A derivation of some recently discovered relations involving 3-j symbols

1977 J. Phys. A: Math. Gen. 10 1059

(http://iopscience.iop.org/0305-4470/10/7/003)

J. Phys. A: Math. Gen., Vol. 10, No. 7, 1977. Printed in Great Britain. © 1977

A derivation of some recently discovered relations involving 3-*j* symbols

John D Morgan III†

Theoretical Chemistry Department, University of Oxford, 1 South Parks Road, Oxford OX1 3TG, UK

Received 23 December 1976, in final form 18 March 1977

Abstract. Some recently discovered identities involving 3-j symbols are derived from the equation $1=r_{12}/r_{12}$. Although the derivation applies only to non-negative even z, the result is extended to complex z since a rational function which has infinitely many zeros vanishes identically. A few summations similar to the previously discovered ones are discussed, and it is noted that application of the Regge symmetry to this class of summations brings them into a more familiar form.

Recently it has been proved that

$$S_{l,J}(z)=\sum_{l'=0}^{l}\left(\frac{z(2l+z+1)}{(2l+z)(z-1)}\frac{1}{2l'+z+1}-\frac{1}{2l'+z-1}\right)\begin{pmatrix} l & l'+J & l-l'+J \\ 0 & 0 & 0 \end{pmatrix}^2=0 \tag{1}$$

for all non-zero z such that the sum makes sense, where J is a natural number and l is a natural number divided by 2 (Morgan 1976, to be referred to as II). The particular cases of $z=0$ and $z=2$ have been discussed previously (Morgan 1975, Rashid 1976, Vanden Berghe and De Meyer 1976). A derivation of these summations is presented for non-negative even z, and the result is then extended to appropriate complex z by a simple argument.

The critical equation is the trivial identity $1=r_{12}/r_{12}$, where r_{12} is the distance between the two vectors $\boldsymbol{r}_1$ and $\boldsymbol{r}_2$. We employ the Neumann expansions for $1/r_{12}$ (Gradshteyn and Ryzhik 1965, p 1027)

$$\frac{1}{r_{12}}=\frac{1}{r_>}\sum_{j=0}^{\infty}u^jP_j(\cos\theta) \tag{2}$$

and for r_{12} (Jen 1933, pp 542–3)

$$r_{12}=r_>\sum_{j=0}^{\infty}\left(-\frac{u^j}{2j-1}+\frac{u^{j+2}}{2j+3}\right)P_j(\cos\theta), \tag{3}$$

where the P_j are Legendre polynomials of the cosine of the angle between $\boldsymbol{r}_1$ and $\boldsymbol{r}_2$ and $u=r_</r_>$, where $r_<$ and $r_>$ are the lesser and greater of r_1 and r_2, respectively. Hence

$$1=\frac{r_{12}}{r_{12}}=\sum_{k=0}^{\infty}\sum_{j=0}^{\infty}u^k\left(-\frac{u^j}{2j-1}+\frac{u^{j+2}}{2j+3}\right)P_j(\cos\theta)P_k(\cos\theta). \tag{4}$$

† Present address: Department of Chemistry, University of California, Berkeley, Ca. 94720, USA.

Since

$$P_j(\cos\theta)P_k(\cos\theta)=\sum_{l=0}^{\infty}(2l+1)\begin{pmatrix} l & j & k \\ 0 & 0 & 0 \end{pmatrix}^2 P_l(\cos\theta), \tag{5}$$

(Messiah 1965, p 1057), equation (4) yields

$$1=\sum_{l=0}^{\infty}(2l+1)P_l(\cos\theta)\sum_{k=0}^{\infty}\sum_{j=0}^{\infty}u^k\left(-\frac{u^j}{2j-1}+\frac{u^{j+2}}{2j+3}\right)\begin{pmatrix} l & j & k \\ 0 & 0 & 0 \end{pmatrix}^2. \tag{6}$$

We now replace k with m, where $m=j+k$, to obtain

$$1=\sum_{l=0}^{\infty}(2l+1)P_l(\cos\theta)\sum_{m=0}^{\infty}\sum_{j=0}^{m}u^m\left(-\frac{1}{2j-1}+\frac{u^2}{2j+3}\right)\begin{pmatrix} l & j & m-j \\ 0 & 0 & 0 \end{pmatrix}^2. \tag{7}$$

The 3-j symbol vanishes unless $l\leqslant j+m-j=m$, so

$$1=\sum_{l=0}^{\infty}(2l+1)P_l(\cos\theta)\sum_{m=l}^{\infty}\sum_{j=0}^{m}u^m\left(-\frac{1}{2j-1}+\frac{u^2}{2j+3}\right)\begin{pmatrix} l & j & m-j \\ 0 & 0 & 0 \end{pmatrix}^2. \tag{8}$$

Let $n=m-l$, so $m=l+n$. Then

$$1=\sum_{l=0}^{\infty}u^l(2l+1)P_l(\cos\theta)\sum_{n=0}^{\infty}\sum_{j=0}^{l+n}u^n\left(-\frac{1}{2j-1}+\frac{u^2}{2j+3}\right)\begin{pmatrix} l & j & l-j+n \\ 0 & 0 & 0 \end{pmatrix}^2. \tag{9}$$

The 3-j symbol vanishes unless $l+j+l-j+n=2l+n$ is even, so $n=2k$, where k is a natural number. Furthermore, the symbol is zero unless $l+j\geqslant l-j+2k$ (i.e., $j\geqslant k$), so

$$1=\sum_{l=0}^{\infty}u^l(2l+1)P_l(\cos\theta)\sum_{k=0}^{\infty}\sum_{j=k}^{l+2k}u^{2k}\left(-\frac{1}{2j-1}+\frac{u^2}{2j+3}\right)\begin{pmatrix} l & j & l-j+2k \\ 0 & 0 & 0 \end{pmatrix}^2. \tag{10}$$

Since the symbol vanishes unless $j\leqslant l+l-j+2k$ (i.e., $j\leqslant l+k$),

$$\begin{aligned}\delta_{l,0}&=\sum_{k=0}^{\infty}\sum_{j=k}^{l+k}u^{2k}\left(-\frac{1}{2j-1}+\frac{u^2}{2j+3}\right)\begin{pmatrix} l & j & l-j+2k \\ 0 & 0 & 0 \end{pmatrix}^2\\ &=\sum_{k=0}^{\infty}\sum_{j=0}^{l}u^{2k}\left(-\frac{1}{2j+2k-1}+\frac{u^2}{2j+2k+3}\right)\begin{pmatrix} l & j+k & l-j+k \\ 0 & 0 & 0 \end{pmatrix}^2.\end{aligned} \tag{11}$$

The coefficient of u^0 is

$$\delta_{l,0}=\sum_{j=0}^{l}\frac{1}{2j-1}\begin{pmatrix} l & j & l-j \\ 0 & 0 & 0 \end{pmatrix}^2, \tag{12}$$

which is equivalent to equation (1) of II. We then obtain

$$\begin{aligned}0=\sum_{k=0}^{\infty}\sum_{j=0}^{l}u^{2k+2}\Bigg(&-\frac{1}{2j+2k+1}\begin{pmatrix} l & j+k+1 & l-j+k+1 \\ 0 & 0 & 0 \end{pmatrix}^2\\ &+\frac{1}{2j+2k+3}\begin{pmatrix} l & j+k & l-j+k \\ 0 & 0 & 0 \end{pmatrix}^2\Bigg).\end{aligned} \tag{13}$$

We now set the coefficients of the powers of u equal to zero:

$$0=\sum_{j=0}^{l}\left(-\frac{1}{2j+2k+1}\begin{pmatrix} l & j+k+1 & l-j+k+1 \\ 0 & 0 & 0 \end{pmatrix}^2 + \frac{1}{2j+2k+3}\begin{pmatrix} l & j+k & l-j+k \\ 0 & 0 & 0 \end{pmatrix}^2\right). \tag{14}$$

Since

$$\begin{pmatrix} l & j+k+1 & l-j+k+1 \\ 0 & 0 & 0 \end{pmatrix}^2 = \frac{(2k+1)(l+k+1)}{(2l+2k+3)(k+1)}\begin{pmatrix} l & j+k & l-j+k \\ 0 & 0 & 0 \end{pmatrix}^2, \tag{15}$$

$$0=\sum_{j=0}^{l}\left(-\frac{1}{2j+2k+1}\frac{(2k+1)(l+k+1)}{(2l+2k+3)(k+1)}+\frac{1}{2j+2k+3}\right)\begin{pmatrix} l & j+k & l-j+k \\ 0 & 0 & 0 \end{pmatrix}^2. \tag{16}$$

From equation (5) of II

$$0=\sum_{j=0}^{l}\left(-\frac{1}{2j+2k+1}\frac{(2k+1)(l+k+1)}{(2l+2k+3)(k+1)}+\frac{1}{2j+2k+3}\right)\begin{pmatrix} l & j & l-j \\ 0 & 0 & 0 \end{pmatrix}^2. \tag{17}$$

If we let $z=2k+2$, we obtain

$$0=\sum_{j=0}^{l}\left(-\frac{1}{2j+z-1}\frac{(z-1)(2l+z)}{(2l+z+1)z}+\frac{1}{2j+z+1}\right)\begin{pmatrix} l & j & l-j \\ 0 & 0 & 0 \end{pmatrix}^2, \tag{18}$$

which is equivalent to equation (3) of II.

It is at first surprising that such apparently complicated expressions can be derived in a straightforward manner from so trivial an identity as $1=r_{12}/r_{12}$.

To generalize equation (18) to complex z such that the summation makes sense, we first note that the expression is a finite sum of rational functions of z, so the expression itself is a rational function of z. It is well known that a rational function which has infinitely many zeros is identically zero. Since equation (18) holds for positive even z, it is valid for all z such that the sum makes sense.

The question arises as to whether more identities can be found by examining the Neumann expansions for the equations $r_{12}^2/r_{12}^2=1$, $r_{12}^3/r_{12}^3=1$, etc. The author worked out the first equation and could not find any interesting identities. However, it was necessary to evaluate the summation

$$\sum_{l'=0}^{l}\begin{pmatrix} l & l' & l-l' \\ 0 & 0 & 0 \end{pmatrix}^2 \tag{19}$$

which was found to equal $(2l)!!/((2l+1)!!)$ by the same recursive process as was used in equations (4) through (10) of II. This result raises the possibility of evaluating any summation of the form

$${}_sM_l(z)=\sum_{l'=0}^{l}\frac{1}{(2l'+z-1)^s}\begin{pmatrix} l & l' & l-l' \\ 0 & 0 & 0 \end{pmatrix}^2 \tag{20}$$

in a similar manner. However, if $s=2$, the only easily evaluable case seems to be $z=0$, in which case the sum equals 1 if $l=0$ and $(2l)!!(2l-2)!!((2l+1)!!(2l-1)!!)^{-1}$ for positive integral l. Because of the difficulty in evaluating the summation for general z and larger s, it was decided to defer further consideration of these summations until they arise in a physical problem.

It has been pointed out (I P Grant, private communication) that one can exploit the Regge symmetry by interchanging rows and columns to see that

$$\begin{pmatrix} l & l' & l-l' \\ 0 & 0 & 0 \end{pmatrix} = \begin{pmatrix} l & \frac{1}{2}l & \frac{1}{2}l \\ 2l'-l & \frac{1}{2}l-l' & \frac{1}{2}l-l' \end{pmatrix} \tag{21}$$

(Landau and Lifshitz 1965, pp 405–6). This symmetry allows us to express our relations in a form involving more familiar sums on the lower indices.

Acknowledgments

I would like to thank D B Abraham, I P Grant, and N C Pyper for their encouragement and advice while I worked on this problem at Oxford. I am also grateful to the Marshall Aid Commemoration Commission for awarding me a scholarship, which made my study at Oxford possible.

References

Gradshteyn I S and Ryzhik I M 1965 *Table of Integrals, Series, and Products* (London: Academic Press)
Jen C K 1933 *Phys. Rev.* **43** 540
Landau L D and Lifshitz E M 1965 *Quantum Mechanics* (Oxford: Pergamon)
Messiah A 1965 *Quantum Mechanics* vol. 2 (Amsterdam: North-Holland)
Morgan III J D 1975 *J. Phys. A: Math. Gen.* **8** L77–9
—— 1976 *J. Phys. A: Math. Gen.* **9** 1231–3
Rashid M A 1976 *J. Phys. A: Math. Gen.* **9** L1–3
Vanden Berghe G and De Meyer H 1976 *J. Phys. A: Math. Gen.* **9** L5–7