Off-Diagonal Hydrogenic r^k Integrals by a Ladder-Operator Procedure

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It is shown that, by applying an "accelerated" or "multi-step" ladder-operatorial procedure, one can obtain, easily, a symmetric closed-form expression for the off-diagonal ($n \neq n'$, $l \neq l'$) hydrogenic r^k matrix elements.

I. INTRODUCTION

Recently, we have shown that the Schrödinger-Infeld-Hull factorization method[1,2] is able not only to give recursion formulas for calculating transition-matrix elements[3,4] but also, when followed by an "accelerated" operatorial formalism or an equivalent matrix procedure, leads to explicit formulas.[3,5] Particularly, without the help of group theory, we obtained[3] a formula in closed form for the general off-diagonal ($n\neq n'$, $l\neq l'$) hydrogenic $\langle nl|r^k|n'l'\rangle$ matrix elements. This explicit expression, which involves only factorials and binomial coefficients, is directly reducible to any particular case, i.e., to available explicit expressions given elsewhere[2,6-8] and moreover exhibits the well-known selection rules such as the Sternheimer-Pasternack selection rule.[9] Nevertheless, as it is not symmetric in (nl) and $(n'l')$, i.e., is valid when the condition $n'-l'\geqslant n-l$ is fulfilled, to calculate any given $\langle nl|r^k|n'l'\rangle$ integral one must use either the formula itself or its counterpart which is formally obtained by interchanging n, l and n', l', respectively. On the other hand, owing to the connection between this matter and finite-difference calculus, one can question if some of the summations which appear in our previous closed-form formula cannot be contracted (not obviously). This possibility suggested to us that there might exist, in the factorization scheme, an alternative "accelerated" operatorial (or equivalent "accelerated" matrix procedure) which can lead to more compact closed-form expressions. In the present paper, it is shown that one can obtain an entirely symmetric [in (nl) and $(n'l')$] explicit expression of the general off-diagonal hydrogenic r^k radial integral.

II. CALCULATION

The radial Schrödinger equation for a Coulomb field, after setting $\psi_{nl}(r)=r^{-1}R_{nl}(r)$ is

$$\left(\frac{d^2}{dr^2}+\frac{2Z}{r}-\frac{l(l+1)}{r^2}-\frac{Z^2}{n^2}\right)R_{nl}(r)=0\,. \tag{1}$$

As has been shown in our previous paper[3] and with use of the same notations, one can obtain the radial wave functions as solutions of a factorizable equation by defining $2Zr=e^x$ and $R(r)=e^{x/2}U(x)$, i.e., the $U(x)$ functions are solutions of the following pair of difference-differential equations:

$$H_S^- U_m^S=[(S-m)(S+m)]^{1/2}U_m^{S-1}\,,\qquad H_S^+ U_m^{S-1}=[(S-m)(S+m)]^{1/2}U_m^S\,, \tag{2}$$

where

$$S=n-\tfrac{1}{2}\,,\qquad m=l+\tfrac{1}{2}\,. \tag{3}$$

The corresponding ladder operators are

$$H_S^\pm=\frac{1}{2n}e^x-S\mp\frac{d}{dx}\,. \tag{4}$$

The necessary condition for the existence of quadratically integrable solutions is

$$S-m=v=\text{integer}=n-l-1\,. \tag{5}$$

In fact, v is the usual radial quantum number $n_r=n-l-1$.

A. "Accelerated" Ladder Operator

Each eigenfunction of the whole discrete set of the quadratically integrable functions $U_m^S=U_m^{m+v}$ is completely characterized by the integer value of v, which fixes its rank starting from the key function $U_m^m(v=0)$, and for each value i of v, the ladder operators in Eq. (2) may be considered as "one-step" ladder operators which generate the eigenfunctions, step by step, downward or upward. Hence, one can define[3] the corresponding "accelerated" or "v-step" operators $\mathcal{H}_v^\pm$, which directly generate any U_m^{m+v} function from/to the key function, so that

$$\mathcal{H}_v^+U_m^m=\mathfrak{N}_vU_m^{m+v}\,,\qquad \mathcal{H}_v^-U_m^{m+v}=\mathfrak{N}_vU_m^m\,, \tag{6}$$

where

$$\mathcal{H}_v^\pm=\prod_{i=1}^{v}H_{m+i}^\pm\,, \tag{7}$$

$$H^{\pm}_{m+i}=\frac{1}{2n}e^x-(m+i)\mp\frac{d}{dx}, \tag{8}$$

$$\mathfrak{N}_v=\prod_{i=1}^{v}[i(i+2m)]^{1/2}=\left(\frac{v!(v+2m)!}{(2m)!}\right)^{1/2}. \tag{9}$$

Using Eq. (8) to express H^+ in terms of H^-, one obtains, particularly, an alternative expression of the "accelerated" operator

$$H_v^+=\prod_{i=1}^{v}\left(\frac{1}{n}e^x-2m-H_m^--i\right) \tag{10}$$

and from Eq. (6), we get

$$U_m^{m+v}=\frac{1}{\mathfrak{N}_v}(\mathcal{H}_v^+U_m^m)$$
$$=\frac{1}{\mathfrak{N}_v}\prod_{i=1}^{v}\left(\frac{1}{n}e^x-2m-H_m^--i\right)U_m^m. \tag{11}$$

In order to introduce the action on U_m^m of the ladder operator H_m^-, one makes use of the following relationship:

$$(-H_m^-)[(1/n)e^x]^tU(x)=[(1/n)e^x]^t(-H_m^-+t)U(x).$$

After rearranging the terms, one gets

$$U_m^{m+v}=\frac{1}{\mathfrak{N}_v}\sum_{i=0}^{v}\binom{v}{i}\left(\frac{1}{n}e^x\right)^i\prod_{u=1}^{v-i}(-2m-H_m^--i-u)U_m^m.$$

Since

$$H_m^-U_m^m=0, \tag{12}$$

one finally obtains the following expression of any function U_m^{m+v} in terms of the key function U_m^m $(v=0)$:

$$U_m^{m+v}(x)=(-)^v\frac{1}{\mathfrak{N}_v}\sum_{i=0}^{v}\binom{v}{i}\left(-\frac{1}{n}e^x\right)^i\frac{(2m+v)!}{(2m+i)!}U_m^m(x). \tag{13}$$

B. Off-Diagonal $(n\neq n')r^k$ Integrals

The general matrix element to be calculated is

$$\langle nl|r^k|n'l'\rangle=\int_0^{+\infty}R_{nl}^*(r)r^kR_{n'l'}(r)\,dr$$
$$=(1/2Z)^{k+1}\mathfrak{M}^k_{v\,v'}(m,m'), \tag{14}$$

where[3]

$$\mathfrak{M}^k_{v,v'}(m,m')=\int_{-\infty}^{+\infty}U_m^{m+v}(x)e^{(k+2)x}U_{m'}^{m'+v'}(x)\,dx. \tag{15}$$

Hence, from the expression (13) of the U_m^{m+v} function, we have

$$\mathfrak{M}^k_{v,v'}(m,m')=\frac{(-1)^v}{\mathfrak{N}_v}\sum_{i=0}^{v}\binom{v}{i}\left(-\frac{1}{n}\right)^i\frac{(2m+v)!}{(2m+i)!}$$
$$\times\mathfrak{M}^{k+i}_{0,v'}(m,m'). \tag{16}$$

As formula (16), for $v'=0$, also gives the expression for $\mathfrak{M}^k_{v,0}$ in terms of the key matrix elements $\mathfrak{M}^k_{0,0}$ and, consequently, its counterpart, i.e., $\mathfrak{M}^k_{0,v'}$ in terms of $\mathfrak{M}^k_{0,0}$ one finally obtains

$$\mathfrak{M}^k_{v,v'}(m,m')=\frac{(-1)^{v+v'}}{\mathfrak{N}_v\mathfrak{N}_{v'}'}\sum_{i=0}^{v}\binom{v}{i}\left(-\frac{1}{n}\right)^i$$
$$\times\sum_{j=0}^{v'}\binom{v'}{j}\left(-\frac{1}{n}\right)^j\frac{(2m+v)!(2m'+v')!}{(2m+i)!(2m'+j)!}$$
$$\times\mathfrak{M}^{k+i+j}_{0,0}(m,m'). \tag{17}$$

The key matrix elements $\mathfrak{M}^w_{0,0}$ have already been calculated in our previous paper.[3] The key functions, which are solutions of Eq. (12) are

$$U_m^m(x)=Cn^{-m}[(2m-1)!]^{-1/2}\exp\left(mx-\frac{1}{2n}e^x\right), \tag{18}$$

where the constant C, when adjusted to match with the usual R_{nl} normalization condition[3] is

$$C=Z^{1/2}n^{-3/2}(2l+1)^{-1/2} \tag{19}$$

and one gets

$$\mathfrak{M}^w_{0,0}(m,m')=CC'\left(\frac{2nn'}{n+n'}\right)^{m+m'+w+2}$$
$$\times\frac{(m+m'+w+1)!}{n^mn'^{m'}[(2m-1)!(2m'-1)!]^{1/2}}. \tag{20}$$

Then, keeping in mind that $v=n-l-1$ and $m=l+\frac{1}{2}$, one finally deduces from Eqs. (14), (17), (19), and (20) the required expression of the general r^k matrix element:

$$\langle nl|r^k|n'l'\rangle=A\sum_{i=0}^{n-l-1}\binom{n-l-1}{i}\left(-\frac{1}{n}\right)^i\sum_{j=0}^{n'-l'-1}\binom{n'-l'-1}{j}\left(-\frac{1}{n'}\right)^j\left(\frac{2nn'}{n+n'}\right)^{i+j}\frac{(l+l'+k+2+i+j)!}{(2l+1+i)!(2l'+1+j)!}, \tag{21}$$

where

$$A=\frac{(-)^{n-l+n'-l'}}{2(2Z)^k}\left(\frac{2nn'}{n+n'}\right)^{l+l'+k+3}\frac{1}{n^{l+2}n'^{l'+2}}\left(\frac{(n+l)!(n'+l')!}{(n-l-1)!(n'-l'-1)!}\right)^{1/2}.$$

Indeed, this result could be obtained by an equivalent "accelerated" matrix method[3]; nevertheless, owing to the evident parallelism of the two methods, we give, in the present paper, only the former one.

III. CONCLUSION

Finally, we have obtained another closed-form expression for the general hydrogenic r^k integral which is entirely symmetric in (nl) and $(n'l')$ and involves only two summations. As it can be shown from the expression [Eq. (13)] of the functions in terms of the key functions [Eq. (18)], the formula obtained must very likely correspond to a crude evaluation of the r^k integral when expressing hydrogenic functions in terms of basic $r^i e^{-(Zr/n)}$ functions. If the formula appears to be easy to handle either by hand calculations or programming, one must point out that it does not directly exhibit, as did our former formula,[3] the existing selection rules.[9] Moreover, analytical reduction of the formula [Eq. (21)] to special particular cases such as $n=n'$, for instance, is not obvious or easy. This last multistep ladder-operatorial procedure seems appropriate to other cases of factorizable equations, particularly, as we have been able to obtain, in the same way, a compact closed-form expression of the Morse-Pekeris nuclear dipole matrix elements.[10] Indeed, we know that this last problem contains the hydrogenic case.

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