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LETTER TO THE EDITOR

An interesting relation involving 3-j symbols

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Abstract. A simple 'pseudo-orthogonality' relation which was encountered in investigating the exact solutions of the helium atom problem is proved. Another set of more complicated summations was obtained but their vanishing has not yet been verified. It is suggested that these relations may arise from some symmetry peculiar to the helium atom.

In the course of investigating recursion relations for the exact solution of the non-relativistic helium atom problem, the following quantity was encountered:

$$S_l = \sum_{l'=0}^{l} \frac{1}{2l'-1}\begin{pmatrix} l & l' & l-l' \\ 0 & 0 & 0 \end{pmatrix}^2 = \sum_{l'=0}^{l} \frac{1}{2l-2l'-1}\begin{pmatrix} l & l' & l-l' \\ 0 & 0 & 0 \end{pmatrix}^2. \tag{1}$$

This sum is -1 for $l = 0$ and 0 for $l = 1$. We shall now show by induction that it vanishes for any $l \geqslant 1$.

Lemma

If $S_l = 0$ for a particular l, then $S_{l,J} = 0$ as well, where

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

The proof is trivial since

$$\begin{pmatrix} l & l'+J & l-l'+J \\ 0 & 0 & 0 \end{pmatrix}^2 = \binom{l+J}{J}^2 \binom{2l+2J+1}{2J}^{-1} \begin{pmatrix} l & l' & l-l' \\ 0 & 0 & 0 \end{pmatrix}^2. \tag{3}$$

We know that $S_l = 0$ for $l = 1$. Now assume that $S_l = 0$ and examine

$$S_{l+1} = \sum_{l'=0}^{l+1} \frac{1}{2l'-1}\begin{pmatrix} l+1 & l' & l+1-l' \\ 0 & 0 & 0 \end{pmatrix}^2$$

$$= \frac{1}{(2l+1)(2l+3)} + \sum_{l'=0}^{l} \frac{1}{2l'-1}\begin{pmatrix} l+1 & l' & l+1-l' \\ 0 & 0 & 0 \end{pmatrix}^2. \tag{4}$$

It is readily verified (Landau and Lifshitz 1965) that

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

so

$$S_{l+1}=\frac{1}{(2l+1)(2l+3)}+\sum_{l'=0}^{l}\frac{2l-2l'+1}{(2l'-1)(l-l'+1)}\begin{pmatrix} l & l'+1 & l-l'+1 \\ 0 & 0 & 0 \end{pmatrix}^2$$

$$=\frac{1}{(2l+1)(2l+3)}+\sum_{l'=0}^{l}\frac{2l'+1}{(2l-2l'-1)(l'+1)}\begin{pmatrix} l & l'+1 & l-l'+1 \\ 0 & 0 & 0 \end{pmatrix}^2. \tag{6}$$

We next separate the $l'=0$ term from the rest in (4).

$$S_{l+1}=-\frac{1}{2l+3}+\sum_{l'=1}^{l+1}\frac{1}{2l'-1}\begin{pmatrix} l+1 & l' & l+1-l' \\ 0 & 0 & 0 \end{pmatrix}^2$$

$$=-\frac{1}{2l+3}+\sum_{l'=0}^{l}\frac{1}{2l'+1}\begin{pmatrix} l+1 & l'+1 & l-l' \\ 0 & 0 & 0 \end{pmatrix}^2$$

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

Using (5),

$$S_{l+1}=-\frac{1}{2l+3}+\sum_{l'=0}^{l}\frac{1}{l-l'+1}\begin{pmatrix} l & l'+1 & l-l'+1 \\ 0 & 0 & 0 \end{pmatrix}^2$$

$$=-\frac{1}{2l+3}+\sum_{l'=0}^{l}\frac{1}{l'+1}\begin{pmatrix} l & l'+1 & l-l'+1 \\ 0 & 0 & 0 \end{pmatrix}^2. \tag{8}$$

We then subtract (6) from (8) to obtain

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

$$=-\frac{2(l+1)}{(2l+1)(2l+3)}+2\sum_{l'=0}^{l}\frac{(l+1)-2(l'+1)}{(l'+1)(2l-2l'-1)}\begin{pmatrix} l & l'+1 & l-l'+1 \\ 0 & 0 & 0 \end{pmatrix}^2. \tag{9}$$

We note that the latter part of the sum vanishes because of the induction hypothesis and our lemma, so

$$\frac{1}{(2l+1)(2l+3)}=\sum_{l'=0}^{l}\frac{1}{(l'+1)(2l-2l'-1)}\begin{pmatrix} l & l'+1 & l-l'+1 \\ 0 & 0 & 0 \end{pmatrix}^2. \tag{10}$$

We now add $0=2\cdot S_{l,1}$ to the right-hand side of (8) to obtain

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

$$=-\frac{1}{2l+3}+\sum_{l'=0}^{l}\frac{2l+1}{(l'+1)(2l-2l'-1)}\begin{pmatrix} l & l'+1 & l-l'+1 \\ 0 & 0 & 0 \end{pmatrix}^2=0 \tag{11}$$

because of (10). Thus $S_l=0$ for any $l\geqslant 1$, and from the lemma, $S_{l,J}=-(2J+1)^{-1}\delta_{l0}$, and therefore other identities are readily obtained from (4) and (6)–(8).

Neither this sum nor any similar expression nor indeed anything which pertains to these quantities could be found in any of the standard references on angular momentum theory (Biedenharn and van Dam 1965, Brink and Satchler 1971, Englefield 1972, Yutsis *et al* 1962). Of course, any identity involving integral quantities can be written in terms of 3-j symbols, but it does not necessarily follow that such an equality is most easily or even can be proved by examining the symmetries of the full rotation group. In fact, these sums were generated by solving for the first few lowest coefficients of the power series expansions for the radial functions corresponding to helium S states, and it was necessary to demand that the radial functions satisfy Schrödinger's equation and have continuous derivatives with respect to the radial coordinates except at Coulomb singular points in order to find these coefficients. Also, if the r_{12}^{-1} potential were replaced with a different potential (eg one which vanished everywhere), these sums would not have been obtained, so it would not be surprising if this 'pseudo-orthogonality' relation was generated by some symmetry peculiar to the helium atom with Coulomb interelectronic repulsion.

Another set of considerably more complicated summations has been obtained by similar means:

$$\bar{S}_l = \sum_{l'=0}^{l} \frac{1}{2l'+3}\begin{pmatrix} l & l' & l-l' \\ 0 & 0 & 0 \end{pmatrix}^2 - \sum_{l'=0}^{l} \frac{1}{2l'+1}\begin{pmatrix} l & l'+1 & l-l'+1 \\ 0 & 0 & 0 \end{pmatrix}^2. \tag{12}$$

The $\bar{S}_l$ vanish for $l = 0, 1, 2, 3, 4$, so one is tempted, especially in light of the previous result, to conjecture that these sums vanish for any natural number l. Unfortunately a proof has not yet been obtained because of the greatly increased number of equivalent forms of these quantities which apparently need to be used in verifying this conjecture.

We note that the S_l and $\bar{S}_l$ vanish if l is half-integral since the 3-j symbols then vanish identically.

In conclusion, an exact treatment of the helium atom problem appears to be considerably more fruitful and interesting than has been imagined previously.

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