1973

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Recommended Citation

Blanchard, P. and Drake, Gordon W. F.. (1973). Energies and Z-expansion coefficients for the D states in the helium sequence. *Journal of Physics B: Atomic and Molecular Physics*, 6 (12), 2495-2503.
https://scholar.uwindsor.ca/physicspub/47

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1973 J. Phys. B: At. Mol. Phys. 6 2495

(http://iopscience.iop.org/0022-3700/6/12/015)

J. Phys. B: Atom. Molec. Phys., Vol. 6, December 1973. Printed in Great Britain. © 1973

Energies and Z-expansion coefficients for the D states in the helium sequence

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Received 10 July 1973

Abstract. Non-relativistic variational energies for the $1s3d(^{1,3}D)$ states of the helium isoelectronic sequence are calculated with a 50-term correlated basis set for $Z = 2-10$, where Z is the nuclear charge, and the corresponding Z-expansion coefficients found through sixth order by fitting the energies to a series in Z^{-1}. A variational-perturbation calculation of these coefficients through eleventh order (with the same basis set) is presented for comparison, and agreement is satisfactory. The 3d energies obtained by summing the Z-expansion perturbation series are found to yield excellent approximations to the variational values. The calculations are extended to the $1s4d(^{1,3}D)$ states to furnish variational energies for neutral helium and perturbation energies for the higher sequence members. All of these results are the most accurate yet reported.

1. Introduction

The present work is an off-shoot of an earlier, unpublished study of the $1s3d(^{1,3}D)$ energies in the helium sequence undertaken to provide estimates of the coefficients E_k in the Z-expansion series

$$E(Z) = Z^2E_0 + ZE_1 + E_2 + Z^{-1}E_3 + \dots \tag{1}$$

where $E(Z)$ is the non-relativistic total energy and Z is the nuclear charge. Here, E_0 is trivial and E_1 may be found exactly (Layzer 1959). The correlated, two-electron coefficients $E_2(3^{1,3}D)$ are required in the calculation of three-electron $1s^23d$ energies through second order in Z^{-1}, and preliminary values of E_2 furnished by our previous work were used in this connection by Horak *et al* (1969). We are now able to report more accurate and extensive values of the energies and E_k coefficients for the 1s3d states, together with results for the 1s4d states.

The higher-order Z-expansion coefficients may be found in two ways. In the first method (that used in our earlier work), calculated energies $E(Z)$ are fitted to a series of the form (1) through the differencing technique of Scherr *et al* (1962). To obtain the coefficients to high order, however, one requires $E(Z)$ values known to many significant figures, and the resulting E_k are good approximations to the exact non-relativistic values only if the energies are also highly accurate. Previously reported 1s3d energies (Green *et al* 1965, Weiss 1967, Brown 1968) are inadequate in one or both respects. We have obtained improved 3d energies through $Z = 10$ by direct variational calculations with a 50-term correlated basis set and are able to estimate the coefficients E_2–E_6 by the series-fit method.

The E_k may also be calculated directly to high order by the variation-perturbation method of Scherr and Knight (1963) and Dalgarno and Drake (1969). The latter authors obtained the 3d coefficients E_2–E_5 using a 40-term basis set. With the 50-term basis we have determined the perturbation-theory $E_k(3^{1,3}\mathrm{D})$ more accurately through $k = 11$ and find satisfactory agreement with the series-fit values. Although the latter more closely approximate the exact non-relativistic values, a summation of series (1) with the E_k furnished by perturbation theory yields strikingly good approximations to the variational energies.

Encouraged by this finding, we have performed similar but less extensive calculations for the 1s4d(^{1,3}D) states. Variational values of $E(Z)$ are presented for helium only; for $Z \geqslant 3$, we list approximations to $E(Z)$ obtained by summing the Z-expansion series (1) with the E_k furnished through $k = 9$ by perturbation theory. These results are slightly more accurate than those previously reported (Green *et al* 1965, Brown and Cortez 1971).

2. Calculations

The correlated basis set is of the Hylleraas type described by Drake *et al* (1969), in which the basis functions are symmetrized combinations of terms of the form $\mathrm{e}^{-\alpha r_1 - \beta r_2} r_1^m r_2^n r_{12}^k$ multiplied by angular factors. Here r_1 and r_2 are the radial coordinates of the two electrons, r_{12} is the interelectronic separation, and α, β are non-linear variational parameters. In the direct variational calculations, we found that departures of α from the value Z (corresponding to a hydrogen-like 1s core) had very little effect upon the total energy minimum and α was set equal to Z here. Much effort was expended, by trial and error, in selecting those basis functions that yielded the lowest 3d energies for optimum choices of β. The 50-term set adopted contains 36 functions with sd angular-momentum dependence, the remainder being pp′ states. For best results, we found it necessary to include many sd functions involving high powers of r_2.

In the usual approach, one first orthonormalizes the basis set and then diagonalizes the hamiltonian matrix to obtain the complete spectrum of eigenvalues. As only a single eigenvalue is desired here, we have employed a variation of the 'power method' which yields the eigenvalue closest to any initial guess both rapidly and accurately.

Energies are given in atomic units (au) throughout.

3. Results and discussion

3.1. *The 3d states*

We first treated the case of neutral helium to investigate the convergence of the 3d variational energy eigenvalues with increasing basis set size and the results appear in table 1. The 20-, 30-, and 40-term subsets of the full 50-term basis are those found to yield the lowest energies for the indicated numbers of terms, with the parameter β optimized for each. The experimental results are taken from a recent compilation of He term values by Martin (1973) and suggest an absolute accuracy of a few parts in 10^8 for the 50-term calculation. The 3^1D energies converge more rapidly, but the 3^3D energies are less sensitive to the choice of basis and appear to be more accurate. Our 50-term He I values are 6×10^{-6} au lower than the best configuration-interaction energies (Green *et al*

Table 1. Convergence of the He I variational energies with increasing basis set size (in au)

Number of terms	$E(3^1\mathrm{D})$	$E(3^3\mathrm{D})$
20	−2·055617617	−2·055634878
30	−2·055619734	−2·055635661
40	−2·055620049	−2·055635881
50	−2·055620115	−2·055635968
exp.†	−2·0556209	−2·0556364

† Martin (1973).

1965, Brown 1968) and agree with the six figures quoted by Weiss (1967) for the results of a 52-term Hylleraas calculation.

Table 2 presents the 50-term $3\mathrm{d}(^{1,3}\mathrm{D})$ variational energies for the helium sequence through $Z = 10$. The calculations were extended to 12 or 13 significant figures to permit a determination of the corresponding Z-expansion coefficients through E_6. This level of numerical accuracy required a four-figure optimization of β, but the observation that the optimum values follow the series expansion $\beta/Z = \beta_0+\beta_1/Z+\beta_2/Z^2+\ldots$ (expected from simple scaling arguments) led quickly to nearly-exact estimates for the higher sequence members. For $Z \geqslant 3$, the most accurate energies previously reported are those of Brown (1968), who also presents a comparison with observation. As the observed energies contain relativistic contributions which increase rapidly with Z, the appropriate comparison is that between different non-relativistic calculations. Our $3^1\mathrm{D}$ energies are lower than the corresponding Brown (1968) values by amounts ranging from 1×10^{-5} au ($Z = 3$) to 5×10^{-5} au ($Z = 10$). The best previous $3^3\mathrm{D}$ values are those of Weiss (1967), who gives results to five decimal places; our $3^3\mathrm{D}$ energies are in agreement with these through $Z = 7$ but lower by 1×10^{-5} au for $Z \geqslant 8$.

In the first columns of tables 3 and 4 we list the higher-order E_k coefficients found by fitting the $E(Z)$ values of table 2 to a series of the form (1). Here, $E_0(3^{1,3}\mathrm{D}) = -5/9$ au and

$$E_1(3^1\mathrm{D}) = 0{\cdot}111\,270\,141\,6\ \mathrm{au}$$

$$E_1(3^3\mathrm{D}) = 0{\cdot}110\,775\,756\,8\ \mathrm{au}$$

Table 2. $1\mathrm{s}3\mathrm{d}(^{1,3}\mathrm{D})$ variational energies in the helium sequence (in au)

Z	$E(3^1\mathrm{D})$	$E(3^3\mathrm{D})$
2	−2·05562011467	−2·05563596801
3	−4·72238996527	−4·72252648764
4	−8·50021450157	−8·50058187867
5	−13·38909872662	−13·38977109501
6	−19·38905734362	−19·39008298339
7	−26·50010131501	−26·50151264274
8	−34·72223798011	−34·72405759390
9	−44·05547224610	−44·05771645075
10	−54·4998074641	−54·5024883784

Table 3. Z-expansion coefficients $E_k(3^1\mathrm{D})$ determined two ways (in au)

k	Variational energy series fit	Perturbation theory
2	−0·0574822	−0·05747078
3	0·006076	0·00597447
4	−0·00845	−0·00812158
5	0·0060	0·00556448
6	−0·002	−0·00231828
7		0·00081629
8		0·00014593
9		−0·00066468
10		0·00074237
11		−0·00071843

Table 4. Z-expansion coefficients $E_k(3^3\mathrm{D})$ determined two ways (in au)

k	Variational energy series fit	Perturbation theory
2	−0·0546193	−0·05461705
3	−0·000713	−0·00073180
4	0·00002	0·00007374
5	−0·0000	−0·00008786
6	0·0001	0·00017709
7		0·00006971
8		−0·00029496
9		0·00009888
10		0·00022185
11		0·00005668

(Sanders and Scherr 1965). We determined the E_k to higher order by applying a modification of the differencing procedure of Scherr *et al* (1962) as described in Appendix A. The error in the E_k arising from uncertainties in the series fit is perhaps one unit (but at most two units) in the last digit quoted. To this accuracy, our second-order coefficients

$$E_2(3^1\mathrm{D}) = -0{\cdot}057\,482\,2\ \mathrm{au} \tag{2}$$

$$E_2(3^3\mathrm{D}) = -0{\cdot}054\,619\,3\ \mathrm{au} \tag{3}$$

are upper bounds to the exact non-relativistic values. These are the best E_2 estimates available and replace our preliminary results used in connection with the $1s^2 3d$ states of the lithium sequence (Horak *et al* 1969; see this reference also for a summary of earlier estimates of the E_2 coefficients). It appears that $E_5(3^3\mathrm{D}) < 0$, with $|E_5(3^3\mathrm{D})| < 5\times 10^{-15}$ au, but as the data do not allow a more exact determination we list this value as zero to four decimal places.

In the second columns of tables 3 and 4 we present the higher-order $E_k(3^{1,3}\mathrm{D})$ coefficients calculated from variational-perturbation theory with the 50-term basis set used before. The values for k = 2–5 supersede those obtained by Dalgarno and Drake

(1969), who describe the procedure. There are no other estimates of these coefficients for $k \geqslant 7$. We consider the overall agreement between the two sets of coefficients satisfactory; part of the discrepancy in the cases of the 3^3D coefficients E_4 and E_5 arises from their small magnitudes, a slight absolute difference leading here to a large fractional change in value. However, in the perturbation calculation one must set $\alpha = 1$ and $\beta = 1/3$ in order to reproduce the correct values of E_0 and E_1, so that the additional accuracy to be gained by a variation of β is forfeited. Hence for $k \geqslant 2$ the perturbation-theory E_k do not approximate the exact non-relativistic values so well as the series-fit E_k, as is clear from the higher E_2 coefficients.

Where comparisons may be made, we note that the perturbation E_k are systematically higher than the series-fit values for even k but lower for odd k. As a result, the 3d perturbation energies are better approximations to the corresponding variational energies than the comparisons of tables 3 and 4 suggest. We do not tabulate these, as the variational results are to be preferred; further, the perturbation energies are not necessarily upper bounds to the exact values except for sufficiently large Z. For $Z = 2$, the perturbation-series partial sums through $k = 11$ have not yet converged, and we can verify agreement with the He I variational energies only to five (3^1D) and six (3^3D) decimals. For $Z \geqslant 3$ the convergence is satisfactory. The perturbation energies are lower than the table 2 values by 4×10^{-7} au and 1×10^{-7} au for the $3^{1,3}$D states of Li II and by 5×10^{-8} au for the 3^3D state of Be III. In all other cases the perturbation results lie above the variational values by amounts increasing with Z from 1×10^{-7} au to 4×10^{-6} au for the 3^1D states and from 1×10^{-7} au to 8×10^{-7} au for the 3^3D states. Thus the 3d perturbation energies are at least as accurate as those of previous calculations and agree with the variational values within the estimated absolute error of the latter.

3.2. *The 4d states*

Here the same 50-term basis set was employed; however, as this set was chosen specifically to optimize the 3d variational energies, comparable accuracy cannot be expected in the 4d case. Our direct variational calculation for He I yields the values

$$E(4^1\mathrm{D}) = -2{\cdot}031\,277\,2 \text{ au} \tag{4}$$

$$E(4^3\mathrm{D}) = -2{\cdot}031\,287\,3 \text{ au} \tag{5}$$

compared to the best previous estimates of $-2{\cdot}031\,277$ au, $-2{\cdot}031\,286$ au (Green *et al* 1965) and the experimental values $-2{\cdot}031\,279\,9$ au, $-2{\cdot}031\,288\,9$ au (Martin 1973) for the $4^{1,3}$D states, respectively. In the Z-expansion series (1) we now have $E_0 = -17/32$ au and

$$E_1(4^1\mathrm{D}) = 0{\cdot}062\,582\,034 \text{ au}$$

$$E_1(4^3\mathrm{D}) = 0{\cdot}062\,318\,318 \text{ au}$$

(Sanders and Scherr 1965). The higher-order $E_k(4^{1,3}\mathrm{D})$ obtained from the perturbation procedure (with $\alpha = 1$, $\beta = 1/4$) are listed through $k = 9$ in table 5. There are no previous estimates of these coefficients. The Z-expansion series converges more slowly here than in the 3d case and for He I we can verify agreement with the values (4) and (5) only within one unit in the fifth decimal place. The 4d perturbation energies for $Z \geqslant 3$ are given in table 6. Configuration-interaction energies for this sequence have been calculated by Brown and Cortez (1971) who also present a comparison with observation. We obtain agreement with the Li II 4^1D energy of Brown and Cortez (1971), but in all

Table 5. Z-expansion coefficients $E_k(4^{1,3}D)$ from perturbation theory (in au)

k	$E_k(4^1D)$	$E_k(4^3D)$
2	−0·03212168	−0·03067137
3	0·00244471	−0·00066606
4	−0·00263634	0·00043907
5	0·00064430	−0·00034391
6	0·00102581	−0·00039242
7	−0·00153298	0·00182846
8	0·00155331	−0·00066390
9	−0·00114809	−0·00155556

Table 6. $1s4d(^{1,3}D)$ perturbation energies in the helium sequence (in au)

Z	$E(4^1D)$	$E(4^3D)$
3	−4·625072	−4·625151
4	−8·281334	−8·281543
5	−13·000072	−13·000448
6	−18·781292	−18·781862
7	−25·625000	−25·625780
8	−33·531200	−33·532202
9	−42·499893	−42·501126
10	−52·531082	−52·532551

other cases the energies of table 6 are lower by amounts ranging from 1×10^{-6} au to 2×10^{-6} au for the 4^1D states and from 1×10^{-6} au to 4×10^{-6} au for the 4^3D states.

3.3. *The case Z = 1*

We obtain a useful check on the Z-expansion coefficients by summing the series (1) with $Z = 1$ to find the d-state energies of the H^- ion. As it is very unlikely that these states are bound, we should obtain $-0{\cdot}5$ au in all cases (the energy of a 1s hydrogen atom and a free electron). Convergence is poor, but the partial sums fluctuate with decreasing amplitude about the expected value. For the 3d states, we find convergence to

$$-0{\cdot}5000 \pm 0{\cdot}0003 \text{ au}$$

with the perturbation-theory E_k and to $-0{\cdot}500$ au with the less extensive series-fit E_k. For the 4d states, with the E_k of table 5, we find the value $-0{\cdot}500 \pm 0{\cdot}001$ au. A similar, oscillatory approach to $-0{\cdot}5$ au has been noted for $Z = 1$ by Sanders and Scherr (1969) in the $2^{1,3}P$ cases in their perturbation study of helium-sequence s and p states.

3.4. *Further remarks on the 3d states*

We may draw tentative conclusions as to the exact nonrelativistic $E_k(3^{1,3}D)$ values by comparing the 40-term perturbation values of Dalgarno and Drake (1969), the present 50-term perturbation values, and the E_k found from the variational-energy series fit; these results form a sequence of increasing absolute accuracy. The E_2 coefficients appear to be converging to values near those of equations (2) and (3), and the convergence of the $E_3(^1D)$ coefficient is also satisfactory. In general, however, our best estimates of the higher-order E_k do not yet provide adequate approximations to the exact values. For example, the $E_3(^3D)$ values furnished by the above calculations are $-0{\cdot}000\,76$, $-0{\cdot}000\,732$, and $-0{\cdot}000\,713$ au, respectively, exhibiting only one-digit convergence. The convergence of the small-magnitude 3^3D coefficients E_4 and E_5 is even worse and precludes any exact-value estimates. It seems clear that even more elaborate calculations than those presented here are required to determine the higher-order E_k to acceptable absolute accuracy, although the improvements in total energy would be expected to be slight.

4. Conclusions

Because of its accuracy and economy, the perturbation procedure of Dalgarno and Drake (1969) appears to be worthy of further refinement and application; a minimal value of E_2 could serve here as a criterion for the choice of basis functions. As convergence is apt to be unsatisfactory for $Z = 2$, however, accurate variational results for neutral helium will continue to be of interest.

Acknowledgments

This research has been supported in part by the United States Air Force under AFOSR Grant 71-2132 and in part by the National Research Council of Canada. We wish to thank the Tufts University Computation Center staff for helpful discussions concerning the Z-expansion analysis of the 3d variational energies carried out in double precision (16 significant figures) on the Decsystem 10 computer.

Appendix A. The differing technique

We describe in this appendix a modification of the differencing technique of Scherr *et al* (1962) used to obtain the higher order energy coefficients from the variational eigenvalues. After subtracting the zero- and first-order contributions, which are known exactly, the eigenvalues are expanded in a series of the form

$$A(Z) = \sum_{k=0}^{\infty} a_k Z^{-k} \tag{A.1}$$

with $a_0 = E_2$ etc. Suppose that $A(Z)$ is known for several values of its argument

$$Z = Z_0, Z_0+1, \dots, Z_0+N.$$

Then the nth order difference function $A_n(Z)$ is defined by

$$A_n(Z) = \frac{1}{n!}\Delta^n(Z^n A(Z)) \tag{A.2}$$

where Δ^n is the nth order differencing operator defined by

$$\begin{aligned} \Delta^n f(Z) &= \Delta^{n-1} f(Z+1) - \Delta^{n-1} f(Z) \\ \Delta^0 f(Z) &= f(Z) \end{aligned} \tag{A.3}$$

for an arbitrary function $f(Z)$. It can be shown that

$$A_n(Z) = a_0 + \sum_{k=n+1}^{\infty} a_k C_{nk}(Z) \tag{A.4}$$

where

$$C_{nk}(Z) = \frac{1}{n!}\Delta^n(Z^{n-k}) \qquad (k \geqslant n+1). \tag{A.5}$$

Since $C_{nk}(Z)$ is $O(Z^{-k})$ for large $Z(k \geqslant n+1)$, then

$$A_n(Z) = a_0 + O(Z^{-n-1}) \qquad \text{for large } Z. \tag{A.6}$$

For $n = 0$ we recover the original series $A(Z)$, but for $n \geqslant 1$ the contaminations due to a_1 through a_n have been removed. Thus the sequence $A_1(Z)$, $A_2(Z)$, ... provides in principle a sequence of increasingly better approximations to a_0, at least for large Z. A practical limit on the accuracy attainable is set by the value of N (which limits n) and by the number of significant figures in the $A(Z)$-values being differenced (which limits the accuracy of the calculated values of A_n for large Z).

In the 'standard procedure' of Scherr *et al* (1962), one differences first the values $A(Z)$ to find a_0, then the values $Z(A(Z)-a_0)$ to find a_1, and so on. Experience shows that this procedure leads to accurate values for the first few coefficients a_k when their magnitudes decrease steadily with k, and particularly when they are all of the same sign. When such is not the case, however, the initial approximations $A_n(Z)$ to a_0 converge more slowly, and a_0 is not so well determined; at the same time, the values obtained for the higher-order coefficients become markedly sensitive to the a_0 value adopted, so that these are even less reliable. (We remark that the best value of a_0 is not necessarily that which yields the most concordant estimates of a_1. The influence of higher-order terms may conspire with inaccuracies in the data to lead one into a polynomial approximation to $A(Z)$ instead of an independent estimate of the higher-order coefficients.)

To avoid this difficulty we formulate an 'alternate procedure' which yields estimates of the higher-order coefficients directly from the data when such values are known to sufficient numbers of significant figures. For $1 \leqslant n \leqslant N$, we note that the quantities

$$B_n(Z) = \frac{(-)^n}{n}\left(\prod_{j=0}^{n}(Z+j)\right)[A_{n-1}(Z+1) - A_{n-1}(Z)] \tag{A.7}$$

may be calculated from the known $A_n(Z)$ values of equation (A.2). On the other hand, it can be shown that

$$B_n(Z) = a_n + (-)^n\left(\prod_{j=0}^{n}(Z+j)\right)\sum_{k=n+1}^{\infty} C_{n,k+1}(Z)a_k \tag{A.8}$$

and

$$B_n(Z) = a_n + O(Z^{-1}) \qquad \text{for large } Z. \tag{A.9}$$

Thus the $B_n(Z)$ provide approximations to a_n directly. Further, for large Z, the deviation of a_n from $B_n(Z)$ becomes a series in Z^{-1} so that the values $B_n(Z)$ may themselves be differenced to yield better approximations to a_n, at least for large Z. A variant of this alternate procedure provides a consistency check on any coefficient a_n (and sometimes a better value) if an approximate value a'_{n+1} for a_{n+1} can be first found directly. Then the bulk of the effect of a_{n+1} upon $B_n(Z)$ may be subtracted off; from equation (A.8) we see that the terms on the left-hand side of the relation

$$B_n(Z)-(-)^n\left(\prod_{j=0}^{n}(Z+j)\right)C_{n,n+2}(Z)a'_{n+1}$$
$$= a_n+(-)^n\left(\prod_{j=0}^{n}(Z+j)\right)C_{n,n+2}(Z)(a_{n+1}-a'_{n+1})+\dots \quad \text{(A.10)}$$

provide better approximations to a_n than the $B_n(Z)$ alone. Greater accuracy is of course achieved if the main effects of two or more higher-order coefficients can be eliminated in this way. In practice, one compares estimates of the a_k from both the standard and alternate procedures to find the most precise values consistent with the accuracy of the data.

In applying the foregcing procedures to the variationally calculated 3d energies $E(Z)$ of the helium sequence $(2 \leqslant Z \leqslant 10)$, we subtract away the known contributions of E_0 and E_1 to form the series

$$A(Z) = E(Z)-Z^2E_0-ZE_1 = E_2+Z^{-1}E_3+Z^{-2}E_4+\dots$$

putting $a_k = E_{k+2}$ with $Z_0 = 2$, $N = 8$. Scherr *et al* (1962) have shown that an analysis in powers of $(Z+\sigma)^{-1}$ where $\sigma = -E_1/2E_0$ can be expected to give more accurate results than an analysis in Z^{-1}. In the present case, however, this approach produced no significant increase in accuracy, perhaps because of the small value of $\sigma(\sigma \sim 0{\cdot}1)$.

Note added in proof. The experimental 3d and 4d He I energies given here are based on the Martin (1973) He I term values and the non-relativistic 1s ionization energy of 2au for He II.

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