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Further relations involving 3-j symbols

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Abstract. A general form of two earlier relations involving 3-j symbols was found through further investigation of the helium atom problem. These relations are proved, and a very general summation is evaluated which should be most useful in summing any similar series found in connection with the helium atom problem.

In an earlier letter (Morgan 1975) it was proved that

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

and conjectured that

$$\bar{S}_{l,J}=\sum_{l'=0}^{l}\left(\frac{1}{2l'+3}-\frac{l+1}{2l+3}\frac{1}{2l'+1}\right)\begin{pmatrix} l & l'+J & l-l'+J \\ 0 & 0 & 0 \end{pmatrix}^2=0 \tag{2}$$

for the non-negative integral and $\frac{1}{2}$-integral l and integral J. Recently two articles on these relations appeared in this journal (Rashid 1976, Vanden Berghe and De Meyer 1976).

Rashid's letter contains an error (in equation (5) for '$\Gamma(z+1)$' read '$\Gamma(z+\frac{1}{2})$' (Gradshteyn and Ryzhik 1965, p 938)), but he appears to have used the proper formula in his manipulations. A more serious consideration is that his equation (8) is of the form $0\times\infty$ and equations (9) and (10) are of the form $0\times\infty\times 0$ for integral $l\geq l'$, which is the case under investigation. Although it is easy to see that the limit exists in (8), because $\sin \pi l$ has a simple zero and $\Gamma(l'-l)$ a simple pole for integral $l\geq l'$, the existence of the limit in the case of the hypergeometric functions is not immediately obvious, and perhaps a justification of these formulae should have been included.

Recently a more general form of equations (1) and (2) was obtained in investigating recursion relations for the exact solution of the non-relativistic helium atom problem:

$$S_{l,J}(z)=\sum_{l'=0}^{l}\left(\frac{z(2l+z+1)}{(2l+z)(z-1)}\frac{1}{2l'+z+1}-\frac{1}{2l'+z-1}\right)\begin{pmatrix} l & l'+J & l-l'+J \\ 0 & 0 & 0 \end{pmatrix}^2 \tag{3}$$

for integral J, non-negative integral and $\frac{1}{2}$-integral l, and complex $z\neq 1-2k$, where k is a natural number less than or equal to $l+1$, and $z\neq -2l$. It will be shown that $S_{l,J}(z)=0$ for all such $z\neq 0$. For $z=0$, equation (3) reduces to equation (1).

First let us consider

$$M_{l,J}(z)=\sum_{l'=0}^{l}\frac{1}{2l'+z-1}\begin{pmatrix} l & l'+J & l-l'+J \\ 0 & 0 & 0 \end{pmatrix}^2$$
$$=\sum_{l'=0}^{l}\frac{1}{2l-2l'+z-1}\begin{pmatrix} l & l'+J & l-l'+J \\ 0 & 0 & 0 \end{pmatrix}^2 \tag{4}$$

under the above restrictions on l, J, and z. We note that $M_{l,J}(0)=S_{l,J}$ in equation (1). Since

$$\begin{pmatrix} l & l'+J & l-l'+J \\ 0 & 0 & 0 \end{pmatrix}^2=\binom{l+J}{J}^2\binom{2l+2J+1}{2J}^{-1}\begin{pmatrix} l & l' & l-l' \\ 0 & 0 & 0 \end{pmatrix}^2, \tag{5}$$

$$M_{l,J}(z)=\binom{l+J}{J}^2\binom{2l+2J+1}{2J}^{-1}M_{l,0}(z). \tag{6}$$

Now

$$M_{l+1,0}(z)=\sum_{l'=0}^{l+1}\frac{1}{2l'+z-1}\begin{pmatrix} l+1 & l' & l-l'+1 \\ 0 & 0 & 0 \end{pmatrix}^2$$
$$=\frac{1}{(2l+z+1)(2l+3)}+\sum_{l'=0}^{l}\frac{1}{2l'+z-1}\begin{pmatrix} l+1 & l' & l-l'+1 \\ 0 & 0 & 0 \end{pmatrix}^2. \tag{7}$$

Since

$$\begin{pmatrix} l+1 & l' & l-l'+1 \\ 0 & 0 & 0 \end{pmatrix}^2=\frac{2l-2l'+1}{l-l'+1}\begin{pmatrix} l & l'+1 & l-l'+1 \\ 0 & 0 & 0 \end{pmatrix}^2, \tag{8}$$

$$M_{l+1,0}(z)=\frac{1}{(2l+z+1)(2l+3)}+\sum_{l'=0}^{l}\frac{1}{2l'+z-1}\,\frac{2l-2l'+1}{l-l'+1}\begin{pmatrix} l & l'+1 & l-l'+1 \\ 0 & 0 & 0 \end{pmatrix}^2$$
$$=\frac{1}{(2l+z+1)(2l+3)}+\sum_{l'=0}^{l}\frac{1}{2l-2l'+z-1}\,\frac{2l'+1}{l'+1}\begin{pmatrix} l & l'+1 & l-l'+1 \\ 0 & 0 & 0 \end{pmatrix}^2$$
$$=\frac{1}{(2l+z+1)(2l+3)}+2\times M_{l,1}(z)$$
$$-\sum_{l'=0}^{l}\frac{1}{(2l-2l'+z-1)(l'+1)}\begin{pmatrix} l & l'+1 & l-l'+1 \\ 0 & 0 & 0 \end{pmatrix}^2$$
$$=\frac{1}{(2l+z+1)(2l+3)}+2\times M_{l,1}(z)$$
$$-\sum_{l'=0}^{l}\frac{1}{2l+z+1}\left(\frac{2}{2l-2l'+z-1}+\frac{1}{l'+1}\right)\begin{pmatrix} l & l'+1 & l-l'+1 \\ 0 & 0 & 0 \end{pmatrix}^2$$
$$=\frac{1}{2l+z+1}\left(\frac{1}{2l+3}-\sum_{l'=0}^{l}\frac{1}{l'+1}\begin{pmatrix} l & l'+1 & l-l'+1 \\ 0 & 0 & 0 \end{pmatrix}^2\right)$$
$$+2\left(1-\frac{1}{2l+z+1}\right)M_{l,1}(z)$$
$$=\frac{2(2l+z)}{2l+z+1}M_{l,1}(z), \tag{9}$$

because of equation (8) of the first letter. Using (6),

$$M_{l+1,0}(z)=\frac{2(2l+z)}{2l+z+1}\frac{l+1}{2l+3}M_{l,0}(z). \tag{10}$$

Thus, since $M_{0,0}(z)=(z-1)^{-1}$,

$$M_{l,J}(z)=\binom{l+J}{J}^2\binom{2l+2J+1}{2J}^{-1}\left(\prod_{i=1}^{l}\frac{2i+z-2}{2i+z-1}\right)\frac{2^l l!}{(2l+1)!!}\frac{1}{z-1} \tag{11}$$

where it is understood that $\Pi_{i=1}^{0}=1$. For integral $z\geqslant 2$, the product in equation (11) can be written as $(2l+z-2)!!(z-1)!!((z-2)!!(2l+z-1)!!)^{-1}$. Use of equation (11) with $J=0$ for z and $z+2$ in equation (3) yields the result that $S_{l,J}(z)=0$ for the appropriate $z\neq 0$, and we have already seen that $S_{l,J}(0)=-(2J+1)^{-1}\delta_{l,0}$. We also note that $\bar{S}_{l,J}=(2l+3)(l+1)^{-1}S_{l,J}(2)$.

$M_{l,J}(z)$ is 0 for $\frac{1}{2}$-integral l since the 3-j symbols then vanish identically.

The finding of expression (11) for $M_{l,J}(z)$ enables us to evaluate any summation of the form

$$\sum_{l'=0}^{l} f(l,z,l')\begin{pmatrix} l & l'+J & l-l'+J \\ 0 & 0 & 0\end{pmatrix}^2 \tag{12}$$

provided that the function $f(l, z, l')$ can be written as a linear combination of reciprocals of terms linear in l'. In particular, we shall be able to evaluate easily any similar summations encountered in our study of the helium atom problem.

We note that $M_{l,J}(z)$ is analytic everywhere except for $z=1-2k$, where k is a natural number less than or equal to 1, with radius of convergence minimum $\{|z+2k-1|\,|k$ is a natural number between 0 and $l\}$. It has simple poles at its singular points.

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