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ON RECURRENCE RELATIONS FOR RADIAL WAVE FUNCTIONS FOR THE N-TH DIMENSIONAL OSCILLATORS AND HYDROGENLIKE ATOMS: ANALYTICAL AND NUMERICAL STUDY*

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Abstract. Using a general procedure for finding recurrence relations for hypergeometric functions and polynomials introduced by Cardoso et al. [J. Phys. A, 36 (2003), pp. 2055-2068] we obtain some new recurrence relations for the radial wave functions of the N-th dimensional isotropic harmonic oscillators as well as the hydrogenlike atoms. A numerical analysis of such recurrences is also presented.

Key words. wave functions, linear recurrence relations, Laguerre polynomials

AMS subject classifications. 33C45, 11B37, 81V45, 81Q99

1. Introduction. There are many applications in modern physics that require the knowledge of the wave functions of hydrogenlike atoms and isotropic harmonic oscillators (see e.g. [13, 16] and references therein). Of particular interest is the numerical implementation of such functions. The most natural, efficient and fast way for generating such functions is to use recurrence relations. In fact, although the explicit expressions are known, their numerical implementations are usually very unstable.

In this paper we will continue the research started in [8] for obtaining recurrence relations and ladder-type operators for the N-th dimensional isotropic harmonic oscillators and the hydrogenlike atoms. In fact, using the technique of [8] we will obtain some new recurrences on one hand, and on the other we will present a comparative numerical analysis of the obtained recurrence relations for generating numerically the corresponding eigenfunctions. The numerical analysis of the linear recurrences, i.e., the rounding errors bounds, stability of the scheme, etc. is, in general, very complicate (see the nice paper [5] and references therein). So we will restrict ourselves to the discussion of the numerical examples. Even in this framework of no rigorous numerical analysis it is possible to conclude what kind of relations are more useful for numerical computations and what are not. This is the main original contribution of the present paper. Finally, let us mention that the present method for finding recurrence relations can be extended to any quantum system whose (radial) wave function are proportional to hypergeometric-type functions (see e.g. [4]).

The structure of the paper is as follows: In sections 2 and 3 the isotropic oscillator and hydrogenlike atoms radial wave functions are introduced. In both cases we include some new recurrence relations as well as the detailed discussion of their computational applications. Finally, an appendix with the required formulas of the Laguerre polynomials is included.

2. The isotropic harmonic oscillator. The N-dimensional isotropic harmonic oscillator (I.H.O.) is described by the Schrödinger equation

$$\left(-\Delta + \frac{1}{2}\lambda^2 r^2\right)\Psi = E\Psi, \qquad \Delta = \sum_{k=1}^{N} \frac{\partial^2}{\partial x_k^2}, \quad r = \sqrt{\sum_{k=1}^{N} x_k^2}\,.$$

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Its solutions are of the form $\Psi = R_{nl}^{(N)}(r) Y_{lm}(\Omega_N)$, where $R_{nl}^{(N)}(r)$ is the radial part, usually called the *radial wave functions*, defined by (see e.g. [3, 6])

$$R_{nl}^{(N)}(r) = \mathcal{N}_{nl}^{(N)}\ r^l e^{-\frac{1}{2}\lambda r^2} L_n^{l+\frac{N}{2}-1}(\lambda r^2), \quad \mathcal{N}_{nl}^{(N)} = \sqrt{\frac{2n!\lambda^{l+\frac{N}{2}}}{\Gamma\left(n+l+\frac{N}{2}\right)}}, \tag{2.1}$$

being $n = 0, 1, 2, \dots$ and $l = 0, 1, 2, \dots$, the quantum numbers, and $N \geq 3$ the dimension of the space. The angular part $Y_{lm}(\Omega_N)$ are the so-called Nth-spherical or hyperspherical harmonics [3, 14]. In the following, we will assume that the parameters n, l, N are nonnegative integers.

2.1. Recurrence relations for the I.H.O. radial functions. For the functions (2.1) the following theorem hold [8]

THEOREM 2.1. *Let $R_{nl}^{(N)}(r)$, $R_{n+n_1,l+l_1}^{(N)}(r)$ and $R_{n+n_2,l+l_2}^{(N)}(r)$ be three different radial functions of the N-th dimensional isotropic harmonic oscillator, where n_1, n_2 and l_1, l_2 are integers such that*

$$\min\left(n+n_1, n+n_2, l+l_1, l+l_2\right) \geq 0.$$

Then, there exist three all non vanishing polynomials in r, A_0, A_1, and A_2, such that

$$A_0(r) R_{n,l}^{(N)}(r) + A_1(r) R_{n+n_1,l+l_1}^{(N)}(r) + A_2(r) R_{n+n_2,l+l_2}^{(N)}(r) = 0. \tag{2.2}$$

The proof of this theorem can be found in [8]. A key point on the proof was the recurrence relation,

$$C_0(s) L_n^{l+\frac{N}{2}-1}(s) + C_1(s) L_{n+n_1}^{(l+l_1)+\frac{N}{2}-1}(s) + C_2(s) L_{n+n_2}^{(l+l_2)+\frac{N}{2}-1}(s) = 0, \tag{2.3}$$

where $s = \lambda r^2$, and $C_i(s)$, $i = 0, 1, 2$, are not all three vanishing polynomials. Moreover, in [8] it was shown that

$$\begin{aligned} A_0(r) &= \left(\mathcal{N}_{n,l}^{(N)}\right)^{-1} C_0(\lambda r^2) r^{l_1+l_2}, \\ A_1(r) &= \left(\mathcal{N}_{n+n_1,l+l_1}^{(N)}\right)^{-1} C_1(\lambda r^2) r^{l_2}, \\ A_2(r) &= \left(\mathcal{N}_{n+n_2,l+l_2}^{(N)}\right)^{-1} C_2(\lambda r^2) r^{l_1}. \end{aligned} \tag{2.4}$$

From the above theorem and the relation (2.3) it is very simple to obtain *à la carte* relations between three different *radial functions* of the I.H.O. Let us point out that, in general, it is not easy to obtain the coefficients C_i in (2.3), nevertheless, combining in a certain way the known relations of the Laguerre polynomials (see the appendix A) they can be found. This has been shown in [7, 8]. We will show here how this works in one of the new examples, for the others the computations are similar. Here we present some examples. The first four can be found in [8] and the other five seem to be new.

• $n_1 = -1, n_2 = 1, l_1 = l_2 = 0$ [8, page 2059]

$$\begin{aligned} &\sqrt{n\left(n+l+\frac{N}{2}-1\right)} R_{n-1,l}^{(N)}(r) + \left[\lambda r^2 - \left(2n+l+\frac{N}{2}\right)\right] R_{n,l}^{(N)}(r) \\ &\qquad + \sqrt{(n+1)\left(n+l+\frac{N}{2}\right)} R_{n+1,l}^{(N)}(r) = 0. \end{aligned} \tag{2.5}$$

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• $n_1 = n_2 = 0, l_1 = -1, l_2 = 1$ [8, page 2059]

$$r\sqrt{\lambda\left(n+l+\frac{N}{2}-1\right)}R^{(N)}_{n,l-1}(r) - \left(l+\frac{N}{2}-1+\lambda r^2\right)R^{(N)}_{n,l}(r) + r\sqrt{\lambda\left(n+l+\frac{N}{2}\right)}R^{(N)}_{n,l+1}(r) = 0. \tag{2.6}$$

• $n_1 = 0, n_2 = 1, l_1 = -1, l_2 = 0$ [8, page 2059]

$$r\sqrt{\lambda\left(n+l+\frac{N}{2}-1\right)}R^{(N)}_{n,l-1}(r) + \left(n+1-\lambda r^2\right)R^{(N)}_{n,l}(r) - \sqrt{(n+1)\left(n+l+\frac{N}{2}\right)}R^{(N)}_{n+1,l}(r) = 0. \tag{2.7}$$

• $n_1 = -1, n_2 = 0, l_1 = 0, l_2 = 1$ [8, page 2059]

$$-\sqrt{n\left(n+l+\frac{N}{2}-1\right)}R^{(N)}_{n-1,l}(r) + \left(n-\lambda r^2\right)R^{(N)}_{n,l}(r) + r\sqrt{\lambda\left(n+l+\frac{N}{2}\right)}R^{(N)}_{n,l+1}(r) = 0. \tag{2.8}$$

• $n_1 = -1, n_2 = 1, l_1 = 1, l_2 = -1$, i.e., we are looking for a relation of type (2.2)

$$A_0(r)R^{(N)}_{n,l}(r) + A_1(r)R^{(N)}_{n+n_1,l+l_1}(r) + A_2R^{(N)}_{n+n_2,l+l_2}(r) = 0.$$

For finding the polynomials A_i, $i = 0, 1, 2$ we use (2.4) where C_i, $i = 0, 1, 2$ are the polynomials in (2.3). Putting $\alpha = l + \frac{N}{2} - 1$ we have

$$C_0(s)L^{\alpha}_n(s) + C_1(s)L^{\alpha+1}_{n-1}(s) + C_2(s)L^{\alpha-1}_{n+1}(s) = 0.$$

Now we substitute the functions $L^{\alpha+1}_{n-1}(s)$ and $L^{\alpha-1}_{n+1}(s)$ using the relations (A.2)

$$L^{\alpha+1}_{n-1}(s) = \frac{n+\alpha}{s}L^{\alpha}_{n-1}(s) - \frac{n}{s}L^{\alpha}_n(s)$$

and (A.4)

$$L^{\alpha-1}_{n+1}(s) = L^{\alpha}_{n+1}(s) - L^{\alpha}_n(s),$$

respectively. This leads to

$$C_1(s)\frac{n+\alpha}{s}L^{\alpha}_{n-1}(s) + [C_0(s) - \frac{n}{s}C_1(s) - C_2(s)]L^{\alpha}_n(s) + C_2(s)L^{\alpha}_{n+1}(s) = 0.$$

Comparing the last formula with the three-term recurrence relation TTRR (A.5) for the Laguerre polynomials we find

$$C_0(s) = s - \alpha, \quad C_1(s) = s, \quad C_2(s) = n + 1,$$

and therefore for the wave functions we find

$$\begin{aligned}\sqrt{n\lambda}rR^{(N)}_{n-1,l+1}(r) - \left(l+\frac{N}{2}-1-\lambda r^2\right)R^{(N)}_{n,l}(r)\\ +r\sqrt{(n+1)\lambda}R^{(N)}_{n+1,l-1}(r)=0.\end{aligned} \tag{2.9}$$

Analogously, we can find the following three recurrence relations

- $n_1=-1, n_2=1, l_1=-1, l_2=1$

$$A_0(r)R^{(N)}_{n,l}(r)+A_1(r)R^{(N)}_{n-1,l-1}(r)+A_2(r)R^{(N)}_{n+1,l+1}(r)=0, \tag{2.10}$$

where,

$$\begin{aligned}A_0(r) = &-\left[(\lambda r^2-(n+1))(\lambda r^2-n)\left(2n+l+\frac{N}{2}-\lambda r^2\right)+\right.\\ &\left.(2n+1)\left(n+l+\frac{N}{2}\right)(\lambda r^2-n)-n\left(l+\frac{N}{2}-1+\lambda r^2\right)\right],\\ A_1(r) = &\ r(\lambda r^2-(n+1))\sqrt{\lambda n\left(n+l+\frac{N}{2}-2\right)\left(n+l+\frac{N}{2}-1\right)},\\ A_2(r) = &\ r(\lambda r^2-n)\sqrt{\lambda(n+1)\left(n+l+\frac{N}{2}\right)\left(n+l+\frac{N}{2}+1\right)}.\end{aligned}$$

- $n_1=0, n_2=2, l_1=1, l_2=0$

$$\begin{aligned}&\sqrt{n+l+\frac{N}{2}}\left(n+l+\frac{N}{2}+1-\lambda r^2\right)R^{(N)}_{n,l}(r)\\ &-\sqrt{\lambda}\,r\left(2n+l+\frac{N}{2}+2-\lambda r^2\right)R^{(N)}_{n,l+1}(r)\\ &-\sqrt{(n+1)(n+2)\left(n+l+\frac{N}{2}+1\right)}R^{(N)}_{n+2,l}(r)=0.\end{aligned} \tag{2.11}$$

- $n_1=0, n_2=-2, l_1=1, l_2=1$

$$\begin{aligned}&r\sqrt{\lambda}\left(2n+l+\frac{N}{2}-1-\lambda r^2\right)R^{(N)}_{n,l}(r)\\ &-\sqrt{\left(n+l+\frac{N}{2}\right)}\left(n+l+\frac{N}{2}-1-\lambda r^2\right)R^{(N)}_{n,l+1}(r)\\ &+\sqrt{n(n-1)\left(n+l+\frac{N}{2}-1\right)}R^{(N)}_{n-2,l+1}(r)=0.\end{aligned} \tag{2.12}$$

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• $n_1 = -1, n_2 = 1, l_1 = 0, l_2 = 1$

$$\begin{aligned}\sqrt{n\left(n+l+\frac{N}{2}-1\right)}\,\left(\lambda r^2-n-1\right) R^{(N)}_{n-1,l}(r)\\ +\left[n(n+1)-\left(3n+l+\frac{N}{2}+1-\lambda r^2\right)\lambda r^2\right] R^{(N)}_{n,l}(r)\\ +r\sqrt{\lambda(n+1)\left(n+l+\frac{N}{2}\right)\left(n+l+\frac{N}{2}+1\right)}R^{(N)}_{n+1,l+1}(r)=0.\end{aligned}$$

2.2. Ladder-type relations for the I.H.O. radial functions. Another important relations for the functions (2.1) are the so-called ladder operators. The following result was proved in [8].

THEOREM 2.2. *Let $R^{(N)}_{n,l}(r)$ and $R^{(N)}_{n+n_1,l+l_1}(r)$ be two radial functions of the N-th dimensional isotropic harmonic oscillator and let* $\min(n+n_1, l+l_1) \geq 0$ *and* $(n_1)^2 + (l_1)^2 \neq 0$*, where n_1 and l_1 are integers. Then, there exist three not all vanishing polynomials in r, A_0, A_1, and A_2, such that*

$$A_0 R^{(N)}_{n,l}(r) + A_1 \frac{d}{dr} R^{(N)}_{n,l}(r) + A_2 R^{(N)}_{n+n_1,l+l_1}(r) = 0. \tag{2.13}$$

The proof of this theorem can be found in [8]. A key point on the proof was the recurrence relation,

$$B_0(s) L_n^{l+\frac{N}{2}-1}(s) + B_1(s) L_{n-1}^{l+\frac{N}{2}}(s) + B_2(s) L_{n+n_1}^{(l+l_1)+\frac{N}{2}-1}(s) = 0, \tag{2.14}$$

where B_0, B_1, and B_2 are not all three vanishing polynomials. Moreover, (2.13) can be rewritten as

$$\begin{aligned}\left[B_1(s)\frac{d}{dr} + \lambda r\left(B_1(s) - 2B_0(s)\right) - B_1(s)\frac{l}{r}\right] R^{(N)}_{nl}(r)\\ = 2\lambda B_2(s)\frac{\mathcal{N}^{(N)}_{n,l}}{\mathcal{N}^{(N)}_{n+n_1,l+l_1}} r^{1-l_1} R^{(N)}_{n+n_1,l+l_1}(r).\end{aligned} \tag{2.15}$$

To obtain the unknown polynomials B_0, B_1, and B_2 in (2.14) we can proceed as in the previous section, i.e., use the Eqs. (A.1)–(A.5) to transform (2.14) into one of the formulas (A.1)–(A.5) or in a sum of linearly independent Laguerre polynomials and solve the resulting equations for the unknown coefficients. Let us consider some examples. The first two are taken from [8] and the other two are new.

• $n_1 = 0, l_1 = 1$ [8, page 2061]

$$\left[\frac{d}{dr} - \lambda r - \frac{l}{r}\right] R^{(N)}_{n,l}(r) = -2\sqrt{\lambda\left(n+l+\frac{N}{2}\right)} R^{(N)}_{n,l+1}(r). \tag{2.16}$$

• $n_1 = 1, l_1 = 0$ [8, page 2061]

$$\left[r\left(\frac{d}{dr}-\lambda r\right)+(2n+l+N)\right] R^{(N)}_{n,l}(r) = 2\sqrt{(n+1)\left(n+l+\frac{N}{2}\right)} R^{(N)}_{n+1,l}(r). \tag{2.17}$$

• $n_1 = 2, l_1 = 0$. Introducing these values into (2.14) and putting $\alpha = n + \frac{N}{2} - 1$ we get

$$B_0(s) L_n^\alpha(s) + B_1(s) L_{n-1}^{\alpha+1}(s) + B_2(s) L_{n+2}^\alpha(s) = 0\,. \tag{2.18}$$

Now, using relations (A.2) and the TTRR (A.5), (2.18) becomes into

$$B_1(s)\frac{n+\alpha}{s} L_{n-1}^\alpha(s) + \left(B_0(s) - \frac{n}{s}B_1(s) - \frac{n+1+\alpha}{n+2}B_2(s)\right) L_n^{\alpha+1}(s) \\ + B_2(s)\frac{2n+\alpha+3-s}{n+2} L_{n+1}^\alpha(s) = 0\,.$$

Comparing with the TTRR (A.5) we find

$$B_0(s) = (n+1)\left(2n+\frac{N}{2}\right) - \left(3n+2+\frac{N}{2}-s\right)\left(2n+\frac{N}{2}-s\right),$$
$$B_1(s) = s\left(3n+2+\frac{N}{2}-s\right), \quad B_2(s) = (n+1)(n+2),$$

and therefore, for the wave functions we find (see (2.15))

$$\left[\left(3n+2+\frac{N}{2}-\lambda r^2\right)\left(r\frac{d}{dr}+4n+N-l-\lambda r^2\right)-(n+1)(4n+N)\right] R_{n,l}^{(N)}(r) \\ = 2\sqrt{(n+1)(n+2)\left(n+l+\frac{N}{2}\right)\left(n+l+\frac{N}{2}+1\right)}\, R_{n+2,l}^{(N)}(r).$$

• $n_1 = 0, l_1 = 2$ Following the same technique and using now twice, in the resulting (2.14), formulas (A.3) and (A.2) we get

$$\left[\left(n+\frac{N}{2}+\lambda r^2\right)\left(r\frac{d}{dr}-l\right)+\lambda r^2\left(3n+\frac{N}{2}-\lambda r^2\right)\right] R_{n,l}^{(N)}(r) \\ = 2\lambda r^2\sqrt{\left(n+l+\frac{N}{2}\right)\left(n+l+\frac{N}{2}+1\right)}\, R_{n,l+2}^{(N)}(r).$$

2.3. Numerical analysis of the recurrences. In this section we will present the numerical analysis of some of the recurrence relations and ladder-type operators for the I.H.O. We have used the commercial program MATLAB [12].

First of all, let us point out that if we choose the values of n and l large enough and compute the radial wave functions $R_{n,l}^{(N)}(r)$ using the definition (2.1) we observe a picture of an unbounded function that do not corresponds to the real ones. This picture is probably due to numerical instabilities and consequently, we can not directly evaluate these functions for a given r by means of (2.1). In figure 2.1 we represent the maximum value of the parameters n, l for which the direct computation works, i.e., the region below the curve defined by these points is the region of *computational* validity of (2.1). Therefore, if we want to have the values of the radial functions for n, l large *enough*, it is necessary to apply the recurrence relations (RR) in order to calculate them.

From the previous sections it follows that the recurrence relations of the I.H.O. can be classify in three different types:

- RRs which involve functions R_{n_i,l_i} with indices (n,l), $(n\pm1,l)$ (see (2.5)); (n,l), $(n,l\pm1)$ (see (2.6)); (n,l) and $(n\mp1,l\pm1)$ (see (2.9)); and (n,l) and $(n\pm1,l\mp1)$ (see (2.10)). We will call them the *regular* recurrences.

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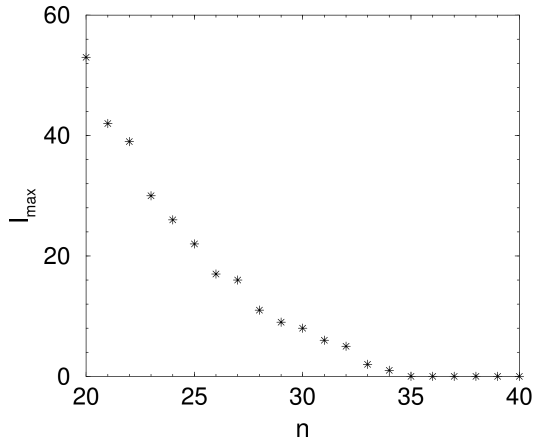

FIG. 2.1. *We plot the maximum value of l versus n, for which the radial wave functions can be calculated by using (2.1).*

- The other RRs, e.g. the ones which involve the indices (n, l), $(n, l-1)$, $(n+1, l)$; (n, l), $(n, l+1)$, $(n-1, l)$; (n, l), $(n, l+1)$, $(n+2, l)$; (n, l), $(n, l+1)$, $(n-2, l)$; etc. (see e.g. (2.7), (2.8), (2.11), (2.12)).
- Relations which involve the derivatives, i.e., ladder-type relations.

In this section we evaluate the radial wave functions by using different recurrence relations with the aim to discuss their effectiveness (based on the time of the numerical simulations and convergence of the formulas). In all the numerical computations of $R_{n,l}(r)$ we use $\lambda = 1$ and $N = 3$.

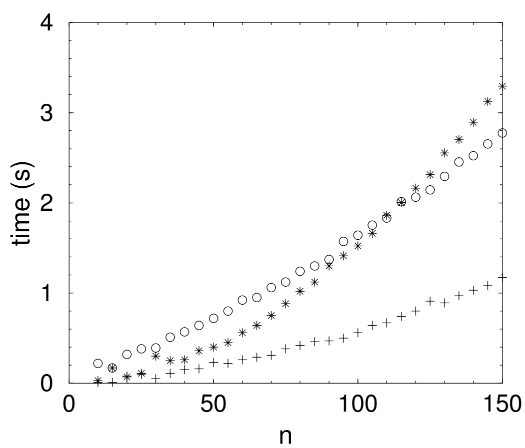

FIG. 2.2. *We represent with pluses, stars and circles the computational time (in seconds) to obtain the radial function versus n from the RRs (2.5), (2.6), and (2.10), respectively. In this case $l = n$ and each function have been evaluated at 1000 points.*

First of all, we evaluate the function $R_{n,l}(r)$ in 1000 points, corresponding to the elements of the vector $r = (4.01, 4.02, \cdots, 14)$ (in the matlab notation $r = [4.01 : 0.01 : 14]$), by using the formulas (2.5), (2.6) and (2.10). In figure 2.2 we compare the computational time to do these operations in each case when $n = l$ (notice that in this case we need to apply the corresponding RR $n-1$ times).

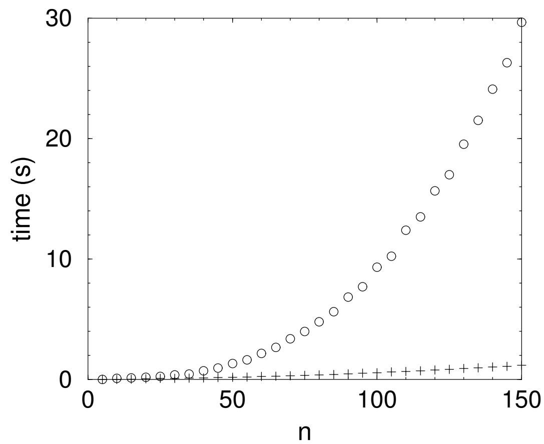

FIG. 2.3. *Computational time versus n for $l = 40$. The pluses refer to the recurrence relation (2.5), whereas the circles are results from (2.11)+(2.5).*

We observe that formula (2.5) allows us to compute these functions faster. The difference in time among these methods is more appreciable when n is bigger. We would like to remark that in order to apply the formula (2.5) to obtain $R_{n,l}(r)$, we fix l and change the first argument from 1 to $n-1$. In addition, we need to know the initial conditions of the RR, which in this case are $R_{0,l}(r)$ and $R_{1,l}(r)$. Both functions are related with the Laguerre polynomials $L_0^{l+N/2-1}(x) = 1$ and $L_1^{l+N/2-1}(x) = x$, respectively, regardless of the value of l. Furthermore, for using the relation (2.6) one should use the initial conditions $R_{n,0}(r)$ and $R_{n,1}(r)$, but they can not be calculated by formula (2.1) for large values of n (see figure 2.1) as already pointed out. So, the initial conditions should be calculated using the recurrence formula (2.5). Moreover, when we use the relation (2.6) we see that there exists an interval close to $r = 0$ where $R_{n,l}(r)$ diverges (oscillates without any pattern) and this interval becomes larger when n increases. This divergence, at the vicinity of zero, also appears when we use (2.10). In the last case, one should also use (2.5) to obtain the initial condition.

The recurrences (2.7), (2.8), (2.11) and (2.12) are even more complicated to use than (2.6) and (2.10). They should be used together with (2.5), not only because the initial conditions, but also because their own nature (they mix both indices). Let us check if $R_{n,l}(r)$ can be obtained faster when we combine for example (2.11) with (2.5), instead of using (2.5) alone. In figure 2.3 we show the computer time to obtain $R_{n,l}(r)$ versus n (and fixing $l = 40$) for the relation (2.5) alone, and combining (2.11) and (2.5) together. Both functions are computed in 1000 points corresponding to the elements of the vector $[0.01 : 0.01 : 10]$. From this figure we conclude that the formula (2.5) is the best one for computing $R_{n,l}(r)$.

Concerning the ladder-type relations, let us mention that the relations (2.16) and (2.17) behave numerically unstable for large values of l and n, respectively. Therefore, they are not useful to compute numerically the radial wave functions but instead of this we can use them, together with (2.5) for finding the derivative of the radial wave functions (see figure 2.4).

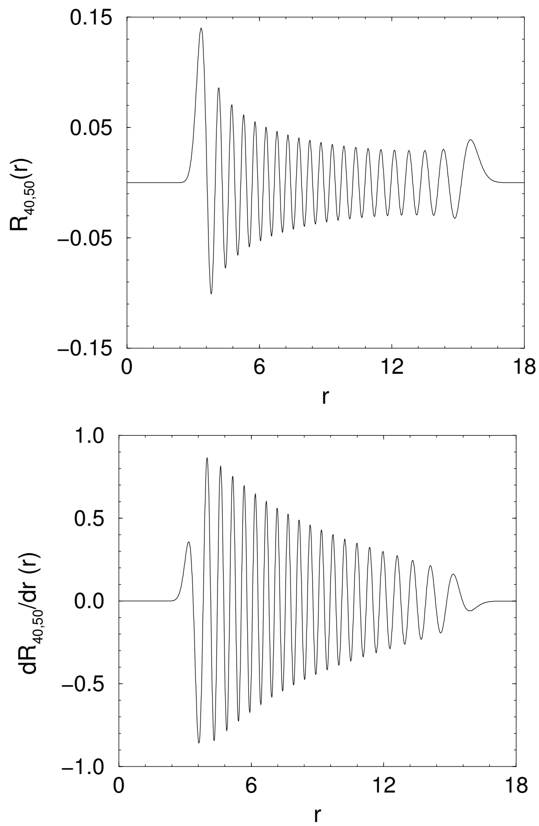

FIG. 2.4. *In the top panel we show the* $R_{40,50}(r)$ *computed by using the recurrence relation (2.5). In the bottom panel we represent the derivative of this function computed from the ladder-type relation (2.16).*

3. Radial functions for the Hydrogen atom. In this section we will provide a similar study for the Hydrogen atom described by the Schrödinger equation

$$\left(-\Delta - \frac{1}{r}\right)\Psi = E\Psi, \qquad \Delta = \sum_{k=1}^{N} \frac{\partial^2}{\partial x_k^2}, \quad r = \sqrt{\sum_{k=1}^{N} x_k^2}.$$

The solution is given by $\Psi = R_{nl}^{(N)}(r) Y_{lm}(\Omega_N)$, where the radial part $R_{nl}^{(N)}(r)$ is defined by [2, 9]

$$R_{nl}^{(N)}(r) = \mathcal{N}_{n,l}^{(N)} \left(\frac{r}{n+\frac{N-3}{2}}\right)^{l} \exp\left(\frac{-r}{2\left(n+\frac{N-3}{2}\right)}\right) L_{n-l-1}^{2l+N-2}\left(\frac{r}{n+\frac{N-3}{2}}\right). \tag{3.1}$$

Here $n = l+1, l+2, \ldots$ and $l = 0, 1, 2, \ldots$ are the quantum numbers, $N \geq 3$ is the dimension of the space, and the normalizing constant $\mathcal{N}_{n,l}^{(N)}$ is

$$\mathcal{N}_{n,l}^{(N)} = \sqrt{\frac{(n-l-1)!}{(n+l+N-3)!}}\,\frac{2}{\left(n+\frac{N-3}{2}\right)^2}.$$

As we already pointed out in [8], the Laguerre polynomials that appear in the expression of the radial functions are not the classical ones $L_n^{\alpha}(x)$ in the sense that the parameter α as

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well as the variable x depend on the degree of the polynomials, n. When the parameters of the classical polynomials depend on n, the polynomials are orthogonal with respect to a *variant weights* (for more details see e.g. [10, 11, 18]). Nevertheless, as we showed in [8], using the algebraic properties of the classical Laguerre polynomials (A.1)–(A.5) one can derive the algebraic relations of the radial wave functions.

3.1. Recurrence relations and ladder-type operators for the radial functions. In [8] we proved the following

THEOREM 3.1. *Let the functions* $R^{(N)}_{nl}\left[\left(n+\frac{N-3}{2}\right)r\right]$, $R^{(N)}_{n+n_1,l+l_1}\left[\left(n+n_1+\frac{N-3}{2}\right)r\right]$ *and* $R^{(N)}_{n+n_2,l+l_2}\left[\left(n+n_2+\frac{N-3}{2}\right)r\right]$ *be three different radial functions of the N-th Hydrogen atom and n_1, n_2 and l_1, l_2 integers such that*

$$\min\,(n+n_1, n+n_2, l+l_1, l+l_2) \geq 0.$$

Then, there exist not all three vanishing polynomials in r, A_0, A_1, and A_2, such that

$$A_0(r)R^{(N)}_{nl}\left[\left(n+\frac{N-3}{2}\right)r\right] + A_1(r)R^{(N)}_{n+n_1,l+l_1}\left[\left(n+n_1+\frac{N-5}{2}\right)r\right] + A_2(r)R^{(N)}_{n+n_2,l+l_2}\left[\left(n+n_2+\frac{N-1}{2}\right)r\right] = 0.$$

Moreover, the expressions for the polynomial coefficients in the above formula are given by [8, Eq. (4.7) page 2063]

$$A_0(r) = A_0^*(r)\left(\mathcal{N}^{(N)}_{n,l}\right)^{-1} r^{l_1+l_2}, \quad A_1(r) = A_1^*(r)\left(\mathcal{N}^{(N)}_{n+n_1,l+l_1}\right)^{-1} r^{l_2},$$
$$A_2(r) = A_2^*(r)\left(\mathcal{N}^{(N)}_{n+n_2,l+l_2}\right)^{-1} r^{l_1},$$

where A_0^*, A_1^*, and A_2^*, are the non all three vanishing polynomials of the linear relation

$$A_0^*(r)L^{\alpha}_m(r) + A_1^*(r)L^{\alpha+2l_1}_{m+n_1-l_1}(r) + A_2^*(r)L^{\alpha+2l_2}_{m+n_2-l_2}(r) = 0,$$

and $\alpha = 2l+N-2$, $m = n-l-1$.

As examples of recurrences obtained by using the Theorem 3.1 we have the following (the first two are taken from [8], the other five are seem to be new). Other cases can be obtained in the same way.

- $n_1 = 1, n_2 = -1, l_1 = l_2 = 0$ [8, page 2063]

$$\sqrt{(n-l-1)(n+l+N-3)}\left(\frac{2n+N-5}{2n+N-3}\right)^2 R^{(N)}_{n-1,l}\left[\left(n+\frac{N-5}{2}\right)r\right] - (2n+N-3-r)R^{(N)}_{n,l}\left[\left(n+\frac{N-3}{2}\right)r\right] + \sqrt{(n-l)(n+l+N-2)}\left(\frac{2n+N-1}{2n+N-3}\right)^2 R^{(N)}_{n+1,l}\left[\left(n+\frac{N-1}{2}\right)r\right] = 0. \tag{3.2}$$

- $n_1 = n_2 = 0, l_1 = -1, l_2 = 1$ [8, page 2064]

$$(2l+N-1)\sqrt{(n-l)(n+l+N-3)}\,rR^{(N)}_{n,l-1}(r) + (2l+N-2)\times \left[(2n+N-3)r - (2l+N-3)(2l+N-1)\left(n+\frac{N-3}{2}\right)\right]R^{(N)}_{n,l}(r) + (2l+N-3)\sqrt{(n-l-1)(n+l+N-2)}\,rR^{(N)}_{n,l+1}(r) = 0. \tag{3.3}$$

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• $n_1 = 1, n_2 = 1, l_1 = 0, l_2 = 1$

$$\sqrt{n-l}(1-r)r\,R^{(N)}_{n+1,l}\left[\left(n+\frac{N-1}{2}\right)r\right] + \sqrt{n+l+N-2}\,(2l+N-1)\left(\frac{2n+N-3}{2n+N-1}\right)^2 r\,R^{(N)}_{n,l}\left[\left(n+\frac{N-3}{2}\right)r\right] - \left[(2l+N-1)^2+(1-r)(2l+N-1-r)\right]\sqrt{n+l+N-1}\times \times R^{(N)}_{n+1,l+1}\left[\left(n+\frac{N-1}{2}\right)r\right]=0,$$

• $n_1 = -1, n_2 = 1, l_1 = 1, l_2 = -1$

$$\{(2l+N-1-r)\left[(2l+N-3)(2l+N-2)+r(r+2)\right]+2r(n-l-1-r)\}\times \times R^{(N)}_{n,l}\left[\left(n+\frac{N-3}{2}\right)r\right] - \sqrt{(n-l-2)(n-l-1)}\left(\frac{2n+N-5}{2n+N-3}\right)^2(2l+N-3-r)r\,R^{(N)}_{n-1,l+1}\left[\left(n+\frac{N-5}{2}\right)r\right] - \sqrt{(n-l)(n-l+1)}\left(\frac{2n+N-1}{2n+N-3}\right)^2(2l+N-1-r)r\,R^{(N)}_{n+1,l-1}\left[\left(n+\frac{N-1}{2}\right)r\right]=0,$$

• $n_1 = -1, n_2 = 1, l_1 = -1, l_2 = 1$

$$A_0(r)R^{(N)}_{n,l}\left[\left(n+\frac{N-3}{2}\right)r\right]+A_1(r)\,R^{(N)}_{n-1,l-1}\left[\left(n+\frac{N-5}{2}\right)r\right] + A_2(r)R^{(N)}_{n+1,l+1}\left[\left(n+\frac{N-1}{2}\right)r\right]=0, \tag{3.4}$$

where,

$$A_0(r) = (2l+N-1+r)\left[-(2l+N-3)(2l+N-2)+(2(n-l-1)-r)\,r\right] - 2(n-l-1-r)r,$$

$$A_1(r) = \sqrt{(n+l+N-4)(n+l+N-3)}\left(\frac{2n+N-5}{2n+N-3}\right)^2(2l+N-1+r)r,$$

$$A_2(r) = \sqrt{(n+l+N-2)(n+l+N-1)}\left(\frac{2n+N-1}{2n+N-3}\right)^2(2l+N-3+r)r.$$

• $n_1 = 0, n_2 = 2, l_1 = 1, l_2 = 0$

$$A_0(r)R^{(N)}_{n,l}\left[\left(n+\frac{N-3}{2}\right)r\right]+A_1(r)\,R^{(N)}_{n,l+1}\left[\left(n+\frac{N-3}{2}\right)r\right] + A_2(r)R^{(N)}_{n+2,l}\left[\left(n+\frac{N+1}{2}\right)r\right]=0, \tag{3.5}$$

where,

$$A_0(r) = \sqrt{n+l+N-2}\left[(2l+N-1)(n+l+N-1-r)+(2n+N-1-r)r\right],$$

$$A_1(r) = \sqrt{n-l-1}\,(2n+N-1-r)r,$$

$$A_2(r) = (2l+N-1)\sqrt{(n-l)(n-l+1)(n+l+N-1)}\left(\frac{2n+N+1}{2n+N-3}\right)^2.$$

• $n_1 = 2, n_2 = 2, l_1 = 0, l_2 = 1$

$$A_0(r)R^{(N)}_{n,l}\left[\left(n+\frac{N-3}{2}\right)r\right] + A_1(r)R^{(N)}_{n+2,l}\left[\left(n+\frac{N+1}{2}\right)r\right] + A_2(r)R^{(N)}_{n+2,l+1}\left[\left(n+\frac{N-3}{2}\right)r\right] = 0, \tag{3.6}$$

where,

$$\begin{aligned} A_0(r) &= -(2l+N-1)\sqrt{(n-l)(n+l+N-2)(n+l+N-1)}\left(\frac{2n+N-3}{2n+N+1}\right)^2, \\ A_1(x) &= \sqrt{n-l+1}\,[(2l+N-1)(n-l-r)+(2n+N-1-r)r], \\ A_2(r) &= \sqrt{n+l+N}\,(2n+N-1-r)r. \end{aligned}$$

3.2. Ladder-type relations for the radial functions of the Hydrogen atom. Our starting point is the following

THEOREM 3.2. *Let $R^{(N)}_{nl}\left[\left(n+\frac{N-3}{2}\right)r\right]$, and $R^{(N)}_{n+n_1,l+l_1}\left[\left(n+n_1+\frac{N-3}{2}\right)r\right]$ two different radial functions of the Hydrogen atom and $\frac{d}{dr}R^{(N)}_{nl}\left[\left(n+\frac{N-3}{2}\right)r\right]$, the first derivative with respect to r, where n_1 and l_1 are integers such that $\min(n+n_1, l+l_1) \geq 0$, $(n_1)^2+(l_1)^2 \neq 0$. Then, there exist not all three vanishing polynomials in r, A_0, A_1 and A_2, such that*

$$A_0(r)R^{(N)}_{nl}\left[\left(n+\frac{N-3}{2}\right)r\right] + A_1(r)\frac{d}{dr}R^{(N)}_{nl}\left[\left(n+\frac{N-3}{2}\right)r\right] + A_2(r)R^{(N)}_{n+n_1,l+l_1}\left[\left(n+n_1+\frac{N-3}{2}\right)r\right] = 0. \tag{3.7}$$

The proof is similar to the one of Theorem 2.2 and was given in [8]. In fact in this case the relation (3.7) becomes into (see [8, (4.13) page 2064])

$$r^{l_1}\left(B_1(r)\frac{d}{dr} - B_1(r)\left(\frac{l}{r}-\frac{1}{2}\right) - B_0(r)\right)R^{(N)}_{nl}\left[\left(n+\frac{N-3}{2}\right)r\right] = B_2(r)\frac{\mathcal{N}^{(N)}_{n,l}}{\mathcal{N}^{(N)}_{n+n_1,l+l_1}}R^{(N)}_{n+n_1,l+l_1}\left[\left(n+n_1+\frac{N-3}{2}\right)r\right], \tag{3.8}$$

where the polynomials B_0, B_1, and B_2 are such that

$$B_0(z)L^{\alpha}_m(z) + B_1(z)L^{\alpha+1}_{m-1}(z) + B_2(z)L^{\alpha+2l_1}_{m+n_1-l_1}(z) = 0, \tag{3.9}$$

and $z = r/n + \frac{N-3}{2}$, $\alpha = 2l+N-2$, $m = n-l-1$.

Again, from the above theorem it is easy to obtain several relations for the radial wave functions of the Hydrogen atom and, in particular, the ladder operators in n and l, respectively. We will present here some of them. The first three are taken from [8] and the other two are seem to be new.

• $n_1 = 0, l_1 = 1$ [8, page 2065]

$$\left[\left(l+\frac{N-1}{2}\right)\left(\frac{d}{dr}-\frac{l}{r}\right)+\frac{1}{2}\right]R^{(N)}_{nl}(r) = -\frac{1}{2}\sqrt{1-\left(\frac{l+(N-1)/2}{n+(N-3)/2}\right)^2}\,R^{(N)}_{n,l+1}(r). \tag{3.10}$$

• $n_1 = 1, l_1 = 1$ [8, page 2065]

$$\begin{aligned}\left[(2l+N-1+r)\left(\frac{d}{dr}-\frac{l}{r}-\frac{1}{2}\right)+(n+l+N-2)\right] R_{nl}^{(N)}\left[\left(n+\frac{N-3}{2}\right)r\right] = \\ -\sqrt{(n+l+N-1)(n+l+N-2)}\left(\frac{n+(N-1)/2}{n+(N-3)/2}\right)^2 R_{n+1,l+1}^{(N)}\left[\left(n+\tfrac{N-1}{2}\right)r\right].\end{aligned} \tag{3.11}$$

• $n_1 = 1, l_1 = 0$ [8, page 2066]

$$\begin{aligned}\left[r\left(\frac{d}{dr}-\frac{1}{2(n+(N-3)/2)}\right)+(n+N-2)\right] R_{nl}^{(N)}(r) = \\ \sqrt{(n-l)(n+l+N-2)}\left(\frac{n+(N-1)/2}{n+(N-3)/2}\right)^2 R_{n+1,l}^{(N)}\left[\left(\frac{n+(N-1)/2}{n+(N-3)/2}\right)r\right].\end{aligned} \tag{3.12}$$

• $n_1 = 0, l_1 = 2$. Introducing these values into (3.9) and putting $\alpha = 2l+N-2$, $m = n-l-1$ and $z = \frac{r}{n+\frac{N-3}{2}}$, we get

$$B_0(z)L_m^{\alpha}(z) + B_1(z)L_{m-1}^{\alpha+1}(z) + B_2(z)L_{m-2}^{\alpha+4}(z) = 0\,. \tag{3.13}$$

Now, using three times relations (A.4) and (A.2), (3.13) becomes into

$$\begin{aligned}&\left[B_0(z) - B_1(z) + B_2(z)\frac{(m+\alpha+2)(m+\alpha+1)}{z^2}\right] L_{m-2}^{\alpha+2}(z) \\ &+\left[-2B_0(z) + B_1 z - 2B_2(z)\frac{(m+\alpha+2)(m-1)}{z^2}\right] L_{m-1}^{\alpha+2}(z) \\ &\qquad+\left[B_0(z) + B_2(z)\frac{(m-1)m}{z^2}\right] L_m^{\alpha+2}(z) = 0\,.\end{aligned}$$

Comparing with the TTRR (A.5) we find

$$\begin{aligned}B_0(z) = m - \frac{m(m-1)}{(\alpha+2)(\alpha+3)}z\,, \qquad B_2(z) = \frac{z^3}{(\alpha+2)(\alpha+3)}\,, \\ B_1(z) = -\frac{(\alpha+1)(\alpha+3)-(2m+\alpha+1)z}{\alpha+3}\end{aligned}$$

and therefore (see (3.8)), for the wave functions we find

$$\begin{aligned}&\left[(2l+N)\left(2r-(2l+N-1)(2l+N+1)\right)\left(\frac{d}{dr}-\frac{l}{r}+\frac{1}{2}\right)-\right. \\ &\left.(n-l-1)\left((2l+N)(2l+N+1)+\frac{n-l-2}{n+\frac{N-3}{2}}r\right)\right] R_{n,l}^{(N)}\left[\left(n+\frac{N-3}{2}\right)r\right] \\ &= \frac{r\sqrt{(n-l-1)(n-l-2)(n+l+N-1)(n+l+N-2)}}{\left(n+\frac{N-3}{2}\right)^3} R_{n,l+2}^{(N)}\left[\left(n+\frac{N-3}{2}\right)r\right].\end{aligned}$$

• $n_1 = 2, l_1 = 0$

$$\begin{aligned}&\left\{\left[2\left(n+\frac{N-3}{2}\right)\left(n+\frac{N-1}{2}\right)-r\right]\left[r\frac{d}{dr}-l-\frac{r}{2}+\left(n+\frac{N-3}{2}\right)(n+l+N-2)\right]\right. \\ &\qquad\left.-\left(n+\frac{N-3}{2}\right)^2(n-l)(n+l+N-2)\right\} R_{n,l}^{(N)}\left[\left(n+\frac{N-3}{2}\right)r\right] = \\ &\left(n+\frac{N+1}{2}\right)^2\sqrt{(n-l)(n-l+1)(n+l+N-2)(n+l+N-3)}R_{n+2,l}^{(N)}\left[\left(n+\frac{N+1}{2}\right)r\right].\end{aligned}$$

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3.3. Numerical analysis of the recurrences. As in the previous case, the radial wave functions for n and l large enough, calculated by using the functions (3.1) (by means of the Laguerre polynomials), behave as an unbounded function, and therefore we can not directly evaluate these functions for a given r. In figure 3.1 we show the critical values of n_{max} for a given l for which the radial functions can be computed using the explicit expression (3.1). The region where the explicit formula works is the one defined by the two curves in figure 3.1, (it is defined the values $l + 1 \leq n \leq n_{max}$).

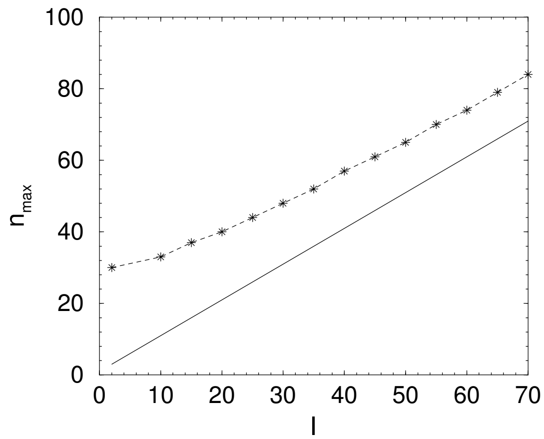

FIG. 3.1. *We represent with solid line the function $n = l + 1$ (this line represent the minimum value of n) and with the stars joint by the dashed line the maximum value of n for a given l for which the radial wave functions can be calculated using (3.1).*

Again we have studied numerically how to obtain the radial wave functions applying the recurrence relations (RR) of two types: the first ones are represented by the formulas (3.2), (3.3) and (3.4) and the second ones correspond to the ladder-type RRs (3.10), (3.11) and (3.12). For the former RRs we observe that

- the relation (3.2) is the most useful one because the initial conditions $R_{l+1,l}$ and $R_{l+2,l}$ can be calculated by using the Laguerre polynomials (notice that in this case we fix l and start with $n = l + 2$).
- in the relation (3.3) we fix n and increase the value of l in each step up to its maximum value. From figure 3.1 we conclude that for large value of n, we can not use the initial condition calculated by using Laguerre polynomials (formula (3.1)) and instead of this we should use the RR (3.2). For this reason, this relation can not be used alone (the same is true for the RR (3.4)). In addition, notice that the initial conditions are two radial functions, $R_{n,l-1}$ and $R_{n,l}$ evaluated at r, whereas (3.2) gives us the same functions but at nr (this implies a rescaling of the argument).
- From figure 3.2 we observe that the computational time is less when we use the formula (3.2). Moreover, the formulas (3.3) and (3.4) are numerically unstable at the vicinity of zero and this region becomes larger when n and l increases.
- As in the case of the I.H.O. the higher order relation (3.5) and (3.6) are not useful for numerical evaluation of the Radial functions.

For the ladder-type relations we would like to point out the following remarks

- Notice that the expression (3.12) involves two wave functions evaluated at different points, so in each step to calculate $R_{n+1,l}[(n+1)r/n]$ we need to know $R_{n,l}(r)$, but in the previous step we calculate $R_{n,l}$ at $nr/(n-1)$, not at r. For this reason

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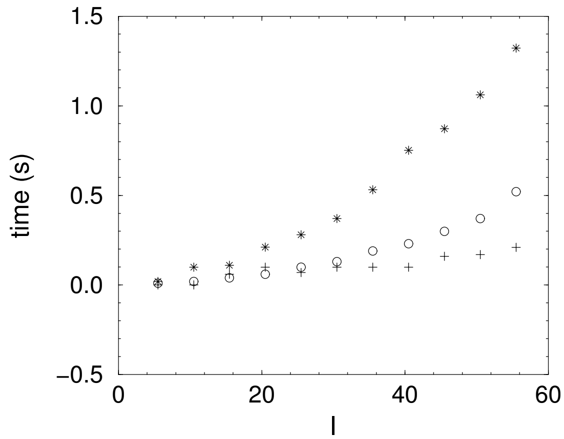

FIG. 3.2. *We represent with pluses, stars and circles the computational time versus* l *(*$n = 2\,l - 1$*) to compute the radial wave functions by using (3.2), (3.3) and (3.4), respectively.*

this RRs it is not useful for obtaining numerically the radial wave functions.

- As in the previous case, we can use the ladder-type relations (3.10), (3.12) and (3.11) together to (3.2), to compute the derivative of the radial wave function. As an example see the figure 3.3, where we plot the radial wave function and its derivative by using (3.10) for $n = 60$ and $l = 50$.

In general we verify that the ladder-type RRs are not useful in order to compute numerically the radial wave functions. Nevertheless they can be used, together with (3.2) for finding the derivative of the radial wave functions.

Programs. For the numerical simulations presented here we have used the commercial program MATLAB. The used source code can be obtained by request via e-mail to `niurka@euler.us.es` or `ran@us.es`.

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Appendix. The Laguerre polynomials. The Laguerre polynomials L_n^α defined by the hypergeometric series

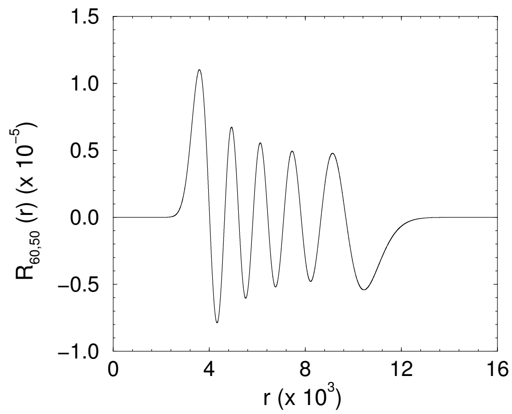
$$L_n^\alpha(x) = \frac{(\alpha+1)_n}{n!}\,{}_1\mathrm{F}_1\left(\begin{array}{c} -n \\ \alpha+1 \end{array}\Bigg|\, x\right) = \frac{(\alpha+1)_n}{n!}\sum_{k=0}^{n}\frac{(-n)_k}{(\alpha+1)_k}\frac{x^k}{k!},$$

$$(a)_0 := 1, \quad (a)_k := a(a+1)\cdots(a+k-1), \quad k = 1,2,3,\ldots .$$

These polynomials satisfy the following useful recurrence and differential-recurrence relations (see e.g. [1, 15, 17])

$$\frac{d}{dx}L_n^\alpha(x) = -L_{n-1}^{\alpha+1}(x), \tag{A.1}$$

$$xL_n^{\alpha+1}(x) = (n+\alpha+1)L_n^\alpha(x) - (n+1)L_{n+1}^\alpha(x), \tag{A.2}$$



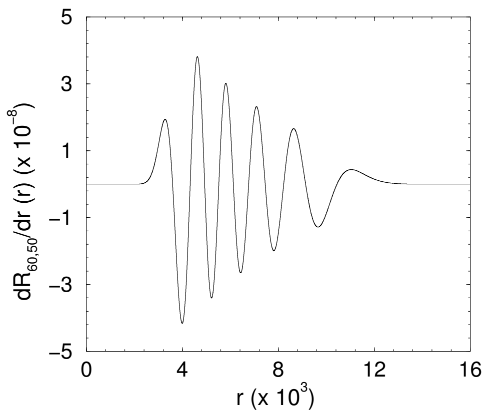


FIG. 3.3. *In the top panel we show the $R_{60,50}(r)$ computed by using the recurrence relation (3.2), whereas in the bottom panel we represent the derivative of this function computed from the ladder-type relation (3.10).*

$$xL_n^{\alpha+1}(x) = (n+\alpha)L_{n-1}^{\alpha}(x) - (n-x)L_n^{\alpha}(x), \tag{A.3}$$

$$L_n^{\alpha-1}(x) = L_n^{\alpha}(x) - L_{n-1}^{\alpha}(x), \tag{A.4}$$

$$(n+1)L_{n+1}^{\alpha}(x) - (2n+\alpha+1-x)L_n^{\alpha}(x) + (n+\alpha)L_{n-1}^{\alpha}(x) = 0. \tag{A.5}$$

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