Matrix-element calculations for hydrogenlike atoms

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The method of factorization, together with the hypervirial theorem, is shown to be appropriate for calculating matrix elements of operators that are functions of r, between hydrogenic radial wave functions that may belong to different atoms. Some numerical results are tabulated for matrix elements of the form $\langle n'l'|r^k|nl\rangle$. The expressions given are valid for both diagonal- and off-diagonal matrix-element calculations with no limitation on the values of the n and l quantum number or in the power of the operator, which can have either positive or negative values.

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I. INTRODUCTION

There are many applications in atomic physics where the calculation of matrix elements using hydrogenic wave functions is of great importance. The first publication [1] on the subject dates therefore from the beginnings of quantum mechanics and it is still of interest in recent years. Some of the applications are as follows: excitation cross sections [2], threshold differential oscillator strengths [3], Lamb shift [4–6], hydrogen recombination spectrum [7], stopping power of inner-shell electrons [8,9], opacity of elements [10], irregular electric multipoles [11], etc.

In principle, the calculation of these elements could be carried out by resolving the integral analytically [1,12–14]. It is indisputable that, when n is much greater than l, Gordon's formula or other analytically expanded formulas are not only hard to use but are of no numerical validity for large n, due to the successive cancellations between positive and negative terms [11].

Several alternative methods have therefore been developed: asymptotic expansions [2,3,15], the use of relationships among the Laguerre polynomials [16–19], algebraic methods such as the joint use of the hypervirial theorem and sum rule [20], hypervirial and Hellmann-Feynman theorems [21], group theory with second-quantization formalism [22–24], and, finally, the use of ladder operators [25,26]. None of them, however, has solved the most complicated and general case, which is that in which the states involved differ in the principal quantum number: $\langle n'l'|\hat{g}(r)|nl\rangle$.

The methods we have chosen to follow are the joint use of the method of factorization [27] and the hyperviral theorem, applied with success in other systems such as the harmonic oscillator and the Morse oscillator [28–30] and even in certain special cases for hydrogenic atoms [31]. The equations that we derive are easy to manage and serve to calculate both diagonal and off-diagonal matrix elements and even matrix elements in which the functions belong to different hydrogenic atoms ($Z'\neq Z$) with operators that are functions of r, $\hat{g}(r)$.

II. DERIVATION OF THE RECURRENCE RELATIONS

The radial Schrödinger equation for hydrogenic atoms, in Hartree units, making $u(r)=r^{-1}R(r)$, has the form

$$\frac{d^2}{dr^2}u_{nl}-\frac{l(l+1)}{r^2}u_{nl}+\frac{2Z}{r}u_{nl}-E(n)u_{nl}=0\ , \tag{1}$$

where $E(n)$ and u_{nl} are the eigenvalues and eigenfunctions, respectively.

This is a second-order differential equation which is factorizable according to the technique of Infeld and Hull [27], yielding the following ladder operators [31]:

$$^{-}L(n,l)=\frac{nl}{Z(n^2-l^2)^{1/2}}\left[\frac{l}{r}-\frac{Z}{l}+\frac{d}{dr}\right]\ , \tag{2}$$

$$^{+}L(n,l)=\frac{n(l+1)}{Z[n^2-(l+1)^2]^{1/2}}\left[\frac{l+1}{r}-\frac{Z}{l+1}-\frac{d}{dr}\right]\ . \tag{3}$$

These act on the secondary quantum number (with $l\neq 0$), raising and lowering it by one unit, while n remains constant

$$^{+}L(n,l+1)u_{nl}=u_{n\,l+1}\ , \tag{4}$$

$$^{-}L(n,l)u_{nl}=u_{n\,l-1}\ . \tag{5}$$

Using the expressions given for the ladder operators (2) and (3) with a differentiable function $g(r)$, in combination with the functions $|n,l\rangle$ and $\langle n',l'|$, one obtains the equations

$$\begin{aligned}\langle n'l'|r^{-1}g(r)|nl\rangle=&\frac{^{+}A}{2l+1}\langle n'l'|g(r)|n\ l+1\rangle\\&+\frac{^{-}A}{2l+1}\langle n'l'|g(r)|n\ l-1\rangle\\&+\frac{Z}{l(l+1)}\langle n'l'|g(r)|nl\rangle\ ,\end{aligned} \tag{6}$$

$$\left\langle n'l' \left| g'(r)\frac{d}{dr} \right| nl \right\rangle = -\frac{{}^{+}A}{2}\langle n'l'|g'(r)|n\ l+1\rangle + \frac{{}^{-}A}{2}\langle n'l'|g'(r)|n\ l-1\rangle + \tfrac{1}{2}\langle n'l'|r^{-1}g'(r)|nl\rangle + \frac{Z}{l(l+1)}\langle n'l'|g'(r)|nl\rangle , \quad (7)$$

where ${}^{+}A$ and ${}^{-}A$ are coefficients coming from ${}^{+}L$ and ${}^{-}L$, respectively, and depend on n, l, and Z.

Defining H' and H as two hydrogenic Hamiltonians, which in the most general case may belong to two different atomic species, one can write the following expression, which can be considered a generalization of the hypervirial theorem to the two-center case:

$$\langle n'l'|H'g(r)-g(r)H|nl\rangle = \Delta E\langle n'l'|g(r)|nl\rangle . \quad (8)$$

Expanding the left-hand side, one obtains the following recursion relations:

$$\left\langle n'l' \left| g'(r)\frac{d}{dr} \right| nl \right\rangle = -\tfrac{1}{2}\langle n'l'|g''(r)|nl\rangle + \frac{\Delta l}{2}\langle n'l'|r^{-2}g(r)|nl\rangle - \Delta Z\langle n'l'|r^{-1}g(r)|nl\rangle + \frac{\Delta E}{2}\langle n'l'|g(r)|nl\rangle . \quad (9)$$

Exchanging $|nl\rangle$ for $|n'l'\rangle$ and $\langle n'l'|$ for $\langle nl|$, one arrives at another three recurrence relations analogous to (6), (7), (9).

A suitable combination of these six equations, (6), (7), (9), and their analogs, allows some terms to be eliminated and leads to two recurrence relations of great utility,

$$\left[(2+l')\frac{Z}{l(l+1)}-\frac{Z'}{l'+1}\right]\langle n'l'|g'(r)|nl\rangle + \left[\frac{l'-l+1}{2l+1}\right]{}^{+}A\langle n'l'|g'(r)|n\ l+1\rangle + \left[\frac{l'+l+2}{2l+1}\right]{}^{-}A\langle n'l'|g'(r)|nl-1\rangle - {}^{+}A'\langle n'\,l'+1|g'(r)|nl\rangle + \langle n'l'|g''(r)|nl\rangle = 0 , \quad (10)$$

$$\left[(2+l)\frac{Z'}{l'(l'+1)}-\frac{Z}{l+1}\right]\langle n'l'|g'(r)|nl\rangle + \left[\frac{l-l'+1}{2l'+1}\right]{}^{+}A'\langle n'\,l'+1|g'(r)|nl\rangle + \left[\frac{l+l'+2}{2l'+1}\right]{}^{-}A'\langle n'\,l'-1|g'(r)|nl\rangle - {}^{+}A\langle n'l'|g'(r)|n\ l+1\rangle + \langle n'l'|g''(r)|nl\rangle = 0 . \quad (11)$$

These equations relate matrix elements with secondary quantum numbers differing by one unit. Using them alternately, one can evaluate all the matrix elements $\langle n'l'|g'(r)|nl\rangle$. Firstly, knowing $\langle n'\,n'-1|g'(r)|n\ n-1\rangle$, which is calculated straightforwardly as indicated in the Appendix, one calculates with Eq. (10) the terms with fixed l' (initially $l'=n'-1$) and l running from $n-1$ to 0 (row of the matrix). Then, with Eq. (11), one calculates the elements with fixed l (initially $l=n-1$) and l' with values running from $n'-1$ to 0 (column of matrix). For the remaining rows and columns one will go on using Eqs. (10) and (11) alternately, calculating first the rows and then the columns from the terms calculated previously.

It must be noted that the strategy in the implementation of these equations is very important. At the beginning, the idea was to program using Eq. (10) to calculate all the elements of the last row of the matrix from the same initial element indicated above. Then, with these terms and Eq. (11), we could simply calculate the rest of the terms columnwise. In principle, this form of program is simpler, but the numerical results that it gave were wrong for the case of high quantum numbers n' and n.

III. SOME CASES OF PARTICULAR OPERATORS

Some particular cases of r-dependent operators are of special interest, such as exponentials (e^{sr}), powers (r^k), and combinations of them with the derivative (d^n/dr^n). The recurrence relations presented above reduce in these cases to the following expressions:

$$\left[(2+l'+k)\frac{Z}{l(l+1)}-\frac{Z'}{l'+1}+s\right]\langle n'l'|r^k e^{sr}|nl\rangle + \left[\frac{l'-l+1+k}{2l+1}\right]{}^{+}A\langle n'l'|r^k e^{sr}|n\ l+1\rangle + \left[\frac{l'+l+2+k}{2l+1}\right]{}^{-}A\langle n'l'|r^k e^{sr}|n\ l-1\rangle - {}^{+}A'\langle n'\,l'+1|r^k e^{sr}|nl\rangle = 0 , \quad (12)$$

$$\left[(2+l+k)\frac{Z'}{l'(l'+1)}-\frac{Z}{l+1}+s\right]\langle n'l'|r^k e^{sr}|nl\rangle + \left[\frac{l-l'+1+k}{2l'+1}\right]{}^{+}A'\langle n'\,l'+1|r^k e^{sr}|nl\rangle + \left[\frac{l+l'+2+k}{2l'+1}\right]{}^{-}A'\langle n'\,l'-1|r^k e^{sr}|nl\rangle - {}^{+}A\langle n'l'|r^k e^{sr}|n\ l+1\rangle = 0 , \quad (13)$$

$$\left\langle n'l' \left| r^k e^{sr} \frac{d^n}{dr^n} \right| nl \right\rangle = -\frac{{}^{+}Al}{2l+1} \left\langle n'l' \left| r^k e^{sr} \frac{d^{n-1}}{dr^{n-1}} \right| n\,l+1 \right\rangle + \frac{-A(l+1)}{2l+1} \left\langle n'l' \left| r^k e^{sr} \frac{d^{n-1}}{dr^{n-1}} \right| n\,l-1 \right\rangle - \frac{Z}{l(l+1)} \left\langle n'l' \left| r^k e^{sr} \frac{d^{n-1}}{dr^{n-1}} \right| nl \right\rangle . \quad (14)$$

To calculate matrix elements when the operate is r^k or e^{sr}, one needs to use Eqs. (12) and (13), as we explained in Sec. II, alternately and starting from the matrix element where the secondary quantum numbers are greatest, $n'-1$ and $n-1$, respectively. Morales, Peña, and Lopez-Bonilla [19] recently obtained expressions very similar to Eqs. (12) and (13) when the exponential terms vanishes ($s=0$). These are their Eqs. (41) and (43). Nevertheless, they coincide only for the cases which are diagonal in n. In the same reference, another two recurrence relations are deduced, (34) and (35), where the secondary quantum numbers are fixed while n' and n vary by one unit. Nonetheless, we do not believe that either these equations or (40) and (42) of the same work represent any novelty or improvement on those referred to earlier as (41) and (43). There must also exist misprints in all of them since the results they yield are inadequate.

In the case of terms with the derivative d^n/dr^n, one works analogously for the calculation of the initial matrix element required in Eq. (14), by means of which one can obtain the rest of the elements which involve the derivative.

The numerical stability of the recurrence relations obtained may be tested by verifying that the orthonormality conditions do not deteriorate numerically, and also by comparing our results with those obtained by other procedures. Given the great importance of the operator r^k and the more abundant information that is available for it, we have particularized our expressions for this operator.

A. Expectaction values $\langle nl|r^k|nl\rangle$

Comparison of our results with those derived by other procedures [18,32] shows that Eqs. (12) and (13) work well. From the generalized expression of the hypervirial theorem, one may deduce the expression

$$(k-1)\left[-\frac{k}{2}(k-2)+2l(l+1)\right] \times \langle r^{k-3}\rangle_{nl} - 2Z(2k-1)\langle r^{k-2}\rangle_{nl} + 2E(n)k\langle r^{k-1}\rangle_{nl} = 0 . \quad (15)$$

This will yield the expectation values of powers of r as long as one known *a priori* at least one of them which may be calculated by means of the Hellmann-Feynman theorem

$$\langle r^{-1}\rangle_{nl} = \frac{Z}{n^2} , \quad (16)$$

$$\langle r^{-2}\rangle_{nl} = \frac{Z^2}{n^3(l+\frac{1}{2})} . \quad (17)$$

Equation (15) is self-sufficient, and it has an ideal structure for programming on an algebraic processor such as muMath or REDUCE. By way of example, we have obtained the analytical expressions for the expectation values of r^k ($k=-7,\ldots,5$), which coincide exactly with those published by Bockasten [17] and Drake and Swainson [33].

The expectation values calculated by means of these analytical expressions and the values given by Shertzer [32] are compared with those resulting from Eqs. (12) and (13). There is seen to be absolute concordance even to the twelfth significant figure.

In calculating the matrix elements with $l=0$, the recurrence relations (12) and (13) are used $(n-1)+2\sum_{i=1}^{n-1}(n-i)$ times. This confirms therefore the numerical stability of the expressions being used. The results have also allowed us to verify the recurrence relation put forward by Blanchard [18], which relates two matrix elements whose operators are nonconsecutive powers of r.

B. Matrix elements of the form $\langle nl'|r^k|nl\rangle$

As the recurrence relations work by calculating matrix elements from previously calculated ones, it is to be expected that if the diagonal elements maintain their stability, off-diagonal elements should do likewise. Hence, the elements that are off-diagonal in l may be taken to be already tested in light of the results of the previous section. But there also exist other checks that can be made on them.

Reference [32] gives some analytical expressions for matrix elements where $n'=n$; $l'=l+1$, $l+2=n-1$, $n-5$. The corresponding numerical results are compared with those obtained from our recurrence relations and we have again appreciated absolute concordance in the first twelve significant figures.

But this is insufficient to demostrate unequivocally the stability of our equations, since these elements are those that are calculated at the start. The toughest test that Eqs. (12) and (13) can be subjected to, as we noted before, is the calculation of the matrix elements with values $l=0$, 1, or 2, i.e., s, p, or d levels. The fulfillment of the orthogonality conditions which are known for them is the only test that can be made. Pasternack and Sterheimer [16], Armstrong [22], Cunningham [23], Herrick and Sinanoğlu [24], and Badawi *et al.* [34] demonstrated with different procedures the orthogonality condition later generalized by Blanchard [18],

$$\langle nl'|r^{-p-2}|nl\rangle = 0 \quad (l'\neq l) , \quad p=0,1,\ldots,|l-l'|-1 . \quad (18)$$

A check of this equation was made even for a case as extreme as that of $n=500$, with no deviations greater than 10^{-18} being observed.

C. Matrix elements $\langle n'l'|r^k|nl\rangle$

Infeld and Hull [27] obtained two recursion equations relating matrix elements for the operator r. Storey and Hummer [35] programmed these equations, giving tables of some results for the matrix elements that we have been dealing with. We have been able to compare them with the results from our recursion equations (12) and (13) for terms which are off-diagonal in the principal quantum number. The numbers are listed in Table I where it can be seen that there are no appreciable differences.

Whether or not the orthogonality condition

$$\langle n'l|nl\rangle=\delta_{n'n}$$

is satisfied represents an alternative way of checking the matrix elements. We have again chosen extreme cases to put our recurrence relations to the test, which led us to discover a small limitation in their use: for matrix elements with $\Delta n=n'-n$ greater than 10, when the principal quantum numbers are large (n' or $n=30$), the error which is made with respect to the orthogonality conditions begins to be greater than 10^{-18}.

IV. CONCLUSIONS

We have obtained a set of recurrence relations for calculating matrix elements between hydrogenic functions for nay operator $\hat{g}(r)$ that is a differentiable function of r.

We have particularized these recurrence relations for distinct operators: r^k, d^n/dr^n, e^{sr}, and combinations of them.

With the joint use of ladder operators and the hypervirial theorem we obtained a self-sufficient set of recursion equations permitting the calculation of all matrix elements of the form $\langle n'l'|\hat{g}(r)|nl\rangle$ for the aforementioned operators, starting from a knowledge of $\langle n'\,n'-1|\hat{g}(r)|n\,n-1\rangle$. This matrix element is calculated straightforwardly, through the wave functions of both states.

We conclude by saying that the present method represents an ideal procedure for tackling the calculation of a great number of matrix elements for different operators $\hat{g}(r)$ of interest in quantum mechanics, between hydrogenic radial wave functions. The different tests that we submitted our equations to allow us to affirm that they present a high degree of numerical stability, comparable to the analytical expresions, and yet with the advantage of being easier to implement on a computer program in which the equations that appear in the present work are developed [36].

TABLE I. Elements that are off diagonal in n and l: $\langle n'l'|r|nl\rangle$.

	$l'=l-1$	$l'=l$	$l'=l+1$
		$n'=2;n=3$	
$l=0$		−1.851 108 792 498	0.938 404 237 739 8[a]
			0.938 404 2[b]
$l=1$	3.064 815 406 571	−1.769 472 000 000	
	3.064 815		
$l=2$	4.747 991 611 539		
	4.747 992		
		$n'=9;n=10$	
$l=0$		−29.159 151 031 48	25.150 758 079 32
			25.150 76
$l=1$	33.491 154 246 21	−29.154 232 503 42	21.431 004 044 51
	33.491 15		21.431 00
$l=2$	38.184 810 709 27	−29.114 024 589 87	17.967 585 914 73
	38.184 81		17.967 59
$l=3$	43.281 633 318 56	−28.973 149 893 03	14.730 410 355 91
	43.281 63		14.730 41
$l=4$	48.827 020 709 28	−28.620 101 271 80	11.690 944 568 25
	48.827 02		11.690 94
$l=5$	54.870 703 024 95	−27.874 257 638 59	8.820 931 912 864
	54.870 70		8.820 932
$l=6$	61.467 226 020 62	−26.435 855 393 55	6.088 550 890 421
	61.467 23		6.088 551
$l=7$	68.676 480 330 84	−23.756 983 054 19	3.438 808 528 265
	68.676 48		3.438 809
$l=8$	76.564 282 256 87	−18.569 566 052 63	
	76.564 28		
$l=9$	85.203 012 472 43		
	85.203 01		

[a]Equations (12) and (13).

[b]Storey and Hummer (Ref. [35]).

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APPENDIX: CALCULATION OF THE INITIAL MATRIX ELEMENTS

We shall evaluate the matrix elements $\langle n'l'|r^k e^{sr}|nl\rangle$ starting from the expression given for the radial wave function of the hydrogenic atom [37]

$$u_{nl}=N_{nl}\varphi_n^{l+1}\exp(-\tfrac{1}{2}\varphi_n)L_{n-l-1}^{2l+1}(\varphi_n)\ , \tag{A1}$$

where L_{n-l-1}^{2l+1} is the associated Laguerre polynomial, φ a variable, and N_{nl} the normalization constant,

$$\varphi=\frac{2Zr}{n}\ , \tag{A2}$$

$$N_{nl}=\left[Z\frac{(n-l-1)!}{n^2(n+l)!}\right]^{1/2}\ . \tag{A3}$$

With the expansion of the Laguerre polynomials as a finite sum [38],

$$L_a^b(x)=\sum_{t=0}^{a}(-1)^t\begin{bmatrix}a+b\\a-t\end{bmatrix}\frac{x^t}{t!}\ , \tag{A4}$$

we obtain the following expression for the matrix elements of the operator $g(r)=r^k e^{sr}$:

$$\langle n'l'|r^k e^{sr}|nl\rangle=N_{n'l'}N_{nl}\sum_{m=0}^{n'-l'-1}\sum_{j=0}^{n-l-1}\frac{(-1)^{m+j}}{m!j!}\begin{bmatrix}n'+l'\\n'-l'-1-m\end{bmatrix}\begin{bmatrix}n+l\\n-l-1-j\end{bmatrix}\left[\frac{2Z'}{n'}\right]^{l'+m}\left[\frac{2Z}{n}\right]^{l+j}$$
$$\times\int_0^\infty r^{k+l'+l+m+j+2}\exp\left[-\left[\frac{Z'}{n'}+\frac{Z}{n}-s\right]r\right]dr\ . \tag{A5}$$

With the change of variable $t=(Z'/n'+Z/n-s)r$, the integral reduces to the gamma function [$\Gamma(x)$], and hence

$$\langle n'l'|r^k e^{sr}|nl\rangle=N_{n'l'}N_{nl}\sum_{m=0}^{n'-l'-1}\sum_{j=0}^{n-l-1}\frac{(-1)^{m+j}}{m!j!}\begin{bmatrix}n'+l'\\n'-l'-l-m\end{bmatrix}\begin{bmatrix}n+l\\n-l-1-j\end{bmatrix}\left[\frac{2Z'}{n'}\right]^{l'+m}\left[\frac{2Z}{n}\right]^{l+j}$$
$$\times\left[\frac{Z'}{n'}+\frac{Z}{n}-s\right]^{-(k+l'+l+m+j+3)}\Gamma(k+l'+l+m+j+3)\ . \tag{A6}$$

In the case that k is a negative integer, recalling that the Γ function can be expressed in the form $\Gamma(y)=(y-1)!$, k cannot take value less than $-(l'+l+3)$.

When l' and l take their maximum values, $l'=n'-1$ and $l=n-1$, the expression (A6) simplifies to

$$\langle n'\,n'-1|r^k e^{sr}|n\,n-1\rangle=\left[\frac{2^3Z'^3}{n'^3(2n')!}\right]^{1/2}\left[\frac{2^3Z^3}{n^3(2n)!}\right]^{1/2}\frac{\left[\frac{2Z'}{n'}\right]^{n'-1}\left[\frac{2Z}{n}\right]^{n-1}}{\left[\frac{Z'}{n'}+\frac{Z}{n}-s\right]^{v+1}} \tag{A7}$$

where $v=k+n+n'$, and the Γ function has the value $\Gamma(v+1)=v!$, when k is an integer.

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