PHYSICAL REVIEW A **86**, 062514 (2012)

Exact nonrelativistic polarizabilities of the hydrogen atom with the Lagrange-mesh method

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(Received 6 November 2012; published 26 December 2012)

Exact analytical expressions of the dipole polarizabilities of the nonrelativistic hydrogen atom in spherical coordinates are derived with the help of the Lagrange-mesh numerical method. This method can provide exact energies and wave functions for well-chosen conditions of calculation. Exact dipole polarizabilities are obtained after an unambiguous rounding up to at least principal quantum numbers around $n = 30$. The scalar polarizability of any nl level is given by $n^4[4n^2 + 14 + 7l(l + 1)]/4$ and its tensor polarizability is given by $-n^4[3n^2 - 9 + 11l(l + 1)]l/4(2l + 3)$, which allows the calculation of the polarizability of any hydrogen state nlm.

DOI: 10.1103/PhysRevA.86.062514 PACS number(s): 31.15.ap, 32.10.Dk, 02.70.Hm, 02.70.Jn

I. INTRODUCTION

The nonrelativistic hydrogen atom is one of the most studied and best-known problems of quantum mechanics [1]. Since the wave functions are known exactly, many of its properties can be derived analytically. An interesting example is given by static dipole polarizabilities for which a general analytical expression as a function of the quantum numbers nlm related to spherical coordinates requires very complicated calculations (see references in Ref. [2]). A polarizability is the response of the electron cloud to some external field [3,4] that can be represented as a multipole operator. Polarizabilities appear in, e.g., the Stark effect, interactions between an electron and an atom, and van der Waals forces.

The dipole polarizability of the ground state of the hydrogen atom has been known for a long time [5]. In parabolic coordinates, the general analytical expression for the hydrogen atom is well known [4] as

$$\alpha^{(n_1 n_2 m)} = \tfrac{1}{8} n^4 [17n^2 - 3(n_1 - n_2)^2 - 9m^2 + 19], \tag{1}$$

in atomic units, where $n_1 n_2 m$ are the parabolic quantum numbers and the principal quantum number is given by $n = n_1 + n_2 + |m| + 1$. These polarizabilities allow calculating the Stark effect at the second order of perturbation theory. The results are valid when the electric field is not too large but large enough so that the fine-structure splitting can be neglected. The calculation of these polarizabilities involves states of mixed parity resulting from the famous degeneracy of the nonrelativistic hydrogen atom. First-order perturbation theory mixes the degenerate states which enter into the second-order polarizabilities.

For the spherical quantum numbers nlm, the situation is different. Polarizabilities $\alpha^{(nlm)}$ can be defined mathematically for each unmixed state nlm. They are useful in different respects. They provide exact limits for vanishing frequencies of the dynamical polarizabilities which are useful in various processes [2,4]. They are also a useful testing ground for numerical techniques [6,7], in particular because of the similarity of simple models of alkali-metal atoms with hydrogen. However, contrary to the alkali-metal case, the hydrogen atom polarizabilities are unrealistic in the sense that degenerate states are excluded. Rigorous treatments must take into account transitions towards states with the same principal quantum number n. These states are separated by the small spin-orbit and Lamb-shift splittings. The nonrelativistic polarizabilities are then useful as a good approximation of the part of the realistic polarizabilities involving different principal quantum numbers and the continuum [8].

For ns states, a general analytical result has been derived by McDowell [9],

$$\alpha^{(ns)} = \tfrac{1}{4} n^4 (2n^2 + 7). \tag{2}$$

For $|m| = n - 1$, l is also equal to $n - 1$ and one deduces from Eq. (1) [4]

$$\alpha^{(n,l=n-1,|m|=n-1)} = \tfrac{1}{4} n^4 (n + 1)(4n + 5). \tag{3}$$

General expressions have been derived by Krylovetsky, Manakov, and Marmo but are not easily accessible (see references in Ref. [2]). For $m = 0$, they obtain

$$\alpha^{(nl0)} = n^4 \frac{n^2[19l(l+1) - 12] + 13l(l+1)[3l(l+1)+2] - 42}{4(2l-1)(2l+3)}. \tag{4}$$

Otherwise, explicit values of static polarizabilities of the hydrogen atom are given for a limited number of states in Refs. [6,7].

The Lagrange-mesh method is an approximate variational method involving a basis of Lagrange functions and using the associated Gauss quadrature for the calculation of matrix elements [10–12]. Lagrange functions are continuous functions that vanish at all points of a mesh but one. The principal simplification appearing in the Lagrange-mesh method is that the potential matrix is diagonal and only involves values of the potential at mesh points. The kinetic-energy matrix can be calculated exactly or approximated with the Gauss quadrature. The remarkable property of the Lagrange-mesh method is that the accuracy of the variational method is essentially preserved despite the use of the Gauss quadrature [13].

Strikingly, for well-chosen conditions of the calculation, the Lagrange-mesh method with exact expressions for the overlaps and kinetic-energy matrix elements can provide the exact values of the hydrogen energies and wave functions and thus, as explained below, of polarizabilities. Since computers

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have a limited number of digits, the numerical results differ from the exact values by rounding errors.

The aim of this paper is to derive exact analytical dipole polarizabilities by fitting numerical results obtained with a variational calculation using a Lagrange basis, which is exact in principle. The rounding required because of the limited accuracy of the computer can be performed unambiguously up to high values of n. In passing, it is observed that a calculation with the simplest version of the Lagrange-mesh method leads to numerical values of the polarizabilities more accurate than those of the variational calculation, despite additional Gauss quadrature approximations.

In Sec. II, general expressions for the polarizabilities induced by multipole fields are summarized and analyzed. In Sec. III, the Lagrange-Laguerre basis is introduced and the corresponding variational calculation is shown to lead to exact results. The difference with the Lagrange-mesh method is explained. Numerical results for the dipole polarizabilities are presented in Sec. IV and their exact analytical expressions are deduced. Concluding remarks are presented in Sec. V.

II. POLARIZABILITIES OF THE HYDROGEN ATOM

The wave functions of the nonrelativistic hydrogen atom are separated in spherical coordinates as $r^{-1}\psi_{nl}(r)Y_{lm}(\Omega)$. The radial functions ψ_{nl} with principal quantum number n are eigenfunctions of the radial Hamiltonian of the hydrogen atom for partial wave l,

$$H_l = \frac{1}{2}\left[-\frac{d^2}{dr^2} + \frac{l(l+1)}{r^2}\right] - \frac{1}{r} \tag{5}$$

(in atomic units), and correspond to energy $-1/2n^2$.

The polarizabilities are often defined by series involving the continuum. These series can be summed in a compact form with the method of Dalgarno and Lewis [14]. Let us consider the polarization by a multipole operator $r^\lambda C^{(\lambda)}_\mu$, where $C^{(\lambda)}_\mu(\Omega) = \sqrt{4\pi/(2\lambda+1)}Y^{(\lambda)}_\mu(\Omega)$. For partial wave l, the radial functions $\psi^{(1)}_{nll'}$ at the first order of perturbation theory are solutions of the inhomogeneous radial equations

$$(H_{l'} - E)\,\psi^{(1)}_{nll'}(r) = r^\lambda \psi_{nl}(r), \tag{6}$$

where ψ_{nl} is the radial wave function of the studied state. The polarizability of state lm for component μ of the multipole operator is given by

$$\alpha^{(nlm)}_{\lambda\mu} = (2l+1)\sum_{l'}\begin{pmatrix} l & \lambda & l' \\ m & \mu & -m-\mu\end{pmatrix}^2 \alpha^{(nll')}_\lambda. \tag{7}$$

This expression allows a calculation for any μ and m from $3jm$ coefficients and $\lambda+1$ reduced polarizabilities. These reduced polarizabilities read

$$\alpha^{(nll')}_\lambda = 2(2l'+1)\begin{pmatrix} l' & \lambda & l \\ 0 & 0 & 0\end{pmatrix}^2 \int_0^\infty \psi^{(1)}_{nll'}(r) r^\lambda \psi_{nl}(r) dr. \tag{8}$$

The sum in Eq. (7) is thus restricted to $|l-\lambda| \leqslant l' \leqslant l+\lambda$, with $l+\lambda+l'$ even and $l' \geqslant |m+\mu|$. The average or scalar polarizabilities defined by

$$\alpha^{(nl)}_\lambda = \frac{1}{2l+1}\sum_{m=-l}^{l} \alpha^{(nlm)}_{\lambda\mu} \tag{9}$$

do not depend on μ and can easily be calculated with

$$\alpha^{(nl)}_\lambda = \frac{1}{2\lambda+1}\sum_{l'=|l-\lambda|}^{l+\lambda}{}' \alpha^{(nll')}_\lambda, \tag{10}$$

where the prime means that the sum runs by steps of 2 and contains in general $\lambda+1$ terms.

The right-hand side of Eq. (6) is a polynomial of degree $n+\lambda$ multiplied by $\exp(-r/n)$. It behaves near the origin as $r^{\lambda+l+1}$. The solution of such an equation is elementary. It is a polynomial of degree $n+\lambda+1$ multiplied by the same exponential. It behaves near the origin as $r^{l'+1}$. Hence the integrand in Eq. (8) is a polynomial of degree $2n+2\lambda+1$ multiplied by $\exp(-2r/n)$ and the integral can be calculated exactly.

An unusual problem arises in the calculation of the static polarizabilities for the hydrogen atom because of the degeneracies in the level scheme. The differential equation (6) has no solution when transitions are possible toward a degenerate state. For dipole polarizabilities, this occurs when $l' = l-1$ and $|m+\mu| \leqslant l'$ or when $l' = l+1$ and $n > l+1$. Degenerate energies must be excluded from the calculation of polarizabilities. By projecting out the degenerate state [7], Eq. (6) is modified into

$$(H_{l'} - E)\,\psi^{(1)}_{nll'}(r) = r^\lambda\psi_{nl}(r) - \langle\psi_{nl'}|r^\lambda|\psi_{nl}\rangle\psi_{nl'}(r). \tag{11}$$

The reduced polarizability is obtained with Eq. (8) where $\psi^{(1)}_{nll'}$ is the solution of Eq. (11), orthogonalized to $\psi_{nl'}$. For particular cases, analytical calculations are quite feasible but the structure of a general formula is not obvious.

III. LAGRANGE-MESH AND VARIATIONAL METHODS

The Lagrange-Laguerre mesh points x_i are defined for $i=1$ to N by [10]

$$L_N(x_i) = 0, \tag{12}$$

where $L_N(x)$ is a Laguerre polynomial of degree N. The corresponding Gauss-Laguerre quadrature

$$\int_0^\infty g(x)\,dx \approx \sum_{k=1}^{N}\lambda_k g(x_k) \tag{13}$$

involves the Gauss-Laguerre weights λ_k [15]. It is exact if $g(x)$ is a polynomial of degree at most $2N-1$ times $\exp(-x)$ [16]. The regularized Lagrange functions read [12,17]

$$f_i(x) = (-1)^i x_i^{-1/2}\frac{xL_N(x)}{x-x_i}e^{-x/2}. \tag{14}$$

These basis functions are polynomials of degree N multiplied by $\exp(-x/2)$. They vanish at the origin. They satisfy the Lagrange property

$$f_i(x_j) = \lambda_i^{-1/2}\delta_{ij}. \tag{15}$$

At the Gauss approximation, the matrix elements of a function $V(x)$ are diagonal,

$$\int_0^\infty f_i(x)V(x)f_j(x)\,dx \approx \sum_{k=1}^{N} \lambda_k f_i(x_k)V(x_k)f_j(x_k) = V(x_i)\delta_{ij}, \tag{16}$$

because of the Lagrange properties (15). Matrix elements of x^{-1} and x^{-2} are exact since they involve polynomials of respective degrees $2N-1$ and $2N-2$, but not those of 1 since they involve a polynomial of degree $2N$. This basis is thus not orthonormal [13],

$$\mathcal{N}_{ij} = \langle f_i|f_j\rangle = \delta_{ij} + \frac{(-1)^{i-j}}{\sqrt{x_i x_j}}, \tag{17}$$

where the Dirac notation represents an integral from 0 to ∞. The matrix elements $T_{ij} = \langle f_i|T|f_j\rangle$ of $T = -d^2/dx^2$ read at the Gauss approximation [17]

$$T^G_{i\neq j} = (-1)^{i-j}\frac{x_i + x_j}{\sqrt{x_i x_j}(x_i - x_j)^2} \tag{18}$$

and

$$T^G_{ii} = -\frac{1}{12x_i^2}\left[x_i^2 - 2(2N+1)x_i - 4\right]. \tag{19}$$

The superscript G indicates the use of the Gauss approximation in a case where it is not exact. Here it is not exact since the integrand is a polynomial of degree $2N$ times $\exp(-x)$. However, the exact matrix elements of T can be obtained as

$$T_{ij} = T^G_{ij} - (-1)^{i-j}\frac{1}{4\sqrt{x_i x_j}}, \tag{20}$$

with a simple correction to the Gauss approximation [11,13].

The regularized Lagrange-Laguerre basis plays a special role for the hydrogen atom since, for some well-chosen scaling parameter h, the exact radial wave functions can be expressed exactly as a finite combination of these Lagrange functions. The radial functions ψ_l are expanded as

$$\psi_l(r) = h^{-1/2}\sum_{i=1}^{N} c_{li} f_i(r/h). \tag{21}$$

This expression is a polynomial of degree N times $\exp(-r/2h)$. For $h = n/2$, the functions $\psi^{(1)}_{nll'}(r)$ and $\psi_{nl}(r)$ can be reproduced exactly by expansion (21) if N is large enough.

The exact variational equations for orbital momentum l with basis (21) read

$$\sum_{j=1}^{N}(\mathcal{H}_{lij} - E\mathcal{N}_{ij})c_{lj} = 0 \tag{22}$$

for $i = 1$ to N, where

$$\mathcal{H}_{lij} = \frac{1}{2h^2}T_{ij} + \left[\frac{l(l+1)}{2h^2x_i^2} - \frac{1}{hx_i}\right]\delta_{ij} \tag{23}$$

is the matrix element $\langle f_i|H_l|f_j\rangle$ calculated exactly with Eq. (20) for the kinetic energy. A crucial property is that the Gauss quadrature is exact for the Coulomb and centrifugal terms. The system (22) is then an exact variational calculation with a basis chosen in a space supporting the exact solution for $n = 2h$ if $2h$ is an integer. Each eigenvalue $-1/2n^2$ can be reproduced exactly but for different values of the scaling parameter h. When the energy is exact, the corresponding expansion (21) is exact. In this case, the notations E_n, c_{nl}, and ψ_{nl} referring to the exact wave function can be used.

Like in Eq. (21), the functions $\psi^{(1)}_{nll'}$ are expanded as

$$\psi^{(1)}_{nll'}(r) = h^{-1/2}\sum_{j=1}^{N} c^{(1)}_{nll'j} f_j(r/h). \tag{24}$$

Eq. (6) leads to the algebraic system

$$\sum_{j=1}^{N}(\mathcal{H}_{l'ij} - E_n\mathcal{N}_{ij})c^{(1)}_{nll'j} = (hx_i)^\lambda c_{nli}, \tag{25}$$

where $\mathcal{H}_{l'ij}$ is the matrix element (23) with l replaced by l'. For $h = n/2$, it can give the exact solution corresponding to ψ_{nl} if N is large enough. With the Gauss quadrature, Eq. (8) provides the reduced polarizabilities

$$\alpha^{(nll')}_\lambda = 2(2l'+1)\begin{pmatrix} l' & \lambda & l \\ 0 & 0 & 0\end{pmatrix}^2 h^\lambda \sum_{j=1}^{N} c^{(1)}_{nll'j}x_j^\lambda c_{nlj}. \tag{26}$$

The Gauss quadrature is exact for $N \geqslant n + \lambda + 1$. Since in this case the c_{nlj} and $c^{(1)}_{nll'j}$ provide the exact functions ψ_{nl} and $\psi^{(1)}_{nll'}$, the polarizabilities are exact.

The algebraic system (25) becomes singular when transitions are possible toward a degenerate state. The degeneracy problem can easily be solved numerically with the Lagrange-mesh method by removing the degenerate eigenvalue. When solving system (25), the inverse of the matrix in the left-hand member is replaced according to

$$(\boldsymbol{\mathcal{H}}_{l'} - E_n\boldsymbol{\mathcal{N}})^{-1} \rightarrow {\sum_k}' \boldsymbol{v}^{(k)}(E^{(k)} - E_n)^{-1}\boldsymbol{v}^{(k)T}, \tag{27}$$

where $E^{(k)}$ and $\boldsymbol{v}^{(k)}$ are the eigenvalues and eigenvectors of the generalized eigenvalue problem $(\boldsymbol{\mathcal{H}}_{l'} - E^{(k)}\boldsymbol{\mathcal{N}})\boldsymbol{v}^{(k)} = 0$ and T means transposition. The prime in the sum indicates that the term with $|E^{(k)} - E_n| < \epsilon$ is dropped, where ϵ is, for example, chosen as 10^{-10} in double precision.

A standard Lagrange-mesh calculation would involve the Gauss approximation everywhere, i.e., the replacements

$$\mathcal{N}_{ij} \rightarrow \delta_{ij} \quad \text{and} \quad T_{ij} \rightarrow T^G_{ij} \tag{28}$$

in Eqs. (22), (23), (25), and (27). We shall see that this approximation essentially leads to the same results despite the Gauss approximation. In fact, we shall even observe that it is more accurate. The propagation of rounding errors is indeed less important in the standard Lagrange-mesh calculation, probably because the overlap matrix $\boldsymbol{\mathcal{N}}$ is diagonal and the eigenvalue problem is not generalized.

TABLE I. Energies and scalar and tensor dipole polarizabilities obtained in a variational calculation with $N = n+2$ Lagrange-Laguerre basis functions and $h = n/2$ for principal quantum numbers $n \leqslant 4$. Atomic units are used.

nl	h	N	E_n	$\alpha_0^{(nl)}$	$\alpha_2^{(nl)}$
$1s$	0.5	3	−0.499 999 999 999 999 7	4.500 000 000 000	0
$2s$	1.0	4	−0.124 999 999 999 999 9	120.000 000 000 000	0
$2p$			−0.124 999 999 999 999 8	175.999 999 999 999	−19.999 999 999 999
$3s$	1.5	5	−0.055 555 555 555 555 52	1012.500 000 000 018	0
$3p$			−0.055 555 555 555 555 59	1295.999 999 999 986	−161.999 999 999 997
$3d$			−0.055 555 555 555 555 64	1862.999 999 999 988	−485.999 999 999 997
$4s$	2.0	6	−0.031 250 000 000 000 00	4991.999 999 999 993	0
$4p$			−0.031 249 999 999 999 98	5887.999 999 999 932	−780.799 999 999 996
$4d$			−0.031 249 999 999 999 95	7680.000 000 000 189	−1920.000 000 000 067
$4f$			−0.031 249 999 999 999 90	10 367.999 999 999 27	−3647.999 999 999 685

IV. NUMERICAL AND DEDUCED ANALYTICAL DIPOLE POLARIZABILITIES

For dipole polarizabilities, the subscripts $\lambda = 1$ and $\mu = 0$ are dropped. Expression (7) is usually written as

$$\alpha^{(nlm)} = \alpha_0^{(nl)} + \alpha_2^{(nl)} \frac{3m^2 - l(l+1)}{l(2l-1)}, \tag{29}$$

where $\alpha_0^{(nl)}$ and $\alpha_2^{(nl)}$ are known as the scalar and tensor polarizabilities, respectively [4]. The average polarizability defined in Eq. (9) is the scalar polarizability $\alpha_0^{(nl)}$. Exact expressions for $\alpha_0^{(nl)}$ and $\alpha_2^{(nl)}$ will be deduced from accurate numerical results.

As we have seen, when $2h$ takes an integer value n, the wave function ψ_{nl} given by Eq. (21) is exact. The exact wave functions in the right-hand side of Eq. (6) are exponentials $\exp(-r/n)$ multiplied by polynomials. The exact solution of an inhomogeneous equation such as Eq. (6) is also a polynomial times the same exponential (see examples in Ref. [6]). Hence, this equation can also be solved exactly, i.e., the coefficients $c_{nll'j}^{(1)}$ obtained from system (25) give the exact functions $\psi_{nll'}^{(1)}(r)$ when $h = n/2$. The reduced polarizabilities (8) are then obtained with the Gauss quadrature (26) which is exact for $N \geqslant n + \lambda + 1$. With an infinite number of digits, the polarizability would be exact. Here they will contain rounding errors related to the double-precision computer accuracy.

The variational energies for $n \leqslant 4$ are presented in Table I. The scalar and tensor dipole polarizabilities obtained with the variational calculation are also displayed in Table I. The conditions of the calculation are $N = n + 2$ and $h = n/2$. The obtained values are close to integers or simple fractions, which can easily be guessed. The $1s$ polarizability has been known for a long time [5]. For $l = 0$, the results agree with the exact values (2) of Ref. [9]. For $l = n - 1$, they also agree with the exact values (3). The $2p0$ and $3d0$ polarizabilities calculated with Eq. (29) and Table I reproduce those obtained from a numerical calculation with B splines in Ref. [6]. It is remarkable that the Lagrange-mesh method with four and five mesh points gives a better accuracy than 80 B splines in Ref. [6]. Other cases do not seem to be available in the literature.

With the standard double precision, exact scalar polarizabilities can be obtained up to $n = 30$, at least, as exemplified by Table II. Strikingly, the Lagrange-mesh results, obtained with the Gauss approximation, are more accurate than the variational ones; i.e., they are closer to integer values. The tensor polarizabilities can be obtained with the same accuracy and hence the polarizabilities of any state nlm as a function of m. Scalar polarizabilities can be safely obtained up to $n = 40$. However, beyond $n \approx 30$, multiprecision should be used to avoid ambiguities in the non-necessarily integer values of the tensor polarizabilities.

From small subsets of values, analytical expressions for the polarizabilities can easily be extracted. These formulas can be tested with all other values. The two reduced dipole polarizabilities read

$$\alpha^{(nll+1)} = \frac{l+1}{4(2l+1)} n^4 [6(2n^2+7) + (5n^2+58)l + 24l^2 + 3l^3] \tag{30}$$

and

$$\alpha^{(nll-1)} = \frac{l}{4(2l+1)} n^4 [7n^2 + 5 - (5n^2+19)l + 15l^2 - 3l^3]. \tag{31}$$

They allow calculating the separate contributions of $l' = l + 1$ and $l' = l - 1$ for any nlm state and $\mu = -1$, 0, or 1.

TABLE II. Typical scalar dipole polarizabilities $\alpha_0^{(nl)}$ for $n = 30$ levels. Comparison of variational and Lagrange-mesh results with exact formula (32).

n	l	Variational	Lagrange mesh	Eq. (32)
30	0	731 834 999.9998	731 835 000.0002	731 835 000
	1	734 669 999.9984	734 670 000.0000	734 670 000
	2	740 339 999.9730	740 340 000.0000	740 340 000
	3	748 845 000.0436	748 845 000.0001	748 845 000
	4	760 184 999.9699	760 184 999.9999	760 185 000
	25	1 653 210 000.1764	1 653 210 000.0003	165 3210 000
	26	1 726 919 998.8397	1 726 920 000.0004	1 726 920 000
	27	1 803 465 000.8468	1 803 464 999.9983	1 803 465 000
	28	1 882 845 000.0327	1 882 845 000.0014	1 882 845 000
	29	1 965 059 999.9875	1 965 059 999.9998	1 965 060 000

The scalar dipole polarizability of level nl is given by three times the sum of expressions (30) and (31),

$$\alpha_0^{(nl)} = \tfrac{1}{4} n^4 [4n^2 + 14 + 7l(l+1)]. \qquad (32)$$

For $l = 0$, the formula (2) of McDowell [9] is recovered. See Table II for a comparison with numerical results at $n = 30$. The tensor dipole polarizability of level nl reads

$$\alpha_2^{(nl)} = -\frac{n^4 l}{4(2l+3)} [3n^2 - 9 + 11l(l+1)]. \qquad (33)$$

These results reproduce those of Krylovetsky, Manakov, and Marmo [2]: combining Eqs. (29), (32), and (33) for $m = 0$ provides Eq. (4). For $l = n - 1$, the sum $\alpha_0^{(n,n-1)} + \alpha_2^{(n,n-1)}$ agrees with Eq. (3). The $2p0$ and $3d0$ polarizabilities of Ref. [6] (216 and 2349, respectively) are easily reproduced with Eq. (29).

V. CONCLUDING REMARKS

The central results of this work are the analytical expressions (30) to (33). They allow a simple calculation of the dipole polarizability for any state nlm of the hydrogen atom. The computer-aided technique used to derive these analytical formulas is unusual. In a numerical sense, they are fully established since they agree with all results obtained with a numerical method which would be exact in a computation with an infinite number of digits. The roundings made necessary by the limited computer accuracy are unambiguous for all states up to $n = 30$ at least. Expressions (32) and (33) are confirmed by Ref. [2].

This is a special example of use of the Lagrange-mesh method. To ensure the exactness of the energies and wave functions, the calculations are performed with the exact overlap and kinetic-energy matrix elements. As already noticed in other cases [13,18], calculations with the usual Gauss quadrature approximation for these matrix elements lead to the same results with often a better accuracy. An excellent accuracy has also been obtained in calculations of polarizabilities of the confined hydrogen atom [19] and the hydrogen molecular ion [20]. The originality here is that a rare case where the method is exact leads to general analytical results.

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