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Some classes of 'nontrivial zeroes' of angular momentum addition coefficients

T A Heim[1], **J Hinze**[2,4] **and A R P Rau**[3]

[1] University of Applied Sciences Northwestern Switzerland, Steinackerstrasse 5, CH-5210 Windisch, Switzerland

[2] Theoretische Chemie, Fakultät für Chemie, Universität Bielefeld, D-33615 Bielefeld, Germany

[3] Department of Physics and Astronomy, Louisiana State University, Baton Rouge, LA 70808, USA

E-mail: thomas.heim@unibas.ch and arau@phys.lsu.edu

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Abstract

Angular momentum coupling in quantum physics obeys obvious symmetries of rotation and reflection so that the Clebsch–Gordan (vector coupling) coefficients or Wigner $3j$-symbols describing the coupling vanish unless these symmetries are satisfied. However, it has long been observed that there are 'accidental' or 'nontrivial' zeroes of some coefficients even when the obvious symmetries are satisfied. Partial explanations and conjectures on the systematics of some of these zeroes have been advanced. We provide some more and propose as well 'near zeroes' which, while not exactly vanishing, are extremely small in magnitude. Connections are made to zeroes of Legendre and hypergeometric polynomials and to classical and semi-classical pictures for the addition of angular momenta. A convenient ordering scheme for $3j$'s that incorporates Regge symmetries also emerges. Further aspects of our analysis concern radial matrix elements of powers of r in a Coulomb potential that have analogous expressions to $3j$'s as a result of a non-compact $O(2,1)$ counterpart of the $O(3)$ group symmetry of rotations. Some remarks are made on possible realization in actual physical systems.

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1. Introduction

The addition of two angular momenta j_1 and j_2 in quantum physics to yield a third j_3 is familiar throughout physics. These are restricted to integer or half-odd integer values and the

[4] Deceased 10 October 2008.

three quantities must form a 'triad', that is, their magnitudes must be representable as three sides of a triangle. Only such triplets can occur as legitimate Clebsch–Gordan or Wigner coefficients for quantum angular addition or in the equivalent, somewhat more symmetric, form called $3j$-symbols [1–5],

$$\begin{pmatrix} j_1 & j_2 & j_3 \\ m_1 & m_2 & m_3 \end{pmatrix}. \tag{1}$$

Here, m are the projection quantum numbers of the corresponding angular momentum on the quantization z-axis (with reversed sign in one case), with $|m| \leqslant j$, and satisfy the requirement $m_1 + m_2 + m_3 = 0$.

Extensive tables[5] [4, 6, 7] and computer programs are available for these $3j$-symbols which record only those triplets which satisfy the above basic requirements. A glance through such a table will show zeroes in the values of certain $3j$'s, an example being

$$\begin{pmatrix} 3 & 3 & 2 \\ 2 & -2 & 0 \end{pmatrix}. \tag{2}$$

There is no obvious reason why this should vanish, in that it represents the addition of two angular momenta of magnitude 3 with equal and opposite m which can lead to an angular momentum 2 with zero z-projection. Hence, they are referred to as 'accidental zeroes' [4, 8]. We will return to this particular coefficient later but note that it arises in quadrupolar coupling and thus has concrete realizations, especially in nuclear E2 transitions (p 415 of [8]). Similar results on nontrivial zeroes obtain for other angular momentum coefficients such as $6j$ but we confine our discussion to the $3j$.

In the 1980s, several authors [9–14] observed whole classes of nontrivial zeroes of $3j$'s, an example being $\left(\begin{smallmatrix} j_1 & j_2 & j_1+j_2-1 \\ m_1 & m_2 & -(m_1+m_2) \end{smallmatrix}\right)$, when $m_1/j_1 = m_2/j_2$ [9]. In a usual geometrical picture of angular momentum j as a vector lying on a cone about the z-axis, with m its projection onto that axis, this would indicate that the conical angle or 'tilt' must be preserved[6]. Further, the familiar Regge symbol and symmetries [6, 15] expressed by the recasting of a $3j$-symbol in (1) as

$$\begin{pmatrix} -j_1+j_2+j_3 & j_1-j_2+j_3 & j_1+j_2-j_3 \\ j_1-m_1 & j_2-m_2 & j_3-m_3 \\ j_1+m_1 & j_2+m_2 & j_3+m_3 \end{pmatrix}, \tag{3}$$

places a unity at the top right corner of this matrix for such a $3j$. Calling the lowest entry in the Regge matrix (3) the 'weight' [10] ('degree' in some places [13, 14], 'order' in others) which we denote by c, this particular vanishing $3j$-symbol was seen as describing all non-trivial zeroes of weight 1. The proof involved solving a Diophantine equation, but alternative proofs relating the $3j$-symbol to a hypergeometric function ${}_3F_2$ with five indices and argument $z = 1$ have also been given, and we will also provide simpler proofs below. Some zeroes were also investigated for higher weights [11–14, 16] and we will present results for general c.

Another set of conjectured zeroes consists of[7]

$$\begin{pmatrix} j_1 & j_2 & j_3 \\ 1 & -1 & 0 \end{pmatrix}, \tag{4}$$

[5] Equation (1.11) of [6] should have all signs of m on the right-hand side reversed and in equation (1.12), the second and third columns should be interchanged. Furthermore, the last factor in the square root in equation (1.52) should read $(L - 2l_3)$.

[6] This concept was advanced by U Fano as a geometrical element, that 'shape' is conserved but, in discussions with one of the authors (ARPR), the word 'tilt' was chosen as a better term.

[7] The original conjecture by S Brudno was modified by one of the authors (ARPR) to incorporate some necessary constraints.

when $j_3(j_3+1) = j_1(j_1+1) + j_2(j_2+1)$ and $j_1 + j_2 + j_3$ is even. Examples include $\begin{pmatrix} 3 & 5 & 6 \\ 1 & -1 & 0 \end{pmatrix}$, $\begin{pmatrix} 6 & 9 & 11 \\ 1 & -1 & 0 \end{pmatrix}$ and $\begin{pmatrix} 14 & 14 & 20 \\ 1 & -1 & 0 \end{pmatrix}$, which have respective weights 2, 4 and 8. This observation is an interesting complement to a known result (corrected equation (1.52) in [6]; see footnote 5 on p 2) that establishes a proportionality between $\begin{pmatrix} j_1 & j_2 & j_3 \\ 1 & -1 & 0 \end{pmatrix}$ and $\begin{pmatrix} j_1 & j_2 & j_3+1 \\ 0 & 0 & 0 \end{pmatrix}$ applicable for odd $j_1 + j_2 + j_3$, such $3j$'s having no accidental zeroes.

In this paper, we collect together these various observations on nontrivial zeroes, systematize them and analyze in terms of different weights, and connect to the hypergeometric function and other special functions to bring out the structures in a simple fashion and, at the same time, extend to other classes of such zeroes. We will also connect to the 'classical limit' of high values of angular momenta [2, 17–22] when the $3j$'s are known to reduce to rotation functions (appendix 2 of [1, 23–26]) and Legendre polynomials (equation (1.59) of [6], p 77 of [27], problem 5.5 of [5, 28, 29]), which sheds further light on the vanishing of certain $3j$'s and points to 'near zeroes' which, while not exactly vanishing are almost so, taking sometimes astonishingly low numerical values. An example is $\begin{pmatrix} 15 & 15 & 3 \\ 12 & -12 & 0 \end{pmatrix}$, with absolute value 0.000 29. Another is the whole family

$$\begin{pmatrix} d^2 & 2d^2-d & d^2 \\ (d-1)(d+2)/2 & -(d-1)(d+2)/2 & 0 \end{pmatrix}, \tag{5}$$

which is exactly zero for $d = 1, 2, 3$, takes the absolute value 0.002 03 for $d = 4$, reaches a small peak absolute value of 0.011 at $d = 9$, declining continuously after that to zero, falling below 0.0001 at $d = 19$.

2. Standardized classification by 'weight' and accidental zeroes

A $3j$-symbol has five independent parameters because of the constraint that the bottom entries sum to zero. Its Regge form in (3) has similarly five parameters which, with the weight c in the upper right corner, can be arranged as

$$\begin{pmatrix} & & c \\ p & q & \\ r & s & \end{pmatrix}, \tag{6}$$

with $p = j_1 - m_1, q = j_2 - m_2, r = j_1 + m_1, s = j_2 + m_2$. The remaining entries can be filled in easily as $(q + s - c)$, $(p + r - c)$ in the first row and $(r + s - c)$, $(p + q - c)$ in the last column. As in (3), each row and column in the Regge matrix sum to the same value, $p + q + r + s - c = j_1 + j_2 + j_3$.

We note first that a Regge matrix with two rows or columns identical, and with the sum of all entries odd, is a trivial zero because it can always be recast as the symbol $\begin{pmatrix} j_1 & j_2 & j_3 \\ 0 & 0 & 0 \end{pmatrix}$, with $j_1 + j_2 + j_3$ odd which vanishes [6]. This is called a symmetry under parity (see equation (10.15) of [3]) in the permutation of j_1 and j_2 and under 'frame reversal', that is, reversal of the sign of all m indices (section 5.1.4 of [5]). Nearly all the zeroes that occur in these tables [6] are such trivial zeroes with only six distinct exceptions.

With $j_3 = j_1 + j_2 - c$ in (1), and casting in the above standard form of weight c, apart from non-vanishing factors, the $3j$ in (1) involves the factor (see equation (5.9) or (5.15) of [5])

$$\sum_{n=0}^{c} (-1)^n \binom{c}{n} \binom{2j_1 - c \equiv b}{j_1 - m_1 - n} \binom{2j_2 - c \equiv a}{j_2 + m_2 - n}, \tag{7}$$

each of the three factors a binomial coefficient. Any zero can only result from a vanishing of this expression. Defining[8] the 'tilt' as $x \equiv m/j$, we can now systematize (7) for various values of c.

Thus, for $c = 1$, (7) reduces to two terms,

$$\left(\frac{1+x_1}{1-x_1}\frac{1-x_2}{1+x_2} - 1\right). \tag{8}$$

Clearly, this vanishes only for $x_1 = x_2$, that is, equal tilt as observed in [14] but proved previously [9] by more complicated methods.

For $c = 2$, (7) has three terms,

$$\frac{(1+x_1)(1-x_2)}{(1-x_1)(1+x_2)}\frac{(1+x_1-1/j_1)(1-x_2-1/j_2)}{(1-x_1-1/j_1)(1+x_2-1/j_2)} - 2\frac{(1+x_1)(1-x_2)}{(1-x_1-1/j_1)(1+x_2-1/j_2)} + 1. \tag{9}$$

Note first, that in the classical limit of large j_1 and j_2, (9) reduces to the square of (8) and thus vanishes for the same condition as before, that the tilts x are equal. Indeed, this holds true in general for large angular momenta because the expression in (7) reduces to $\sum_{n=0}^{c}(-1)^n\binom{c}{n}$ and thereby vanishes for all $c \neq 0$. This proves that the only non-zero $3j$ is for $c = 0$, that is $j_3 = j_1 + j_2$, or for the same tilt.

The non-triviality of the above result is worth noting, that it applies to all c, that is, all values of j_3 for a given (j_1, j_2), both large. A more straightforward conclusion due to the parity symmetry noted already applies for $j_1 = j_2$ (whether large or not), with $x_1 = x_2$, that all $3j$ for odd c vanish. In this case, the first two columns of the Regge matrix are identical and, as noted, can be mapped into a $3j$ with all m values zero which vanishes when $j_1 + j_2 + j_3$ is odd. But the preservation of tilt, that only the $3j$ with $c = 0$ is non-zero, so that the tilt x_3 equals $x_1 = x_2$ is a stronger conclusion.

Other cases of zeroes or near-zeroes for $c = 2$ can be read off easily from (9). For $x_1 = x_2$, there is no exact zero in general although for large j_1 and j_2, the expression nearly vanishes. For $x_1 = 0$, that is, when one tilt is zero, a zero occurs when

$$x_2 = \sqrt{(j_1 + j_2 - 1)/(j_2(2j_1 - 1))}, \tag{10}$$

an example being $\begin{pmatrix} 4 & 4 & 6 \\ 0 & 2 & -2 \end{pmatrix}$.

For $x_1 = -x_2$, that is, opposite tilts, a zero occurs when

$$x_2 = \sqrt{(j_1 + j_2 - 1)/(8j_1 j_2 - 3j_1 - 3j_2 + 1)}, \tag{11}$$

while for $x_1 j_1 = -x_2 j_2$, that is, 'opposite projections' $m_1 = -m_2$, a zero occurs for

$$m_1 = -m_2 = \sqrt{j_1 j_2/(2(j_1 + j_2) - 1)}, \tag{12}$$

an example being $\begin{pmatrix} 5 & 3 & 6 \\ 1 & -1 & 0 \end{pmatrix}$, a zero already encountered as an example of (4).

Similar results pertain to $c = 3$. Again, for $x_1 = x_2$, there are only trivial zeroes for $x_1 = x_2 = 0$ or $j_1 = j_2$ but, for large angular momenta, near zeroes occur associated with the result in the classical limit. For $x_1 = 0$, a zero occurs for

$$x_2 = \sqrt{\left(3j_1 j_2 + 3j_2^2 - j_1 - 6j_2 + 2\right)/\left(j_2^2(2j_1 - 1)\right)}, \tag{13}$$

[8] Alternatives to the ratio that have been used elsewhere in the literature are $m/\sqrt{j(j+1)}$ and the semi-classical replacement $m/(j + 1/2)$. All have merit in appropriate contexts, as we also use in this paper, but in results such as (10)–(14), the use of the entries m and j themselves that occur in the $3j$ prove appropriate.

examples being $\binom{3\ 6\ \ 6}{0\ 5\ -5}$ and $\binom{9\ 9\ \ 15}{0\ 5\ -5}$ although the former is actually a weight-one zero. For 'opposite projections' $m_1 = -m_2$, a zero occurs for

$$m_1 = -m_2 = \sqrt{(3j_1j_2 - j_1 - j_2)/(2j_1 + 2j_2 - 3)}, \tag{14}$$

an example provided by $\binom{23/2\ \ 13/2\ \ 15}{5/2\ \ -5/2\ \ 0}$.

Sometimes, a zero of lower weight is more easily viewed in terms of the next higher entry in (6). Thus, $\binom{7/2\ \ 15/2\ \ 9}{1/2\ \ -5/2\ \ 2}$ is a weight $c = 2$ zero, but it does not belong to any of the categories in (9)–(12). However, in its Regge form in (6), it has two equal entries that can be brought to the positions p and r through Regge symmetries and thus a $3j$ with vanishing entry m_1, $\binom{5\ \ 13/2\ \ 17/2}{0\ \ -9/2\ \ 9/2}$, and in this case of 'pseudo-weight' three, which vanishes as per (13) for such an ($c = 3, x_1 = 0$) object.

3. Connection to hypergeometric polynomials

Consider next the connection to the hypergeometric polynomials ${}_3F_2$ with argument unity [30, 31]. This well-known relationship (p 428 of [8, 13, 32, 33]) has already been used to analyze for nontrivial zeroes [13]. Since ${}_3F_2$ is an analytic function of its argument, this connection has important implications. The expression in (7) can be recast, again to within non-zero multiplicative factors, as

$${}_3F_2(-c, -r, -q; p + 1 - c, s + 1 - c; 1), \tag{15}$$

the search for zeroes becoming one of searching for when this function vanishes. Indeed, all non-trivial zeroes for $c \geqslant 1$ occur through zeroes of ${}_3F_2$. Note that this symbol also depends, of course, on five parameters. Since permutation among the first three 'numerator' and next two 'denominator' entries (12 in all) trivially leave the value unchanged, of the 72 symmetries of the hypergeometric polynomial, we are left with six different ones in agreement with the similar six when viewed in terms of Regge symmetries [6, 15].

For any c, the expression for this ${}_3F_2$ in terms of the Pochhammer symbols, $(a)_n \equiv a(a+1)\cdots(a+n-1)$, has $(c+1)$ terms,

$$\sum_{n=0}^{c} \frac{(-c)_n(-r)_n(-q)_n}{n!(p+1-c)_n(s+1-c)_n} = \left(1 - \frac{(-r)(-q)}{(p+1-c)(s+1-c)}\right)^c, \tag{16}$$

where the right-hand side is a binomial-like expansion but with Pochhammer symbols in place of powers, $a^n \to (a)_n$. These finite expansions can now be analyzed for their zeroes. As examples, it is easily verified that $\binom{4\ 4\ \ 6}{0\ 2\ -2}$ and $\binom{9\ 9\ \ 15}{0\ 5\ -5}$ are zeroes. It is based on this that we first conjectured and then established the generalization in (5) that applies to general weight d.

For $c = 1$, the zero occurs for $rq = ps$ which gives the previous result that the only zeroes of weight 1 are for $x_1 = x_2$. Also, as observed earlier, in the classical limit of large j_1 and j_2, when $p \approx r \approx j_1$ and $q \approx s \approx j_2$, with m and c dropped as negligible in comparison, we have the expression in (16) vanish for all $c \neq 0$.

This occurrence of $rq = ps$ suggests a convenient systematics for viewing $3j$ zeroes that incorporates Regge symmetries so that all equivalent ones related through these symmetries are grouped together. Tables such as in [6] order $3j$'s with the first entry the largest j but this does not incorporate Regge symmetries. To do so, tables can be drawn up with the five parameters arranged as follows: (i) c, the weight and the least value in the Regge matrix; (ii) the determinant of its minor in (6) which is indeed $(ps - qr)$; (iii) the minimum among those four elements of the minor, (iv) followed in order by the other two members that share a row or column with it. Thus, the weight $c = 4$ zero, $\begin{pmatrix} 11 & 15/2 & 15/2 \\ 3 & -5/2 & -1/2 \end{pmatrix}$, whose Regge form is $\begin{pmatrix} 11 & 11 & 4 \\ 10 & 8 & 8 \\ 5 & 7 & 14 \end{pmatrix}$, would be classified as (4, 30, 5, 7, 10). Note that the occurrence of equal entries in the Regge matrix allows this to be written as a $3j$ with one zero m-value, $\begin{pmatrix} 15/2 & 8 & 21/2 \\ -7/2 & 0 & 7/2 \end{pmatrix}$, which would be a pseudo-weight five zero with $x_2 = 0$. Similarly, the $c = 4$ zeroes, $\begin{pmatrix} 9 & 8 & 8 \\ 5 & -4 & -1 \end{pmatrix}$ and $\begin{pmatrix} 21/2 & 8 & 13/2 \\ 7/2 & -1 & -5/2 \end{pmatrix}$, are both described in this systematization as (4, 27, 4, 7, 9). An alternative scheme has been used in the rapid and efficient computation of $3j$-symbols which also uses the smallest element c in the Regge matrix as the lead element [34, 35]. It does not, however, use the determinant of its minor as suggested here if the focus is on zeroes. There is no obviously best schematization scheme but those that incorporate Regge symmetries lead, of course, to more economical groupings. Ansari [36–38] has extensive discussions of Regge and alternative forms and 'quasi-binomial' representations such as (16).

4. Connection to Legendre polynomials

Using (15) and (16), we can write

$$\begin{pmatrix} j & J & J \\ 0 & M & -M \end{pmatrix} = \sqrt{\frac{(2J-j)!}{(2J+j+1)!}} \sum_{n=0}^{j} \binom{j}{n}^2 (-J+M)_n (J+M+1+n-j)_{j-n}$$

$$= \sqrt{\frac{(2J-j)!}{(2J+j+1)!}} \sum_{n=0}^{j} (-1)^{j-n} \binom{j}{n}^2 (-J+M)_n (-J-M)_{j-n}. \tag{17}$$

It is instructive to examine this for specific j. For $j = 1$, the casting as the Legendre polynomial P_1 is the well-known expression as in equation (1.59) of [6]. For $j = 2$, the sum is proportional to $(3M^2 - J(J+1))$, or the Legendre polynomial of degree 2 as in the known result

$$2\sqrt{2J+1} \begin{pmatrix} 2 & J & J \\ 0 & M & -M \end{pmatrix} = \sqrt{\frac{J(J+1)}{(J-1/2)(J+3/2)}} \left(\frac{3M^2}{J(J+1)} - 1 \right). \tag{18}$$

In particular, it vanishes at the zero of the $P_2(\cos\theta)$ last term, where $\cos\theta = M/\sqrt{J(J+1)}$, an example being $\begin{pmatrix} 2 & 3 & 3 \\ 0 & 2 & -2 \end{pmatrix}$. This is a zero of weight 1 as discussed earlier and may have physical realization in the vanishing of a quadrupole coupling between nuclear states of $J = 3$. The next example with $3M^2 = J(J+1)$ for integer values occurs for $J = 48$, $M = 28$, its $3j$ a zero of weight 2.

For $j = 3$, (17) is proportional to $[M/\sqrt{J(J+1)}][3 - (5M^2+1)/(J(J+1))]$ together with non-vanishing factors involving J, again in agreement with a known result [28, 29] for $\begin{pmatrix} 3 & J & J \\ 0 & M & -M \end{pmatrix}$. Except for the small 'correction' 1 to $5M^2$, this resembles $P_3(\cos\theta)$ which vanishes for $\cos^2\theta = 3/5$. Indeed, with $J = 15$, this gives $M = 11.992$ so that $\begin{pmatrix} 3 & 15 & 15 \\ 0 & 12 & -12 \end{pmatrix}$ is a 'near zero', having the value $-0.000\,29$. Likewise, (17) for $j = 4$ closely approximates the polynomial $P_4(\cos\theta)$ with a near zero for $M^2 = 4J(J+1)/35$, an example being $\begin{pmatrix} 4 & 9 & 9 \\ 0 & 3 & -3 \end{pmatrix} \approx 0.0093$.

The above relationship to Legendre polynomials is general, as can be seen from the close resemblance of the general expression in (17) to a known, if less familiar, expression for these polynomials [39],

$$P_j(x) = \frac{1}{2^j j!}\frac{\mathrm{d}^j}{\mathrm{d}x^j}(x^2-1)^j = 2^{-j}\sum_{n=0}^{j}\binom{j}{n}^2 (x-1)^n(x+1)^{j-n}, \tag{19}$$

with Pochhammer symbols replaced by powers. Note also that a $3j$-symbol is a ${}_3F_2$ series with five parameters (its argument being fixed at unity) whereas a Legendre polynomial is a ${}_2F_1$ function which has four parameters (among them its argument, not fixed at unity). The reduction of the number of parameters by one is reflected in M and J occurring only in a single combination of their ratio, the tilt (see footnotes 6 and 8) as the argument of the Legendre polynomial.

Yet another approach to connect $3j$ coefficients to Legendre polynomials is through three-term recurrence relations obeyed by these (and also $6j$) coefficients. Indeed, the most efficient way of computing the coefficients, especially for large values of j, is through such recurrence algorithms. Thus, the coefficient in (17) obeys a three-term recurrence relation given in [40] for the function $g(M)$ with $m_1 = 0$ and $j_2 = j_3 = J$, the entries of the three terms listed in the middle column of the paper's table 1. Using an additional phase factor in the definition so that $g(M) = (-1)^M \left(\begin{smallmatrix} j & J & J \\ 0 & M & -M\end{smallmatrix}\right)$, this difference equation is

$$\begin{aligned}(J-M)(J+M+1)g(M+1) - [2J(J+1) - j(j+1) - 2M^2]g(M)\\ +(J-M+1)(J+M)g(M-1) = 0.\end{aligned} \tag{20}$$

Through a procedure for casting difference equations as differential equations [41, 42], by writing $g(M\pm 1) = g(x) \pm g' + g''/2$, where primes denote differentiation with respect to $x = \cos\theta = M/\sqrt{J(J+1)}$, a continuous variable between -1 and $+1$ for large J, $g(x)$ is seen to obey the Legendre differential equation for $P_j(\cos\theta)$, thus again establishing the equivalence for large J. Interestingly, if instead of this viewing of the above $3j$ as a function of M at fixed j and J which gives P_j, an analogous conversion of the recurrence relation in the first column of table 1 of [40] to a differential equation but now for fixed J and M and varying j expresses the $3j$ as a Bessel function $J_0(u)$, with $u \equiv (j+1/2)/(J+1/2)$. These results bear on the topic in the following section associated with the semi-classical connection to rotation matrices.

5. Connection to rotation matrices and semi-classical pictures

The reduction of a $3j$ in the classical limit to Wigner reduced rotation matrices, $d^j_{mm'}(\theta)$, has also long been recognized (see appendix 2 of [1, 2, 26], and problem 5.5 of [5]). Again, as in the previous section's reduction to Legendre polynomials, the similar reduction of parameters here by one is because M and J appear only in the form of the ratio, the tilt $\cos\theta$. A host of interesting relationships of these rotation d matrices in various limiting cases to special functions such as Legendre, Bessel, Hermite and Laguerre is also known; see, especially, equations (11.48), (13.11) and (13.36) of [25].

Heisenberg's correspondence principle has also been used to examine such classical limits and the reduction of $3j$ (and, again, also $6j$'s) to a reduced rotation matrix element [43, 44]. Actually, it is rather the Clebsch–Gordan coupling coefficient that shows this correspondence but it is simply related to the $3j$. With two values of j fixed, the behavior either as a function of the other j or an m value, shows oscillations in the 'classically allowed' region and monotonic decay into the 'classically forbidden' zone, these zones defined by the classical vector addition rule [17, 18, 21, 23, 45, 46]. These plots resemble those of the special functions noted

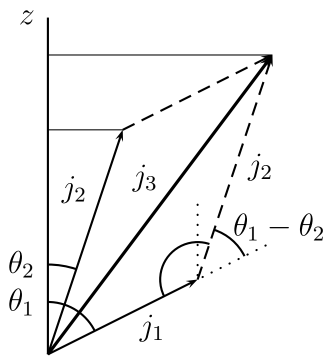

Figure 1. Vector coupling diagram (classical picture).

above. Accurate results for $3j$ in classically allowed and forbidden regions have been given in [17].

The classical diagram [2, 21, 45] for adding two angular momentum vectors according to the parallelogram rule, as shown in figure 1, gives for tilts x_1 and x_2 and corresponding tilt angles θ_1 and θ_2, the tilt of the sum through simple geometry as

$$x_3 = \frac{m_3}{j_3} = \frac{j_1 x_1 + j_2 x_2}{\sqrt{j_1^2 + j_2^2 + 2 j_1 j_2 \left(x_1 x_2 + \sqrt{1 - x_1^2}\sqrt{1 - x_2^2}\right)}}. \tag{21}$$

In the classical limit, the coupling coefficient for this value will be dominant. As an example, for ($j_1 = j_2 = 4, m_1 = 3, m_2 = 0$), this coefficient for the allowed values $j_3 = 3, 4, \ldots, 8$ is largest for $j_3 = 7$ as per the prediction of (21). As another example, $\begin{pmatrix} 2 & 4 & j_3 \\ 1 & 2 & -3 \end{pmatrix}$, with tilts $x_1 = x_2 = 1/2$, has its peak value for $j_3 = 6$. Indeed, this $3j$ has a weight $c = 1$ zero for $j_3 = 5$, both these results in conformity with our initial discussion in the introduction that tilt is conserved.

The semi-classical picture of $3j$ or Clebsch–Gordan coefficients also sheds light on their nontrivial zeroes and near-zeroes. Another example, with larger values for its entries than that in the previous paragraph, illustrates the point. The $3j$-symbol for ($j_1 = 6, j_2 = 9/2, m_1 = 2, m_2 = 3/2, m_3 = -7/2$) as a function of j_3 takes the values -0.128, 0.121, 0.031, -0.107, -0.008, 0.104, 0, -0.127 for $j_3 = 7/2, 9/2, \ldots, 21/2$. Note the oscillation as a function of j_3. This being another example of equal tilt, $x_1 = x_2 = 1/3$, there is a weight $c = 1$ zero at $j_3 = j_1 + j_2 - c = 19/2$. Descending from that value in steps of two, the values are again small although not exactly zero. As a function of a continuous parameter, oscillations in the classically allowed region have zeroes, only one of them coinciding with the physically allowed value of integer or half-odd integer. Other physically allowed values that lie near a zero of the classical oscillations exhibit the near-zero values in the above set of numbers. Note also that the dominant value occurs at the highest j_3 which has the same tilt of $1/3$ and is also the value given by (21), representing the classical turning point in this example. Interestingly, the lowest allowed $j_3 = 7/2$ value for this set is the other turning point, given by the same expression in (21) but with a plus sign in front of the last square root, which makes its coefficient relatively large instead of a near-zero. This illustrates another familiar feature, as best illustrated by harmonic oscillator wavefunctions of high quantum numbers, of a peaking near the classical turning points. Many other nice examples of such oscillations, zeroes and peaking near the edges in Clebsch–Gordan coefficients are shown in [21, 46].

6. Connection to expectation values of r^k for the hydrogen atom

Expressions similar to those discussed in previous sections have also long been known for matrix elements of r^k for the quantum-mechanical hydrogen atom. Several authors have noted that the expectation value of such an operator can be written as a sum over a product of three binomial factors, just as in (7) (see [47], section 3 of [48, 49–51]). Others have written the expectation value as a $_3F_2$ with argument unity [50], again analogous to (15) for $3j$. Semi-classical renderings [52, 53], this time through the Coulomb–Kepler orbit, to cast the expectation value as a Legendre polynomial are also known [54, 55]. All these features for just the radial or dynamical aspects of the hydrogen atom, not its angular momentum aspects, may at first sight seem surprising, given no obvious rotational symmetry considerations for the radial equation. However, they are understood through the recognition that the radial problem has the symmetry of the non-compact group $O(2, 1)$ [56, 57]. This group's closed triplet of operators under commutation is very similar, apart from sign changes in the structure factors, to those of the angular momentum's $O(3)$ triplet, which explains the appearance of such Clebsch–Gordan coefficients in radial matrix elements.

Among illustrations of this correspondence between expectation values of powers of the radial coordinate and results in previous sections are the very familiar ones in textbooks for a hydrogenic state $|nlm\rangle$ (we use atomic units),

$$\langle r\rangle = \frac{1}{2}(3n^2 - l(l+1)), \qquad \langle r^2\rangle = \frac{n^2}{2}(5n^2 - 3l(l+1) + 1). \tag{22}$$

These are, of course, reminiscent of the Legendre polynomials P_2 and P_3 as in (18) and in the discussion following, down to the quantum 'correction' 1 to the semi-classical in P_3 as discussed there. More extensive powers are given in [50] and a general semi-classical expression for the expectation value is (see equation (12.11a) of [5])

$$\langle r^k\rangle = n^{2k}\left(\frac{l+1/2}{n}\right)^{k+1} P_{k+1}\left(\frac{n}{l+1/2}\right). \tag{23}$$

Note that the roles of (l, m) in angular momentum are now played by (l, n) so that the tilt m/l is now replaced by $n/(l+1/2)$. Again, as in alternatives for the tilt (see footnote 8), in some contexts one can use n/l or even $(n-1/2)/(l+1/2)$. The former is related to the eccentricity ϵ of the orbit, given by $(1-\epsilon^2)^{-1/2} = n/l = a/b$ [52] while the latter takes the limiting value of unity for 'circular' orbits, $l = n-1$. a and b are the major and minor axes of the orbit and these connections establish an analogy between tilt and eccentricity.

Nearly all discussions have been for the expectation values or diagonal matrix elements, where $\langle r^k\rangle$ are given by $\begin{pmatrix} k+1 & l & l \\ 0 & n & -n\end{pmatrix}$. We suggest that the off-diagonal elements for differing n and l may be rendered as the corresponding $3j$ with more general entries. Indeed, the above expectation value which involves a radial integral over an exponential, a power and a square of a Laguerre polynomial, is given by [58, 59]

$$\langle r^k\rangle = \frac{n^{k-1}}{2^{k+1}}\frac{(n+l+k+1)!}{(n+l)!}\,{}_3F_2(-k-1, -k-1, l+1-n; 1, -n-l-k-1; 1), \tag{24}$$

which is related through (15) to $3j$ noted above. A more general radial integral with the two Laguerre polynomials in the integrand differing in one index has been noted [59, 60]:

$$\int_0^\infty \mathrm{e}^{-x} x^{k+\alpha} L_m^{(\alpha)}(x) L_n^{(\alpha)}(x)\,\mathrm{d}x = (-k)_{n-m}\frac{\Gamma(\alpha+k+m+1)}{(n-m)!m!} \times {}_3F_2(-k, -k+n-m, -m; n-m+1, -k-m-\alpha; 1). \tag{25}$$

Such expressions and further generalizations could provide off-diagonal matrix elements of powers of r. Another version but without explicit ${}_3F_2$ is given in appendix F of [61] and versions with Appell functions and others involving two variables are also known [62–64] but the above bear the closest relationship to results in previous sections.

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