# Matrix elements $<n_2l_2|r^k|n_1l_1>$ for the Coulomb interaction

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We show that the Gregory-Newton infinite expansion for equidistant interpolation gives a simple approach to Laplace transform of Laguerre polynomials, which has an immediate usefulness to determine radial matrix elements for hydrogen-like atoms.

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## Introduction

In quantum mechanics it is important (for example, in the calculation of the electromagnetic transition probability) to have exact expressions for the matrix elements:

$$< n_2 l_2 \left| r^k \right| n_1 l_1 > \equiv \int_0^\infty g_{n_2 l_2}(r) r^k g_{n_1 l_1}(r) dr, \qquad \mathrm{k} = \text{integer} \tag{1}$$

where $\frac{1}{r} g_{nl}$ is the radial wave function verifying the Schrödinger equation for the Coulomb potential, n and l denoting the total and orbital quantum numbers, respectively.

As $g_{nl}$ is proportional to Laguerre polynomials $L_q^p$, then (1) essentially is the Laplace transform $L$ of these polynomials. Thus in Sec. 2 we employ the Gregory-Newton infinite interpolation to study $L\left\{u^{x+p} L_m^p\left(u\right)\right\}$, and in Sec. 3 we apply this result to calculate (1).

## Laplace transform of Laguerre polynomials via Gregory-Newton interpolation.

We know [1] that if $g\left(t\right)$ can be written in terms of Laguerre polynomials [2]:

$$g(t) = \sum_{k=0}^{\infty} g_k L_k^p(t), \qquad \mathrm{p} > -1 \tag{2}$$

then defined by the integral transform:

$$f(x) = \frac{1}{(x+p)!} \int_0^\infty t^{x+p} e^{-t} g(t) dt, \qquad x \geq 0 \tag{3}$$

accepts the Gregory-Newton infinite expansion:

$$f(x) = \sum_{k=0}^{\infty} (-1)^k g_k \binom{x}{k}, \tag{4}$$

where $(x+p)!$ means the gamma function $\Gamma\left(x+p+1\right)$.

Here we show that a suitable choice for $g(t)$ generates a simple approach to Laplace transform of Laguerre polynomials. In fact, if we consider:

$$g(t) = L_m^p\left(\frac{t}{s}\right), \quad \text{p > -1, s > 0, m = 0, 1,...} \tag{5}$$

then by a known identity [2] it adopts the form (2) with:

$$g_k = \binom{m+p}{k+p}\frac{(s-1)^{m-k}}{s^m}, \tag{6}$$

therefore $g_j = 0,\ j = m+1,\ m+2,\ldots$ Thus (3),...,(6) imply the following Laplace transform:

$$L\left\{u^{x+p}L_m^p(u)\right\} \equiv \int_0^\infty e^{-su}u^{x+p}L_m^p(u)du, \tag{7}$$

$$= \frac{(x+p)!}{s^{x+p+m+1}}\sum_{k=0}^{m}(-1)^k(s-1)^{m-k}\binom{m+p}{k+p}\binom{x}{k},\ p > -1, s > 0, x \geq 0 \tag{8}$$

The usual method [3] to obtain (8) is to put in (7) the definition [2] of $L_m^p(u)$ and to make directly the corresponding integral; with (7) and (8) we can deduce several particular cases [3] when $p = 0$ or/and $x = 0$. Our procedure exhibits the intimate relationship between Laguerre polynomials, Laplace transform and Gregory-Newton infinite formula for equidistant interpolation.

## Matrix elements $< n_2 l_2 \left| r^k \right| n_1 l_1 >$

The radial part of the Schrödinger equation for hydrogen-like atoms (in natural units with $M = 1, \hbar = 1$) reads [4,5]:

$$-\frac{1}{2}\left[\frac{d^2}{dr^2}-\frac{l(l+1)}{r^2}\right]g_{nl}-\frac{Ze^2}{4\pi\varepsilon_0 r}g_{nl}=-\frac{Z^2e^4}{32\pi^2\varepsilon_0^2n^2}g_{nl} \tag{9}$$

It is very well known that (using the conventions found in [2] for $L_p^q$ ):

$$g_{nl}(r)=\frac{2^{l+1}}{n^{l+2}}\left[\frac{(n-l-1)!}{(n+l)!}\right]^{\frac{1}{2}}\frac{r^{l+1}}{b^{l+\frac{3}{2}}}e^{-\frac{r}{nb}}L_{n-l-1}^{2l+1}\left(\frac{2r}{nb}\right), \tag{10}$$

with $b=\dfrac{4\pi\varepsilon_0}{Ze^2}$ and normalization:

$$\int_0^\infty\left[g_{nl}(r)\right]^2dr=1 \tag{11}$$

Many quantum mechanical applications [4, 6-15] require the calculation of (1). In several publications, computation of these matrix elements for some specific values of $k$ can be found, but, in general, they are restricted to the case $n_1=n_2$ and the computation methods therein are complicated. The analytical method has been used in [4, 11-13] to compute (1) when $n_1=n_2$ for $l_1=l_2$ or $l_2=l_1+1$ for some values of $k$. For our purposes, both sets of quantum numbers and $k$ are arbitrary. Here we show that using the analytical method makes the determination of (1), in general case $n_1\neq n_2$, very simple (compared, for instance, with the operator-factorization technique [16-21] employed in [9,15]). We also derive a closed-form expression from which all the results reported in the literature are particular cases. Such an analytical procedure is direct, since it consists of substitution of (10) into (1) and subsequent integration using (8). In fact, (1) adopts the form:

$$\left\langle n_2 l_2 \,|\, r^k \,|\, n_1 l_1 \right\rangle = \frac{2^{l_1+l_2+2}}{b^{l_1+l_2+3} n_1^{l_1+2} n_2^{l_2+2}} \left[ \frac{(n_1-l_1-1)!(n_2-l_2-1)!}{(n_1+l_1)!(n_2+l_2)!} \right]^{\frac{1}{2}}$$

$$\int_0^\infty e^{-\frac{(n_1+n_2)r}{b n_1 n_2}} r^{l_1+l_2+k+2} L_{n_1-l_1-1}^{2l_1+1}\left(\frac{2r}{bn_1}\right) L_{n_2-l_2-1}^{2l_2+1}\left(\frac{2r}{bn_2}\right) dr \tag{12}$$

where we can use the definition [2] of Laguerre polynomials

$$L_{n_1-l_1-1}^{2l_1+1}\left(\frac{2r}{bn_1}\right) = \sum_{q=0}^{n_1-l_1-1} \frac{(-1)^q}{q!} \binom{n_1+l_1}{n_1-l_1-1-q} \left(\frac{2r}{bn_1}\right)^q, \tag{13}$$

the change of variable $t = \dfrac{2r}{bn_2}$, and the result (8) to obtain the closed-form relation:

$$\left\langle n_2 l_2 \,|\, r^k \,|\, n_1 l_1 \right\rangle = \frac{2^{l_1+l_2+2} b^k (n_2-n_1)^{n_2-l_2-1}}{(n_1+n_2)^{n_2+l_1+k+2}} n_1^{l_2+k+1} n_2^{l_1+k+1}$$

$$\left[ \frac{(n_1-l_1-1)!(n_2-l_2-1)!}{(n_1+l_1)!(n_2+l_2)!} \right]^{\frac{1}{2}} \sum_{q=0}^{n_1-l_1-1} \sum_{m=0}^{n_2-l_2-1} \frac{(-1)^q 2^{q+m} n_1^m n_2^q}{q!(n_1+n_2)^q (n_1-n_2)^m} \tag{14}$$

$$\binom{n_1+l_1}{n_1-l_1-1-q} \binom{n_2+l_2}{2l_2+1+m} \binom{l_1-l_2+k+1+q}{m} (l_1+l_2+k+2+q)!$$

From (14) it is immediate to deduce the following particular expressions:

$$\left\langle nl_2 \,|\, r^k \,|\, nl_1 \right\rangle = \frac{(-1)^{n-l_2-1} b^k}{2^{k+1} n^{1-k}} \left[ \frac{(n-l_1-1)!(n-l_2-1)!}{(n+l_1)!(n+l_2)!} \right]^{\frac{1}{2}}$$
$$\sum_{m=0}^{n-l_1-1} \frac{(-1)^q}{q!} \binom{n+l_1}{n-l_1-1-q} \binom{l_1-l_2+k+1+q}{n-l_2-1} (l_1+l_2+k+2+q)! \quad (15)$$

and

$$\left\langle nl \,|\, r^k \,|\, nl \right\rangle = \frac{(-1)^{n-l-1} b^k (n-l-1)!}{2^{k+1} n^{1-k} (n+l)!}$$
$$\sum_{q=0}^{n-l-1} \frac{(-1)^q}{q!} \binom{n+l}{n-l-1-q} \binom{k+1+q}{n-l-1} (2l+k+2+q)! \quad (16)$$

Comments:

a). Our eq. (14) is equivalent to (56) of [9] (derived by a complicated process based on the factorization method). Notice, however, that in this Ref. [9] three sums have to be performed, increasing the amount of computational work.

b). Our expression (16) reproduces the formula (12) in Sec. 2, Chap. 4 of [11].

c). For $n_1 = n_2$ and $l_2 = l_1 + 1$ when $k = -1,\ -3,\ -4,\ -5$, our eq. (14) yields the result in Appendix B of [8].

d). When $k = -6,\ -5,\ -4,\ \ldots,\ 1,\ 2,\ 3$ formula (16) generates the matrix elements reported in [4, 6, 8, 10-14, 20, 22-28], for example:

$$\left\langle r^{-3} \right\rangle = \frac{2(bn)^{-3}}{l(l+1)(2l+1)}, \qquad \left\langle r^{-2} \right\rangle = \frac{2b^{-2}}{n^3(2l+1)},$$
$$\left\langle r^{-1} \right\rangle = \frac{b^{-1}}{n^2}, \qquad \left\langle r \right\rangle = \frac{b}{2}\left[3n^2 - l(l+1)\right] \quad \text{, etc} \quad (17)$$

and (11) is verified.

e). For $K = -2$, eq.(15) implies the theorem of Pasternack-Sternheimer [8,9]:

$$\left\langle nl_2 \,|\, r^{-2} \,|\, nl_1 \right\rangle = 0, \qquad l_1 \neq l_2 \tag{18}$$

The above remarks and the details of the analytical procedure (employing the Laplace transform (8)) that we used show that this is, indeed, the simplest approach to compute (1). It is very simple and produces a closed-form formula that summarizes all the values of (1) known in the literature.

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