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LETTER TO THE EDITOR

Two-electron Lamb shifts and $1s2s\ ^3S_1-1s2p\ ^3P_J$ transition frequencies in helium-like ions

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Abstract. The leading terms in the $1/Z$ expansion of the two-electron Bethe logarithm are calculated for the states $1s^2\ ^1S_0$, $1s2s\ ^1S_1$, $1s2s\ ^3S_1$, $1s2p\ ^1P_1$ and $1s2p\ ^3P_J$ by the use of a novel finite basis set method. The resulting QED terms are combined with other relativistic and mass polarisation corrections to obtain total transition frequencies. The results are compared with recent measurements in helium-like ions from Li^+ to Fe^{24+} .

Recent high-precision measurements of the $1s2s\ ^3S_1-1s2p\ ^3P_J$ ($J=0, 1, 2$) transition frequencies in high- Z two-electron ions (Davis and Marrus 1977, Holt *et al* 1980, DeSerio *et al* 1981, Buchet *et al* 1981, Stamp *et al* 1981, Livingston and Hinterlong 1982) have stimulated considerable interest in the theoretical calculation of relativistic and quantum electrodynamic (QED) effects in these ions (Goldman and Drake 1983, Hata and Grant 1983a, b, c, 1984). (For a review, see Drake 1982.) Since the non-relativistic energy difference increases only as Z , compared with $\alpha^2 Z^4$ and $\alpha^3 Z^4 \ln(\alpha Z)$ for the relativistic and QED corrections, the corrections become rapidly more important with increasing Z . For example, at $Z=20$, they are about 20% and 1% of the total, respectively. The experimental transition frequency for Cl^{15+} determines the two-electron Lamb shift to an accuracy of $\pm 0.65\%$ (DeSerio *et al* 1981) (assuming that other contributions are accurately known), which is more accurate than corresponding measurements in high- Z one-electron ions. The purpose of this letter is to present new calculations for the Bethe logarithms of the states $1s2s\ ^1S$, $1s2s\ ^3S$, $1s2p\ ^1P$ and $1s2p\ ^3P$, and to compare the resulting transition frequencies with experiment.

Following Kabir and Salpeter (1957), the lowest order (in α) two-electron QED correction is (in atomic units, with $1\text{ au} = \alpha^2 mc^2$)

$$E_{L,2} = \frac{4}{3} Z \alpha^3 \{ \ln(Z\alpha)^{-2} + \ln[Z^2 \text{Ryd}/\epsilon(nLS)] + \frac{19}{30} \} \langle \delta(\mathbf{r}_1) + \delta(\mathbf{r}_2) \rangle \quad (1)$$

where Z is the nuclear charge and $\alpha = 1.137.03596$ is the fine-structure constant. The above includes all terms of $O(Z^4 \alpha^3)$, but neglects terms of $O(Z^3 \alpha^3)$ which are proportional to $\langle \delta(\mathbf{r}_{12}) \rangle$ (Kabir and Salpeter 1957). The latter terms do not contribute to the energy shifts of triplet states in LS coupling because $\langle \delta(\mathbf{r}_{12}) \rangle$ vanishes. The principal uncertainty in the evaluation of (1) is the value of the two-electron Bethe

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logarithm defined by

$$\ln \varepsilon(nLS) = \frac{\sum_m |\langle \psi_0 | \mathbf{t} | \psi_m \rangle|^2 \ln (E_m - E_0) / (E_m - E_0)}{\sum_m |\langle \psi_0 | \mathbf{t} | \psi_m \rangle|^2 / (E_m - E_0)} \quad (2)$$

in the dipole acceleration form where ψ_0 is the wavefunction for the nLS two-electron configuration, $\mathbf{t} = Z \sum_i \mathbf{r}_i / r_i^3$ and the sums are over all intermediate states. The use of standard methods involving discrete variational basis sets to evaluate (2) leads to non-convergent results because of the large contribution from highly excited states. Accurate calculations have been attempted for the ground state with Z up to 10 (Schwartz 1961, Aashamar and Austvik 1976), and estimates have been made for the low-lying excited states of He and Li^+ (Suh and Zaidi 1965, Ermolaev 1975). For other cases, it has become customary to use the lowest-order hydrogenic approximation (DeSerio *et al* 1981, Hata and Grant 1983b)

$$\ln(\varepsilon_0(nLS)) = (1 + \delta_{i,0}/n^3)^{-1} (\ln \varepsilon_0(1s) + n^{-3} \ln \varepsilon_0(nl)) \quad (3)$$

where $\varepsilon_0(nl)$ is the hydrogenic Bethe logarithm for nuclear charge $Z=1$. Recently, Hata and Grant (1984) have devised a semi-empirical fitting procedure to obtain improved values for $\ln(\varepsilon(nLS))$.

In the present work, we write the two-electron Bethe logarithm in the form $\ln \varepsilon(nLS) = A/B$ where A and B are the numerator and denominator of (2) respectively, and insert the $1/Z$ expansions

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

$$B = Z^4 (B_0 + B_1 Z^{-1} + \dots). \quad (5)$$

The coefficients in the expansion of B can be obtained from the identity (in atomic units) $B = 2\pi Z \langle \delta^3(\mathbf{r}_1) + \delta^3(\mathbf{r}_2) \rangle$. The exact values of B_0 and B_1 for the S states are

$$B_0(1^1S) = 4 \quad B_0(2^1S) = \frac{9}{4} \quad B_0(2^3S) = \frac{9}{4}$$

$$B_1(1^1S) = -\frac{19}{4} + 3 \ln 2 \approx -2.670558$$

$$B_1(2^1S) = (-4130 + 6879 \ln 3 - 6720 \ln 2) / 3^7 \approx -0.562686$$

$$B_1(2^3S) = (-4402 + 7647 \ln 3 - 7104 \ln 2) / 3^7 \approx -0.422967.$$

The above B_1 values were obtained with the aid of matrix elements tabulated by Cohen and Dalgarno (1961). Our numerical values for the P states are

$$B_0(2^1P) = 2 \quad B_0(2^3P) = 2$$

$$B_1(2^1P) = 0.0436905(1)$$

and

$$B_1(2^3P) = -0.17190190(3).$$

The value of A_0 is now determined by the condition $A_0/B_0 = \ln \varepsilon_0(nLS)$. Only A_1 requires significant additional calculation. Using $1/r_{12}$ as a first-order perturbation, it is given by (Goldman and Drake 1983, Ermolaev and Swainson 1983)

$$A_1 = \sum_m [2\mathbf{t}_{0,m}^{(0)} \cdot \mathbf{t}_{m,0}^{(1)} \ln \Delta E_m^0 / \Delta E_m^0 + |\mathbf{t}_{0,m}^{(0)}|^2 \Delta E_m^1 (1 - \ln \Delta E_m^0) / (\Delta E_m^0)^2] \quad (6)$$

where

$$\begin{aligned} t_{m,0}^{(0)} &= \langle \psi_m^0 | t | \psi_0^0 \rangle \\ t_{m,0}^{(1)} &= \langle \psi_m^1 | t | \psi_0^0 \rangle + \langle \psi_m^0 | t | \psi_0^1 \rangle \\ \Delta E_m^n &= E_m^n - E_0^n \end{aligned}$$

and ψ_m^1 and E_m^1 are the first-order perturbed two-electron wavefunctions and energies. In general, the sums in (6) are difficult to evaluate because of the presence of the ψ_m^1 given by

$$|\psi_m^1\rangle = \sum_{k \neq m} \frac{|\psi_k^0\rangle \langle \psi_k^0 | r_{12}^{-1} | \psi_m^0 \rangle}{E_m^0 - E_k^0}. \quad (7)$$

However, since t is a sum of one-electron operators, only single-electron excitations from the hydrogenic initial state ψ_0^0 make non-vanishing contributions. We therefore replace the actual summations in (6) and (7) by summations over discrete variational one-electron basis sets of the form

$$\phi_n = \sum_{i=1}^I \sum_{j=1}^J c_{i,j}^{(n)} r^{i-1} \exp(-a_j r) Y_l^m(\theta, \phi) \quad n = 1, 2, \dots, I \times J. \quad (8)$$

The linear variational coefficients $c_{i,j}^{(n)}$ are determined by first orthonormalising the basis set, and then diagonalising the one-electron Hamiltonian.

The presence of multiple exponential parameters α_j in (8) is essential to obtaining convergent results as the number of terms in the basis set is increased. We have devised a novel and highly successful iteration procedure for progressively altering the α_j , depending on the eigenvalue spectrum obtained in the preceding iteration. For the p th iteration, the α_j are calculated from

$$\alpha_j^{(p)} = [2(Z_j^{(p)} - \varepsilon_0 - Z_1^{(p)})]^{1/2} \quad (9)$$

with

$$Z_j^{(p)} = \frac{1}{I} \sum_{i=1}^I \varepsilon_{j+i-1}^{(p-1)} \quad (10)$$

and the $\varepsilon_n^{(p-1)}$ are the variational eigenvalues obtained in the preceding iteration. Successive iterations have the effect of progressively spreading out the eigenvalue spectrum and extending it to higher energies. A quantity such as A_1 calculated from the p th basis set passes through an extremum as a function of p . The interpolated extremum point at a non-integral value of p represents the optimum value of A_1 . Test calculations yielded the known B_1 coefficients, and the 1s and 2s hydrogenic Bethe logarithms, correct to six figures or better with twenty-term basis sets. Typically, fewer than ten iterations were required to find an extremum as a function of p . The method appears to offer a significant advance in computational technique for the evaluation of nearly divergent perturbation sums.

The calculations for A_1 converge to the values $A_1(1^1S) = -6.167410(5)$, $A_1(2^1S) = -1.186594(3)$, $A_1(2^3S) = -0.898450(2)$, $A_1(2^1P) = 0.12393(1)$ and $A_1(2^3P) = -0.37415(5)$. Using expansions (4) and (5), the two-electron Bethe logarithm is

$$\begin{aligned} \ln(\varepsilon(n/S)/\text{Ryd}) &= A_0/B_0 + \ln 2 + 2 \ln Z + [(A_1 B_0 - A_0 B_1)/B_0^2] Z^{-1} + O(Z^{-2}) \\ &= \ln[\varepsilon_0(nLS)(Z - \sigma)^2] + O(Z^{-2}) \end{aligned} \quad (11)$$

with $\sigma = -(A_1 B_0 - A_0 B_1)/(2B_0^2)$. The numerical values are

$$\ln(\varepsilon(1^1S)/\text{Ryd}) = \ln[19.7693(Z - 0.00615)^2]$$

$$\ln(\varepsilon(2^1S)/\text{Ryd}) = \ln[19.3943(Z + 0.02040)^2]$$

$$\ln(\varepsilon(2^3S)/\text{Ryd}) = \ln[19.3943(Z + 0.01388)^2]$$

$$\ln(\varepsilon(2^1P)/\text{Ryd}) = \ln[19.6952(Z + 0.00600)^2]$$

$$\ln(\varepsilon(2^3P)/\text{Ryd}) = \ln[19.6952(Z + 0.00475)^2].$$

The result for the ground state does not differ significantly from our earlier less accurate calculation (Goldman and Drake 1983). Screening constants for the excited states have not been calculated before. From (11) the correction $\Delta \ln \varepsilon_0$ to the zero-order Bethe logarithm is $0.02776/Z$ for the 2^3S state and $0.00951/Z$ for the 2^3P state. The numerical values for $Z > 3$ are much larger than the estimates of Hata and Grant (1984) and, unlike their Z^{-3} dependence, $\Delta \ln \varepsilon_0$ decreases only as Z^{-1} . The values obtained from (11) for neutral helium are 4.371 and 4.365 for the 2^1S and 2^3S states respectively, as compared with 4.345 ± 0.020 and 4.380 ± 0.020 calculated by Suh and Zaidi (1965).

The QED corrections for the $2^3S_1-2^3P_J$ transitions can be compared with experiment after other relativistic effects have been taken into account. This was done by diagonalising the matrix (Drake 1979, 1982)

$$\mathbf{H} = (\mathbf{H}_{\text{NR}} + \mathbf{B}_{\text{P}} + \mathbf{E}_{\text{L},2} + \mathbf{H}_{\text{M}} + \mathbf{H}_{\text{NS}})_{\text{LS}} + \mathbf{R}(\mathbf{H}_{\text{D}} + \mathbf{V}_{12} + \mathbf{B} + \mathbf{E}_{\text{HO}})_{jj} \mathbf{R}^{-1} - \mathbf{\Delta} \quad (12)$$

in the basis set of zero-order degenerate states to obtain relativistic and QED corrected eigenvalues. Here, \mathbf{H}_{NR} is the non-relativistic Hamiltonian, \mathbf{B}_{P} is the Breit-Pauli interaction, $\mathbf{E}_{\text{L},2}$ is the diagonal matrix of lowest order QED terms given by (1), \mathbf{H}_{M} is the mass polarisation correction, \mathbf{H}_{NS} is the nuclear size correction including relativistic (Mohr 1983) and two-electron (Ermolaev 1973) effects, \mathbf{H}_{D} is the sum of one-electron Dirac Hamiltonians, $V_{12} = e^2/r_{12}$, \mathbf{B} is the 16-component Dirac form of the Breit interaction including retardation (Mittleman 1971) and \mathbf{E}_{HO} contains all higher diagonal one-electron QED corrections as calculated by Mohr (1982). Following Ermolaev (1975), the \mathbf{E}_{HO} terms for nS states are multiplied by $n^3(2\pi\langle\delta(r_1)\rangle/Z^3 - 1)$ to correct for the non-hydrogenic electron density at the nucleus. The first group of terms in (12) is calculated with highly accurate variational wavefunctions in LS coupling (Drake 1979, Accad *et al* 1971), while the second group of terms is calculated with hydrogenic products of Dirac spinors in jj coupling for wavefunctions. Finally, \mathbf{R} is the $jj \rightarrow LS$ recoupling transformation and $\mathbf{\Delta}$ subtracts those terms that are counted twice. \mathbf{H} is a 2×2 matrix for the states 2^3P_1 and 2^1P_1 , and is a scalar for the states 2^3S_1 , 2^3P_0 and 2^3P_2 . The significance of (12) is that it contains the (essentially) exact non-relativistic eigenvalues and fine-structure shifts, while summing to infinity the one- and two-electron relativistic corrections of order $\alpha^2 Z^4$, $\alpha^4 Z^6$, ..., and $\alpha^2 Z^3$, $\alpha^4 Z^5$, The leading term not included is of $O(\alpha^4 Z^4)$.

The results are compared with a selection of the more precise experimental measurements for ions up to $Z = 26$ in table 1. The theoretical error estimates are obtained by assuming that uncalculated terms contribute approximately $\pm 0.2 \alpha^4 Z^4 \text{ au} = \pm 1.2(Z/10)^4 \text{ cm}^{-1}$. The coefficient 0.2 is chosen to be similar in magnitude to other known coefficients. The net influence of the screening term in (11) is to decrease the

Table 1. Comparison of theory and experiment for the $1s2p\ ^2P_J-1s2s\ ^3S_1$ transitions of He-like ions (in cm^{-1}). Experimental data which disagree with theory are underlined.

Z	J	Theory ^a	Experiment	Z	Theory	Experiment	
3	0	18 231.30 (1)	18 231.303 (1) ^b	10	78 266.5 (1.2)	78 266.9 (2.4) ^c	
	1	18 226.10 (1)	18 226.108 (1) ^b				78 265.0 (1.2) ^d
	2	18 228.19 (1)	18 228.198 (1) ^b			78 565.3 (1.2)	78 566.3 (2.4) ^c
4	0	26 864.6 (0.1)	<u>26 867.4</u> (0.7) ^c			78 565.7 (1.8) ^d	
	1	26 853.1 (0.1)	26 853.1 (0.2) ^c		80 122.4 (1.2)	80 120.5 (1.3) ^c	
	2	26 867.9 (0.1)	26 867.9 (0.2) ^c			80 123.3 (0.8) ^d	
5	0	35 393.7 (0.1)	35 393.2 (0.6) ^c	14	113 821.2 (4.8)	113 815 (4) ^e	
	1	35 377.4 (0.1)	35 377.2 (0.6) ^c			115 589.5 (4.8)	
	2	35 430.1 (0.1)	35 429.5 (0.6) ^c			122 744.3 (4.8)	122 746 (3) ^e
6	0	43 899.1 (0.2)	43 899.0 (0.1) ^c	15	122 971.6 (6.3)	122 940 (30) ^f	
	1	43 886.4 (0.2)	43 886.1 (0.1) ^c			125 393.3 (6.3)	
	2	44 022.1 (0.2)	<u>44 021.6</u> (0.1) ^c			135 153.4 (6.3)	135 153 (18) ^f
7	0	52 421.1 (0.3)	<u>52 413.9</u> (1.4) ^c	16	132 239.9 (8.2)	<u>132 198</u> (10) ^e	
			52 420.0 (1.1) ^d			135 447.5 (8.2)	
	1	52 429.3 (0.3)	52 429.0 (0.6) ^c			148 499.1 (8.2)	148 493 (5) ^e
		52 428.2 (1.1) ^d	17	141 643 (10)	141 643 (40) ^e		
2	52 720.3 (0.3)	52 719.5 (0.6) ^c			145 771 (10)		
		52 720.2 (0.7) ^d			162 926 (10)	162 923 (6) ^e	
8	0	60 979.9 (0.5)	60 978.2 (1.5) ^c	18	151 189 (13)	151 350 (250) ^g	
			<u>60 978.4</u> (0.6) ^d			156 368 (13)	
	1	61 037.9 (0.5)	61 036.6 (3.0) ^c			178 580 (13)	178 500 (300) ^g
		61 037.6 (0.9) ^d	26	233 616 (57)	<u>232 558</u> (550) ^h		
2	61 589.3 (0.5)	61 588.3 (1.5) ^c			249 797 (57)		
		61 589.7 (0.6) ^d			368 756 (57)	<u>368 960</u> (125) ^h	
9	0	69 592.8 (0.8)	69 586.0 (4.0) ^c				
	1	69 742.8 (0.8)	69 743.8 (3.0) ^c				
	2	70 700.3 (0.8)	70 700.4 (3.0) ^c				

^a Numbers in brackets give the uncertainty in the final figure(s) quoted.

^b Holt *et al* (1980).

^c Older data referenced by DeSerio *et al* (1981).

^d Stamp (1983).

^e DeSerio *et al* (1981).

^f Livingston and Hinterlong (1982).

^g Davis and Marrus (1977).

^h Buchet *et al* (1981).

transition frequencies by approximately $0.77(Z/10)^3 \text{ cm}^{-1}$. The effect is small only because the σ turn out to be much less than unity in magnitude.

Theory and experiment agree within the error limits, except as noted in table 1. A further comparison can be made with a high precision measurement of the $2\ ^3P_2 \rightarrow 2\ ^3P_1$ fine-structure interval in F^{7+} . Here, our calculation gives $957.48 \pm 0.80 \text{ cm}^{-1}$, in agreement with the much more accurate experimental value $957.80 \pm 0.03 \text{ cm}^{-1}$ (Myers *et al* 1981). Hata and Grant (1983c) obtained 957.76 cm^{-1} by including an estimate of the $\alpha^4 Z^4$ contribution. Their (1984) values for the $2\ ^3S-2\ ^3P$ transition frequencies should be decreased because of the $\Delta \ln \epsilon_0$ and finite nuclear size corrections not included in their work. At $Z = 10$, the shifts are -0.77 cm^{-1} and -0.51 cm^{-1} respectively, bringing their results into better agreement with ours. Also, their calculation includes only the spin-dependent part of the $\alpha^6 mc^2$ contribution. There are further uncalculated spin-independent terms (Douglas and Kroll 1974) analogous to those in

the Breit interaction. It is clear that further progress in the comparison between theory and experiment will require a complete calculation of the $\alpha^4 Z^4$ term, which contains the combined effects of electron correlation and higher-order relativistic corrections.

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