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Radial Matrix Elements for Hydrogen-Like Atoms

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Abstract: We show hypergeometric formulae for radial matrix elements under Coulomb potential.

Key words: Hypergeometric functions・Coulomb interaction・Matrix elements

INTRODUCTION

In [1] were obtained the following expressions for the radial matrix elements for hydrogen-like atoms:

$$< n_2 l \,|\, r^k \,|\, n_1 l_1 >= \frac{2^{l_1+l_2+2} b^k (n_2-n_1)^{n_2-l_2-1} n_1^{\,l_2+k+1} n_2^{\,l_1+k+1}}{(n_2+n_1) n_2 + l_1 + k + 2} \sqrt{\frac{(n_2-l_2-1)!(n_1-l_1-1)!}{(n_2+l_2)!(n_1+l_1)!}}. \qquad (1)$$

$$\sum\nolimits_{q=0}^{n_1-l_1-1} \frac{(-2n_2)^q (l_2+l_1+k+2+q)!}{q!(n_2+n_1)^q} \binom{n_1+l_1}{n_1-l_1-1-q} \sum\nolimits_{m=0}^{n_2-l_2-1} \frac{(2n_1)^m}{(n_1-n_2)^m} \binom{n_2+l_2}{2l_2+1+m} \le \binom{l_1+l_2+l+1+q}{m},$$

$$< n l_2 \,|\, r^k \,|\, n l_1 >= \frac{(-1)^{n-l_2-1} b^k}{2^{k+1} n^{1-k}} \sqrt{\frac{(n-l_2-1)!(n-l_1-1)!}{(n+l_2)!(n+l_1)!}} \sum\nolimits_{q=0}^{n-l_1-1} \frac{(-1)^q}{q!} (l_2+l_1+k+2+q)! \qquad (2)$$

$$\binom{n+l_1}{n-l_1-1-q} \binom{l_1-l_2+k+1+q}{n-l_2-1},$$

$$< nl \,|\, r^k \,|\, nl >= \frac{(-1)^{n-l-1} b^k (n-l-1)!}{2^{k+1} n^{1-k} (n+l)!} \sum\nolimits_{q=0}^{n-l-1} \frac{(-1)^q}{q!} \binom{n+l}{n-l-1-q} \binom{k+1+q}{n-l-1} (2l+k+2+q)!, \qquad (3)$$

where $b = \frac{4\pi\varepsilon_0}{ze^2}, k \varepsilon \mathbb{Z}$, with n,l denoting the total and orbital quantum numbers, respectively.

Now we apply the term ratio technique [2, 3] to introduce hypergeometric functions into (1), (2) and (3). In fact:

$$A \equiv \sum\nolimits_{m=0}^{n_2-l_2-1} \frac{(2n_1)^m}{(n_1-n_2)^m} \binom{n_2+l_2}{2l_2+1+m} \binom{l_1-l_2+k+1+q}{m} = \binom{n_2+l_2}{2l_2+1} \sum\nolimits_{m=0}^{\infty} t_m,$$

such that:

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$$t_m = \frac{(2n_1)^m \binom{n_2+l_2}{2l_2+1+m}\binom{l_1+l_2+k+1+q}{m}}{(n_1-n_2)^m \binom{n_2+l_2}{2l_2+1}} \therefore \frac{t_{m+1}}{t_m} = \frac{(m+l_2-n_2+1)(m+l_2-l_1-k-1-q)}{(m+2l_2+2)(m+1)}.\frac{2n_1}{n_1-n_2},$$

thus:

$$A = \binom{n_2+l_2}{2l_2+1}\ {}_2F_1\left(l_2-n_2+1,\ l_2-l_1-k-1-q;\ 2l_2+2; \frac{2n_1}{n_1-n_2}\right), \tag{4}$$

involving the Gauss hypergeometric function ${}_2F_1$ [4]; then (1) adopts the form:

$$< n_2 l_2 \mid r^k \mid n_1 l_1 >= \frac{2^{l_1+l_2+2} b^k (n_2-n_1)^{n_2-l_2-1} n_1{}^{l_2+k+1} n_2{}^{l_1+k+1}}{(2l_2+1)!(n_2+n_1)n^2+l_1+k+2} \sqrt{\frac{(n_2+l_2)!(n_1-l_1-1)!}{(n_1+l_1)!(n_2-l_2-1)!}}.$$

$$\sum_{q=0}^{n_1-l_1-1} \frac{(-2n_2)^q (l_2+l_1+k+2+q)!}{q!(n_2+n_1)^q} \binom{n_1+l_1}{n_1-l_1-1-q}\ {}_2F_1\left(l_2-n_2+1, l_2-l_1-k-1-q; 2l_2+2; \frac{2n_1}{n_1-n_2}\right). \tag{5}$$

Similarly:

$$B = \sum_{q=0}^{n-l_1-1} \frac{(-1)^q (l_2+l_1+k+2+q)!}{q!} \binom{n+l_1}{n-l_1-1-q} \binom{l_1-l_2+k+1+q}{n-l_2-1},$$

$$= \binom{n+l_1}{n-l_1-1}\binom{l_1-l_2+k+1}{n-l_2-1} \sum_{q=0}^{\infty} p_q, \quad p_q = \frac{(-1)^q \binom{n+l_1}{n-l_1-1-q}\binom{l_1-l_2+k+1+q}{n-l_2-1}}{q! \binom{n+l_1}{n-l_1-1}\binom{l_1-l_2+k+1}{n-l_2-1}},$$

therefore:

$$\frac{p_{q+1}}{p_q} = \frac{(q+l_1-n+1)(q+l_2+l_1+k+3)(q+l_1-l_2+k+2)}{(q+2l_1+2)(q+l_1-n+k+3)(q+1)},$$

hence:

$$B = \binom{n+l_1}{n-l_1-1}\binom{l_1-l_2+k+1}{n-l_2-1}\ {}_3F_2(l_1-n+1,\ l_2+l_1+k+3,\ l_1-l_2+k+2;\ 2l_1+2,\ l_1-n+k+3;1), \tag{6}$$

then (2) acquires the structure:

$$< nl_2 \mid r^k \mid nl_1 >= \frac{(-1)^{n-l_2-1} b^k}{2^{k+1} n^{1-k}} \sqrt{\frac{(n+l_1);}{(n+l_2)!(n-l_1-1)!(n-l_2-1)!}}.\frac{(l_1-l_2+k+1)!}{(2l_1+1)!(l_1-n+k+2)!}.$$

$${}_3F_2(l_1-n+1,\ l_2+l_1+k+3,\ l_1-l_2+k+2;\ 2l_1+2,\ l_1-n+k+3;1). \tag{7}$$

Finally, from (7) with $l_1 = l_2$ we deduce the hypergeometric version of (3):

$$< nl \mid r^k \mid nl >= \frac{(-1)^{n-l-1} b^k}{2^{k+1} n^{1-k} (2l+1)!} \binom{k+1}{n-l-1} \, {}_3F_2(l-n+1,\ 2l+k+3,\ k+2;\ 2l+2,\ l-n+k+3;1) \tag{8}$$

The Ref. [5] has abundant literature about radial matrix elements for hydrogen-like atoms.

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