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l-separated Hylleraas basis functions in the perturbation expansion of atomic states: Accurate partial-wave energies of second order in $1/Z$ for the $1s^2$ ground state

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The previously derived method of l-projected Hylleraas basis functions [for calculating the individual partial waves $R_l(r_1,r_2)P_l(\cos\theta)$ of an atomic pair function of first perturbation order in $1/Z$] is analyzed again and improved. It suffices to project, onto $P_l(\cos\theta)$, a subset of Hylleraas functions (the powers of $u=r_{12}$ and $s=r_1+r_2$ alone). The l-separated Hylleras functions give rapid convergence since they possess a similar discontinuity at $r_1=r_2$ as the exact partial wave [C. Schwartz, Phys. Rev. **126**, 1015 (1962)]. The handling of the l projections is easy. The method is applied to the $1s^2$ pair to obtain, at relatively low basis-set dimensions and without using any nonlinear parameter, the heretofore most accurate values of the partial-wave energies E_l^2 $(l=0,1,2,\ldots)$ and of the entire second-order energy E_{He}^2.

I. INTRODUCTION

In the calculation of an n-electron atomic state by perturbation expansion (with respect to the full or screened electronic interaction[1,2]), there are two kinds of mathematically rigorous decoupling which divide the large problem into subproblems that can be solved independently of each other. This decoupling holds for the first perturbation order. It does not hold for the entire eigenfunction, therefore it is not available in a method that is only variational. The first-order eigenfunction $\Psi^1(n)$ (which provides the energy up to the third order) decouples into $\sim\binom{n}{2}$ heliumlike pair functions $\Psi^1(2)$.[3,4,5(a)] Secondly, the perturbation equation for each of the atomic pair functions $\Psi^1(2)$ splits into independent equations for its "partial waves"[6]; for an $(L=0)$ pair the partial-wave decomposition is

$$\Psi^1(2):=\Psi^1(r_1,r_2,\theta)=\sum_{l=0}^{\infty}R_l(r_1,r_2)P_l(\cos\theta) \tag{1}$$

(θ is the angle between the vectors $\mathbf{r}_1$ and $\mathbf{r}_2$, P_l the lth Legendre polynomial).

Both principles have been taken care of in the "method of symmetry-adapted pair functions" (SAPF's) developed by Jankowski *et al.*[7] In the framework of the Hartree-Fock-based perturbation expansion the method has provided very accurate second- and third-order energies for the ten-electron[7(d),7(e)] and larger[7(b)] atoms. The $\Psi^1(n)$ problem for atoms thus reduces to the calculation of individual radial functions like the $R_l(r_1,r_2)$ $(l=0,1,2,3,\ldots)$ in Eq. (1).

The R_l can be approximated in a linear basis set using the variation-perturbation principle.[1,8] Continuing the work of a previous paper[9] (here called paper I), we study basis functions which can compactly represent an R_l. The exact $R_l(r_1,r_2)$ is characterized by a finite discontinuity of the third derivative in the neighborhood of $r_1=r_2$. Therefore the approximation by configuration-interaction-like products of orbitals, e.g., $r_1^n\exp(-\alpha r_1)r_2^m\exp(-\beta r_2)$, must be slowly convergent.[6] The basis set should contain functions which themselves have a discontinuous third derivative. Paper I has shown that such functions arise naturally by projection [onto $P_l(\cos\theta)$] of the Hylleraas basis functions (powers of $u=r_{12}$, $s=r_1+r_2$, and $t=-r_1+r_2$) which are known[1,10,11] to give a good representation of the entire $\Psi^1(2)$.

In the present paper we simplify this "l-Hylleraas method:" It suffices to project a subset of Hylleraas functions (the powers of u and s alone). These still generate a complete set of radial functions. The convergence improves and, furthermore, the method is easier to handle since from the outset there are no linearly dependent projections. We apply the method to the $1s^2$ ground state and calculate accurate values of the partial-wave energies E_l^2 (of second order in $1/Z$). Section II contains the mathematical results, Sec. III the calculations and the comparison with other work. Section IV indicates possible applications. The description of the method in this paper is restricted to the $1/Z$ expansion.[12] However, after the necessary changes the l-separated Hylleraas basis functions must be also applicable to the Hartree-Fock-based expansion.

II. THE CONDENSED l-HYLLERAAS BASIS SET

We consider the $1/Z$ expansion for the ground state of the two-electron atom:

$$\Psi_{\mathrm{He}}=\Psi_{\mathrm{He}}^0+Z^{-1}\Psi_{\mathrm{He}}^1+\cdots \tag{2}$$

where $\Psi_{\mathrm{He}}^0=(1/\pi)\exp(-r_1-r_2)$,

$$E_{\mathrm{He}}=-1+(\tfrac{5}{8})Z^{-1}+E_{\mathrm{He}}^2Z^{-2}+\cdots \tag{3}$$

(unit of length is $1/Z$ bohrs; unit of energy is Z^2 hartree).

Through the partial-wave expansion Eq. (1), the first-order perturbation equation[8] splits into separate equations for $l=0,1,2,\ldots$:

$$(H^0+1)\Psi_l^1+[(1/r_{12})_l-\tfrac{5}{8}\delta_{l,0}]\Psi^0_{\mathrm{He}}=0 \tag{4}$$

[H^0 is the sum of two hydrogenic operators, and $(1/r_{12})_l=(r_<^l/r_>^{l+1})P_l$]. Likewise the variation-perturbation principle decouples[6] into separate principles for the E_l^2 and Ψ_l^1; cf. Eqs. (1)–(5) of paper I.

The Hylleraas basis functions (for representing the entire Ψ^1_{He}) are ($s=r_1+r_2$, $t=-r_1+r_2$, $u=r_{12}$)

$$F_{abc}=u^a s^b t^c X;\quad a,b\in\{0,1,2,\ldots\},\ c\in\{0,2,4,\ldots\}\ . \tag{5}$$

In our calculations we choose the simplest reference function: $X=\Psi^0_{\mathrm{He}}$ for all l. The "l-Hylleraas basis functions" as suggested in paper I arise by projection of the F_{abc} onto $P_l(\cos\theta)$. These projections, which we write as $F_{abc,l}$, are of two types: They are infinitely differentiable in r_1 and r_2 for the even u powers ($a=0,2,4,\ldots$), and finitely (at least two times) differentiable at $r_1=r_2$ for the odd $a=1,3,5,\ldots$. Since in Eq. (4) $(1/r_{12})_l$ has a "cusp" at $r_1=r_2$ (a discontinuous first derivative) the solution Ψ_l^1 must have a discontinuous third derivative. Among the basis functions $F_{abc,l}$ the $F_{1b0,l}$ (which contain the first power of u and do not contain t) are the most important for modeling this cusp behavior of Ψ_l^1; see (c) below. Since $\Psi_l^1\rightarrow\frac{1}{2}(u)_l\Psi^0_{\mathrm{He}}$ for $l\rightarrow\infty$ (Ref. 6) the first basis function $F_{100,l}$ alone is sufficient for representing the partial waves of high l. (The $E^2_{l=6}$, for example, is so approximated with an accuracy of 10^{-7} a.u.)

From these considerations it results that the generating set (5) can be reduced to the subset where $c=0$:

$$F_{ab}=u^a s^b X,\quad a,b\in\{0,1,2,3,\ldots\}\ . \tag{6}$$

For given l, let $\{F_{abc,l}\}$ and $\{F_{ab,l}\}$ denote the sets of the (nonzero) l-projections of the functions (5) and (6), respectively. Our basis sets for the practical calculations will be fixed by the usual conditions

$$a+b+c\leq\hat{M}\quad\text{and}\quad a+b\leq M\ , \tag{7}$$

respectively, where $\hat{M},M\in\{1,2,3,\ldots\}$. These finite sets will be denoted by $\hat{B}_l(\hat{M})$ and $B_l(M)$, respectively. We have the following statements (to be proved subsequently).

(a) For $l=0$ and any M, $\hat{B}_0(M)$ and $B_0(M)$ span the same linear space; i.e., the elimination of linearly dependent projections reduces $\hat{B}_0(M)$ to $B_0(M)$. For $l\geq1$ the linear space of $\hat{B}_1(M)$ is actually larger than that of $B_l(M)$. The observations (b)–(d) refer to all $l\geq0$.

(b) $\{F_{ab,l}\}$ is an (over)complete system, i.e., it can represent the exact partial wave Ψ_l^1.

(c) Through the projections of us^b ($b=0,1,2,\ldots$), $\{F_{ab,l}\}$ is capable of a rapid modeling of Ψ_l^1 near $r_1=r_2$.

(d) All projections in $\{F_{ab,l}\}$ are linearly independent. That is, the elimination of linear dependences as in $\{F_{abc,l}\}$ is no longer necessary.

Observation (a) follows from the fact that, for $l=0$, there is a linear relation[13] between $(u^m t^2)_0$ and the $F_{ab,0}$:

$$[(m+2)u^m t^2-(m+4)u^{m+2}]_{l=0}=-2s^{m+2}\qquad (M=0,1,2,\ldots)\ . \tag{8}$$

For $l\geq1$ the projection $(ut^2)_l$, for example, is linearly independent of the $F_{ab,l}$.

Statement (b) is a consequence of the fact[14] that, in the space of the wave functions $\Psi(r_1,r_2,\theta)$, the subset $u^{2a}s^b t^c$ of (5) with even u exponents is already a complete system. When this subset of Hylleraas functions is projected onto a given l, one obtains complete radial sets consisting, however, of the infinitely differentiable functions only. It is easily seen that each $(u^{2a}s^b t^c)_l$ depends linearly on the projections of the form $(u^{2a}s^b)_l$.

For (c) one examines the projections $F_{abc,l}$ for $a=1,3,5,\ldots$ as functions of (r_1,r_2) in the neighborhood of $r_1=r_2$. The $(us^b)_l$ ($b=0,1,2,3,\ldots$) exhibit a discontinuity in the third derivative. For $(us^b t^2)_l$ and $(u^3 s^b)_l$ the discontinuity moves to the fifth derivative, for $(us^b t^4)_l$, $(u^3 s^b t^2)_l$, and $(u^5 s^b)_l$ to the seventh derivative.

(d) can be proved as follows. Any projection $F_{ab,l}$ has the form

$$F_{ab,l}=y^m q^l A(q)P_l(\cos\theta)\ , \tag{9}$$

where $m=a+b$, $y=r_>$, $q=r_</r_>$, and $A(q)$ is a polynominal in q (which depends on l, a, and b). Because of the y^m in (9) there can be linear dependence at most between functions of the same m. Consider the case of the partial wave $l=0$. For $m=1$ there are two projections

$$(s)_0=s=y(1+q) \tag{10a}$$

and

$$(u)_0=\tfrac{1}{3}y(3+q^2) \tag{10b}$$

which are linearly independent. For higher m one concludes by induction: If the projections of $s^m,us^{m-1},\ldots,u^m$ are independent then the same must be true for the projections of the s-multiplied functions $s^{m+1},\ldots,u^m s$. There is one remaining projection: that of u^{m+1}. For a pure u power the polynomial $A(q)$ in Eq. (9) is nonzero at $q=-1$; so, it cannot be a linear combination of the s-multiplied projections since these vanish at $q=-1$. For the $l\geq1$ the proof works the same way.

TABLE I. Partial wave $l=0$. Calculations using the l-separated Hylleraas functions $\{F_{ab,l=0}\}$ where $a+b\leq M$; cf. Eqs. (6) and (7). dim is the respective basis-set dimension. Energies in 10^{-6} a.u.

M	dim	E
1	1[a]	−124 694.019
2	5	−125 331.192
3	9[b]	−125 333.249
4	14	−125 333.688
5	20	−125 333.789
6	27	−125 333.816
7	35	−125 333.825
8	44	−125 333.828
9	54	−125 333.830

[a] Only function u.

[b] See Ref. 21.

TABLE II. Partial wave $l=1$. Comparison of the full and the condensed l-separated Hylleraas sets (left- and right-hand sides, respectively); cf. Eqs. (5)–(7). Improved convergence for sets fixed by $2a+b\leq N$ (lower right); cf. Eq. (11). All energies in 10^{-6} a.u.

	$\{F_{abc,l=1}\}$			$\{F_{ab,l=1}\}$	
$\hat{M}$	dim	E	M	dim	E
1	1	−24 781.837	1	1	−24 781.837
4	12	−26 489.931	4	10	−26 489.785
5	18	−26 493.644	5	15	−26 493.581
6	25	−26 494.637	6	21	−26 494.610
7	33	−26 494.955	7	28	−26 494.943
8	42	−26 495.072	8	36	−26 495.066
9	52	−26 495.120	9	45	−26 495.117
			N	dim	E
			9	20	−26 494.954
			10	25	−26 495.068
			11	30	−26 495.117
			12	36	−26 495.140
			13	42	−26 495.150
			14	49	−26 495.155
			15	56	−26 495.158

III. CALCULATIONS

The l-projected Hylleraas functions are all of the form (9). The variation principle for E_l^2 and Ψ_l^1 [see Eq. (5) of paper I] leads, as usual, to a system of linear equations. All matrix and vector elements are sums of the James-Coolidge integrals[15] V_{mn} ($\alpha=2$, $\beta=2$); cf. Eq. (18) of I. We set $m+n=\sigma$ and $V_{mn}=U_{m,\sigma}$. The $U_{m,\sigma}$ are computed recursively using the formulas of James and Coolidge.[15] The original procedure, which starts from $U_{0,-1}=\frac{1}{2}\ln 2$ and *ascends* in m and σ, tends to accumulate roundoff error. For reaching higher values of m and σ, it is much safer to *descend*, starting from some "corner value" U_{m_0,σ_0} with $m_0\geq\sigma_0+1$. This U_{m_0,σ_0} can be found by summation of the series Eq. (20) of I. (This series is convergent for all m and σ.) Fifty terms of it provide $U_{50,40}$ with an accuracy of 12 decimal places.

The numerical results for the partial waves $l=0$–15 are collected in Tables I–V. In the case of $l=0$ (Table I) the full l-separated Hylleraas set $\hat{B}_0(M)$ and the condensed set $B_0(M)$ are equal [see (a) of Sec. II]. For the partial waves $l=1$ and 2 Tables II and III give the results from both basis sets for comparison; one can see that the energy is altered very little by the omission of the t-dependent functions, while the dimension reduces. The convergence with rising M of $B_l(M)$, see Eq. (7), is relatively slow for the partial waves $l=1$ and 2. This is owing partly to our rigid choice of reference function Ψ^0_{He} for all l. We have therefore applied sets $B_l'(N)$ which are the subsets of $\{F_{ab,l}\}$ restricted by the condition

$$2a+b\leq N \quad (N=1,2,3,\ldots)\,. \tag{11}$$

These contain relatively more s than u powers and allow for a better modeling of the s dependence of the radial function R_l in a similar way as the substitution of the

TABLE III. Partial wave $l=2$. Similar calculations as Table II; cf. Eqs. (5)–(7) and (11).

	$\{F_{abc,l=2}\}$			$\{F_{ab,l=2}\}$	
$\hat{M}$	dim	E	M	dim	E
1	1	−3832.698	1	1	−3832.698
7	30	−3905.984	7	22	−3905.971
8	39	−3906.065	8	29	−3906.058
9	49	−3906.100	9	37	−3906.096
			N	dim	E
			13	32	−3906.109
			14	38	−3906.120
			15	44	−3906.126
			16	51	−3906.129

TABLE IV. Partial waves $l=3,4,5$ using the l-separated Hylleraas sets $\{F_{ab,l}\}$; cf. Eq. (6).

l	M	dim	E
3	1	1	-1070.190
	8	24	-1077.716
	9	31	-1077.721
	10	39	-1077.724
	11	48	-1077.726
4	1	1	-404.846
	7	16	-406.093
	8	21	-406.095
	9	27	-406.096
	10	34	-406.097
5	1	1	-184.710
	5	9	-184.991
	6	12	-184.993
	7	16	-184.994
	8	20	-184.995

reference function $\exp(-s)$ by $\exp(-ks)$ where k is a free parameter.[10] The lower parts of Tables II and III show for $l=1$ and 2 that $B_l'(N)$ needs considerably fewer basis functions than $B_l(M)$ for the same accuracy of the energy. (For $l=0$ and 3 the use of $B_l'(N)$ gives little advantage.)

For $l=15$ (see Table V) the energy of the "one-function approximation" $\Psi_l^1 = c(l)(u)_l \Psi_{\text{He}}^0$ is -3.029714×10^{-6} a.u.; this differs from the exact energy by only 1×10^{-10} a.u. The one-function approximation, in turn, can be replaced very accurately by the three terms of its asymptotic expansion, Eq. (21) of I. This three-term formula gives -3.029716×10^{-6} a.u. for $l=15$ and, when summed[16,17] over all $l\geq16$, the total of -14.2481×10^{-6} a.u. The difference against the sum of the exact partial-wave energies should be less than 1×10^{-9} a.u.

TABLE V. Partial waves $l\geq6$ using the l-separated Hylleraas sets $\{F_{ab,l}\}$; cf. Eq. (6). The values in the column "converged" are attained with $M=6$ (dim 12) for $l=6$–12, with $M=4$ (dim 6) for $l=13$–15. Sum $l\geq16$ is taken from the asymptotic formula Eq. (21) or Ref. 9.

l	$M=1$ (dim 1)	Converged
6	-95.7082	-95.788
7	-54.3689	-54.396
8	-33.1093	-33.120
9	-21.2898	-21.2941
10	-14.3009	-14.3029
11	-9.9570	-9.9579
12	-7.1432	-7.1437
13	-5.2564	-5.2566
14	-3.9531	-3.9533
15	-3.0297	-3.0298
≥16	-14.2481	-14.2481

For the $l\geq4$ (Tables IV and V) the respective best values of the partial-wave energies are converged within the given number of digits. For $l=0$–3 (Tables I–III) the remaining error appears to be not larger than a few 10^{-9} a.u. in each case. Summation over all l gives the total second-order energy E_{He}^2; cf. Eq. (3). In Table VI, lines 1(A)–1(C), three sums of different accuracy have been formed. The best value, gained with l-separated Hylleraas basis sets of dimension ≤56, is $E_{\text{He}}^2 = -157\,666.425\times10^{-6}$ a.u.

The extrapolated value of Midtdal,[11] see line 4(B) of Table VI, is very close to it. Midtdal's variational result [4(A)] enables the direct comparison between entire and l-separated Hylleraas functions since Midtdal's work, like the present one, uses the nonoptimized reference function $\exp(-ks)$ with $k=1$. The accuracy of the 203 entire functions is reached in l-separated calculations of dimensions ≤30 [see line 1(A)].

Our result 1(B) is close to the best previous values: That of Scherr and Knight[10(b)] (line 7 of Table VI) and Knight's[10(c)] value of $-157\,666.40\times10^{-6}$ a.u. which was obtained in 100 Hylleraas functions with an optimized k. It is well known[10(b)] that the optimization of k saves basis functions; compare also lines 4(A) and 5 of Table VI. Recent l-separated Hylleraas calculations[18] which optimize $k=k_l$ for each l need only 70–50 % of the dimensions of the present ($k=1$) calculations.

Good convergence of the l-separated Hylleraas functions can be seen from the comparison with other radial basis sets. The powers of $r_<$ and $r_>$ [Ref. 18(b)] have been discussed in paper I; see also the present Table VI, line 2. A recent paper by Kutzelnigg[5(b)] explores the partial-wave structure of the remainder wave function which is obtained from either the entire or the first-order perturbation eigenfunction by separation of an r_{12}-proportional part $r_{12}\phi(r_1,r_2)$. The Ψ_l^1 of the $1/Z$ expansion is thus represented by $\frac{1}{2}(r_{12})_l\Psi_{\text{He}}^0$ plus the sum of orbital products (which contain one optimized exponential parameter per l). A set of 55 products gives for $l=1$ the energy of $-26\,494.93\times10^{-6}$ a.u. The same accuracy can be attained with 20 of the l-separated Hylleraas functions (Table II). This indicates that the convergence for the low l is improved by the participation of more of the "cusp functions" $(u)_l s^b \Psi_{\text{He}}^0$ along with the ($b=0$) function; cf. Sec. II. In Kutzelnigg's method a similar improvement is provided for through the optimization of the reference function ϕ.

At the end of this section we should like to underline the observation of Schwartz[6] and Byron and Joachain[19(b)] that a partial wave is approximated only slowly if the radial basis set consists of orbital products $\phi_{ij}(r_1,r_2)=\varphi_i(r_1)\varphi_j(r_2)$ alone. This should also be true[20] for the Møller-Plesset expansion. Orbital products have been used by Jankowski and co-workers[7] for the practical implementation of the SAPF method. For each partial wave of the $1s^2$ pair of the neon atom (Møller-Plesset expansion) a choice of 120 products (which are expressed in 20 Slater orbitals with carefully optimized exponential parameters) gave the E_l^2 (for example, $l=3,4,\ldots,9$) with

TABLE VI. Total second-order energy E^2_{He} (all partial waves included). Results from l-separated variation (lines 1–3) and from entire variation (lines 4–7). Energies in 10^{-6} a.u.

Line	Method	E^2_{He}
1	l-projected Hylleraas functions, exponential parameter $k=1$ (present results):	
(A)	(27,30,27,18,12,12)[a]	$-157\,666.299$
(B)	(44,42,44,31,21,20)[a]	$-157\,666.405$
(C)	(54,56,51,48,34,20)[a]	$-157\,666.425$
2	Powers of $r_<$ and $r_>$, $k=1$, dim 30 for each $l\leq 10$ [Byron *et al.*, Ref. 19(b)]	$-157\,656$
3	$(r_{12})_l$ and orbital products,[b] k opt., dim 55 for the low l [Kutzelnigg, Ref. 5(b)]	$-157\,666.14$
4	Hylleraas functions, $k=1$ (Midtdal, Ref. 11):	
(A)	variational result, dim 203	$-157\,666.239$
(B)	extrapolated value	$-157\,666.428$
5	Hylleraas functions, k opt., dim 70 [Knight and Scherr, Ref. 10(a)]	$-157\,666.149$
6	Hylleraas-like functions, k opt., dim 100 (Sanders and Scherr, Ref. 22)	$-157\,666.38$
7	Kinoshita functions, k opt., dim 100 [Scherr and Knight, Ref. 10(b)]	$-155\,666.405$

[a] In brackets are the respective dimensions for $l=0,1,2,3,4,5$.

[b] Cf. Sec. III.

an accuracy of 10^{-6} a.u. [Table II of Ref. 7(a)]. In order to obtain the E^2_l of the $1/Z$ series with the same accuracy (see also Table II of paper I) very small sets of 8, 5, and 1 l-separated Hylleraas functions are sufficient for $l=3$, 4, and $l\geq 5$, respectively.

IV. CONCLUSION

In this paper the method of the l-separated Hylleraas basis functions (for calculating a partial wave of an atomic pair function) has been analyzed again and simplified. Generating the l projections and evaluating the matrix elements is transparent and straightforward. The application of the method to the $1s^2$ ground state ($1/Z$ expansion) gave the most accurate values to date of the partial-wave energies E^2_l ($l=0,1,2,\ldots$) and of the entire E^2_{He} (Table VI). In order to approximate a partial wave Ψ^1_l with a given accuracy, the basis-set dimension is lower (in some cases much lower) with the l-separated Hylleraas functions than with other previously used basis functions.[5(b),7,19(b)] The 203-dimensional calculation[11] in entire Hylleraas functions is equivalent to individual l-separated calculations, each of dimension ≤ 30. For the low l it would be possible to reduce the basis set dimensions further by optimizing the reference function $X=X_l$ for each l (von Hirschhausen[18]). Further details have been discussed in Sec. III.

The decoupling into partial waves exist also for the pair functions of the second and higher perturbation orders, Ψ^2_{He}, etc. The l-separated Hylleraas functions are then again applicable. Though the variation principle for E^4_l and Ψ^2_l (of some l) contains the first-order partial waves Ψ^1_l of *all* l, the evaluation appears to present no difficulties.

The main field of application of the l-separated Hylleraas basis set is the determination of the first-order eigenfunction of the *n-electron* atom through the separate calculation of the pairs $1s\,2s$ (singlet and triplet S), $2p^2$ (triplet P), etc.; that is, in the framework of the method of "symmetry-adapted pairs"[7] or in the counterpart of it in the $1/Z$ expansion.

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[14]B. Klahn, Theor. Chim. Acta **44**, 27 (1977).

[15]H. M. James and A. S. Coolidge, Phys. Rev. **49**, 688 (1936).

[16]In Table II of paper I (see Ref. 9) the value for the sum over $l \geq 11$ has been given inaccurately. The correct value is -43.588.

[17]*Handbook of Mathematical Functions,* edited by M. Abramowitz and I. A. Stegun (Dover, New York, 1965), pp. 806–808.

[18]H. von Hirschhausen (unpublished).

[19](a) F. W. Byron and C. J. Joachain, Phys. Rev. **146**, 1 (1966); (b) **157**, 1 (1967).

[20]Byron *et al.* [Ref. 18(a)] have calculated the E^2 for helium $(1s^2)$ both for the Hartree-Fock-based and the hydrogenic expansion, using entire Hylleraas functions. Their Table I shows that, with a given number of functions, a similar accuracy is attained for both types of expansion.

[21]In Table I of paper I (see Ref. 9) the linear dependence of $(ut^2)_{l=0}$ has not been taken account of; cf. Eq. (8) and Ref. 13 of the present paper. For $l=0$ and $m=3$ there are only 9 (not 10) functions. The energies given in Tables II and III of paper I remain unaltered.

[22]F. C. Sanders and C. W. Scherr, Phys. Rev. **181**, 84 (1969).