harmonics:

$$\sum_{\lambda\mu} |\lambda\mu\rangle\langle\lambda\mu| = I. \tag{8}$$

Substitution of equation (7) into equation (6) gives

$$S_q^{(N)} = (2l+1)^{-1}(4\pi/3)^N \sum_{m=-l}^{l} \int \mathrm{d}\Omega_{\hat{k}} |\langle \hat{k}|(Y_{1,q})^N|lm\rangle|^2, \tag{9}$$

and this may be transformed further by using a particular case of the addition theorem for spherical harmonics

$$\sum_{m=-l}^{+l} \langle \hat{k}|lm\rangle\langle lm|\hat{k}\rangle = (2l+1)/4\pi, \tag{10}$$

so that

$$S_q^{(N)} = (4\pi)^{-1}(4\pi/3)^N \int \mathrm{d}\Omega_{\hat{k}} |Y_{1,q}(\hat{k})|^{2N}. \tag{11}$$

Since:

$$(4\pi/3)^{1/2} Y_{1,0}(\hat{k}) = \cos\theta, \tag{12a}$$

$$(4\pi/3)^{1/2} Y_{1,\pm1}(\hat{k}) = \pm\sin\theta\, \mathrm{e}^{\pm\mathrm{i}\phi}/\sqrt{2}, \tag{12b}$$

the integration over $\hat{k}$ eventually gives the results stated in equation (1).

Whereas the derivation presented here is very simple indeed, one may question whether equation (2) could be obtained so easily by an entirely algebraic method, on using the machinery of angular momentum theory. In the particular case $N=1$ equation (1) reduces to

$$S_q^{(1)} = \sum_{L,M,m} (2L+1)\begin{pmatrix} L & 1 & l \\ 0 & 0 & 0 \end{pmatrix}^2 \begin{pmatrix} L & 1 & l \\ -M & q & m \end{pmatrix}^2, \tag{13}$$

and the result $S_q^{(1)} = \frac{1}{3}$ follows trivially at once from the usual orthogonality relations for 3-*j* symbols. For $N>1$ the problem seems to be much more involved. An algebraic proof for arbitrary N has been given by Sureau (private communication), who used the graphical method of Yutsis *et al* (1962), but required a large amount of work, in contrast to the analytical approach presented here.

Similar sum rules may be established of course for any multipole operator. Other interesting summation formulae have been worked out by Heno (private communication), who considered various bound–bound multiphoton transitions, instead of bound–free transitions.

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