LETTER TO THE EDITOR

Explicit functional approximations for the Z dependence of self-energy radiative corrections in hydrogen-like atoms

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Abstract. Explicit approximate expressions are developed that accurately represent the self-energy radiative corrections of an electron in a hydrogen-like atom as a function of effective nuclear charge Z. Known perturbation expansions valid for low Z are compared with existing numerical calculations for the 1s, 2s and 2p shifts, and the differences are parameterised to extend their validity to include the Z values of all stable elements. These expansions are applied to make extrapolative predictions for principal quantum numbers $n \leqslant 4$. The results have applications in the semi-empirical study of Rydberg states in complex atoms.

Explicit formal representations of the self-energy radiative corrections in single-electron atoms have applications in the semi-empirical study of Rydberg states in complex atoms. High-resolution spectroscopic analyses must often rely upon isoelectronic extrapolations utilising semi-empirical screening parameter linearisations (such as the regular and irregular doublet laws) to obtain the requisite precision (cf Edlén 1964, Curtis 1985). Long before the development of quantum electrodynamics, correction procedures were empirically formulated in the isoelectronic screening parametrisation of x-ray spectra (Green 1923) that can now be recognised (Curtis 1977) as accounting for self-energy radiative corrections. It has been shown (Edlén 1978) that the linearities exhibited in these systematisations can be enhanced if self-energy radiative corrections are approximately included for these many-electron systems, using the corresponding hydrogen-like estimate with an appropriately screened effective central charge Z.

Such corrections become increasingly important as new experimental techniques permit the extension of precision spectroscopic studies to very heavy and very highly ionised systems, where interactions sensitive to higher powers of Z grow in significance. Although the gross energy of a highly ionised atom with many remaining electrons may resemble a *fully screened* hydrogen-like Balmer system, corrections sensitive to the inner portion of the wavefunction (such as the Breit interaction, the finite size of the nucleus, the relativistic inseparability of the reduced mass and these self-energy radiative corrections) approach more nearly a *fully stripped* highly relativistic system. Where explicit functional expressions for their charge dependences exist, these interactions can be incorporated directly into screening parameter systematisations of the data, both to provide accurate extrapolations and to elucidate the dynamics deep within the charge core.

Explicit perturbation expansions for self-energy corrections in hydrogen-like systems have been formulated (Bethe 1947, Harriman 1956, Garcia and Mack 1965, Erickson 1977) that are valid for $Z \leqslant 20$, and exact numerical calculations have been

reported (Mohr 1974, 1982) for selected values of $Z \leqslant 110$ in the $n = 1$ and 2 shells. To facilitate semi-empirical formulations, we have used these exact calculations to develop explicit corrected approximation formulae that are valid over the entire range of stable elements for the ns and np states with principal quantum number $n \leqslant 4$.

Following the notation of Mohr (1974, 1982), we utilise the fact that the lowest-order self-energy radiative corrections scale with the fine structure as αZ to factor out the dominant Z and n dependences. Thus the self-energy radiative correction E_{nl2j} for a state of orbital and total angular momentum l and j is written as

$$E_{nl2j}(Z) = \frac{2R\alpha^3 Z^4}{\pi n^3} F_{nl2j}(Z).\tag{1}$$

Here R is the Rydberg energy and α is the fine-structure constant. F_{nl2j} is the reduced splitting factor, which is less rapidly varying with Z and n than E_{nl2j}, and hence the quantity chosen for study here.

Garcia and Mack (1965) give perturbative expansions for these shifts that are valid for $Z \leqslant 20$. For $ns_{1/2}$ and $np_{1/2}$ these expansions can be expressed as

$$F_{ns1}^{GM}(Z) = \tfrac{8}{3} \ln(1/\alpha Z) - A_n + 9.6184\alpha Z - (\alpha Z)^2 [4 \ln^2(1/\alpha Z)$$

$$- B_n \ln(1/\alpha Z) + 25.442]\tag{2}$$

$$F_{np1}^{GM}(Z) = -C_n + D_n(\alpha Z)^2 \ln(1/\alpha Z).\tag{3}$$

Garcia and Mack (1965) give a similar expression for $np_{3/2}$, but a more inclusive perturbative expression has been given for the $np_{3/2}$-$np_{1/2}$ fine-structure interval by Erickson (1977), expressed as

$$F_{np3}^{E}(Z) - F_{np1}^{E}(Z) = 0.2496 - \tfrac{3}{16}\pi(\alpha Z)^3 - E_n(\alpha Z)^2 [2 \ln(1/\alpha Z) + \tfrac{11}{24} - 7.476\alpha Z].\tag{4}$$

The n-dependent coefficients can be written as

$$A_n = \tfrac{4}{3} \ln k_{ns} - 0.8438\tag{5}$$

$$B_n = 8 \left(\ln(2/n) + \sum_{q=1}^{n} 1/q - 77/180n^2 \right) + 0.4491\tag{6}$$

$$C_n = \tfrac{4}{3} \ln k_{np} + 0.1664\tag{7}$$

$$D_n = \tfrac{8}{45}(3 - 2/n^2) + \tfrac{14}{5} E_n\tag{8}$$

$$E_n = \tfrac{1}{3}(1 - 1/n^2)\tag{9}$$

where k_{nl} is the mean excitation energy, which has been computed and tabulated for $n = 1$-4 by Harriman (1956). For convenience the numerical values of these coefficients for $n = 1 - 4$ are given in table 1.

We have used these approximate perturbation expansions to attempt to deconvolute from the exact values their dependences on low powers of Z. We have therefore studied the Z variation of the differences Δ between the exact and perturbation values, as defined by

$$F_{ns1}(Z) = F_{ns1}^{GM}(Z) + \Delta_{ns}(Z)\tag{10}$$

$$F_{np1}(Z) = F_{np1}^{GM}(Z) + \Delta_{np1}(Z)\tag{11}$$

and

$$(F_{np3}(Z) - F_{np1}(Z)) = (F_{np3}^{E}(Z) - F_{np1}^{E}(Z)) + \Delta_{nfs}(Z).\tag{12}$$

Table 1. Coefficients for equations (2)-(4) computed from equations (5)-(9) and the table of Harriman (1956).

n	A_n	B_n	C_n	D_n	E_n
1	3.1351	10.572	—	—	—
2	2.9053	11.594	0.126 39	1.1444	0.2500
3	2.8465	11.492	0.115 49	1.3235	0.2963
4	2.8227	11.357	0.100 47	1.3861	0.3125

Ab initio numerical computations of F_{1s1}, F_{2s1}, F_{2p1} and F_{2p3} for specific values of Z (10–110 in intervals of 10) have been reported by Mohr (1974, 1982). This permits parametrisation studies of the Z dependences of Δ_{1s}, Δ_{2s}, Δ_{2p1} and Δ_{2fs}.

Figure 1 displays both Δ_{1s} and Δ_{2s} plotted as a function of $(\alpha Z)^3$. This exposition is interesting in two respects: it reveals that Δ_{ns} is a linear function of this abscissa, and that it possesses only a very weak dependence on principal quantum number. Least-squares fits to a straight line yield an intercept and slope of 0.2164 and 22.49 for 1s and 0.1820 and 23.44 for 2s. On this basis we shall assume that the corresponding quantitites for the $n = 3$ and 4 levels differ negligibly from those of the $n = 2$, and use Δ_{2s} to extrapolate the 3s and 4s shifts.
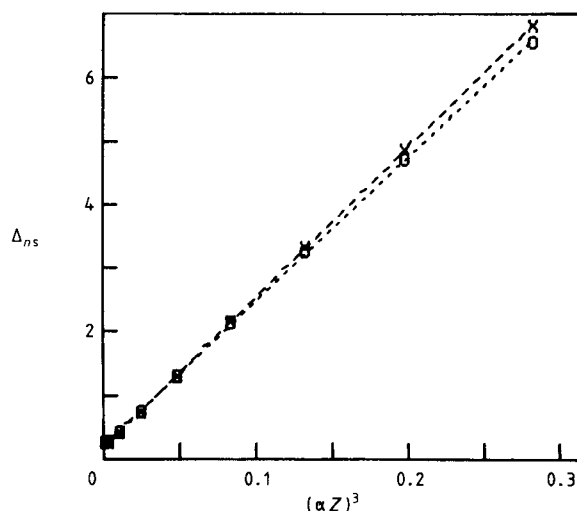

Figure 1. Plot of the differences between the calculations of Mohr (1974, 1982) and the formulae of Garcia and Mack (1965) against $(\alpha Z)^3$ for the reduced splitting of the 1s ($\bigcirc$) and 2s ($\times$) levels. The broken lines represent least-squares fits to straight lines on this plot.

Figure 2 shows Δ_{2p1} plotted as a function of $(\alpha Z)^2$. In this case Δ_{2p1} is seen to be well represented by a parabolic function of the abscissa, as indicated by the least-squares fit. Although no calculations for other $np_{1/2}$ shifts are available, we shall also assume that this quantity has a negligible dependence on n, and use Δ_{2p1} to extrapolate the shifts of the $3p_{1/2}$ and $4p_{1/2}$.

Figure 3 presents Δ_{2fs} plotted as a function of $(\alpha Z)^4$. Here Δ_{2fs} is very accurately represented by a linear function of the abscissa, and the intercept (indicated by a
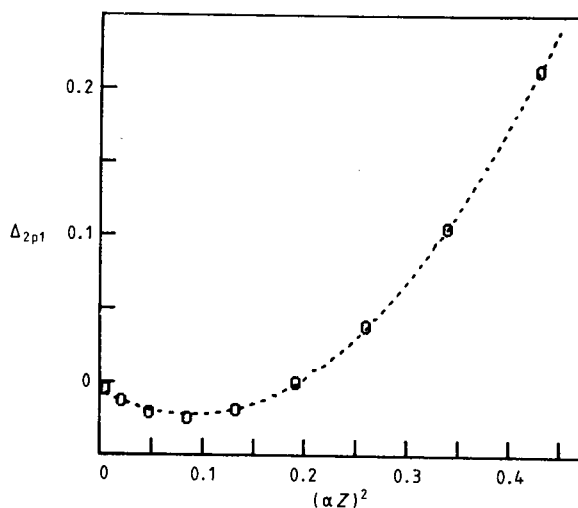
Figure 2. Plot of the difference between the calculations of Mohr (1982) and the formula of Garcia and Mack (1965) against $(\alpha Z)^2$ for the reduced shift of the $2p_{1/2}$ level. The broken curve represents a least-squares fit to a parabola on this plot.
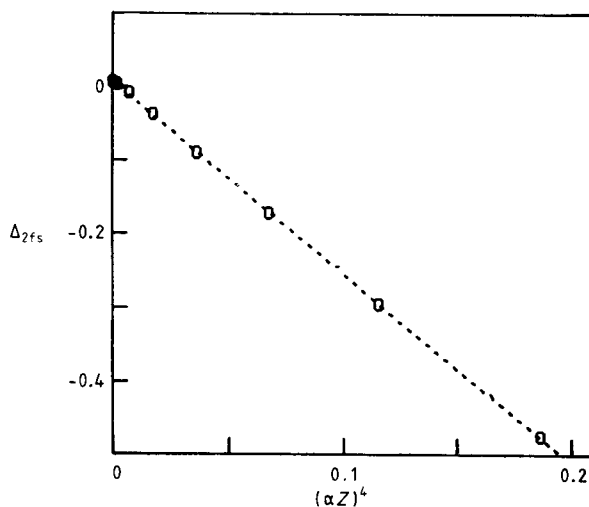

Figure 3. Plot of the difference between the calculations of Mohr (1982) and the formula of Erickson (1977) against $(\alpha Z)^4$ for the reduced shift of the fine structure of the 2p term. The broken line represents a least-squares fit to a straight line on this plot.

least-squares fit) is very close to the origin of the coordinate system. Thus this correction reduces essentially to a simple one-term power law. Again here we shall assume negligible n dependence in this correction.

From these figures it can be seen that the differences between the exact and perturbation values are dominanted by only one or two powers in an αZ expansion. It is interesting to note that for Δ_{ns} and Δ_{2fs} the correction corresponds to a power of αZ one unit higher than was already included in equations (2) and (4), indicating that these expressions are correct (to within a small additive constant) to within the order

of αZ to which they were expanded. In the case of Δ_{2p1}, occurrence of a correction proportional to $(\alpha Z)^2$ indicates that equation (3) requires additional inclusions within the order to which it was expanded. These results suggest that a relatively modest refinement and extension of the *ab initio* perturbation expansion might identify the origin of these corrections.

Assuming the results of these least-squares fits can be extrapolated to higher n, we obtain the following explicit corrections:

$$\Delta_{1s}(Z) = 0.2164 + 22.49(\alpha Z)^3 \tag{13}$$

and for $n > 1$

$$\Delta_{ns}(Z) = 0.1820 + 23.44(\alpha Z)^3 \tag{14}$$

$$\Delta_{np1}(Z) = -0.0057 - 0.3634(\alpha Z)^2 + 2.018(\alpha Z)^4 \tag{15}$$

$$\Delta_{nfs}(Z) = 0.0068 - 2.593(\alpha Z)^4. \tag{16}$$

Thus the substitution of equations (2)–(4) (using table 1) and (13)–(16) in equations (10)–(12) provides an explicit functional representation for F_{nl2j}. A comparison of results using the approximation formula and the exact computations of Mohr (1974, 1982) is given for the 1s and 2s states in table 2. Agreement is generally to within 1%. Assuming the n independence of Δ_{ns} for $n \geq 2$, extrapolative predictions for 3s and 4s are also presented in table 2. Similarly, approximate and exact results for $2p_{1/2}$ and $2p_{3/2}$ are compared in table 3. Agreement for the $2p_{3/2}$ (and the fine-structure difference) is also to within about 1%. The percentage error in $2p_{1/2}$ is slightly larger in the region where it passes through zero, but the absolute agreement is quite good. Assuming negligible n dependence in the correction functions Δ_{np1} and Δ_{nfs}, extrapolative predictions for $3p_{1/2}$, $3p_{3/2}$, $4p_{1/2}$ and $4p_{3/2}$ are also presented in table 3.

The explicit formulae presented here provide a useful means for modelling the core charge scaling of the self-energy radiative corrections in Rydberg states of complex many-electron atoms. They also provide predictions of these corrections for $n = 3$ and 4 states for truly one-electron atoms over all Z, for which no other estimates presently exist. The apparent n independence and the simple power law Z dependence of the corrections to these perturbative expansions raise interesting theoretical questions and motivate the formal calculation of further terms in those expansions.

Table 2. Calculated (Mohr 1974, 1982) and fitted reduced shifts for the 1s and 2s levels and extrapolated fitted shifts for the 3s and 4s levels.

Z	F_{1s1} Mohr	F_{1s1} Fit	F_{2s1} Mohr	F_{2s1} Fit	F_{3s1} Fit	F_{4s1} Fit
10	4.654	4.64	4.893	4.85	4.91	4.93
20	3.246	3.26	3.506	3.50	3.56	3.58
30	2.552	2.58	2.839	2.86	2.91	2.93
40	2.135	2.16	2.455	2.48	2.53	2.54
50	1.864	1.86	2.224	2.24	2.29	2.29
60	1.684	1.66	2.095	2.09	2.14	2.14
70	1.568	1.53	2.044	2.03	2.07	2.07
80	1.503	1.48	2.065	2.05	2.09	2.09
90	1.488	1.53	2.169	2.18	2.22	2.22

Table 3. Calculated (Mohr 1974, 1982) and fitted reduced shifts for the $2p_{1/2}$ and $2p_{3/2}$ levels and extrapolated fitted shifts for the $3p_{1/2}$, $3p_{3/2}$, $4p_{1/2}$ and $4p_{3/2}$ levels.

	F_{2p1}		F_{2p3}		F_{3p1}	F_{3p3}	F_{4p1}	F_{4p3}
Z	Mohr	Fit	Mohr	Fit	Fit	Fit	Fit	Fit
10	−0.1145	−0.1180	0.1303	0.1312	−0.1046	0.1433	−0.0987	0.1488
20	−0.0922	−0.0920	0.1436	0.1443	−0.0738	0.1593	−0.0662	0.1658
30	−0.0641	−0.0616	0.1604	0.1604	−0.0376	0.1802	−0.0280	0.1884
40	−0.0308	−0.0283	0.1794	0.1789	0.0013	0.2056	0.0129	0.2162
50	0.0082	0.0089	0.1999	0.1992	0.0438	0.2356	0.0573	0.2496
60	0.0549	0.0536	0.2215	0.2210	0.0928	0.2706	0.1078	0.2891
70	0.1129	0.1111	0.2440	0.2440	0.1534	0.3106	0.1694	0.3352
80	0.1884	0.1884	0.2671	0.2675	0.2321	0.3558	0.2486	0.3880
90	0.2934	0.2942	0.2906	0.2906	0.3375	0.4060	0.3539	0.4477

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