Self-energy corrections to the K-electron binding in heavy and superheavy atoms*†

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The self-energy corrections of order α to the K-electron binding energy in high-Z atoms are studied numerically throughout the range $Z = 70$–160. Nuclear finite-size effects are included in the electron wave functions and in the electron propagator to avoid the Coulomb singularity at $Z\alpha = 1$. Denoting the self-energy correction by $\Delta E = \alpha(Z\alpha)^4 F(Z\alpha) mc^2/\pi$, it is found that $F(Z\alpha)$ increases smoothly from a minimum near $Z = 90$ through $F(100\alpha) = 1.46 \pm 0.01$ to $F(160\alpha) = 3.34 \pm 0.16$. For comparison purposes, the self-energy corrections in a Coulomb field for Z between 50 and 130 are evaluated, and the values of $F(Z\alpha)$ thus obtained are in close agreement with previously published values; the Coulomb field values of $F(Z\alpha)$ are very close to the finite-nucleus results for $Z < 90$.

I. INTRODUCTION

Quantum electrodynamics (QED) leads, in lowest order, to two types of radiative corrections to the energy levels of an electron bound in an external potential. They are the electron self-energy and the vacuum polarization corresponding to the Feynman diagrams in Figs. 1(a) and 1(b), respectively. In this work, we will address ourselves to the self-energy contributions only; the vacuum polarization corrections have been discussed in detail elsewhere.[1]

In most of the early work on the self-energy, one was interested in the level shifts in light atoms, such as hydrogen, deuterium, or helium, where precise measurements of the Lamb shift could be performed. Thus, the general approach was to expand the self-energy into a series in $Z\alpha$. A comprehensive treatment of this $Z\alpha$ expansion is given by Erickson and Yennie.[2] References to earlier works on the Lamb shift calculations can be found in Ref. 2, as well as in more recent review articles on QED.[3]

In the $Z\alpha$ expansion calculations, the self-energy level shifts ΔE is usually expressed in the form

$$\Delta E = (\alpha/\pi)(Z\alpha)^4 F(Z\alpha) mc^2. \quad (1)$$

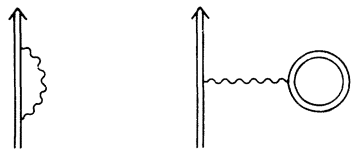

FIG. 1. Feynman diagrams representing the (a) electron self-energy and (b) vacuum polarization. Double lines in these diagrams refer to the propagation of the electron in an external potential.

The function $F(Z\alpha)$ is then expanded into a series involving powers as well as logarithms of $Z\alpha$. The general form of this expansion can be found, for example, in Ref. 2.

The $Z\alpha$ expansion calculation may be a good approximation for small-Z atoms. For $Z \gtrsim 10$, however, contributions from uncalculated terms become so important that successive approximations to the function $F(Z\alpha)$ fail to show signs of convergence. If we want to calculate the level shifts for heavy elements, this $Z\alpha$ expansion is certainly not suitable.

There are various reasons for extending the study of the self-energy radiative corrections to higher-Z atoms. From the purely theoretical point of view, correct prediction of the Z dependence of the level shift by QED is an important test of the theory; this test is especially significant in view of the recent advances in experimental technique which now make possible measurements of the Lamb shift in hydrogenlike systems with Z not small.[4]

From a more practical point of view, though negligibly small in light elements, the self-energy level shift represents a sizeable correction to the binding energies of the inner-shell electrons in heavy and superheavy atoms.[5-7] Thus, the inclusion of the self-energy correction should, in principle, improve the theoretical accuracy of the binding-energy calculations. This, in turn, enables one to estimate the accuracy of present day approximations used in the atomic orbital calculations by direct comparison with precise experimental measurements.

In fact, one may be able to obtain information on the limits of validity of QED in this way. There have been speculations about the possible breakdown of QED at high energy and small interaction distance.[8] An interesting test case will be the study of electrons bound to superheavy nuclei with $Z\alpha$, say, greater than 1. It has been proposed that

if QED is to be replaced by a nonlinear theory with an upper limit to the electric field strength, then for these superheavy elements, there will be dramatic differences between the binding energies calculated from QED and those from the nonlinear theory.[9] Since precise measurements of the binding energies for fermium, $Z=100$, are available,[10] detailed comparisons between the theoretical and experimental inner-shell binding energies for $_{100}$Fm have been made and comparisons show excellent agreement between experiment and the conventional linear version of QED.[11,12] This implies that either we must give up the nonlinear theory completely, or at least that the upper limit of the electric field strength will have to be substantially higher than expected.[13]

In any case, it seems that accurate *ab initio* calculations of atomic binding energies are now possible even in the superheavy atomic region. If we take this for granted, we can then tabulate theoretical x-ray energies to aid in the identification of superheavy elements through their characteristic x-ray spectra. Experiments have been carried out in the identification of elements 102,[14] 104,[15] and recently, 116 and 126,[16] based on the theoretical x-ray energies tabulated from semiempirical calculations.[17] There have been speculations on the possible existence of islands of stability of superheavy nuclei near $Z=114$, 126, and 164.[18] More accurate theoretical calculations of the x-ray energies might aid in the identification of these elements if they are found in nature, or produced artificially.

In spite of all these important applications, our knowledge of the self-energy level shifts in heavy and, especially, superheavy atomic systems is quite inadequate. In what follows, we shall discuss briefly some of the earlier works on the exact evaluation of the self-energy; then we shall turn to the results of the present calculation.

For a pure Coulomb potential, the $1S_{1/2}$ self-energy level shifts for Z in the range 10–110 have been calculated by Mohr, who expanded the bound electron propagator in terms of the known Coulomb radial Green's function.[19] Mohr's study has been extended to L shells[20] and new values for the Lamb shift in hydrogenlike ions have been given.[21] In Fig. 2, the function $F(Z\alpha)$ for the $1S_{1/2}$ state is plotted against the nuclear charge Z. Mohr's values of $F(Z\alpha)$, shown as small closed dots in Fig. 2, illustrate the important point that the self-energy in a pure Coulomb field diverges at $Z\alpha=1$. This divergence is a consequence of the singular behavior of the Coulomb wave functions at $Z\alpha=1$, and has also been pointed out by Labzovskii.[22]

An earlier calculation of the level shift which avoids the $Z\alpha$ expansion has been given by Erickson.[23] The function $F(Z\alpha)$ obtained by Erickson is plotted in the dashed curve of Fig. 2. There remain discrepancies between Erickson's values and those of Mohr which are beyond the stated theoretical uncertainties. In particular, the function $F(Z\alpha)$ given by Erickson decreases with increasing Z, passes smoothly through the Coulomb singularity $Z\alpha=1$, and drops slowly to zero as Z approaches infinity. This, however, is entirely different from Mohr's results, as well as from those of the present calculation, as can be seen in the last section of the present work.

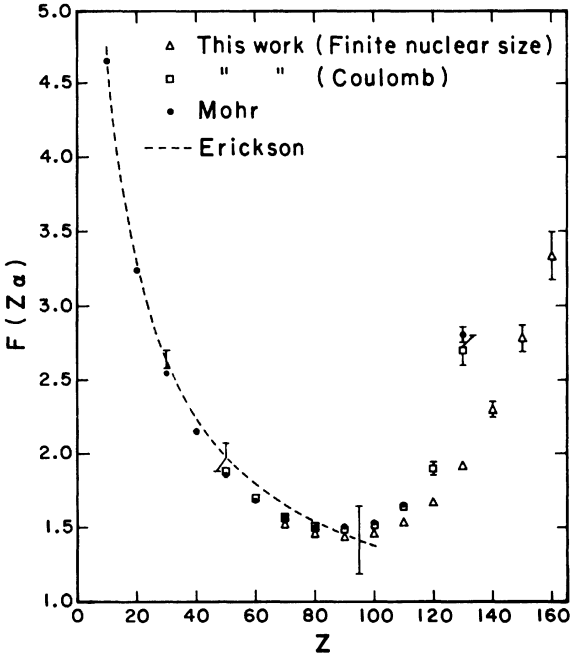

FIG. 2. Values of the function $F(Z\alpha)$ obtained in this calculation and the values of $F(Z\alpha)$ based on the results of Mohr (Ref. 19) and Erickson (Ref. 23).

Among the alternatives to these two approaches, there is the calculation by Desiderio and Johnson[5] (referred to as DJ in the following) based on a method developed by Brown, Langer, and Schaefer.[24] Only values of the $1S_{1/2}$ level shifts for Z between 70 and 90 are given in DJ, and within this range, all three calculations are consistent with each other.

At this point, we would like to mention that there are at least two other calculations on the self-energy level shifts for a wide range of Z. One is the phenomenological approach of Fricke,[25] and the other, a nonrelativistic approximation by Au.[26] These two alternative calculations give results that are of the correct order of magnitude; however, neither seems to be suitable for the treatment of very heavy elements. For our present purposes, we shall not discuss them further.

The method used in the present work is basically the same as that of DJ. There are several advantages associated with this approach. In the first place, the method is concerned with an exact determination of the self-energy term of order α, and expansions in powers of $Z\alpha$ and nonrelativistic approximations are avoided entirely. Since we can extend our numerical evaluations of the level shifts to the superheavy region, we are able to check the results predicted by the other theories near the Coulomb singularity. Moreover, the present method is not limited to pure Coulomb interactions. For example, finite nuclear size effects can be included in the calculation to extend the study of the self-energy level shift beyond the Coulomb limit $Z\alpha = 1$. This is of particular importance in view of the recent rising interests in the superheavy atoms.[16,27,28] In the following sections, we shall first describe the formulation of the DJ method and discuss the associated numerical problems; we shall then present and discuss the results of our calculations.

II. THEORY

In this section, we give a brief description of the formulation of our calculation. Details of the method as well as formulas can be found in DJ and in Ref. 24.

Following DJ, the renormalized self-energy level shift ΔE is given by

$$\Delta E = \Delta E_0 - \Delta E_x + \Delta E_c + \Delta E^{(2)}. \tag{2}$$

Here, ΔE_0 is the self-energy contribution corresponding to Fig. 1(a). The terms ΔE_x, ΔE_c, and $\Delta E^{(2)}$ are all defined in DJ; these terms are introduced to renormalize the electron mass. The term ΔE_x is found from Fig. 1(a) with the bound-electron propagator replaced by a free-electron propagator. Both ΔE_0 and ΔE_x contain linear divergences which cancel, leaving a logarithmically divergent residue. The counter term ΔE_c is also logarithmically divergent, but the sum of the first three terms in Eq. (2) is finite. The fourth term in Eq. (2), $\Delta E^{(2)}$, is also finite and can be evaluated by an independent calculation.

Evaluation of the ΔE_0 term is carried out in Furry's bound interaction representation of QED.[29] The electron wave functions $u_n(\vec{r})$ satisfy the Dirac equation

$$H_0 u_n(\vec{r}) = E_n u_n(\vec{r}), \tag{3}$$

where $H_0 = -i\vec{\alpha}\cdot\vec{\nabla} + \beta m + V(r)$.

Hence, $\vec{\alpha}$ and β are conventional Dirac matrices. Natural units in which $\hbar = c = 1$ are used. $V(r)$ is a time independent external potential. In the numerical calculations to follow, $V(r)$ is chosen either as a pure Coulomb potential, $V(r) = -Z\alpha/r$, or as a Dirac-Hartree-Fock-Slater (DHFS) potential including both finite nuclear size effects and electronic screening; the full Slater average exchange is employed.

To reduce the ΔE_0 term to a form suitable for numerical evaluation, the bound-electron propagator is decomposed into eigenstates of angular momentum using a technique developed by Brown and Schaefer.[30] The angular integration is then carried out, as well as the three-dimensional integration over the photon momentum $\vec{k}$. As a result, ΔE_0 is reduced to a sum of a multipole series over l and an integration over the photon energies ω. For numerical purposes, the path of the ω integration is rotated from the real axis to the imaginary axis in the complex ω plane. One result of the rotation is the appearance of pole terms. ΔE_0 then becomes

$$\Delta E_0 = \Delta E_0' + i\pi R_0 + 2\pi i R_N. \tag{4}$$

Here, $\Delta E_0'$ is the self-energy integral after the path rotation. $i\pi R_0$ and $2\pi i R_N$ are the residues at the poles of the integrand. The expression for the self-energy level shift then becomes

$$\Delta E = (\Delta E_0' - \Delta E_x + \Delta E_c) + \Delta E^{(2)} + i\pi R_0 + 2\pi i R_N. \tag{5}$$

In what follows, we shall refer to the term $(\Delta E_0' - \Delta E_x + \Delta E_c)$ as the main term of our calculation and, as explained before, it is completely finite. Expressions for all the terms in the right-hand side of Eq. (5) can be found in DJ and will not be repeated here. In the next section, we shall discuss some of the numerical aspects of the evaluation of Eq. (5).

III. NUMERICAL CONSIDERATIONS

Since there is no $2\pi i R_N$ term for the $1S_{1/2}$ state, the K-shell self-energy level shift consists of the following three terms:

$$\Delta E = (\text{main term}) + \Delta E^{(2)} + i\pi R_0. \tag{6}$$

The evaluation of the $i\pi R_0$ term is straightforward and involves no essential numerical problems. In the $\Delta E^{(2)}$ term, we have to deal with the Fourier transforms of the electron wave functions. For a Coulomb potential, these transforms can be calculated analytically. For a self-consistent potential, however, the wave functions have to be generated numerically. For high momentum, the integrands of the Fourier transforms oscillate so rapidly that extreme care has to be taken to avoid drastic loss of accuracy as a result of severe numerical cancellation. Upper and lower bounds of the $\Delta E^{(2)}$ term have carefully been es-

timated. The overall error resulting from this term is found to be less than 1% even in the worst cases.

The most difficult part of our numerical program is perhaps the evaluation of the main term. Specifically, we have to deal with the sum of a multipole series and an integration over the photon energy ω. For numerical purposes, we can only carry out the calculation to a finite multipole order l_{max} and to some cutoff energy ω_{max}. Beyond these limits, extrapolation techniques are required.

Gaussian quadrature is used to carry out the ω integration from 0 to ω_{max}. Thus, before any extrapolation, the calculation reduces to the evaluation of a two-dimensional series in l and ω. As an illustration, we refer to Table I of DJ in which the integrand of $-(\Delta E_0' - \Delta E_x)$ is tabulated as a function of ω and l for the K electron of Hg($Z = 80$) in a pure Coulomb potential.

The techniques employed in the extrapolation of the multipole series and those used in the ω integration have been discussed in DJ and will not be repeated here. Essentially, these techniques are designed for the specific forms of the integrand in the asymptotic regions. Accuracy of these extrapolations depends strongly on the cutoff values, l_{max} and ω_{max}. The choice of the cutoff, in turn, results from a compromise between two factors. On the one hand, we always want to choose as high a cutoff as possible to approach closely the asymptotic region and thus to ensure a good start for the extrapolation. On the other hand, the numerical program becomes more and more unstable as l and ω increase, resulting in less and less accurate values for the integrand. In particular, the stability of the numerical program decreases with increasing Z. Various methods have been developed to monitor the accuracy of the extrapolations and to determine the optimum cut-off values, l_{max} and ω_{max}. The extrapolations beyond l_{max} and ω_{max} are believed to be the main causes of our numerical errors. We shall return to this point when we discuss our error estimates in Sec. IV.

IV. RESULTS

For a pure Coulomb potential, the results of our calculation on the $1S_{1/2}$ self-energy level shifts with Z in the range 50–130 are presented in Table I. Comparisons are made with previous calculations; throughout the 50–130 range, our results agree well with Mohr's calculations. In particular, our values of $F(Z\alpha)$ increase very rapidly as $Z\alpha \to 1^-$, in agreement with Mohr's determination.

To go beyond the Coulomb limit $Z\alpha = 1$, finite nuclear size effects have to be included in the calculation. We use a DHFS potential because it has the advantage that the effects of electronic screening are automatically included along with those of finite nuclear size. The nuclear model employed is that of a uniformly charged sphere with a nuclear radius R being given approximately by

$$R \simeq 1.2A^{1/3} \text{ (Fermi)}. \tag{7}$$

Here A refers to the atomic weight of the nucleus; for Z greater than 100, the values of A are obtained from Ref. 27. In Table II, results of the $1S_{1/2}$ level shift including finite nuclear size effect and electronic screening for Z in the range 70–160 are listed. Values of $F(Z\alpha)$ for both the Coulomb and finite nuclear cases are plotted in Fig. 2.

Error estimates are difficult to make in view of the complexity of the numerical program. However, we believe that the main source of error arises from the extrapolation of the integration described in the preceding section. When pos-

TABLE I. Values of the $1S_{1/2}$ self-energy level shifts (in units of Ry) and the function $F(Z\alpha)$ for a pure Coulomb potential.

Z	$i\pi R_0$	$\Delta E^{(2)}$	Main	ΔE	$F(Z\alpha)$ This work	$F(Z\alpha)$ Mohr [a]	$F(Z\alpha)$ Desiderio [b]
50	31.19	−9.84	−18.44	2.91	1.88	1.864	···
60	37.46	−9.61	−22.39	5.46	1.70	1.684	···
70	43.83	−7.97	−26.51	9.35	1.57	1.568	1.53
80	50.41	−4.71	−30.50	15.20	1.50	1.503	1.48
90	57.41	0.35	−33.76	24.00	1.48	1.488	1.45
100	65.24	7.27	−35.12	37.39	1.51	1.532	···
110	74.8	15.4	−30.5 ± 1.0	59.7 ± 1.0	1.65 ± 0.02	1.661	···
120	88.6	20.4	−11.6 ± 2.1	97.4 ± 2.1	1.90 ± 0.04	···	···
130	116.3	−24.3	98.1 ± 11.5	190.1 ± 11.5	2.70 ± 0.10	2.808 ± 0.050 [c]	···

[a] Values except $F(130\alpha)$ are taken from Reference 19.
[b] Reference 5.
[c] Private communication.

TABLE II. Values of the $1S_{1/2}$ self-energy level shifts (in units of Ry) and the function $F(Z\alpha)$ for a DHFS potential including finite nuclear size.

Z	$i\pi R_0$	$\Delta E^{(2)}$	Main	ΔE	$F(Z\alpha)$
70	43.46	−8.12	−26.23	9.11	1.53
80	50.01	−5.23	−29.93	14.85	1.47
90	56.94	−0.57	−33.00	23.37	1.44
100	64.61	5.99	−34.42	36.18	1.46
110	73.67	14.37	−32.53	55.51	1.53 ± 0.02
120	85.45	23.70 ± 0.03	−23.73	85.42	1.67 ± 0.02
130	102.64	31.10 ± 0.05	1.8 ± 2.1	135.5 ± 2.1	1.92 ± 0.03
140	131.3	27.6 ± 0.2	60.0 ± 4.8	218.9 ± 4.8	2.30 ± 0.05
150	179.7	−3.0 ± 0.4	171.5 ± 11.3	348.2 ± 11.3	2.78 ± 0.09
160	257.2	−82.8 ± 0.8	367.0 ± 26.0	541.4 ± 26.0	3.34 ± 0.16

sible, the cutoff energy ω_{max} is so chosen that the extrapolated tail integral is at least two orders of magnitude smaller than the truncated integral. Thus, the overall accuracy of our calculation should not be affected significantly by uncertainties in the extrapolation. For most of our results, errors are believed to be less than 1%.

However, when Z is very large, or when $Z\alpha \simeq 1$ in the case of a pure Coulomb potential, the tail of the ω integration drops off so slowly that the remaining part of the integral, after truncation, is not at all negligible. Since the numerical program is unstable at high energy as explained in the preceding section, we must limit the size of ω_{max}. We can roughly estimate the corresponding numerical errors in terms of the uncertainties in the tail integrals. Our errors estimated from the tail integrals are included in Tables I and II and in Fig. 2.

Of course, from the theoretical point of view, apart from these numerical errors, there are also uncertainties arising from the specific nuclear models chosen and from the values of the nuclear radius employed in the calculations. We believe, however, that the level shifts should be insensitive to these factors. In fact, we have changed the radius R by a few percent and the resulting changes to the level shifts are so small that they are completely negligible in comparison with the numerical uncertainties. We therefore assume that errors arising from other sources are comparatively smaller, and can be absorbed in the rough error estimates already made.

As we have mentioned in the introduction, accurate DHF calculations of the $1S_{1/2}$ electron binding energy including various corrections have been made for fermium $Z = 100$,[11,12] and the theoretical values are in excellent agreement with precise experimental measurements. However, the value of the self-energy correction used in Ref. 11 is obtained from an extrapolation based on the results of DJ for $Z = 70 - 90$. Since a more exact value of the $Z = 100$ self-energy is now available, the theoretical $1S_{1/2}$ binding energy of $_{100}$Fm can be reexamined by replacing the value of the self-energy correction in Ref. 11 by that obtained in the present calculation. As can be seen from Table III, the agreement between the present theoretical value and the experiment is still quite satisfactory. In fact, if the contribution from other binding effects is replaced by that given in Ref. 12 instead of that given in Ref. 11, the theoretical value thus obtained is still consistent with experimental measurements. This shows that the order of magnitude of the present results is reasonable and illustrates the utility of the DHF scheme for calculating the binding energies in the superheavy region.

As we can see in Fig. 2, the function $F(Z\alpha)$ increases rapidly for $Z > 100$. This means, in accordance with Eq. (1), that the rate of increase of the self-energy correction is faster than $(Z\alpha)^4$ in the superheavy region. The level shift at $Z = 100$ already accounts for 0.3% of the $1S_{1/2}$ electron binding energy. In view of the strong Z dependence of this correction, the effect of the level shifts for higher-Z atoms will be even more important. It has been pointed out that for some critical charge $Z_{cr} \simeq 170$, the $1S_{1/2}$ state will reach the lower continuum with binding energy $B = 2mc^2$. Further increase in Z will lead to "diving" of the bound state into the positron continuum.[27,28] Rough estimates based on the extrapolation of our

TABLE III. Comparison of the theoretical and experimental $1S_{1/2}$ electron binding energy (keV) in $_{100}$Fm.

Sum of all other effects [a]	−142.449	−142.449
Self-energy	0.492 [b]	0.484 [a]
$E_{1S}(Z=100)$	−141.957	−141.965
Experimental value [c]	−141.967 ± 0.013	−141.967 ± 0.013

[a] Reference 11.
[b] This work.
[c] Reference 10

present results shows that the self-energy correction will at least be 1% of the $1S_{1/2}$ electron binding energy near the critical region. Together with contributions from other effects, such as the vacuum polarization which has already been examined elsewhere,[31] we expect that the value of the critical charge Z_{cr} will be altered somewhat. This will be of interest because the prediction of the point of diving by QED could be a test of the theory in the presence of a strong external field.

It should be mentioned in closing that Labzovskii (Ref. 22) predicts the Coulomb singularity in self-energy at $Z\alpha = 1$ and estimates the level shift for a finite nucleus at $Z = 137$ to be $\Delta E \simeq 25 \pm 10$ keV. One sees from Table II that the actual value of the self-energy at 137 is an order of magnitude smaller than Labzovskii's estimate.

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