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LETTER TO THE EDITOR

1/Z expansion calculation of the Bethe logarithm for the ground state Lamb shift of two-electron ions

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Abstract. The leading two terms in the $1/Z$ expansion of the two-electron Bethe logarithm are calculated by the application of a new finite basis set method. The results can be expressed in the form

$$\ln \varepsilon (1s^2\ ^1S) = \ln[19.77(Z - 0.0063)^2].$$

The high-Z behaviour appears to differ from that of a previous variational calculation by Aashamar and Austvik.

Recent measurements of transition frequencies in high-Z two-electron ions (Davis and Marrus 1977, Berry *et al* 1978, 1980, O'Brien *et al* 1979, Armour *et al* 1979, Holt *et al* 1980, DeSerio *et al* 1981, Buchet *et al* 1981, Stamp *et al* 1981) are sufficiently accurate to be sensitive to the lowest-order Lamb shift type radiative corrections. The principal uncertainty in the theoretical calculation of the Lamb shift is the value of the two-electron Bethe logarithm defined by

$$\ln \varepsilon (nLS) = \frac{\Sigma_m\ |\langle\psi_0|t|\psi_m\rangle|^2 \ln(E_m - E_0)/(E_m - E_0)}{\Sigma_m\ |\langle\psi_0|t|\psi_m\rangle|^2/(E_m - E_0)} \tag{1}$$

in the dipole acceleration form, where ψ_0 (E_0) is the wavefunction (energy) for the nLS two-electron configuration, $t = Z \Sigma_i r_i/r_i^3$ and the sums are over all intermediate states. The direct evaluation of (1) by standard means is difficult because the dominant contribution comes from very highly excited states. Accurate calculations have been attempted for the ground state with Z up to 10 (Schwartz 1961; Aashamar and Austvik 1976) and for the low-lying excited states of He and Li$^+$ (Suh and Zaidi 1965, Ermolaev 1975). For the heavier two-electron ions, DeSerio *et al* (1981) suggest the *ad hoc* prescription

$$\ln(\varepsilon (1snl)/Ry) = \ln(\varepsilon (1s)/Ry) + n^{-3} \ln(\varepsilon (nl)/Ry) \tag{2}$$

where $\ln \varepsilon (nl)$ is the corresponding one-electron Bethe logarithm and Ry is the Rydberg constant. Although (2) appears to give reasonably good agreement with experiment for the 1s2s $^3S_1$–1s2p $^3P_0$ and $^3P_2$ transitions, it has no rigorous theoretical foundation.

The purpose of this letter is to report the first Z^{-1} expansion calculation of the Bethe logarithm for two-electron ions. The results for the ground state are compared

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with the direct variational calculations of Aashamar and Austvik (1976). We start by inserting the well known Z^{-1} expansions

$$\psi_n = \psi_n^0 + Z^{-1}\psi_n^1 + \ldots \tag{3}$$

$$E_n = Z^2(E_n^0 + Z^{-1}E_n^1 + \ldots) \tag{4}$$

into (1) to obtain

$$\ln \varepsilon (nLS) = A/B \tag{5}$$

with

$$A = Z^4[A_0 + A_1 Z^{-1} + 2(\ln Z)(B_0 + B_1 Z^{-1}) + \ldots] \tag{6}$$

$$B = Z^4(B_0 + B_1 Z^{-1} + \ldots). \tag{7}$$

Here, A and B are the numerator and denominator of (1) respectively. The expansion of B can easily be obtained from the identity (in atomic units)

$$B = 2\pi Z \langle \delta^3(r_1) + \delta^3(r_2) \rangle. \tag{8}$$

Thus $B_0 = 4$ and $B_1 = -2.670\,587$ for the ground state (Dalgarno and Stewart 1960, Aashamar 1970). Since A_0/B_0 is the Bethe logarithm $\ln \varepsilon (1s) = 2.984\,129 - \ln 2$ for hydrogen (in atomic units), this determines $A_0 = 9.1639$. Only A_1 requires significant additional calculation. It is given by

$$A_1 = \sum_m [2\langle \psi_0^0|t|\psi_m^0 \rangle \langle \psi_m^1|t|\psi_0^0 \rangle \ln \Delta E_m^0/\Delta E_m^0$$

$$+ 2\langle \psi_0^0|t|\psi_m^0 \rangle \langle \psi_m^0|t|\psi_0^1 \rangle \ln \Delta E_m^0/\Delta E_m^0$$

$$+ |\langle \psi_0^0|t|\psi_m^0 \rangle|^2 \Delta E_m^1 (1 - \ln \Delta E_m^0)/(\Delta E_m^0)^2] \tag{9}$$

where

$$|\psi_m^1 \rangle = \sum_{k \neq m} \frac{|\psi_k^0 \rangle \langle \psi_k^0|r_{12}^{-1}|\psi_m^0 \rangle}{E_m^0 - E_k^0} \tag{10}$$

$$E_m^1 = \langle \psi_m^0|r_{12}^{-1}|\psi_m^0 \rangle \tag{11}$$

and

$$\Delta E_m^j = E_m^j - E_0^j. \tag{12}$$

Both singly and doubly excited states contribute to the sums over m and k in (9) and (10). However, since t is a sum of one-electron operators, only s- and p-type one-electron excited states make non-vanishing contributions. We therefore introduce discrete variational one-electron basis sets of the form

$$\phi_n = \sum_{i=1}^{I} \sum_{j=1}^{J} c_{i,j}^{(n)} r^{i-1} \exp(-\alpha_j r) Y_l^m(\theta, \phi) \qquad n = 1, 2, \ldots, I \times J \tag{13}$$

for the s and p intermediate states. The linear variational coefficients $c_{i,j}^{(n)}$ are determined by the conditions

$$\langle \phi_m|H|\phi_n \rangle = \varepsilon_m \delta_{m,n} \tag{14}$$

$$\langle \phi_m|\phi_n \rangle = \delta_{m,n} \tag{15}$$

and the α_j form a geometric series according to

$$\alpha_j = \alpha_0 \beta^{j-1} \qquad j = 1, 2, \ldots, J. \tag{16}$$

The infinite sums in (9) and (10) are then replaced by finite sums over two-electron states constructed from antisymmetrised products of the form $(\phi_m(1)\phi_n(2) - \phi_m(2)\phi_n(1))/\sqrt{2}$.

The value of A_1 obtained from the basis set (13) depends not only on the total size of the basis set, $I \times J$, but also on the values of the non-linear parameters α_0 and β. It is therefore important that regions of stability exist with respect to variations in α_0 and β, and that A_1 converges to a definite answer as I or J is increased. We found that these conditions are met only if $J \geq 2$, and the $i = 1$ term in (13) is retained for the p-type basis states. The latter point follows from a consideration of oscillator strength sum rules (Dalgarno and Epstein 1969). The best convergence and stability were obtained with $J = 3$. The multiple exponentials thus introduced into the basis set provide sufficient flexibility to represent adequately both low- and high-energy states. It is then not necessary to treat the two energy regions separately, as done by Schwartz (1961) and Aashamar and Austvik (1976). As a test of the basis set, the hydrogenic Bethe logarithm was calculated by performing directly the summations in (1), with the results shown in table 1. The extrapolated result agrees with the exact value to within the accuracy of the calculation.

The results for A_1 are shown in table 2. The tabulated values correspond to a variational minimum with respect to α_0 and β. The values vary approximately linearly

Table 1. Test calculation for the one-electron Bethe logarithm using basis sets with $J = 3$.

$I \times J$	$\ln[\varepsilon(1s)/Ry]$	Error(%)
6	2.9290	−1.85
9	2.9619	−0.75
12	2.9726	−0.39
15	2.9775	−0.22
18	2.9800	−0.14
Extrapolated	2.9847 ± 0.0010	0.02 ± 0.03
Exact	2.984 129[a]	

[a] Klarsfeld and Maquet (1973).

Table 2. Values of the expansion coefficient A_1 for basis sets with $J = 3$ and optimised values for α_0 and β.

$I \times J$	α_0	β	A_1(au)
6	0.667	5.5	−5.999
9	0.571	8	−6.0972
12	0.500	10	−6.1330
15	0.444	13.5	−6.148 41
18	0.400	16	−6.155 51
21	0.364	20	−6.159 66
Extrapolated			−6.169 ± 0.001

with $1/I^{2.5}$ and extrapolate to

$$A_1 = -6.169 \pm 0.001 \text{ au}$$

as $I \to \infty$. Using expansions (6) and (7) in (5), the two-electron Bethe logarithm is then

$$\ln \frac{\varepsilon(1s^2\,{}^1S)}{Ry} = \frac{A_0}{B_0} + \ln 2 + 2\ln Z + \left(\frac{A_1 B_0 - A_0 B_1}{B_0^2}\right)Z^{-1} + O(Z^{-2})$$

$$= \ln(19.77 Z^2) - (0.0127 \pm 0.002)Z^{-1} + O(Z^{-2})$$

$$\simeq \ln[19.77(Z - 0.0063)^2]. \tag{17}$$

Table 3. Comparison of Bethe logarithms for the ground state of helium-like ions.

Z	Variational[a]	$1/Z$ expansion[b]	$Z^2\Delta$
2	4.37 ± 0.01	4.364	0.02 ± 0.04
3	5.21 ± 0.01	5.177	0.29 ± 0.09
4	5.777 ± 0.003	5.754	0.37 ± 0.05
5	6.214 ± 0.003	6.201	0.33 ± 0.08
6	6.565 ± 0.002	6.566	-0.02 ± 0.07
7	6.864 ± 0.002	6.874	-0.50 ± 0.10
8	7.115 ± 0.002	7.141	-1.70 ± 0.13
9	7.334 ± 0.002	7.377	-3.50 ± 0.16
10	7.525 ± 0.002	7.588	-6.31 ± 0.20

[a] Aashamar and Austvik (1976).
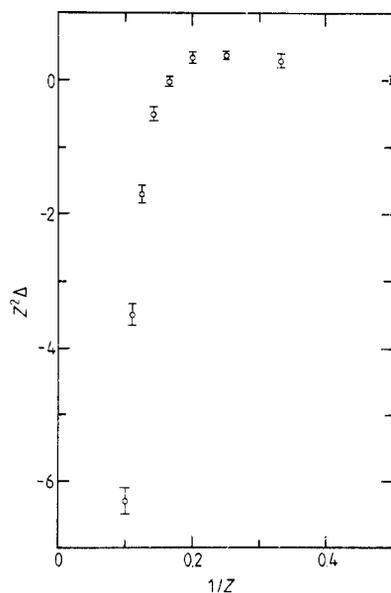[b] $\ln(\varepsilon/Ry) = \ln[19.77(Z - 0.0063)^2]$.

Figure 1. Comparison of results for the two-electron Bethe logarithm as a function of $1/Z$. Δ is the difference between the variational calculation of Aashamar and Austvik (1976) and the value obtained from equation (17).

The last form expresses the result in terms of a screened nuclear charge. The small magnitude of the screening parameter, 0.0063, is in harmony with a semi-empirical estimate by Bethe and Salpeter (1957), but the sign is reversed.

The results obtained from (17) are compared in table 3 with the direct variational calculations of the Bethe logarithm by Aashamar and Austvik (1976). The last column gives the difference Δ between the two sets of results multiplied by Z^2. Thus $Z^2\Delta$ should tend to a constant related to the coefficient of the next term of $O(Z^{-2})$ not included (17). As can be seen from figure 1, the differences for $Z > 5$ deviate strongly from the expected behaviour, indicating that the results of Aashamar and Austvik may be less accurate than their estimated error limits. In this high-Z region, the $1/Z$ expansion values calculated from (17) are probably more accurate. Further results for $Z > 10$ can be obtained immediately from equation (17).

The use of multiple exponential parameters α_j in the basis set (13) plays a crucial role in obtaining stable results with a reasonably small number of terms in the basis set. The technique can be immediately extended to excited states, as will be reported in a future publication.

References

Aashamar K 1970 *Nucl. Instrum. Meth.* **90** 263–8
Aashamar K and Austvik A 1976 *Phys. Norv.* **8** 229–37
Armour I A, Myers E G, Silver J D and Träbert E 1979 *Phys. Lett.* **75A** 45–6
Berry H G, DeSerio R and Livingston A E 1978 *Phys. Rev. Lett.* **41** 1652–5
—— 1980 *Phys. Rev.* A **22** 998
Bethe H A and Salpeter E E 1957 *Quantum Mechanics of One- and Two-Electron Atoms* (Berlin: Springer) § 74γ
Buchet J P, Buchet-Poulizac M C, Denis A, Desesquelles J, Druetta M, Grandin J P and Husson X 1981 *Phys. Rev.* A **23** 3354–6
Dalgarno A and Epstein S T 1969 *J. Chem. Phys.* **50** 2837–9
Dalgarno A and Stewart A L 1960 *Proc. Phys. Soc.* **75** 441
Davis W A and Marrus R 1977 *Phys. Rev.* A **15** 1963–75
DeSerio R, Berry H G, Brooks R L, Hardis H, Livingston A E and Hinterlong S 1981 *Phys. Rev.* A **24** 1872–88
Ermolaev A M 1975 *Phys. Rev. Lett.* **34** 380–3
Holt R A, Rosner S D, Gaily T D and Adam A G 1980 *Phys. Rev.* A **22** 1563–71
Klarsfeld S and Maquet A 1973 *Phys. Lett.* **43B** 201–3
O'Brien R, Silver J D, Jelley N A, Bashkin S, Träbert E and Heckmann P H 1979 *J. Phys. B: At. Mol. Phys.* **12** L41
Schwartz C 1961 *Phys. Rev.* **123** 1700–5
Stamp M F, Armour I A, Peacock N J and Silver J D 1981 *J. Phys. B: At. Mol. Phys.* **14** 3551–61
Suh K S and Zaidi M H 1965 *Proc. R. Soc.* A **29** 94–105