Self-energy correction to one-electron energy levels in a strong Coulomb field

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Results of a precise calculation of the Coulomb self-energy for states with $n = 1$ and 2 for nuclear charge Z in the range 5–110 in increments of 5 are given. Results are also given for some elements that are of particular experimental interest. These values provide improved accuracy over previous calculations.
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The energy eigenvalue of the Dirac equation for an electron in a static Coulomb field gives the energy level as a function of the nuclear charge Z to all orders in $Z\alpha$, where α is the fine-structure constant. This formula is the zeroth-order term in an expansion of the energy levels in powers of α, and quantum electrodynamics (QED) predicts corrections as a power series in α. The first-order corrections are the one-photon self-energy and vacuum polarization which together give this next contribution to all orders in $Z\alpha$. In contrast to the Dirac formula, which can be written in a relatively simple analytical form, the order α corrections, and particularly the self-energy correction, have required extensive numerical calculations to obtain an accurate estimate.

Calculations of the self-energy in a strong Coulomb field have been done by Brown *et al.* [1, 2], Desiderio and Johnson [3], Erickson [4], Mohr [5–7], Cheng and Johnson [8], Soff *et al.* [9], Blundell and Snyderman [10], and Kim and Mohr [11].

The present work is motivated by recent and anticipated increases in precision of spectroscopic measurements that are sensitive to this QED correction. In order for these measurements to provide fundamental tests of QED, rather than checks on computational methods, it is of value to reduce numerical uncertainties in the calculation to a negligible level.

As a step in this direction, a precise calculation of the one-photon Coulomb self-energy for the $n = 1$ and 2 states over a wide range Z has been done, with an improvement in precision over previous theoretical results that ranges from one to four orders of magnitude, depending on the state and Z.

The basic method of calculation has been described in a series of papers [5–7, 11]. Increases in precision reported here are the result of both improvements in numerical methods and increased computing capacity. Most of these calculations were done on the NIST Cray Y-MP computer and an IBM RS/6000 workstation [12]. Results of this calculation are compared with earlier results below.

A division of the self-energy calculation into a low-energy part and a high-energy part, $\Delta E = \Delta E_L + \Delta E_H$, has been described previously [5]. The low-energy part is (in units in which $\hbar = c = m_e = 1$)

$$\Delta E_L = \frac{\alpha}{\pi} E_n - \frac{\alpha}{\pi} \mathrm{P} \int_0^{E_n} dz \int d\mathbf{x}_2 \int d\mathbf{x}_1 \phi_n^\dagger(\mathbf{x}_2) \alpha^j G(\mathbf{x}_2, \mathbf{x}_1, z) \alpha^l \phi_n(\mathbf{x}_1) (\delta_{jl} \boldsymbol{\nabla}_2 \cdot \boldsymbol{\nabla}_1 - \nabla_2^j \nabla_1^l) \frac{\sin[(E_n - z)x_{21}]}{(E_n - z)^2 x_{21}}, \quad (1)$$

where ϕ_n and E_n are the eigenfunction and eigenvalue of the Dirac equation for the bound state n, G is the Green's function for the Dirac equation corresponding to the operator $G = (H - z)^{-1}$, where $H = \boldsymbol{\alpha} \cdot \mathbf{p} + V + \beta$ is the Dirac Hamiltonian, $\mathbf{x}_{21} = \mathbf{x}_2 - \mathbf{x}_1$, and the indices j and l are summed from 1 to 3.

The method of evaluation of Eq. (1) is described in Ref. [11], where it is applied to a calculation of the self-energy of excited states. In the present application, the number of integration points is greater, but the method is otherwise the same. Numerical values are expressed in terms of a function $f_L(Z\alpha)$ defined by

$$\Delta E_L = \frac{\alpha}{\pi} \left[\tfrac{3}{2} E_n + \tfrac{7}{6} \langle V \rangle + \frac{(Z\alpha)^4}{n^3} f_L(Z\alpha) \right]. \quad (2)$$

Table I gives the results of this calculation for the function $f_L(Z\alpha)$. The uncertainties listed in that table are expected to be larger than the actual errors in most cases. These results are consistent with Refs. [6, 7]. Numerical differences between these results and the results in Refs. [6, 7] are due to the difference between the value for α employed there and the value $\alpha = 1/137.036$ employed here.

The high-energy part is

$$\Delta E_H = -\frac{i\alpha}{2\pi} \int_{C_H} dz \int d\mathbf{x}_2 \int d\mathbf{x}_1 \phi_n^\dagger(\mathbf{x}_2) \alpha_\mu G(\mathbf{x}_2, \mathbf{x}_1, z) \alpha^\mu \phi_n(\mathbf{x}_1) \frac{e^{-bx_{21}}}{x_{21}} - \delta m \int d\mathbf{x}\, \phi_n^\dagger(\mathbf{x}) \beta \phi_n(\mathbf{x}), \quad (3)$$

TABLE I. The low-energy part $f_L(Z\alpha)$. Uncertainties shown in parentheses.

Z	$1S_{1/2}$	$2S_{1/2}$	$2P_{1/2}$	$2P_{3/2}$
5	7.523832(1)	7.891283(6)	0.945203(6)	0.692379(5)
10	5.88505566(5)	6.2620372(4)	0.9570601(4)	0.6973815(3)
15	4.99243951(3)	5.38256144(8)	0.97392538(8)	0.70402408(3)
20	4.39937735(1)	4.80561612(2)	0.99520836(2)	0.71187896(2)
25	3.96741817(1)	4.39244335(1)	1.02068761(1)	0.72069263(1)
30	3.63561574	4.08196792	1.05035270	0.73029920(1)
35	3.37189002	3.84209988	1.08434614	0.74058454(1)
40	3.15738959	3.65407179	1.12294256	0.75146824
45	2.98018703	3.50612498	1.16654684	0.76289343
50	2.83233940	3.39057129	1.21570541	0.77482060
55	2.70837201	3.30228645	1.27112956	0.78722354
60	2.60443821	3.23788818	1.33373231	0.80008666
65	2.51783137	3.19527737	1.40468307	0.81340312
70	2.44669656	3.17339358	1.48548706	0.82717347
75	2.38986662	3.17211699	1.57810186	0.84140467
80	2.34678656	3.19229262	1.68511128	0.85610929
85	2.31751431	3.23588581	1.80999162	0.87130482
90	2.30280548	3.30631487	1.95753305	0.88701308
95	2.30431592	3.40906644	2.13453426	0.90325944
100	2.32500108	3.55281704	2.35100541	0.92007211
105	2.36989036	3.75155070	2.62238416	0.93748141
110	2.44766055	4.02883306	2.97394890	0.95551998

where $b = -i[(E_n - z)^2 + i\delta]^{1/2}$, $\mathrm{Re}(b) > 0$, and the contour C_H extends from $-i\infty$ to $0 - i\epsilon$ and from $0 + i\epsilon$ to $+i\infty$, with the appropriate branch of b chosen in each case. Results of this calculation of the high-energy part are given terms the function $f_H(Z\alpha)$, defined by

$$\Delta E_H = \frac{\alpha}{\pi}\left[-\tfrac{3}{2}E_n - \tfrac{7}{6}\langle V\rangle + \frac{(Z\alpha)^4}{n^3}f_H(Z\alpha)\right], \quad (4)$$

in Table II. The method of calculation employed here is described in Ref. [11], with the following modifications. In this calculation, the summation over the electron intermediate angular momentum is terminated when the estimated error is less than 10^{-8}, or in a few cases 10^{-7}; this precision is reached with angular momentum less than 10 000. The method of integration for all Z is the method described in Ref. [11] for the range $Z > 60$,

TABLE II. The high-energy part $f_H(Z\alpha)$. Uncertainties shown in parentheses.

Z	$1S_{1/2}$	$2S_{1/2}$	$2P_{1/2}$	$2P_{3/2}$
5	−1.272205(8)	−1.4065(2)	−1.0680(2)	−0.5668(1)
10	−1.2308934(2)	−1.36759(6)	−1.07189(4)	−0.56703(2)
15	−1.1910287(1)	−1.33168(1)	−1.078474(6)	−0.567457(4)
20	−1.1531218(1)	−1.298968(2)	−1.087727(3)	−0.568040(2)
25	−1.1173140(1)	−1.2694841(7)	−1.099753(1)	−0.568772(1)
30	−1.0836006(1)	−1.2431295(7)	−1.1146829(4)	−0.569652(1)
35	−1.0519140(1)	−1.2197641(7)	−1.1326884(4)	−0.5706836(8)
40	−1.0221612(1)	−1.1992426(7)	−1.1539926(4)	−0.5718734(4)
45	−0.9942433(2)	−1.1814350(7)	−1.1788771(3)	−0.5732303(3)
50	−0.9680651(2)	−1.1662336(7)	−1.2076933(2)	−0.5747669(2)
55	−0.9435417(3)	−1.1535597(7)	−1.2408767(2)	−0.5764989(2)
60	−0.9206025(3)	−1.1433706(6)	−1.2789691(1)	−0.5784456(1)
65	−0.8991950(4)	−1.1356667(6)	−1.3226456(1)	−0.5806302(1)
70	−0.8792891(4)	−1.1305025(6)	−1.3727545(1)	−0.5830809(1)
75	−0.8608825(4)	−1.1280025(6)	−1.4303725(1)	−0.5858315(1)
80	−0.8440091(4)	−1.1283865(6)	−1.4968850(1)	−0.5889232(1)
85	−0.8287517(4)	−1.1320101(6)	−1.5741058(4)	−0.5924066(1)
90	−0.8152636(4)	−1.1394315(6)	−1.6644608(8)	−0.5963453(1)
95	−0.8038037(4)	−1.1515265(6)	−1.771281(2)	−0.6008202(1)
100	−0.7948014(4)	−1.1696948(6)	−1.899294(4)	−0.6059379(1)
105	−0.7889782(7)	−1.196252(2)	−2.055501(5)	−0.6118436(1)
110	−0.787598(1)	−1.235241(5)	−2.250848(6)	−0.6187448(1)

TABLE III. Results for the function $F(Z\alpha)$. Uncertainties shown in parentheses.

Z	$1S_{1/2}$	$2S_{1/2}$	$2P_{1/2}$	$2P_{3/2}$
5	6.251627(8)	6.4848(2)	−0.1228(2)	0.1256(1)
10	4.6541622(2)	4.89445(6)	−0.11483(4)	0.13036(2)
15	3.8014108(1)	4.05088(1)	−0.104549(6)	0.136567(4)
20	3.2462556(1)	3.506648(2)	−0.092519(3)	0.143839(2)
25	2.8501042(1)	3.1229593(7)	−0.079066(1)	0.151921(1)
30	2.5520151(1)	2.8388385(7)	−0.0643302(4)	0.160647(1)
35	2.3199761(1)	2.6223358(7)	−0.0483423(4)	0.1699009(8)
40	2.1352284(1)	2.4548292(7)	−0.0310500(4)	0.1795949(4)
45	1.9859437(2)	2.3246900(7)	−0.0123303(3)	0.1896631(3)
50	1.8642743(2)	2.2243377(7)	0.0080122(2)	0.2000537(2)
55	1.7648303(3)	2.1487267(7)	0.0302529(2)	0.2107246(2)
60	1.6838358(3)	2.0945176(6)	0.0547632(1)	0.2216410(1)
65	1.6186364(4)	2.0596107(6)	0.0820375(1)	0.2327729(1)
70	1.5674075(4)	2.0428911(6)	0.1127325(1)	0.2440925(1)
75	1.5289841(4)	2.0441145(6)	0.1477294(1)	0.2555732(1)
80	1.5027775(4)	2.0639061(6)	0.1882263(1)	0.2671861(1)
85	1.4887626(4)	2.1038757(6)	0.2358858(4)	0.2788982(1)
90	1.4875419(4)	2.1668834(6)	0.2930723(8)	0.2906678(1)
95	1.5005122(4)	2.2575400(6)	0.363253(2)	0.3024393(1)
100	1.5301997(4)	2.3831222(6)	0.451711(4)	0.3141342(1)
105	1.5809122(7)	2.555298(2)	0.566883(5)	0.3256378(1)
110	1.660063(1)	2.793592(5)	0.723101(6)	0.3367752(1)

TABLE IV. Special cases of the function $F(Z\alpha)$. Uncertainties shown in parentheses.

Z	$1S_{1/2}$	$2S_{1/2}$	$2P_{1/2}$	$2P_{3/2}$
26	2.78393814(5)	3.0594657(6)	−0.0762190(5)	0.1536189(4)
36	2.27969676(8)	2.5853631(4)	−0.0449909(2)	0.1718068(2)
54	1.7831410(2)	2.1620498(3)	0.0256366(1)	0.20856976(3)
66	1.6073191(2)	2.0548320(3)	0.0878783(1)	0.23502264(1)
79	1.5070511(3)	2.0584011(3)	0.1796152(2)	0.26485443(1)
82	1.4956900(3)	2.0773446(3)	0.2063172(2)	0.27186113(1)
83	1.4928824(3)	2.0853160(3)	0.2158304(3)	0.27420388(1)
92	1.4909160(3)	2.1994938(3)	0.3193408(4)	0.29537993(1)

TABLE V. Comparison with previous results for the $1S_{1/2}$ state at $Z = 70$, 80, and 90. Uncertainties shown in parentheses.

Reference	$F(70\alpha)$	$F(80\alpha)$	$F(90\alpha)$
Desiderio and Johnson [3]	1.53	1.48	1.45
Mohr [6]	1.5675(4)	1.5032(6)	1.4880(7)
Cheng and Johnson [8]	1.57	1.50	1.48
Blundell and Snyderman [10]	1.5674(3)	1.5031(3)	1.4876(2)
This work	1.5674075(4)	1.5027775(4)	1.4875419(4)

TABLE VI. Comparison with previous results for $F(80\alpha)$ for the $n = 2$ states. Uncertainties shown in parentheses.

Reference	$2S_{1/2}$	$2P_{1/2}$	$2P_{3/2}$
Mohr [7]	2.065(2)	0.1884(3)	0.2671(4)
Blundell and Snyderman [10]	2.064(1)	0.188(1)	0.267(1)
This work	2.0639061(6)	0.1882263(1)	0.2671861(1)

however, in most cases, a greater number of integration points is employed here.

The total self-energy correction is given, in units of the electron rest energy $m_e c^2$, by

$$\Delta E = \frac{\alpha}{\pi}\frac{(Z\alpha)^4}{n^3}F(Z\alpha), \tag{5}$$

where

$$F(Z\alpha) = f_L(Z\alpha) + f_H(Z\alpha). \tag{6}$$

The function $F(Z\alpha)$ is tabulated in Table III, and some special cases with slightly higher precision are listed in Table IV.

Results for the $1S_{1/2}$ state at Z =70, 80, and 90 are compared with previous numerical calculations of the Coulomb self-energy in Table V. A similar comparison for the $n = 2$ states at $Z = 80$ is made in Table VI. For $5 \leq Z \leq 45$, there is only one complete earlier calculation [6, 7], and those results are in agreement with the present work within the quoted error estimates. For $Z \geq 90$, some of the results in Refs. [6, 7] differ from the present results by more than the estimated error, but none differs by more than two times the estimated error.

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