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Improved many-body perturbation-theory calculations of the $n=2$ states of lithiumlike uranium

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A recent calculation of the spectrum of the $n=2$ states of lithiumlike uranium is improved by a more accurate treatment of the effect of finite nuclear size and a more complete calculation of higher-order corrections to Breit and mass-polarization contributions. Predictions for the $2s_{1/2}$-$2p_{1/2}$ and $2p_{1/2}$-$2p_{3/2}$ splittings, incorporating a phenomenological treatment of radiative corrections, are presented.

Quantum electrodynamics (QED) is known to describe with high accuracy the behavior of charged leptons in weak external fields, such as the magnetic fields of Penning traps or the Coulomb potential of the hydrogen nucleus. It is of fundamental interest to test this theory in more extreme environments. For the atomic case, an ideal place to make such tests is in the heaviest long-lived atom, uranium. The simplest system in which tests of the Lamb shift can be made is one-electron uranium, for which accurate theoretical predictions have been made.[1] However, experiments on this system are sufficiently difficult so that to date no measurements have been reported. The next simplest system is heliumlike uranium, and an effect related to the Lamb shift has been measured[2] in this ion. The actual experiment is a measurement of a lifetime sensitive to the $2\,^3P_0-2\,^3S_1$ energy separation that has a QED component, including nuclear finite size, of

$$\Delta E = 71.0(83)\ \text{eV}\ , \tag{1}$$

in agreement with the theoretical value[1,3] 74.3(4) eV.

The purpose of this paper is to improve the theory underlying the determination of the Lamb shift from the spectrum of lithiumlike uranium. This spectrum is decidedly more accessible experimentally because the $2p_{1/2}$ state is part of the ground-state manifold and is easily populated. Indeed, an experiment is presently underway[4] which aims at measuring the $2s_{1/2}$-$2p_{1/2}$ splitting in this system to an accuracy of 0.1 eV, which is 0.2% of the one-electron Lamb shift.

Because three electrons are present, an accurate treatment of the many-body problem is required and, because of the high nuclear charge, a relativistic treatment is appropriate. Relativistic many-body perturbation theory (MBPT) is an ideal tool to treat the spectrum of this ion, because at large Z the perturbation expansion converges very rapidly. In addition, there is a one-to-one correspondence of terms in MBPT with a set of Furry representation[5] QED Feynman graphs, so that the calculations are rigorously based in field theory. Consideration of other QED graphs allow an unambiguous identification of radiative corrections, the most important of which enter in order $Z^4\alpha^3$ a.u. and order $Z^3\alpha^3$ a.u.

In a recent paper,[6] we calculated the energy levels of the $n=2$ states of the lithium isoelectronic sequence starting from the Hartree-Fock potential. In that work, we included only one QED effect, that of retardation on the Breit interaction, but calculated the Coulomb correlation to third order and correlation corrections to the Breit interaction to second order. Mass polarization was accounted for by use of the Hughes-Eckhart formula.[7] Then, by comparing our theory with experiment, we could infer the size of uncalculated QED effects, which were dominated by the one-electron Lamb shift, but which were systematically smaller than that effect. In this paper we make two modifications to that work for the case of $Z=92$. The first is an improved calculation of the nuclear finite-size correction, which we now model using a deformed Fermi distribution. The second is the inclusion of a more sophisticated treatment of mass polarization and of corrections to the Breit interaction which we developed for use on the sodium isoelectronic sequence.[8] These effects result in small, but significant, changes from our previous theory. We also include the results of a treatment of nuclear polarization by Plunien *et al.*[9] After we describe these modifications, we will also incorporate radiative corrections in a phenomenological manner. To give a sense of the relative importance of the new calculations, we will compare them in the following with the point nucleus one-electron Lamb shift (referred to in the following as the point Coulomb shift) for the $2s_{1/2}$-$2p_{1/2}$ splitting, which is 1.572 a.u., or 42.78 eV.

In our previous treatment, the effect of nuclear finite size was accounted for by solving the Hartree-Fock equations in the presence of the Coulomb field of a nucleus with a spherically symmetric Fermi distribution of charge. The Fermi parameters were taken from a fit designed[10] for the entire periodic table obtained from fitting both electron scattering data and muonic x-ray

TABLE I. MBPT contributions to $n=2$ energy levels of lithiumlike ^{238}U; units of a.u.

State	$2s_{1/2}$	$2p_{1/2}$	$2p_{3/2}$
$E^{(0)}_{\text{point nucleus}}$	−1211.028 91(2)	−1199.305 71(2)	−1043.786 26
$E_{\text{nuclear size}}$	1.316 40(33)	0.128 83(3)	−0.008 23(2)
$E^{(2)}$	−0.010 72(1)	−0.030 66(1)	−0.012 27(1)
$E^{(3)}$	−0.000 03	−0.000 08	−0.000 05
$B^{(1)}_{\text{Breit}}$	1.263 83	2.628 51	0.926 09
$B^{(1)}_{\text{ret}}$	0.023 93	0.010 42	−0.235 35
$B^{(2)}$	−0.007 69	−0.013 42	−0.003 64
$B^{\text{RPA a}}$	−0.005 79	−0.018 83	−0.009 01
$B^{(3)}$	0.000 04	0.000 20	0.000 03
$P^{(1)}$	0.000 00	−0.001 25(125)	−0.001 34(134)
$P^{(2)}$	0.000 00	0.000 01	0.000 00
Reduced mass	0.002 79	0.002 76	0.002 41
E^{total}	−1208.446 15(33)	−1196.599 22(125)	−1043.127 62(134)

[a]Random-phase approximation.

measurements. However, the uranium nucleus has been carefully studied through a high-accuracy muonic x-ray experiment, and for the purposes of this paper we adopt the parameters determined from that work.[11] Specifically, we use a modified Fermi distribution

$$\rho(\mathbf{r})=\frac{\rho_0}{1+e^{(\mathbf{r}-R)/a}}\ ,$$

$$R=c[1+\beta_2 Y_{20}(\hat{\mathbf{r}})+\beta_4 Y_{40}(\hat{\mathbf{r}})]\ ,$$

with $c=7.0110(12)$ fm, $a=0.5046(9)$ fm, $\beta_2=0.2653(14)$, and $\beta_4=0.0672(49)$. Because the ground state of ^{238}U has $J=0$, we take a spherical average of this distribution, and then solve the Hartree-Fock equations in the corresponding potential. The results are presented in Table I. The change from the previous calculation is most significant for the $2s_{1/2}$ state, giving a positive 0.032-a.u. shift, which is 2% of the point Coulomb shift: the $2p_{1/2}$ state shifts upwards by 0.19%, while the $2p_{3/2}$ state shifts by a negligible amount. While the nuclear finite size effect is quite large, being 84% of the point Coulomb shift for the $2s_{1/2}$ state, because of the high accuracy of the muonic x-ray experiment the uncertainties coming from finite size are only 0.02% of that shift. Note also that a measurement of the fine-structure splitting is less sensitive by an order of magnitude to such uncertainties.

Although the change in the Hartree-Fock potential resulting from use of the more realistic nuclear charge distribution is relatively small, we have recalculated all of the many-body perturbation theory corrections considered in Ref. 6, except for $E^{(3)}$, using the new potential. In addition, we have incorporated the higher-order terms described in Ref. 8 for the Breit interaction and have also treated mass polarization as in that reference, replacing the use of the Hughes-Eckhart formula.[7] In this case the changes are quite small, never entering above the level of 0.02% of the point Coulomb shift. The results are shown in Table I. We now, however, separate the lowest-order exchange of a transverse photon into the instantaneous Breit interaction and its retardation correction; only the sum of these two was tabulated in Ref. 6. Note that the retardation term $B^{(1)}_{\text{ret}}$ is relatively small compared to the point Coulomb shift for the $2s_{1/2}$ and $2p_{1/2}$ states, but is quite large for the $2p_{3/2}$ state. We have assigned a 100% error estimate for reduced-mass effects because we have found considerable sensitivity to the form of the momentum operator used in the mass-polarization operator. Specifically, significantly different answers are found depending on whether one uses the Dirac form $\mathbf{p}/m \rightarrow c\boldsymbol{\alpha}$, which was used for the present calculation, or the gradient form $\mathbf{p}/m \rightarrow -i\nabla/m$. This sensitivity is presumably associated with the fact that uncalculated corrections of order $(Z\alpha)^2$ are quite large at $Z=92$. Because of the small size of reduced-mass effects in this ion, this uncertainty contributes under 0.1% of the point Coulomb shift. Another nuclear effect that must be considered is nuclear polarizability. The ^{238}U nucleus has relatively low-lying excited states that can be virtually excited and give rise to nuclear polarization energy shifts. The size of the polarization correction has recently been estimated by Plunien *et al.*[9] for the 1s state; the calculation included the effect of both low-lying rotational states and giant resonances. If one scales the result of Ref. 9 by $1/n^3$, an additional nuclear structure effect of 0.004 63 a.u. results for the $2s_{1/2}$ state, which is tabulated in Table II. No error estimate is given for that entry because the calcula-

TABLE II. MBPT, nuclear polarization, and extrapolated radiative correction contributions to $n=2$ splittings in lithiumlike ^{238}U; units of eV. Note that while there are no error bars given for nuclear polarization and radiative corrections, they have systematic uncertainties as discussed in the text.

	$2p_{1/2}$-$2s_{1/2}$	$2p_{3/2}$-$2p_{1/2}$
MBPT	322.374(35)	4176.21(5)
Nuclear polarization	−0.126	
Extrapolated QED	−41.225	2.15
Total	281.023(35)	4178.36(5)

tion of Ref. 9 is correct only in order of magnitude. The difficulty of accurately calculating nuclear polarizability is likely to limit the ultimate precision of QED tests available from ^{238}U.

We now consider uncalculated radiative corrections. As mentioned above, Furry representation[5] QED offers a consistent framework for the calculation of these effects. Briefly, what is required is (i) a recalculation of the one-electron Lamb shift in whatever potential the MBPT calculation is carried out in, which contributes in order $Z^4\alpha^3$; (ii) an extension of the QED graphs in which two Coulomb photons are exchanged, which give rise to the second-order MBPT energy, to graphs in which transverse photons are also exchanged, which leads to effects of order $Z^3\alpha^3$ a.u.; and finally (iii) vertex and self-energy corrections to one photon exchange, which also enter in order $Z^3\alpha^3$. (A further radiative correction associated with three-body forces has been shown to be very small.[12]) These calculations are all comparable in difficulty to the Lamb shift calculation itself. Because this undertaking will take some time, it is of interest to find other means of estimating the size of radiative corrections. We choose to utilize the information available from experiments on lower-Z lithiumlike ions. The control of correlation effects at under the level of experimental uncertainties allows the unambiguous determination of the size of radiative corrections for ions with $Z \leq 36$. We formed using the tables of the one-electron Lamb shift in Ref. 10 a function $F(Z)$ valid for noninteger Z using a fifth-order interpolation method, and then made a least-squares fit of the inferred radiative corrections (the difference between theory and experiment in Ref. 6) to the function $F(Z-\beta)$. This was done for both the $2s_{1/2}$-$2p_{1/2}$ and $2p_{1/2}$-$2p_{3/2}$ splittings, leading to the respective values for β of 0.9560 and 1.422. We then used $F(Z-\beta)$ to extrapolate the radiative corrections to $Z=92$. The results are presented in Table II. While this is a significant extrapolation, the dominant effect of the one-electron Lamb shift is, of course, correctly described; however, if the behavior of the screening corrections is significantly different, a systematic error will be introduced. We note that Seely[13] has recently taken the results of Ref. 6, together with a different method of estimating radiative corrections based on the use of Grant's code[14] for ions with $Z \leq 54$, achieving a good fit to the data. We find from Grant's code the value -1.536 a.u. at $Z=92$ for the $2s_{1/2}$-$2p_{1/2}$ radiative corrections. This value can be compared to -1.515 a.u., determined by our extrapolation procedure. The discrepancy between the two values is to be expected, since both come from phenomenological arguments, and do not represent first principles QED calculations. We would interpret the difference of 0.57 eV, which is 1.3% of the point Coulomb shift, as a measure of theoretical uncertainty arising from the lack of such calculations. Because experiment is likely to reach this level of precision in the near future, this strongly emphasizes the need for carrying out calculations of the radiative corrections, which, although difficult, are well defined and unambiguous. Once they are carried out, the study of the spectrum of lithiumlike uranium will provide a stringent test of our understanding of QED and the many-body problem in intense Coulomb fields.

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