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# Closed-Form Hydrogenic Radial $r^k$ Matrix Elements and the Factorization Method

M. Badawi,* N. Bessis, G. Bessis, and G. Hadinger
*Laboratoire de Spectroscopie et de Luminescence, Universite Claude Bernard, Lyon I, 69621 Villeurbanne, France*
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It is shown that the factorization method, when introducing accelerated ladder operators or accelerated ladder matrices, leads to a formula in closed form for the general off-diagonal ($n \neq n'$) hydrogenic $r^k$ matrix elements. This explicit expression, which involves only factorials and binomial coefficients, is directly reducible to any particular case. The well-known selection rules follow from the formula. The method seems appropriate to other cases of factorizable equations. Its extension to the Dirac-Coulomb, generalized Kepler problems, and the discrete-continuous case is considered.

## INTRODUCTION

If, for special cases, hydrogenic radial $r^k$ integrals have been calculated many times, either using the generating function of Laguerre polynomials,[1,2] or using both the factorization method and algebraic manipulations,[3] or both the factorization method and group theory,[4-7] the evaluation of the general matrix element is known to be rather difficult and intricate, owing to the quantum-number-$n$ dependence of the variable. Recently, we have questioned whether the factorization method is solely able to give recursion formulas or whether it can also give explicit formulas without the help of group theory, and we have shown[8] that this method, when followed by an "accelerated" operatorial formalism or an equivalent matrix procedure, leads to formulas in closed form for calculating diatomic vibrational-transition matrix elements. While investigating this last question, it appeared that it contained the hydrogenic case with two slight changes: On the one hand, the key matrix elements are trivial, as they merely reduce to factorials or to Euler complex-Γ functions (for the discrete-continuous key matrix elements); on the other hand, one must be careful when normalizing the wave functions.[3]

A preliminary investigation has shown that the difficulties for evaluating the diagonal or the off-diagonal matrix elements are of the same kind; in the present paper, we consider, the general ($n \neq n'$) hydrogenic radial $r^k$ integral. Other particular cases are merely a reduction of this last case. In Sec. I the recursion formulas we use are derived. In Sec. II, it is shown how the operator formalism and the alternative matrix procedure work, and we give the hydrogenic radial $\langle nl | r^k | n'l' \rangle$ matrix elements in closed form. The results are given and discussed in Sec. III.

## I. RECURSION FORMULAS

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

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

If one defines $2Zr = e^x$ and $R(r) = e^{x/2} U(x)$, Eq. (1) transforms to

$$\left(\frac{d^2}{dx^2} - \frac{1}{4n^2} e^{2x} + e^x - (l + \tfrac{1}{2})^2\right) U(x) = 0 . \tag{2}$$

Equation (2) is factorizable,[3,9] i.e., one can write the following pair of difference-differential equations equivalent to Eq. (2):

$$\left(\frac{1}{2n}e^x - S - \frac{d}{dx}\right)\left(\frac{1}{2n}e^x - S + \frac{d}{dx}\right)U_m^S = (S^2 - m^2)U_m^S ,$$

$$\left(\frac{1}{2n}e^x - (S+1) + \frac{d}{dx}\right)\left(\frac{1}{2n}e^x - (S+1) - \frac{d}{dx}\right)U_m^S = [(S+1)^2 - m^2]U_m^S , \tag{3}$$

where

$$S = n - \tfrac{1}{2} \text{ and } m = l + \tfrac{1}{2}. \tag{4}$$

Thus, the corresponding ladder operators are defined

$$H_S^- U_m^S = \left(\frac{1}{2n}e^x - S + \frac{d}{dx}\right)U_m^S = [(S-m)(S+m)]^{1/2} U_m^{S-1},$$

$$H_S^+ U_m^{S-1} = \left(\frac{1}{2n}e^x - S - \frac{d}{dx}\right)U_m^{S-1} = [(S-m)(S+m)]^{1/2} U_m^S . \tag{5}$$

The necessary condition for the existence of quadratically integrable solutions is[3]

$$S - m = v = \text{integer} = n - l - 1 . \tag{6}$$

The key eigenfunctions are obtained for $S = m \to v = 0$ and are solutions of the first-order differential equation

$$\left(\frac{1}{2n}e^x - m + \frac{d}{dx}\right)U_m^m = 0 . \tag{7}$$

One gets

$$U_m^m = Cn^{-m}[(2m-1)!]^{-1/2}\exp(mx - (1/2n)e^x) , \tag{8}$$

where $C$ is a constant which shall be adjusted further to match with the usual $R_{nl}$ normalization condition. As has been previously shown,[3] the ladder operators are defined so that they preserve not only the quadratic integrability but also the normalization of the eigenfunctions $U_m^{m+v}$ and

$$C^2 = \int_{-\infty}^{+\infty} (U_m^m)^2 dx = \int_{-\infty}^{+\infty} (U_m^{m+v})^2 dx . \tag{9}$$

Each eigenfunction of the whole discrete set of quadratically integrable solutions of Eq. (2) is now completely characterized by the integer value of $v$, which fixes its rank starting from the key function $U_m^m$[Eq. (8)], labeled $v=0$. The quantum number $v$ is just the usual radial quantum number $n_r = n - l - 1$.

The radial matrix elements to be calculated are

$$\langle nl | r^k | n'l' \rangle = \int_0^{+\infty} R_{nl}^* r^k R_{n'l'}\, dr , \tag{10}$$

when the $R_{nl}(r)$ radial wave functions are assumed to be normalized to unity. By introducing the $U_m^{m+v}(x)$ wave functions, one gets

$$\langle nl | r^k | n'l' \rangle = [CC'/(2Z)^{k+1}]\mathfrak{M}_{v,v'}^k(m,m') , \tag{11}$$

where

$$\mathfrak{M}_{v,v'}^k(m,m') = (1/CC') \times \int_{-\infty}^{+\infty} U_m^{m+v}(x) e^{(k+2)x} U_{m'}^{m'+v'}(x)\, dx . \tag{12}$$

As pointed out before, the values of the constant $C$(or $C'$) must be adjusted to match with the usual $R_{nl}(r)$ normalization condition. One gets

$$C^2 = (2Z)^{-1}\int_0^{+\infty} (R_{nl})^2 r^{-2} dr = [Z/n^3(2l+1)] , \tag{13}$$

so that

$$C = Z^{1/2} n^{-3/2}(2l+1)^{-1/2} . \tag{14}$$

It should be noted that for $k=-2$ and $m+v=m'+v'$, i.e., $n=n'$, owing to the orthogonality of the $U_m^{m+v}$ functions,[8] the matrix element $\langle nl | r^{-2} | n'l' \rangle$ vanishes unless $m=m'$, i.e., $l=l'$. One finds again the well-known result of Feinberg,[10] which appears as the limit of the Pasternack-Sternheimer[11] condition which will be re-established further.

Now, one must calculate the general matrix element $\mathfrak{M}_{v,v'}^k(m,m')$[Eq. (12)] and derive recursion relationships, giving its determination in terms of the key matrix elements

$$\mathfrak{M}_{0,0}^k(m,m') = \left(\frac{2nn'}{n+n'}\right)^{m+m'+k+2} \times \frac{(m+m'+k+1)!}{n^m n'^{m'}[(2m-1)!(2m'-1)!]^{1/2}} . \tag{15}$$

Obviously, from (15), the only nonvanishing key matrix elements are obtained for $k \geq -(m+m'+1)$, i.e., $k > -(l+l'+1)$.

Using Eq. (5) with the quantification condition $S = m+v$, and owing to the mutual adjointness of the ladder operators, we find for $v>0$:

$$\mathfrak{M}_{v,v'}^k(m,m') = [v(v+2m)]^{-1/2}\int_{-\infty}^{+\infty} (H_{m+v}^+ U_m^{m+v}) e^{(k+2)x} U_{m'}^{m'+v'}\, dx$$
$$= [v(v+2m)]^{-1/2}\int_{-\infty}^{+\infty} U_m^{m+v-1}(H_{m+v}^- e^{(k+2)x} U_{m'}^{m'+v'})\, dx . \tag{16}$$

In order to always have the ladder operator $H^-_{m+v}$ acting directly on the wave function, we note that there exist the following pair of relationships which are valid for any value of the constant "$a$" and of the quantum numbers "$m$" or "$v$" (this relation will be used systematically):

$$H^{\pm} e^{ax} U(x) = e^{ax}(\mp a + H^{\pm})U(x) . \qquad (17)$$

Then, remarking that

$$H^-_{m+v} U(x) = [H^-_{m'+v'} + (m' - m + v' - v) + (1/2n - 1/2n')e^x] U(x) , \qquad (18)$$

one finally obtains the following required recursion formula ($v' \geq v$):

$$\mathfrak{M}^k_{v,v'}(m,m') = [v(v+2m)]^{-1/2} \times \{[v'(v'+2m')]^{1/2} \mathfrak{M}^k_{v-1,v'-1}(m,m') + (k+2+m'-m+v'-v)\mathfrak{M}^k_{v-1,v'}(m,m') + (1/2n - 1/2n')\mathfrak{M}^{k+1}_{v-1,v'}(m,m')\} \qquad (19)$$

and its counterpart ($v \geq v'$), which is formally obtained by interchanging respectively $v$, $n$, $m$ and $v'$, $n'$, $m'$. By repeated use of the recursion relationship [Eq. (19)] and its counterpart, any matrix element $\mathfrak{M}^k_{v,v'}(m,m')$ can be finally expressed in terms of the key matrix elements $\mathfrak{M}^i_{0,0}(m,m')$ [Eq. (15)] ($i \geq k$).

It should be noted that for $n = n'$ and $v' = 0$, the relationship in Eq. (19) merely reduces to

$$\mathfrak{M}^k_{i,0}(m,m') = \frac{(k+2+m'-m-i)}{[i(i+2m)]^{1/2}} \mathfrak{M}^k_{i-1,0}(m,m') \qquad (1 \leq i \leq v). \qquad (20)$$

Thus

$$\mathfrak{M}^k_{v,0}(m,m') = \left(\prod_{i=1}^{v} \frac{(k+2+m'-m-i)}{[i(i+2m)]^{1/2}}\right) \mathfrak{M}^k_{0,0}(m,m') . \qquad (21)$$

For the diagonal element, i.e., $n = n'$, and for $v' = 0$, i.e., $m' - m = v = l' - l > 0$, the matrix element $\mathfrak{M}^k_{v,0}(m,m')$ vanishes when $2 < -k < 1 + (l' - l)$. This is the Pasternack-Sternheimer[11] selection rule.

Using Eqs. (11), (14), and (15), one finally gets

$$\langle nl | r^k | n\, n-1 \rangle = \left(\prod_{i=1}^{n-l-1} (1+k+i)\right) \times \frac{n^{k-1}(l+n+k+1)!}{2(2Z)^k[(2n-1)!(n-l-1)!(n+l)!]^{1/2}} , \qquad (22)$$

where

$$\prod_{i=1}^{n-l-1} (1+k+i) = \frac{(n-l+k)!}{(1+k)!} \quad \text{for } k > \max\begin{cases}-2\\ l-n\end{cases}$$
$$= (-1)^{n-l-1} \frac{(-k-2)!}{(-k+l-n-1)!} \quad \text{for } k < \min\begin{cases}-2\\ l-n\end{cases} . \qquad (23)$$

## II. CALCULATION OF MATRIX ELEMENTS

Although the recursion formula (19) is valid even for discrete-continuous matrix elements,[3,12,13] we limit ourselves hereafter to discrete-discrete matrix elements.

### A. Operatorial Procedure

For each value $i$ of the quantum number $v$, Eqs. (5) may be rewritten

$$H^-_{m+i} U^{m+i}_m = \left(\frac{1}{2n} e^x - (m+i) + \frac{d}{dx}\right) U^{m+i}_m = N_i U^{m+i-1}_m , \qquad (24)$$

$$H^+_{m+i} U^{m+i-1}_m = \left(\frac{1}{2n} e^x - (m+i) - \frac{d}{dx}\right) U^{m+i-1}_m = N_i U^{m+i}_m ,$$

where

$$N_i = [i(i+2m)]^{1/2}$$

and (25)

$$N'_i = [i(i+2m')]^{1/2} .$$

The ladder operators in (24) may be considered as "one-step" ladder operators which generate the eigenfunctions, step by step, upward or downward. Let us define the "accelerated" or "$v$ step" operators

$$\mathcal{H}^{\pm}_v = \prod_{i=1}^{v} H^{\pm}_{m+i} . \qquad (26)$$

Since, obviously, the ladder operators $H^{\pm}_{m+i}$ and $H^{\pm}_{m+j}$, respectively, commute among themselves, one gets

$$\mathcal{H}^+_v U^m_m = \mathfrak{N}_v U^{m+v}_m , \qquad \mathcal{H}^-_v U^{m+v}_m = \mathfrak{N}_v U^m_m , \qquad (27)$$

where

$$\mathfrak{N}_v = \prod_{i=1}^{v} [i(i+2m)]^{1/2} = \left[\frac{v!(v+2m)!}{(2m)!}\right]^{1/2} . \qquad (28)$$

Then the matrix element [Eq. (12)] may be rewritten

$$\mathfrak{M}^k_{v,v'}(m,m') = \mathfrak{N}_v^{-1} \int_{-\infty}^{+\infty} (\mathcal{H}^+_v U^m_m) e^{(k+2)x} U^{m'+v'}_{m'} \, dx . \qquad (29)$$

Owing to the mutual adjointness of the ladder operators, we get

$$\mathfrak{M}^k_{v,v'}(m,m') = \frac{1}{\mathfrak{N}_v}\int_{-\infty}^{+\infty} U^m_m(\mathcal{K}^-_v e^{(k+2)x} U^{m'+v'}_{m'})\,dx$$
$$= \frac{1}{\mathfrak{N}_v}\int_{-\infty}^{+\infty} U^m_m\left(\prod_{i=1}^{v} H^-_{m+i}\right) e^{(k+2)x} U^{m'+v'}_{m'}\,dx\,. \tag{30}$$

Using Eqs. (17) and (18), and noting that

$$H^-_{m'+i} = H^-_{m'} - i \tag{31}$$

one gets, when introducing the abbreviated notation

$$k_0 = k + 2 + m' - m$$

and

$$n_0 = (1/2n - 1/2n')\,; \tag{32}$$

$$\mathfrak{M}^k_{v,v'}(m,m') = \frac{1}{\mathfrak{N}_v}\int_{-\infty}^{+\infty} U^m_m e^{(k+2)x}$$
$$\times\prod_{i=1}^{v}(k_0 + n_0e^x + H^-_{m'} - i)U^{m'+v'}_{m'}\,dx\,. \tag{33}$$

Using Eq. (17) once more, and rearranging the terms, one deduces

$$\prod_{i=1}^{v}(k_0 + n_0e^x + H^-_{m'} - i)\,U^{m'+v'}_{m'}$$
$$= \sum_{i=0}^{v}\binom{v}{i}(n_0e^x)^{v-i}\prod_{u=1}^{i}(k_0 + H^-_{m'} - u)\,U^{m'+v'}_{m'}\,. \tag{34}$$

One must now introduce upon $U^{m'+v'}_{m'}$ the action of the successive one-step down $H^-_{m'+v'}$ ⋯ operators. The finite-difference mathematical nature of this quantification problem suggests the use of the Vandermonde[14] formula [Eq. (35)] to transform the product factor of [Eq. (34)]:

$$\prod_{u=1}^{i}(a + b - u)$$
$$= \sum_{j=0}^{i}\binom{i}{j}\prod_{u=1}^{i-j}(a + u - i - 1)\prod_{w=1}^{j}(b + w - 1)\,. \tag{35}$$

We apply the Vandermonde formula for $a = k_0 + v'$ and $b = H^-_{m'} - v' = H^-_{m'+v'}$, since, obviously, $k_0$ commutes with $H^-_{m'}$. Hence, we get

$$\prod_{i=1}^{v}(n_0e^x + k_0 + H^-_{m'} - i)\,U^{m'+v'}_{m'} = \sum_{i=0}^{v}\binom{v}{i}(n_0e^x)^{v-i}\sum_{j=0}^{i}\binom{i}{j}\left(\prod_{u=1}^{i-j}(k_0 + v' + u - i - 1)\right)\left(\prod_{w=1}^{j}H^-_{m'+v'} + w - 1\right)U^{m'+v'}_{m'}\,, \tag{36}$$

so that now, since

$$\prod_{w=1}^{j}(H^-_{m'+v'} + w - 1)\,U^{m'+v'}_{m'} = \left(\prod_{u=1}^{j}N'_{v'-u+1}\right)U^{m'+v'-j}_{m'}$$
$$= \left(\frac{\mathfrak{N}'_{v'}}{\mathfrak{N}'_{v'-j}}\right)U^{m'+v'-j}_{m'}\,. \tag{37}$$

One finally obtains

$$\mathfrak{M}^k_{v,v'}(m,m')$$
$$= \frac{1}{\mathfrak{N}_v}\sum_{i=0}^{v}\binom{v}{i}\sum_{j=0}^{i}\binom{i}{j}\left(\prod_{u=1}^{i-j}(k_0 + v' - i + u - 1)\right)$$
$$\times\frac{\mathfrak{N}'_{v'}}{\mathfrak{N}'_{v'-j}}\,n_0^{v-i}\,\mathfrak{M}^{k+v-i}_{0,v'-j}(m,m')\,. \tag{38}$$

Expression (38) can be used twice, not only because it gives the evaluation of the general matrix element $\mathfrak{M}^k_{v,v'}(m,m')$ in terms of the simpler ones $\mathfrak{M}^{k+v-i}_{0,v'-j}(m,m')$, but also because it gives the determination of these last matrix elements in terms of the already calculated [Eq. (15)] key matrix elements $\mathfrak{M}^u_{0,0}(m,m')$. Indeed, for $v' = 0$, involving $j = 0$, expression (38) reduces to

$$\mathfrak{M}^k_{v,0}(m,m')$$
$$= \frac{1}{\mathfrak{N}_v}\sum_{i=0}^{v}\binom{v}{i}\left(\prod_{u=1}^{i}(k_0 - i + u - 1)\right)n_0^{v-i}\,\mathfrak{M}^{k+v-i}_{0,0}(m,m')\,. \tag{39}$$

Hence, using both Eq. (38) and the counterpart of Eq. (39), (for $v' \to v' - j$) one obtains the required expression of the general matrix element in terms of the key matrix elements

$$\mathfrak{M}^k_{v,v'}(m,m') = \frac{1}{\mathfrak{N}_v}\sum_{i=0}^{v}\binom{v}{i}\sum_{j=0}^{i}\binom{i}{j}\left(\prod_{u=1}^{i-j}(k_0 + v' - i + u - 1)\right)n_0^{v-i}$$
$$\times\frac{\mathfrak{N}'_{v'}}{\mathfrak{N}'^2_{v'-j}}\sum_{w=0}^{v'-j}\binom{v'-j}{w}\left(\prod_{u=1}^{w}(k_0 + v - i - u)\right)(-)^{v'-w-j}\,n_0^{v'-w-j}\,\mathfrak{M}^{k+v-i+v'-j-w}_{0,0}\,. \tag{40}$$

Before explicitly deriving the corresponding final expression of $\langle nl \mid r^k \mid n'l' \rangle$, we investigate its alternative determination by a matrix procedure.

### B. Matrix Procedure

Before investigating the general case $n \neq n'$, let us first, for the sake of clarity and simplicity, consider how the matrix procedure works for the diagonal case $n = n'$.

#### 1. *Diagonal Matrix Elements $n = n'$*

For $n = n'$, the set of the $[(v+1)\times(v'+1)]$ successive recursion formulas [Eqs. (19)] ($i = 0, v$ and $j = 0, v'$) reduces to

$$\mathfrak{M}^k_{i,j}(m,m') = N_i^{-1}[N'_j \, \mathfrak{M}^k_{i-1,j-1}(m,m') + (k_0 + j - i)\mathfrak{M}^k_{i-1,j}(m,m')], \quad (41)$$

where $N_i$, $N'_j$, and $k_0$ have been defined by Eqs. (25) and (32), respectively.

For each current value $i$ of $v$, this set of equations can be replaced by the action of a one-step square matrix $[H(i)]$ acting on a $(v'+1)$-dimensional vector $|V^k_{i-1}|$ in which, for convenience, the successive normalization constants $N'_j$ are incorporated. This last procedure produces, as will be seen later, a substantial simplification in the final result.

Indeed, let us define the following square matrix, and vector

$$[H] = \begin{bmatrix} k_0 & & & & \\ 1 & k_0+1 & & & \\ & \ddots & \ddots & & \\ & & \ddots & \ddots & \\ & & & 1 & k_0+v' \end{bmatrix} \quad |V^k_i| = \begin{vmatrix} V^k_{i,0} \\ V^k_{i,1} \\ \vdots \\ \vdots \\ V^k_{i,v'} \end{vmatrix}, \quad (42)$$

where the $(j+1)$th component is

$$V^k_{i,j} = \left(\prod_{u=0}^{v'-j-1} N'_{v'-u}\right)\mathfrak{M}^k_{i,j} = \frac{\mathfrak{N}'_{v'}}{\mathfrak{N}'_j}\mathfrak{M}^k_{i,j}. \quad (43)$$

Hence, for each current value $i$ of $v$, the matrix equation

$$[V^k_i] = N_i^{-1}[H(i)]|V^k_{i-1}|, \quad [H(i)] = [H] - i \quad (44)$$

is equivalent to the set of recursion formulas [Eq. (41)] when multiplying both sides successively by $N'_{v'}$, $N'_{v'-1} \ldots N'_1$, when $j$ decreasing from $v' = 1$.

Then, one can relate $|V^k_v|$ to $|V^k_0|$, i.e., $\mathfrak{M}^k_{v,v'}$ to the $\mathfrak{M}^k_{0,j}$ $(j = 0, v')$, by the action on the "accelerated" or "$v$ step-down" matrix

$$[\mathcal{K}_v] = \prod_{i=1}^{v}[H(i)], \quad (45)$$

so that

$$|V^k_v| = \mathfrak{N}_v^{-1}[\mathcal{K}_v]|V^k_0|, \quad (46)$$

and particularly

$$V^k_{v,v'} = \mathfrak{M}^k_{v,v'} = \sum_{j=0}^{v'}(\mathcal{K})_{v',v'-j}V^k_{v'-j}. \quad (47)$$

Owing to the particular structure of the commuting successive square matrices $[H(i)]$, the current element of the last row of the accelerated matrix $[\mathcal{K}_v]$ is $(v' \geq v)$

$$(\mathcal{K}_v)_{v',v'-j} = \binom{v}{j}\prod_{u=1}^{v-j}(k_0 + v' - v + u - 1) \quad (j = 0, v'). \quad (48)$$

One finally obtains the following expression which is valid for $n = n'$ and $v' \geq v$:

$$\mathfrak{M}^k_{v,v'} = (1/\mathfrak{N}_v)\sum_{j=0}^{v'}\binom{v}{j}\prod_{u=1}^{v-j}(k_0 + v' - v + u - 1) \times(\mathfrak{N}'_{v'}/\mathfrak{N}'_{v'-j})\mathfrak{M}^k_{0,v'-j}. \quad (49)$$

As shown in the preceding section, successive use of expression (49) and of its counterpart for $v = 0$, allows the determination of $\mathfrak{M}^k_{v,v'}$ in terms of the key matrix elements $\mathfrak{M}^k_{0,0}$.

#### 2. *Off-Diagonal Matrix Elements $n \neq n'$*

Let us consider the general case $n \neq n'$. The corresponding set of the $[(v+1)(v'+1)]$ successive recursion formulas ($i = 0, v$ and $j = 0, v'$) is now

$$\mathfrak{M}^{k+u}_{i,j}(m,m') = N_i^{-1}[N'_j \mathfrak{M}^{k+u}_{i-1,j-1} + (k_0 + u + j - i)\mathfrak{M}^{k+u}_{i-1,j} + n_0\mathfrak{M}^{k+u+1}_{i-1,j}], \quad (50)$$

where $N_i$, $N'_j$ and $k_0$, $n_0$ have been defined by Eqs. (25) and (32), respectively.

For each current value $i$ of $v$, this set of equations can be replaced by the action of a one-step rectangular supermatrix $[[G(i)]]$ with $[(v - i + 1) \times (v'+1)]$ rows and $[(v - i + 2)(v'+1)]$ columns acting on a $[(v - i + 2)(v'+1)]$-dimensional supervector $\|W_{i-1}\|$. Indeed, let us consider the following supermatrix and the corresponding supervector, in which, for convenience, the successive powers of the constant $n_0$ are incorporated:

$$[[G(i)]] = \begin{bmatrix} [1] & [H(2i-v)] & & & \\ & [1] & \ddots & & \\ & & \ddots & \ddots & \\ & & & [1] & [H(i-1)] \\ & & & & [1] \; [H(i)] \end{bmatrix} \quad \| W_i \| = \begin{vmatrix} n_0^{v-i} | V_i^{k+v-i} | \\ \vdots \\ n_0 | V_i^{k+1} | \\ | V_i^k | \end{vmatrix} , \tag{51}$$

where $[H(i)] = [H] - i \ldots$ and $[H]$ is the preceding $(v'+1)$-dimensional square matrix (42) and the supervector $\| W_i \|$ is built up from the preceding vectors $| V_i^k |$ [Eq. (42)]. With these definitions, Eq. (50) is equivalent to the matrix equation

$$\| W_i \| = N_i^{-1} [[G(i)]] \, \| W_{i-1} \| \; . \tag{52}$$

Hence one can define, in the same way as before, the accelerated supermatrix

$$[[\mathcal{G}]] = \frac{1}{\mathfrak{N}_v} \prod_{i=1}^{v} [[G(i)]] \, , \tag{53}$$

so that, introducing the accelerated matrices $[\mathcal{H}_i]$ [Eq. (45)], one gets the matrix relation

$$| V_v^k | = \frac{1}{\mathfrak{N}_v} \sum_{i=0}^{v} \binom{v}{i} [\mathcal{H}_i] n_0^{v-i} | V_0^{k+v-i} | \, , \tag{54}$$

and then

$$V_{v,v'}^k = \frac{1}{\mathfrak{N}_v} \sum_{i=0}^{v} \binom{v}{i} n_0^{v-i} \sum_{j=0}^{i} (\mathcal{H}_i)_{v',v'-j} V_{0,v'-j}^{k+v-i} \, , \tag{55}$$

where the scalar matrix element $(\mathcal{H}_i)_{v',v'-j}$ is given by Eq. (48).

Finally, using Eq. (43), one finds again expression (38) that was derived by the operator procedure. Of course, as expected, the operator and the matrix procedures correspond step by step. Nevertheless, as pointed out elsewhere,[8] from a computational point of view, the matrix derivation seems more advantageous than the use of an explicit expression.

## III. RESULTS

In order to derive the final $\langle nl | r^k | n' l' \rangle$ matrix element we make successive use of expressions (11), (14), and (15) and substitute the definitions of $\mathfrak{N}_v$ [Eq. (28)] $k_0$ and $n_0$ [Eq. (32)]. Then, keeping in mind that $v = n_r = n - l - 1$, $v' = n'_r = n' - l' - 1$, $m = l + \frac{1}{2}$, and $m' = l' + \frac{1}{2}$, one obtains the following formula which is valid for $v' \geq v$:

$$\langle nl | r^k | n' l' \rangle = A \sum_{i=0}^{v} \binom{v}{i} \sum_{j=0}^{v-i} \binom{v-i}{j} \left( \prod_{u=1}^{v-i-j} (k+1+n'-n+i+u) \right) \frac{1}{(n'-l'-1-j)!(n'+l'-j)!}$$
$$\times \sum_{t=0}^{v'-j} \binom{v'-j}{t} (-)^t \left( \frac{n'-n}{n'+n} \right)^{i+t} (l+l'+k+2+i+t)! \left( \prod_{u=1}^{v'-j-t} (l-l'+k+2+i-u) \right) , \tag{56}$$

where

$$A = \frac{1}{4Z} \left( \frac{n+n'}{4Z} \right)^{k-1} \left( \frac{2n}{n'+n} \right)^{l'+k+1} \left( \frac{2n'}{n+n'} \right)^{l+k+1} \left( \frac{(n'-l'-1)!(n'+l')!}{(n-l-1)!(n+l)!} \right)^{\frac{1}{2}} . \tag{57}$$

We have written formula (56) with the $\prod$ symbol rather than with the equivalent ratios of factorials to keep the same expression for any value of $k$. Furthermore, selection rules are apparent.

Setting $n = n'$, the only nonvanishing contribution in Eq. (56) corresponds to $i + t = 0$ (i.e., $t = 0$ and $i = 0$) and we obtain

$$\langle nl | r^k | nl' \rangle = A_1 \sum_{j=0}^{v} \binom{v}{j} \left( \prod_{u=1}^{v-j} (k+1+u) \right) \left( \prod_{u=1}^{v'-j} (l-l'+k+2-u) \right) \frac{1}{(n-l'-1-j)!(n+l'-j)!} , \tag{58}$$

where

$$A_1 = \frac{1}{4Z} \left( \frac{n}{2Z} \right)^{k-1} \left( \frac{(n-l'-1)!(n+l')!}{(n-l-1)!(n+l)!} \right)^{1/2} (l+l'+k+2)! \; . \tag{59}$$

Formulas (56) and (58) have been checked with the available explicit expressions given elsewhere.[2,3,12,15]

## IV. CONCLUSION

It appears that the factorization method, when using accelerated ladder operators or accelerated matrices becomes a powerful tool for calculating matrix elements. We have shown that the problem of calculating hydrogenic radial $r^k$ integrals for any value of the quantum numbers, i.e., for $n \neq n'$, $l \neq l'$, and any value of $k$ can be completely solved. Up to now, even using group theory, closed-form formulas for the general case have not been given except for the particular cases $k=1$ or $k=-1$.[1,2,15] (See also Infeld and Hull.[3]) It should be emphasized that our recursion formulas [Eq. (19)] and, correspondingly, our explicit expression (56) of the radial $r^k$ integral, which are established for the general case $n \neq n'$ are "continuous" when $n=n'$ and then, as was shown in Sec. III, can be reduced to any particular case. As pointed out by Landau and Lifshitz (see Ref. 2, p. 159), Gordon's formulas are not directly valid for $n=n'$ owing to the presence of the variable $-4nn'/(n-n')^2$ in the hypergeometric function.

By introducing a direct factorization closely related to Schrödinger's technique,[9] we have overcome, without introducing either a dilatation operator[6] or a nonphysical two-variable wave function[4]—the well-known difficulty that the radial variable is not $r$ but $r/n$.

We find again, for $n=n'$, the Pasternack-Sternheimer[11] selection rules by directly considering the nonvanishing conditions of products appearing in expression (58). By inspection of our general expression (56), it seems that for $n \neq n'$, these selection rules do not hold. The same conclusions occur for discrete-continuous matrix elements. This last case as well as the extension of our results to the Dirac-Coulomb and the generalized Kepler problem will be given elsewhere.

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*On leave from the Physics Department, Damas University, Syria.

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