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LETTER TO THE EDITOR

**Two-electron QED corrections in helium-like ions**

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**Abstract.** The calculation of two-electron QED energy shifts in helium-like ions is discussed in order to correct a number of errors and misunderstandings which have appeared in the literature. New results are presented for the terms involving  $\langle r_{12}^{-3} \rangle$  in the ground and low-lying excited states for ions up to  $Z = 10$ . A detailed comparison is made with the high-precision measurement by Martin and a calculation by Hata for the  $1s2p\ ^1P_1 - 1s2p\ ^3P_1$  transition of helium.

The basic theory of the lowest-order quantum electrodynamic (QED) contributions in two-electron ions was developed in the early papers of Kabir and Salpeter (1957), Araki (1957) and Sucher (1958). Recent high-precision measurements of transition frequencies among the  $n = 2$  states of helium (Sansonetti and Martin 1984, Martin 1984) and  $\text{Li}^+$  (Holt *et al* 1980, Englert *et al* 1982) have stimulated renewed interest in the precise calculation of the two-electron QED terms. The purpose of this Letter is to correct some errors and misunderstandings which have appeared in the literature, and to present new results for the  $1s2p\ ^1P_1 - 1s2p\ ^3P_1$  transition in helium.

Following the conventional notation, the leading QED energy shifts in a two-electron ion are (in atomic units, with  $1\text{ au} = \alpha^2 mc^2$ )

$$\Delta E_L = E_{L,2} + E_{L,2}^{\text{HO}} + E'_{L,2} \quad (1)$$

where

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

$$E_{L,2}^{\text{HO}} = \frac{4}{3} Z \alpha^3 \left\{ 3\pi Z \alpha \left( \frac{427}{384} - \frac{1}{2} \ln 2 \right) + (Z\alpha)^2 \left[ -\frac{3}{4} \ln^2(Z\alpha)^{-2} + O(\ln Z\alpha) \right] \right. \\ \left. + (\alpha/\pi)(0.4042 + O(Z\alpha)) + O(\alpha^2/\pi^2) \right\} \langle \delta(\mathbf{r}_1) + \delta(\mathbf{r}_2) \rangle \quad (3)$$

$$E'_{L,2} = \alpha^3 \left( \frac{14}{3} \ln \alpha + \frac{164}{15} \right) \langle \delta(\mathbf{r}_{12}) \rangle - \frac{14}{3} \alpha^3 Q \quad (4)$$

with

$$Q = 1/4\pi \lim_{a \rightarrow 0} \langle r_{12}^{-3}(a) + 4\pi(\gamma + \ln a)\delta(\mathbf{r}_{12}) \rangle \quad (5)$$

$$r_{12}^{-3}(a) = \begin{cases} r_{12}^{-3} & |\mathbf{r}_1 - \mathbf{r}_2| > a \\ 0 & |\mathbf{r}_1 - \mathbf{r}_2| \leq a. \end{cases} \quad (6)$$

Here,  $\ln \varepsilon(nLS)$  is the two-electron Bethe logarithm (Goldman and Drake 1984) and  $\gamma$  is Euler's constant. The term  $E_{L,2}^{\text{HO}}$  represents an approximate extension of the higher-order one-electron QED energy shifts to the two-electron case by incorporating the correct electron density at the nucleus (Goldman and Drake 1984, Hata 1984a).

The terms shown in (3) as  $O(\ln Z\alpha)$ ,  $O(Z\alpha)$  and  $O(\alpha^2/\pi^2)$  are too small to affect the comparison with experiment in neutral helium.

The main point of this Letter concerns the calculation of  $Q$ . Ermolaev (1973) suggested the approximate formula

$$Q = -\langle \delta(\mathbf{r}_{12}) \rangle \ln[Z + (Z-1)/n] + O(Z^3) \quad (7)$$

and this has subsequently been used in a number of recent papers. Equation (7) is valuable as an asymptotic formula that can be used to estimate the order of magnitude of  $Q$  for large  $Z$ . However, as shown below, it is an extremely poor approximation at low  $Z$  for singlet states, and of no use at all for triplet states because  $\langle \delta(\mathbf{r}_{12}) \rangle$  vanishes. The usual approach in the literature has been to set  $Q = 0$  for triplet states.

We present here detailed calculations of  $Q$  using correlated variational wavefunctions constructed from radial functions of the form  $r_1^i r_2^j r_{12}^k \exp(-\alpha r_1 - \beta r_2)$ . Considerable care must be exercised in treating the singular integrals required for the evaluation of equation (5). For example, it can be shown that the definition (6) for  $r_{12}^{-3}(a)$  is equivalent to

$$r_{12}^{-3}(a) = \begin{cases} r_{12}^{-3} & |r_1 - r_2| > a \\ 4\pi\delta(\mathbf{r}_{12}) & |r_1 - r_2| \leq a \end{cases} \quad (8)$$

when the vector difference  $|\mathbf{r}_1 - \mathbf{r}_2|$  is replaced by the scalar difference in defining the cut-off for singular terms. Equation (8) leads to simpler integration formulae because the  $r_{12}$  integration can be done first instead of leaving it to the last as required by (6).

A detailed study of the contributions to  $Q$  with wavefunctions written as a  $1/Z$  expansion shows that  $Q$  can be expressed in the form

$$Q = -\langle \delta(\mathbf{r}_{12}) \rangle \left\{ \ln Z + \frac{1}{4} \ln \left[ \frac{4}{n} \left( 1 + \frac{1}{n} \right)^2 \right] - 1 \right\} + \frac{Z^3}{4\pi} (A_0 + A_1 Z^{-1} + \dots). \quad (9)$$

Values of  $Q$  obtained with 50-term variational wavefunctions are listed in table 1 for several low-lying states of the helium sequence. The approximation (7) does not even give the correct sign for small values of  $Z$ , although asymptotically the  $\ln Z$  term eventually dominates.

Values for the complete two-electron term  $E'_{L,2}$  are listed in table 2. The ground-state results agree with, but are more accurate than those of Hata (1984b) and earlier calculations referenced by him. No comparable calculations incorporating accurate values for  $Q$  have been published for the excited states. The numerical values for the

Table 1. Values of  $Q$  for low-lying states of the helium sequence in  $\text{au}^3$ .

$Z$	$1s^2 \ ^1S$	$1s2s \ ^1S$	$1s2s \ ^3S$	$1s2p \ ^1P$	$1s2p \ ^3P$
2	0.078 05	0.005 3	0.003 81	0.003 34	0.003 09
3	0.011 61	-0.007 8	0.024 9	0.021 4	0.015 56
4	-0.609 9	-0.116	0.075 6	0.053 2	0.043 64
5	-2.316	-0.423	0.168 2	0.086 3	0.093 58
6	-5.712	-1.05	0.315 1	0.100 7	0.171 7
7	-11.456	-2.12	0.528 5	0.071 6	0.284 2
8	-20.255	-3.79	0.821 1	-0.029 9	0.437 4
9	-32.852	-6.20	1.205	-0.234 7	0.637 6
10	-50.023	-9.52	1.693	-0.578 9	0.891 0

<sup>a</sup> To find the contribution to the energy, multiply the entries by  $-14\alpha^3/3 \text{ au} = -0.3980 \text{ cm}^{-1}$ .

**Table 2.** Values of the two-electron QED contribution  $E'_{L,2}$  for low-lying states of the helium sequence (in  $\text{cm}^{-1}$  with  $1 \text{ au} = 219\,474.6 \text{ cm}^{-1}$ ).

Z	$1s^2\ ^1S$	$1s2s\ ^1S$	$1s2s\ ^3S$	$1s2p\ ^1P$	$1s2p\ ^3P$
2	-0.140 17	-0.011 0	-0.001 54	-0.002 09	-0.001 23
3	-0.552 18	-0.064	-0.009 93	-0.018 6	-0.006 19
4	-1.319 6	-0.175	-0.030 1	-0.063 6	-0.017 4
5	-2.476	-0.35	-0.067 0	-0.147 6	-0.037 2
6	-4.027	-0.60	-0.125 4	-0.278 9	-0.068 3
7	-5.953	-0.90	-0.210	-0.463	-0.113
8	-8.219	-1.26	-0.327	-0.706	-0.174
9	-10.774	-1.67	-0.480	-1.010	-0.254
10	-13.554	-2.10	-0.674	-1.379	-0.355

singlet states differ by more than an order of magnitude from those of Ermolaev (1973) obtained with equation (7). For the  $1s2p\ ^1P$  state of He, the present value of  $-0.002\,09 \text{ cm}^{-1}$  is much larger than  $-0.000\,48 \text{ cm}^{-1}$  obtained by Hata (1984a).

A further point of misunderstanding concerns the anomalous magnetic moment correction in the tabulations of Accad *et al* (1971). Although this correction is included in the  $^3P$  fine-structure splittings  $\Delta\nu_{01}$  and  $\Delta\nu_{21}$  listed in his table XXVI, it is *not* included in the relativistic shift  $E_J$  to the ionisation potential of  $^3P_1$  states in tables XII-XX. (To verify this, compare with the calculations of Schwartz 1964.) The anomalous magnetic moment shifts for the  $^3P_1$  states (Drake 1982) must be added separately.

As an instructive example, the theoretical  $2^1P_1$ - $2^3P_1$  splitting is compared with Martin's (1984) high-precision measurement, and with Hata's (1984a) calculation in table 3. The non-relativistic energy difference used in the present work was obtained

**Table 3.** Contributions to the  $1s2p\ ^1P_1$ - $1s2p\ ^3P_1$  transition frequency of helium in  $\text{cm}^{-1}$ . The value of the Rydberg used is  $109\,722.2731 \text{ cm}^{-1}$  (Martin 1984).

Contribution	Present work	Hata (1984a) <sup>c</sup>	Difference
$\Delta E_{NR}$	2045.465 53 <sup>a</sup>	2045.464 86	0.000 67
$\Delta E_{rel}$	-0.782 52	-0.782 52	0
$\Delta E_{st}$	0.000 317	0.000 317	0
$\Delta E_{mass\ pol}$	3.327 785	3.327 785	0
$\Delta E_{anom\ mag}$	0.000 62	0	0.000 62
$\Delta E_{L,2}^0 + \Delta E_{L,2}^{HO}$	-0.043 83	-0.043 83	0
$\Delta E_{L,2}^\sigma$	-0.000 75	0	-0.000 75
$\Delta E'_{L,2}$	-0.000 86	-0.000 48	-0.000 38
$\Delta E_{nuc\ size}$	0.000 11	0	0.000 11
$\Delta E_{RR}(\text{Stone})$	-0.000 49	0	-0.000 49
Total	2048.053 58(50)	2048.053 80(5)	-0.000 22
Experiment <sup>b</sup>	2048.053 79(11)		

<sup>a</sup> Obtained from the extrapolated non-relativistic energies

$$E(2^1P) = -2.123\,843\,0863 \text{ au}$$

and

$$E(2^3P) = -2.133\,164\,1907 \text{ au (Schiff *et al* 1965).$$

<sup>b</sup> Martin (1984).

<sup>c</sup> See also Hata (1984c) for his revised values of  $\Delta E_{NR}$  and  $\Delta E_{L,2}^\sigma$ .

by extrapolating the eigenvalue calculations of Schiff *et al* (1965) to larger basis sets. The result differs by  $0.000\ 67\ \text{cm}^{-1}$  from Hata's extrapolation because he used the data tabulated by Accad *et al* (1971) which contain fewer significant figures. The difference is substantial. The terms  $\Delta E_{\text{rel}}$ ,  $\Delta E_{\text{mass pol}}$  and  $\Delta E_{\text{st}}$  (the singlet-triplet mixing term) are the same as used by Hata, while  $\Delta E_{\text{anom mag}}$  is the anomalous magnetic moment correction to the  $2^3\text{P}_1$  state (Drake 1982) not included by Hata. The term  $\Delta E_{L,2}^0$  is given by equation (2) with the simple hydrogenic approximation  $\ln(\varepsilon/\text{Ryd}) = \ln(19.6952Z^2)$  for the Bethe logarithm of both P states. The result is  $\Delta E_{L,2}^0 = 0.043\ 15\ \text{cm}^{-1}$ . The combination  $\Delta E_{L,2}^0 + \Delta E_{L,2}^{\text{HO}}$  is in agreement with Hata, but he did not include  $\Delta E_{L,2}^{\sigma}$ , which is the shift due to electron screening in the one-electron Bethe logarithm (Goldman and Drake 1984). For this term, one writes

$$\ln(\varepsilon(2^{1,3}\text{P})\text{Ryd}) = \ln[19.6952(Z - \sigma)^2]$$

with  $\sigma(2^1\text{P}) = -0.006\ 00$  and  $\sigma(2^3\text{P}) = -0.004\ 75$ . In a subsequent paper, Hata (1984c) included the  $\Delta E_{L,2}^{\sigma}$  term and corrected his extrapolation for  $\Delta E_{\text{NR}}$ . The two-electron term  $\Delta E_{L,2}^{\sigma}$  is nearly twice as large as Hata's. Finally,  $\Delta E_{\text{RR}}(\text{Stone})$  is the relativistic recoil shift of  $O(\alpha^2 Z^4 m/M)$  arising from finite nuclear mass corrections to the Breit interaction as derived by Stone (1963). However, there are further uncalculated contributions arising from second-order cross terms between the Breit interaction and the mass polarisation operator (Lewis and Serafino 1978) which could be equally as large. We therefore take the theoretical uncertainty to be  $\pm \Delta E_{\text{RR}}(\text{Stone})$ . Higher-order relativistic corrections of  $O(\alpha^4 Z^6)$  and  $O(\alpha^4 Z^5)$  do not contribute more than  $\pm 0.000\ 10\ \text{cm}^{-1}$ . The total agrees with Martin's (1984) observed value to within the accuracy of the calculation. The closer agreement obtained by Hata (1984a) should be modified because of the terms he did not consider.

A more extensive discussion of the results for other transitions and comparison with experimental data will be presented in a future publication.

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