Title

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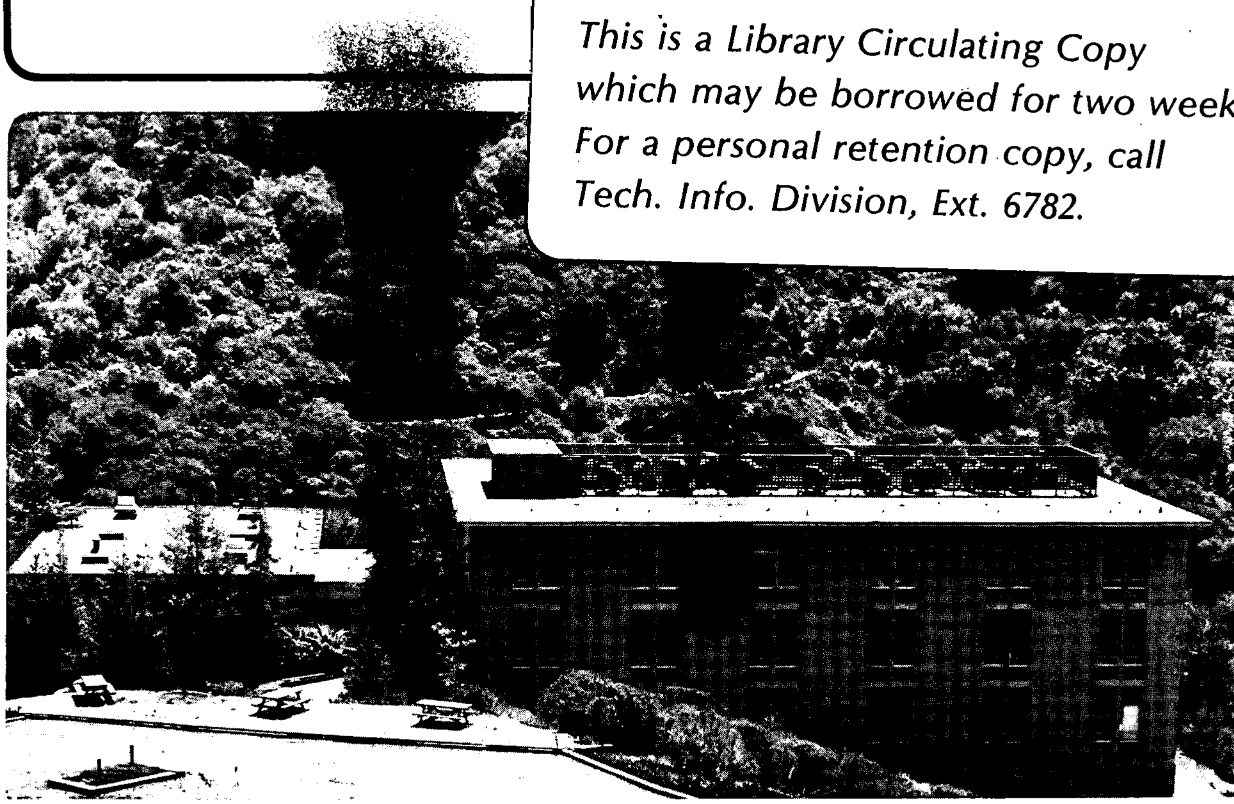

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Two-electron Lamb Shifts and 1s2s $^3S_1$ - 1s2p ^3P_J Transition Frequencies in Helium-like Ions

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Abstract

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

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Recent high precision measurements of the 1s2s $^3S_1$ - 1s2p ^3P_J (J = 0,1,2) transition frequencies in high Z two-electron ions[1-6] have stimulated considerable interest in the theoretical calculation of relativistic and quantum electrodynamic (QED) effects in these ions[7-10]. Since the nonrelativistic energy difference increases only as Z, compared with α^2Z^4 and $\alpha^3Z^4\ln(\alpha Z)$ 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 $C\ell^{15+}$ determines the two-electron Lamb shift to an accuracy of ±0.65%[3] (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 1s2s $^1S_0$ and $^3S_1$ states, and to compare the resulting transition frequencies with experiment.

Following Kabir and Salpeter[11], the lowest order (in α) two-electron QED correction is (in atomic units, with 1 a.u. = α^2mc^2)

$$E_{L,2} = \frac{4}{3}Z\alpha^3\{\ \ln(Z\alpha)^{-2} + \ln[Z^2Ry\ /\varepsilon(nLS)] + \frac{19}{30}\} <(\vec{r}_1) + \ \ (\vec{r}_2)> \qquad (1)$$

where Z is the nuclear charge and α = 1/137.03596 is the fine structure constant. The principal uncertainty in the evaluation of (1) is the value of the two-electron Bethe logarithm defined by

$$\ln\varepsilon(nLS) = \frac{\sum_m |<\psi_0|\vec{t}|\psi_m>|^2 \ln(E_m - E_0)/(E_m - E_0)}{\sum_m |<\psi_0|\vec{t}|\psi_m>|^2/(E_m - E_0)} \qquad (2)$$

in the dipole acceleration form where ψ_0 is the wave function for the nLS two-electron configuration, $\vec{t} = Z\sum_i \vec{r}_i/r_i^{\ 3}$ and the sums are over all imtermediate 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,[12,13] and estimates have been made for the low lying excited states of He and Li^+.[14,15] For other cases, it has become customary to use the lowest order hydrogenic approximation[3,9]

$$\ln[\varepsilon_0(nLS)] = (1 + \delta_{\ell,0}/n^3)^{-1}[\ln\varepsilon_0(1s) + n^{-3}\ln\varepsilon_0(n\ell)] \tag{3}$$

where $\varepsilon_0(n\ell)$ is the hydrogenic Bethe logarithm for nuclear charge Z = 1.

In the present work, we write the two-electron Bethe logarithm in the form

$$\ln\varepsilon(nLS) = A/B \tag{4}$$

where A and B are the numerator and denominator of (2) respectively, and insert the 1/Z expansions

$$A = Z^4[A_0 + A_1Z^{-1} + 2(\ln Z)(B_0 + B_1Z^{-1}) + \cdots] \tag{5}$$

$$B = Z^4[B_0 + B_1Z^{-1} + \cdots] . \tag{6}$$

The coefficients in the expansion of B can be obtained from the identity (in atomic units)

$$B = 2\pi Z\langle\delta^3(\vec{r}_1) + \delta^3(\vec{r}_2)\rangle . \tag{7}$$

The exact values of B_0 and B_1 are

$$B_0(1\ ^1S) = 4,\ B_0(2\ ^1S) = 9/4,\ B_0(2\ ^3S) = 9/4$$

$$B_1(1\ ^1S) = -19/4 + 3\ln 2 \simeq -2.670558$$

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

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

The above B_1 values were obtained with the aid of matrix elements tabulated by Cohen and Dalgarno.[16] The value of A_0 is now determined by the condition

$$A_0/B_0 = \ln\varepsilon_0(nLS) . \tag{8}$$

Only A_1 requires significant additional calculation. Using $1/r_{12}$ as a first order perturbation, it is given by[8,10]

$$A_1 = \sum_m [2\vec{t}^{(0)}_{0,m}\cdot\vec{t}^{(1)}_{m,0}\ \ln\Delta E^0_m/\Delta E^0_m + |\vec{t}^{(0)}_{0,m}|^2 \Delta E^1_m (1 - \ln\Delta E^0_m)/(\Delta E^0_m)^2] \qquad (9)$$

where $\vec{t}^{(0)}_{m,0} = \langle\psi^0_m|\vec{t}|\psi^0_0\rangle$,

$\vec{t}^{(1)}_{m,0} = \langle\psi^1_m|\vec{t}|\psi^0_0\rangle + \langle\psi^0_m|\vec{t}|\psi^1_0\rangle$,

$\Delta E^n_m = E^n_m - E^0_m$

and ψ^1_m and E^1_m are the first order perturbed two-electron wave functions and energies. In general, the sums in (9) are difficult to evaluate because of the presence of the ψ^1_m given by

$$|\psi^1_m\rangle = \sum_{k\neq m} \frac{|\psi^0_k\rangle\langle\psi^0_k|r_{12}{}^{-1}|\psi^0_m\rangle}{E^0_m - E^0_k} \ . \qquad (10)$$

However, since $\vec{t}$ 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 (9) and (10) by summations over discrete variational one-electron basis sets of the form

$$\phi_n = \sum_{i=1}^{I}\sum_{j=1}^{J} c^{(n)}_{i,j}\ r^{i-1}\exp(-\alpha_j r)Y^m_\ell(\theta,\phi), \quad n = 1,2,\cdots,I\times J \ . \qquad (11)$$

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

The presence of multiple exponential parameters α_j in (11) is essential to obtaining convergent results as the number of terms in the basis set is increased.[8] We have devised a novel and highly successful iteration procedure for progressively altering the α_j, depending on the eigenvalue spectrum obtained in the preceeding iteration. For the p'th iteration, the α_j are calculated from

$$\alpha_j^{(p)} = [2(Z_j^{(p)} - \mathcal{E}_0 - Z_1^{(p)}]^{1/2} \tag{12}$$

with $$Z_j^{(p)} = \frac{1}{I}\sum_{i=1}^{I} \mathcal{E}_{j+i-1}^{(p-1)} \tag{13}$$

and the $\mathcal{E}_n^{(p-1)}$ are the variational eigenvalues obtained in the preceeding 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 6 figures or better with 20 term basis sets. Typically, fewer than 10 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 $A_1(1\ ^1S) = -6.167410(5)$, $A_1((2\ ^1S) = -1.186594(3)$ and $A_1(2\ ^3S) = -0.898450(2)$. Using expansions (5) and (6) in (4), the two-electron Bethe logarithm is

$$\begin{aligned}\ln[\varepsilon(nLS)/Ry] &= A_0/B_0 + \ln 2 + 2\ln Z + [(A_1B_0 - A_0B_1)/B_0^{\,2}]Z^{-1} + O(Z^{-2}) \\ &= \ln[\varepsilon_0(nLS)(Z-\sigma)^2] + O(Z^{-2})\end{aligned} \tag{14}$$

with $\sigma = -(A_1B_0 - A_0B_1)/(2B_0^{\,2})$. The numerical values are

$$\ln[\varepsilon(1\ ^1S)/Ry] = \ln[19.7693(Z - 0.00615)^2]$$

$$\ln[\varepsilon(2\ ^1S)/Ry] = \ln[19.3943(Z + 0.02040)^2]$$

$$\ln[\varepsilon(2\ ^3S)/Ry] = \ln[19.3943(Z + 0.01388)^2]\ .$$

The result for the ground state does not differ significantly from our earlier less accurate calculation.[8] Screening constants for the excited states have not been calculated before. The values obtained from (14) 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.[14]

The QED corrections for the $2\ ^3S_1 - 2\ ^3S_J$ transitions can be compared with experiment after other relativistic effects have been taken into account. This was done by diagonalizing the matrix[7,17]

$$\underline{H} = (\underline{H}_{NR} + \underline{B}_P + \underline{E}_{L,2} + \underline{H}_M + \underline{H}_{NS})_{LS} + \underline{R}(\underline{H}_D + \underline{V}_{12} + \underline{B} + \underline{E}_{HO})_{jj}\underline{R}^{-1} - \underline{\Delta} \tag{15}$$

in the basis set of zero-order degenerate states to obtain relativistic and QED corrected eigenvalues. Here, H_{NR} is the nonrelativistic Hamiltonian, $\underline{B}_P$ is the Breit-Pauli interaction, $\underline{E}_{L,2}$ is the diagonal matrix of lowest order QED terms given by (1), H_M is the mass polarization correction, $\underline{H}_{NS}$ is the nuclear size correction calculated by Ermolaev[18], H_D is the sum of one-electron Dirac Hamiltonians, $V_{12} = e^2/r_{12}$, B is the 16-component Dirac form of the Breit interaction including retardation[19], and $\underline{E}_{HO}$ contains all higher order diagonal one-electron QED corrections as calculated by Mohr.[20] The first group of terms in (15) is calculated with highly accurate variational wave functions in LS coupling,[17,21] while the second group of terms is calculated with hydrogenic products of Dirac spinors in jj-coupling for wave functions. Finally, $\underline{R}$ is the jj → LS recoupling transformation and $\underline{\Delta}$ subtracts those terms that are counted twice. $\underline{H}$ 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 (15) is that it contains the (essentially) exact nonrelativistic eigenvalues and fine structure shifts, while summing to infinity the one- and two-electron relativistic corrections of order α^2Z^4, α^4Z^6, $\cdots$, and

$\alpha^2 Z^3$, $\alpha^4 Z^5$, $\cdots$. 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 $\pm 0.2\alpha^4 Z^4$ a.u. = $\pm 1.2(Z/10)^4$ cm^{-1}. The coefficient 0.2 is chosen to be similar in magnitude to other known coefficients. The influence of the screening term in (14) is to decrease the transition frequencies by approximately $1.11(Z/10)^3$ cm^{-1}. The effect is small only because $|\sigma|$ turns out to be much less than unity for the 1s2s $^3S_1$ state. It is presumably even smaller for the 1s2p ^3P_J states.

Except for a few notable exceptions, theory and experiment agree within the error limits.[22] 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, theory gives 957.48 ± 0.80 cm^{-1} in agreement with the much more accurate experimental value[23] 957.80 ± 0.03 cm^{-1}. It is clear that further progress in the comparison between theory and experiment will require a 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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References

1. W. A. Davis and R. Marrus, Phys. Rev. A 15, 1963 (1977).
2. R. A. Holt, S. D. Rosner, T. D. Gaily and A. G. Adam, Phys. Rev. A 22,1563 (1980).
3. R. Deserio, H. G. Berry, R. L. Brooks, H. Hardis, A. E. Livingston and S. Hinterlong, Phys. Rev. A 24, 1872 (1981).
4. J. P. Buchet, M. C. Buchet-Poulizac, A. Denis, J. Desesquelles, M. Druetta, J. P. Grandin and X. Husson, Phys. Rev. A 23, 3354 (1981).
5. M. F. Stamp, I. A. Armour, N. J. Peacock and J. D. Silver, J. Phys. B14,3551 (1981).
6. A. E. Livingston and S. J. Hinterlong, Nucl. Instrum. Meth. 202, 103 (1982).
7. For a review, see G. W. F. Drake, Advan. At. Mol. Phys. 18, 399 (1982).
8. S. P. Goldman and G. W. F. Drake, J. Phys. B16, L183 (1983).
9. J. Hata and I. P. Grant, J. Phys. B16, 507 and 523 (1983).
10. A. M. Ermolaev and R. A. Swainson, J. Phys. B 16, L35 (1983).
11. P. K. Kabir and E. E. Salpeter, Phys. Rev. 108, 1256 (1957).
12. C. Schwartz, Phys. Rev. 123, 1700 (1961).
13. K. Aashamar and A. Austvik, Phys. Norv. 8, 229 (1976).
14. K. S. Suh and M. H. Zaidi, Proc. Roy. Soc. A 29, 94 (1965).
15. A. M. Ermolaev, Phys. Rev. Lett. 34, 380 (1975).
16. M. Cohen and A. Dalgarno, Proc. Roy. Soc. A 261, 565 (1961).
17. G. W. F. Drake, Phys. Rev. A 19, 1387 (1979).
18. A. M. Ermolaev, Phys. Rev. A 8, 1651 (1973).
19. M. H. Mittleman, Phys. Rev. A 4, 897 (1971).
20. P. J. Mohr, Phys. Rev. A 26, 2338 (1982) and At. Data Nucl. Data Tables, in press (1983).
21. Y. Accad, C. L. Pekeris and B. Schiff, Phys. Rev. A 4, 516 (1971).
22. See ref. 10 for a discussion of the caclulations of Hata and Grant (ref. 9).
23. E. G. Myers, P. Kuske, H. J. Andrä, I. A. Armour, N. A. Jelley, H. A. Klein, J. D. Silver and E. Träbert, Phys. Rev. Lett. 47, 87 (1981).

Table 1. Comparison of theory and experiment for the 1s2p ^3P_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	18231.30(1)	18231.303(1)[2]	10	78265.0(1.2)	78266.9(2.4)[b], 78265.0(1.2)[c]
	1	18226.10(1)	18226.108(1)[2]		78563.7(1.2)	78566.3(2.4)[b], 78565.7(1.8)[c]
	2	18228.19(1)	18228.198(1)[2]		80120.8(1.2)	80120.5(1.3)[b], 80123.3(.8)[c]
4	0	26864.6(.1)	26867.4(.7)[b]	14	113814.9(4.8)	113815(4)[3]
	1	26853.0(.1)	26853.1(.2)[b]		115583.3(4.8)	
	2	26867.9(.1)	26867.9(.2)[b]		122738.2(4.8)	122746(3)[3]
5	0	35393.7(.1)	35393.2(.6)[b]	15	122963.4(6.3)	122940(30)[6]
	1	35377.4(.1)	35377.2(.6)[b]		125385.2(6.3)	
	2	35430.0(.1)	35429.5(.6)[b]		135145.3(6.3)	135153(18)[6]
6	0	43898.9(.2)	43899.0(.1)[b]	16	132229.5(8.2)	132198(10)[3]
	1	43886.2(.2)	43886.1(.1)[b]		135437.1(8.2)	
	2	44021.9(.2)	44021.6(.1)[b]		148488.7(8.2)	148493(5)[3]
7	0	52420.7(.3)	52413.9(1.4)[b],52420.0(1.1)[c]	17	141630(10)	141643(40)[3]
	1	52429.0(.3)	52429.0(.6)[b], 52428.2(1.1)[c]		145758(10)	
	2	52719.9(.3)	52719.5(.6)[b], 52720.2(.7)[c]		162913(10)	162923(6)[3]
8	0	60979.2(.5)	60978.2(1.5)[b],60978.4(.6)[c]	18	151173(13)	151350(250)[1]
	1	61037.3(.5)	61036.6(3.0)[b],61037.6(.9)[c]		156352(13)	
	2	61588.7(.5)	61588.3(1.5)[b],61589.7(.6)[c]		178564(13)	178500(300)[1]
9	0	69591.8(.8)	69586.0(4.0)[b]	26	233554(57)	232558(550)[4]
	1	69741.8(.8)	69743.8(3.0)[b]		249730(57)	
	2	70699.3(.8)	70700.4(3.0)[b]		368695(57)	368960(125)[4]

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

[b] Older data referenced by DeSerio et al.[3] [c] M. F. Stamp, D. Phil. Thesis, Oxford (1983).

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