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Correlation Effects in Two- and Three-Electron Systems

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Correlation effects in the lithium isoelectronic series $(1s)^2 2s\,{}^2S$ have been studied by computing the expectation values of a number of one- and two-electron operators. Calculations were performed using both Hartree-Fock and configuration interaction wave functions. The operators considered are $\sum r_i^N$ ($N=-2$, -1, 2, 4), $\sum\delta^3(\mathbf{r}_i)$, $\sum p_i^2$, $\sum_{i>j}\delta^3(\mathbf{r}_{ij})$, $\sum_{i>j}(\mathbf{r}_i\cdot\mathbf{r}_j)$, and $\sum_{i>j}(\mathbf{p}_i\cdot\mathbf{p}_j)$. Computations were performed for $Z=3$, 4, 5, and 8. For comparison purposes the same expectation values were computed from configuration interaction wave functions of comparable accuracy for the two-electron systems $(1s)^2\,{}^1S$ with $Z=2$, 3, 4, 5, and 8. The results of the two-electron computations show reasonable agreement with more accurate computations and with empirical estimates. For the three-electron systems the main conclusions are: (a) Correlation has little effect on the one-electron expectation values, (b) the expectation values of $\sum_{i>j}(\mathbf{r}_i\cdot\mathbf{r}_j)$ and $\sum_{i>j}(\mathbf{p}_i\cdot\mathbf{p}_j)$ are proportionately larger for three- than for two-electron systems, and (c) the configuration interaction approach probably gives poor estimates of the expectation value of $\sum_{i>j}\delta^3(\mathbf{r}_{ij})$ even though this value appears to converge as the number of terms in the wave function is increased.

I. INTRODUCTION

RECENT computations of wave functions for low-lying states of two-electron atomic systems[1,2] has led to accurate expectation values for a number of quantum mechanical operators. The purpose of such bound-state calculations has been primarily to obtain the total energy for a given state directly by approximate solution of the nonrelativistic Schrödinger equation. It appears that at present this can be done for two electron low-lying states about as accurately as spectral term values can be measured. From this point of view expectation values of operators other than the Hamiltonian represent a useful by-product of such calculations which can be compared with experimental results. Most of the interest in such values has been in attempts to compute relativistic corrections to the energy.[3–5] The success of such efforts, coupled with the satisfactory agreement of other theoretically determined expectation values with observed quantities,[6] indicates that basically the properties of such two-electron systems are well understood.

For systems with three or more electrons, the best bound-state calculations presently available yield total energies several orders of magnitude less accurate than those for two electrons.[7] While the wave functions obtained from such calculations give a moderately realistic spatial description of the electronic charge cloud, expectation values derived from them do not always agree with experimentally measured quantities. For example, the expectation value of $(\sum\mathbf{r}_i)^2$ can be obtained by an analysis of experimental refractive index data.[8] This method yields results for the rare gases which lie 4 to 6% below the quantities computed from Hartree-Fock wave functions. For other properties, such as the hyperfine splitting,[9–11] discrepancies between calculated and measured values tend to be much larger even when wave functions superior to Hartree-Fock functions are used.

The differences between experimental and calculated values mentioned above are, of course, due to the use of approximate wave functions which ignore important correlation effects between electrons. While such effects can be studied in some detail for two-electron systems, very little has been done for systems of three or more electrons. It is the purpose of this paper to make a start in this direction by studying correlation effects for the lithium isoelectronic series $(1s)^2 2s\,{}^2S$. Such a study is possible since wave functions for this series have recently been computed[12] using the configuration interaction approach which is expected to include most of the interelectron correlation. In addition, Hartree-Fock wave functions for the sequence are also available.[13]

With the above in mind, we have computed the expectation values for a number of one and two electron operators using both of the above-mentioned sets of wave functions. In order to shed further light on the effects of correlation, we have computed the same expectation values using wave functions of comparable accuracy for the two electron $(1s)^2\,{}^1S$ isoelectronic

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[1] C. Pekeris, Phys. Rev. **112**, 1649 (1959); **115**, 1216 (1959); **126**, 1470 (1962).

[2] T. Kinoshita, Phys. Rev. **105**, 1490 (1957); **115**, 368 (1959).

[3] A. Dalgarno and A. L. Stewart, Proc. Phys. Soc. (London) **A76**, 49 (1960).

[4] C. Schwartz, Phys. Rev. **123**, 1700 (1961).

[5] E. E. Salpeter and M. H. Zaidi, Phys. Rev. **125**, 248 (1962).

[6] For example, Pekeris computes a value of 1.320355 for $\delta^3(\mathbf{r}_1)$ compared with a measured value of 1.320345±0.000091 obtained from hyperfine splitting measurements for the $2\,{}^3S$ state of He. While discrepancies still exist between computed and measured values {see, for example, R. Ya. Damburg and E. M. Iolin, Zh. Eksperim. i Teor. Fiz. **42**, 820 (1961) [translation: Soviet Phys.—JETP **15**, 572 (1962)]}, the above agreement is typical of what one should expect from accurate two-electron bound-state calculations.

[7] Variations of 0.01 atomic units in the total energy from the experimental values are typical for such systems. See, for example, R. E. Watson, Phys. Rev. **119**, 170 (1960).

[8] A. Dalgarno and A. E. Kingston, Proc. Roy. Soc. (London) **A259**, 424 (1960).

[9] N. Bessis, H. Lefebvre-Brion, and C. M. Moser, Phys. Rev. **124**, 1124 (1961).

[10] R. K. Nesbet, Phys. Rev. **118**, 681 (1960).

[11] A. J. Freeman and R. E. Watson, Phys. Rev. **127**, 2058 (1962).

[12] A. W. Weiss, Phys. Rev. **122**, 1826 (1961).

[13] C. C. J. Roothaan, L. M. Sachs, and A. W. Weiss, Rev. Mod. Phys. **32**, 186 (1960).

series. The results for these two-electron systems are of some interest by themselves since, although accurate values are available for He and Li^+, a complete study has not been made for larger values of Z.

II. EXPECTATION VALUES CONSIDERED AND COMPUTATIONAL DETAILS

The operators we consider are the one-electron operators $\sum r_i^N$ ($N=2$, -1, 2, and 4), $\sum \delta^3(\mathbf{r}_i)$, and $\sum p_i^2$ and the two-electron operators $\sum_{i>j}(\mathbf{r}_i\cdot\mathbf{r}_j)$, $\sum_{i>j}(\mathbf{p}_i\cdot\mathbf{p}_j)$, and $\sum_{i>j}\delta^3(\mathbf{r}_{ij})$, where $\mathbf{r}_i$ is the radius vector between the ith electron and the nucleus, $\mathbf{r}_{ij}$ the vector between the ith and jth electrons, and $\mathbf{p}_i$ the momentum of the ith electron. The radial moments were chosen to gauge the effects of the correlation on the spatial distribution of the electron cloud described by the wave functions. The operators $\sum r_i^2$, $\sum_{i>j}\mathbf{r}_i\cdot\mathbf{r}_j$, $\sum p_i^2$, $\sum_{i>j}(\mathbf{p}_i\cdot\mathbf{p}_j)$, and $\sum\delta^3(\mathbf{r}_i)$ have special significance since the minus first, first, and second moments of the spectral distribution of oscillator strengths for transitions from the ground state are proportional to $\langle(\sum\mathbf{r}_i)^2\rangle$, $\langle(\sum\mathbf{p}_i)^2\rangle$, and $\langle\sum\delta^3(\mathbf{r}_i)\rangle$, respectively. The deviations of expectation values such as $\langle\sum r_i^2\rangle$ from experimental determinations such as those mentioned for the rare gases in the previous sections can be interpreted as being due to the approximation ignoring the correlation factor $\langle\sum_{i>j}(\mathbf{r}_i\cdot\mathbf{r}_j)\rangle$. Similarly, the correlation term $\langle\sum_{i>j}(\mathbf{p}_i\cdot\mathbf{p}_j)\rangle$ is ignored in computing the mean squared momentum $\langle(\sum\mathbf{p}_i)^2\rangle$ using Hartree-Fock functions. The expectation value $\langle\sum_{i>j}\delta^3(\mathbf{r}_{ij})\rangle$ is a measure of the depth of the "hole" surrounding individual electrons due to correlation effects and the exclusion principle.[14] The expectation value $\langle\sum p_i^2\rangle$ provides a check on the computations since it must equal twice the total energy of the system due to the virial theorem. This equality was verified to at least four-place accuracy for all cases considered.

The details of the functional form of the configuration interaction wave functions are described in detail in Weiss' paper.[12] Briefly, he uses a linear combination of Slater determinants, the one-electron wave functions of each determinant being orbitals of the Slater type represented by

$$\psi_{nlm}=\frac{(2\zeta)^{n+1/2}}{[(2n)!]^{1/2}}r^{n-1}e^{-\zeta r}Y_{lm}(\theta,\phi)\,. \tag{1}$$

For wave functions of this form, the evaluation of expectation values such as those listed above for a two- or three-electron system reduces to evaluating linear combinations of expressions of the form:

$$\langle\psi_{n_1l_1m_1}(1)\psi_{n_2l_2m_2}(2)\psi_{n_3l_3m_3}(3)\,|O|\,\psi_{n_1'l_1'm_1'}(1)\psi_{n_2'l_2'm_2'}(2)\psi_{n_3'l_3'm_3'}(3)\rangle\,. \tag{2}$$

In the above expression, O is an arbitrary many-electron operator. For one-electron operators $O(1)$, the above form reduces immediately to the form

$$\langle\psi_{n_1l_1m_1}(1)|O(1)|\psi_{n_1'l_1'm_1'}(1)\rangle S_{n_2n_2'}S_{n_3n_3'}\,, \tag{3}$$

where the quantities $S_{n_2n_2'}$ represent "overlap" integrals of the form $\langle\psi_{n_2l_2m_2}|\psi_{n_2'l_2'm_2'}\rangle$. These overlap integrals vanish unless $l_2=l_2'$, $m_2=m_2'$ and can in each case be reduced to simple expressions involving r_α, r_α', ζ_α, and ζ_α'. For all of the operators considered except $\delta^3(\mathbf{r}_{ij})$, the whole expression (2) can be reduced to linear combinations of products of overlap integrals. For $\delta^3(\mathbf{r}_{ij})$ a similar reduction occurs. Thus, the process of evaluating such expectation values reduces to a straightforward but tedious job of evaluating linear combinations of products of simple functions. Since the number of configurations is large (Weiss uses 35 for two- and 45 for three-electron systems) such calculations are only practical when a large-scale computer is available. However, since only direct evaluation of given expressions is involved, the amount of computing time required is quite small.[15]

For the Hartree-Fock wave functions the evaluation of expectation values for one-electron operators is a simple straightforward task. The only nonzero two-electron operator we consider is $\sum_{i>j}\delta^3(\mathbf{r}_{ij})$. While an analytic evaluation of this is possible we found it easier to evaluate the operator by direct numerical integration of the expression

$$\langle\sum_{i>j}\delta^3(\mathbf{r}_{ij})\rangle=\int d\tau_1 u_{1s}^4(\mathbf{r}_1)+\int d\tau_1 u_{1s}^2(\mathbf{r}_1)u_{2s}^2(\mathbf{r}_1)\,,$$

where $u_{1s}(\mathbf{r}_1)$ and $u_{2s}(\mathbf{r}_1)$ are the wave functions of the $1s$ and $2s$ electrons, respectively. The two integrals represent the relative contributions to the expectation value from the overlap of the core electrons and from the overlap of the valence electron and the core electron of antiparallel spins, respectively.

III. RESULTS FOR TWO-ELECTRON SYSTEMS

In Table I we present the ground-state expectation values for two-electron ^1S systems with $Z=2$, 3, 4, 5, and 8. Also shown in the table are "exact" values for Li^+ and He as computed by Pekeris[1] and Kinoshita[2] and approximate values computed from perturbation expansions given by Cohen and Dalgarno[16] and by Dalgarno and Stewart.[17] The table shows that for $Z=2$ all expectation values except $\langle\delta^3(\mathbf{r}_{12})\rangle$ agree with the "exact" values to better than 3 places. For $\langle\delta^3(\mathbf{r}_{12})\rangle$ the Weiss wave functions overestimate the value by about

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[14] This phenomenon is called the "Coulomb hole" when due to electrostatic repulsion and the "Fermi hole" when due to the vanishing of second-order density matrix elements for electrons of parallel spin. See P. O. Löwdin, in *Advances in Chemical Physics* (Interscience Publishers, Inc., New York, 1959), Vol. II.

[15] For example, the computation of all nine expectation values considered for a 45-configuration wave function of given Z required less than 2 min on the IBM 7090.

[16] M. Cohen and A. Dalgarno, Proc. Roy. Soc. (London) **A261**, 565 (1961).

[17] A. Dalgarno and A. L. Stewart, Proc. Roy. Soc. (London) **A247**, 245 (1958).

TABLE I. Two-electron expectation values.

Operator \ Z		2	3	4	5	8
r_1^{-2}	[a]	6.0187	14.930	27.843	44.759	119.51
	[b]	5.8290	14.744	27.659	44.574	119.32
	[c]	6.0174				
r_1^{-1}	[a]	1.6882	2.6880	3.6878	4.6878	7.6878
	[b]	1.6875	2.6875	3.6875	4.6875	7.6875
	[c]	1.6883				
r_1^2	[a]	1.1922	0.4461	0.2320	0.1419	0.0520
	[b]	1.049	0.4130	0.2249	0.1391	0.0515
	[c]	1.1935	0.4463			
r_1^4	[a]	3.9379	0.5276	0.1402	0.0520	0.0069
$\mathbf{r}_1\cdot\mathbf{r}_2$	[a]	−0.06455	−0.0172	−0.00686	−0.00340	−0.00079
	[b]	−0.0624	−0.0170	−0.00686	−0.00342	−0.00075
	[c]	−0.06474				
$\mathbf{p}_1\cdot\mathbf{p}_2$	[a]	0.1597	0.2898	0.4213	0.5533	0.9520
	[c]	0.1591	0.2890	0.4205	0.5528	0.9510
$\delta^3(\mathbf{r}_1)$	[a]	1.8156	6.8626	17.217	34.789	149.90
	[b]	1.696	6.681	16.971	34.476	149.37
	[c]	1.8104	6.8520	17.198	34.759	149.83
$\delta^3(\mathbf{r}_{12})$	[a]	0.1319	0.6127	1.6858	3.5903	16.675
	[b]	0.106	0.587	1.671	3.597	16.813
	[c]	0.1064	0.5337	1.5230	3.3126	15.871
$-E$ (H.F.)	[a]	2.9032	7.2792	13.6548	22.030	59.1557
	[b]	2.8617	7.2364	13.6113	21.986	59.1111
	[c]	2.9037	7.2799	13.6556	22.031	59.1566

[a] This paper.
[b] Empirical estimates from Refs. 16 and 17.
[c] "Exact" values from Refs. 1 and 2.

TABLE II. Expectation values for three-electron systems. Rows labeled 1*s* and 2*s* are Hartree-Fock (H.F.) contributions for single 1*s* and 2*s* electrons and rows labeled "Sum" are the total Hartree-Fock estimates. Rows labeled C.I. represent expectation values for the whole atom computed from Weiss' 45-configuration wave function.

Operator \ Z		3	4	5	8
Σr_i^{-2}	1*s*	14.913	27.766	44.637	119.24
	2*s*	0.435	1.450	2.982	10.61
	Sum	30.261	56.982	92.256	249.09
	C.I.	30.244	56.999	92.270	249.12
Σr_i^{-1}	1*s*	2.6885	3.6825	4.6806	7.6776
	2*s*	0.3454	0.6075	0.8633	1.6212
	Sum	5.7224	7.9725	10.2245	16.9764
	C.I.	5.7175	7.9728	10.2252	16.9781
Σr_i^2	1*s*	0.4456	0.2330	0.1427	0.0522
	2*s*	17.7140	6.0833	3.1263	0.9328
	Sum	18.6051	6.5494	3.4117	1.0372
	C.I.	18.3722	6.5314	3.4069	1.0371
Σr_i^4	1*s*	0.53	0.143	0.0530	0.0070
	2*s*	561.01	63.618	16.546	1.4477
	Sum	562.06	63.903	16.652	1.4616
	C.I.	545.80	63.706	16.636	1.4630
$\Sigma\delta^3(\mathbf{r}_i)$	1*s*	6.8307	17.1519	34.671	149.52
	2*s*	0.1660	0.8082	2.155	12.80
	Sum	13.8274	35.112	71.497	311.84
	C.I.	13.8661	35.1510	71.534	316.16
$\Sigma_{i>j}\delta^3(\mathbf{r}_{ij})$	1*s*	0.7682	1.9827	4.0729	17.9885
	1*s*–2*s*	0.0013	0.0106	0.0301	0.1955
	Sum	0.7695	1.9933	4.1030	18.1840
	C.I.	0.5916	1.6582	3.5396	16.5396
$\Sigma_{i>j}(\mathbf{r}_i\cdot\mathbf{r}_j)$	C.I.	−0.1834	−0.0835	−0.0426	−0.0101
$\Sigma_{i>j}(\mathbf{p}_i\cdot\mathbf{p}_j)$	C.I.	0.9056	1.3634	1.8263	3.2182
$\Sigma p_i^2/2$	C.I.	7.4765	14.3218	23.4226	64.2343
$-E$ (H.F.)		7.4327	14.2774	23.3760	64.1780
$-E$ (C.I.)		7.4771	14.3235	23.4231	64.2266
$-E$ (Exact)		7.4781	14.3248	23.4248	64.2292

25% for $Z=2$ and by about 5% for $Z=8$. The close agreement between our values and the empirical estimates of Dalgarno *et al.*[16,17] (which, for one-electron operators, are merely estimates of the Hartree-Fock values) should be noted. For most practical purposes these estimates lie close enough to our more accurate values to eliminate the need for further computations of this type.

IV. RESULTS FOR THREE-ELECTRON SYSTEMS

The expectation values for three-electron ^2S systems are given in Table II. Also shown are individual contributions by 1*s* and 2*s* electrons to the one-electron expectation values computed from Hartree-Fock functions.[13] A comparison of the results for one-electron operators obtained from both calculations shows that correlation has very little effect on the spatial distribution of the electronic charge cloud. The largest deviation between the Hartree-Fock and the configuration interaction results occurs for $Z=3$ for $\sum r_i^2$ and $\sum r_i^4$ and amounts to a difference of only 2 or 3%. As with two-electron systems, the agreement is better for higher values of Z.[18] The over-all agreement is about what one would expect. The addition of configuration interaction lowers the total energy of the system by about 0.04 atomic unit (a.u.) for $Z=3$ from the Hartree-Fock value. The decrease in energy is accompanied by a slight contraction of the charge cloud. The portion of the charge cloud close to the nucleus remains practically unaffected by the electron correlation.

As mentioned previously, the quantities $\langle(\sum\mathbf{r}_i)^2\rangle$ and $\langle(\sum\mathbf{p}_i)^2\rangle$ are related to moments of the spectral distribution of oscillator strengths. We can obtain an estimate of the effect of correlation on these quantities by studying the ratios $\langle(\sum\mathbf{r}_i)^2\rangle_{\text{C.I.}}/\langle(\sum\mathbf{r}_i)^2\rangle_{\text{H.F.}}$ and $\langle(\sum\mathbf{p}_i)^2\rangle_{\text{C.I.}}/\langle(\sum\mathbf{p}_i)^2\rangle_{\text{H.F.}}$. The ratios include two effects of correlation. The first is due to the slight changes in $\langle\sum r_i^2\rangle$ and $\langle\sum p_i^2\rangle$. The second and dominant effect is due to the cross terms $\langle\sum_{i>j}\mathbf{r}_i\cdot\mathbf{r}_j\rangle$ and $\langle\sum_{i>j}(\mathbf{p}_i\cdot\mathbf{p}_j)\rangle$ which vanish in the Hartree-Fock approximation. In Table III we list these ratios. We have used $-2E$ for the Hartree-Fock values of $\langle\sum p_i^2\rangle$ since the virial theorem is satisfied by a Hartree-Fock calculation. Also shown in the table are the mean squared momentum

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[18] For large Z all expectation values must approach the values for hydrogen-like systems, so this behavior is quite general.

TABLE III. Ratios of expectation values computed using configuration-interaction wave functions to those computed using Hartree-Fock wave functions.

Operator \ Z	3	4	5	8
$(\sum \mathbf{r}_i)^2$ (3-electron)	0.968	0.971	0.973	0.980
$(\sum \mathbf{p}_i)^2$ (3-electron)	1.128	1.098	1.080	1.050
$(\sum \mathbf{p}_i)^2$ (2-electron)	1.046	1.034	1.027	1.016
$\sum_{i>j}\delta^3(\mathbf{r}_{ij})$ (3-electron)	0.768	0.827	0.856	0.899

ratios $\langle(\sum\mathbf{p}_i)^2\rangle_{\text{exact}}/\langle(\sum\mathbf{p}_i)^2\rangle_{\text{H.F.}}$ for two-electron systems, where $\langle(\sum_i\mathbf{p}_i)^2\rangle_{\text{exact}}$ were computed using the "exact" values of Table I and the Hartree-Fock values were obtained from Ref. 13.

Table III illustrates the importance of correlation in evaluating expectation values of this kind. Notice that the correlation causes a much larger change in $\langle(\sum \mathbf{p}_i)^2\rangle$ (about 13% for Li) than one would expect from the change in $\langle(\sum \mathbf{p}_i)^2\rangle$ of the ion core (which is less than 5% for Li^+). The percentage changes for $\langle(\sum \mathbf{p}_i)^2\rangle$ are much larger than the changes for $\langle(\sum \mathbf{r}_i)^2\rangle$ when correlation is included as is the case for two-electron systems.

Ratios of the expectation values for $\sum_{i>j}\delta^3(\mathbf{r}_{ij})$ are also shown in Table III. The decrease of this value when configuration interaction is introduced corresponds to the correlation increasing the depth of the "hole" mentioned previously. However, our results for two-electron systems indicate that wave functions of this type do not predict $\langle\sum_{i>j}\delta^3(\mathbf{r}_{ij})\rangle$ very accurately. For helium, for example, our result of 0.132 lies about midway between the Hartree value of[19] 0.188 and the "exact" value 0.106. This would seem to indicate that our configuration interaction values are still about 10–40% above the true values, the accuracy increasing with Z.

In order to estimate the accuracy of the values given in Table II, all expectation values for $Z=3$ were computed using 35- and 41-term wave functions.[20] The results are shown in Table IV. The only value which shows substantial deviations is $\langle\sum_{i>j}\mathbf{r}_i\cdot\mathbf{r}_j\rangle$. However, the fluctuations of this quantity are about the same size as those of $\langle\sum r_i^2\rangle$. Note also that $\langle\sum r_i^2\rangle$ and $\langle\sum r_i^4\rangle$ become larger as the number of configurations is increased, even though the total energy is lowered.

TABLE IV. Expectation values for 35-, 41-, and 45-term wave functions of Li.

Operator	35 terms	41 terms	45 terms
$\sum r_i^{-2}$	30.317	30.247	30.244
$\sum r_i^{-1}$	5.7360	5.7171	5.7175
$\sum r_i^2$	17.6299	18.4455	18.3722
$\sum r_i^4$	511.341	549.618	545.801
$\delta^3(\mathbf{r}_i)$	13.8980	13.8685	13.8661
$\sum_{i>j}\delta^3(\mathbf{r}_{ij})$	0.6093	0.5911	0.5916
$\sum_{i>j}(\mathbf{r}_i\cdot\mathbf{r}_j)$	−0.0484	−0.0886	−0.1834
$\sum_{i>j}(\mathbf{p}_i\cdot\mathbf{p}_j)$	0.8872	0.8739	0.9056
$-E$	7.4740	7.4762	7.4771

V. FINAL REMARKS

The results of the preceding section show that correlation may produce large changes in the expectation values of three-electron systems even though the change in total energy is extremely small. While the same is true for two-electron systems, the variations appear to be less extreme in that case. Consequently, estimates of the effects of correlation in many electron systems based upon our knowledge of analogous effects in two-electron systems are likely to be substantially in error.

The accuracy of the values reported here is difficult to estimate. While Table IV shows that most of the expectation values we compute appear to remain more or less stationary, this should not be interpreted to mean that these values are correct. In particular, the value of $\langle\sum_{i>j}\delta(\mathbf{r}_{ij})\rangle$ remains stationary to about 3% in going from 35 to 45 terms in the wave function, yet from our two-electron results we expect even the 45-term value to be a considerable overestimate of this quantity.

ACKNOWLEDGMENT

The authors gratefully acknowledge the aid of Dr. A. W. Weiss in carrying out the computations described in this paper.

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[19] H. Bethe and E. E. Salpeter, *Quantum Mechanics of One- and Two-Electron Systems* (Academic Press Inc., New York, 1957), p. 164.

[20] These wave functions are not tabulated by Weiss. However, the total energy corresponding to this calculation is given in Table VI of his paper.