Nuclear-Size Effects on Vacuum Polarization in Muonic Pb†

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The effect of finite nuclear size on the vacuum-polarization charge density is studied. The results to third order $\alpha(Z\alpha)^3$, and to all orders $\alpha(Z\alpha)^n$, $n \geq 3$, are presented with special attention focused on the $5g_{9/2}$-$4f_{7/2}$ transition in muonic Pb. In addition, the accuracy of analytic calculations exploiting the smallness of the electron mass and of the nuclear radius is discussed.

One of the major tests of quantum electrodynamics lies in the calculation of transition energies in high-Z muonic atoms. The most important radiative corrections to these transition energies come from vacuum polarization (VP). Even the higher-order $\alpha(Z\alpha)^n, n \geq 3$, VP is important because of the high resolution of recent experiments. Since discrepancies between theory and experiment have been observed,[1] most notably in $_{56}$Ba and $_{82}$Pb, several workers[2-4] have looked at the higher-order VP in more detail. In particular, the effect of finite nuclear size on the VP charge density has been studied. However, complete agreement on the size of this effect has not yet been reached. In the hope of eliminating this uncertainty, this Letter presents the results of an independent numerical study of the problem.

In muonic Pb, a 42 ± 20 eV discrepancy[3] exists between theory and experiment for the $5g_{9/2}$-$4f_{7/2}$ transition when the theoretical contribution to the transition energy due to higher-order VP is calculated for a point nucleus. For a finite-size nucleus, characterized by a radius R, the VP charge density $\rho(R,r)$ differs from its point-nucleus form in such a way as to increase the transition energy. This has the effect of increasing the discrepancy between theory and experiment. For the $5g$-$4f$ transition this increase was calculated numerically by Rinker and Wilets[2] to be 16 eV. On the other hand, the analytic calculations of Arafune[3] and Brown *et al.*,[4] using the approximations based on the smallness of m_e and the ratio of the nuclear radius to the muonic orbit R/a_0, gave 5 eV.

The calculation reported in this Letter gives 6 eV for the energy shift of the $5g$-$4f$ transition. The central assumption in this calculation is that the finite nuclear size is felt only by the $j=\frac{1}{2}$ electrons in the VP density. It is shown that this assumption leads to an error of less than 0.5 eV in the calculated 6 eV. The third order $\alpha(Z\alpha)^3$ contribution and the contribution to all orders, $\alpha(Z\alpha)^n$, $n \geq 3$, are studied separately. This provides a check on the internal consistency of the final results since the numerical techniques required to calculate each are quite distinct. As a further check, the point-nucleus limit $R \to 0$ is examined and compared to the results of Wichmann and Kroll[5] and of Blomqvist.[6] Finally, setting $m_e = 0$ and expanding to lowest order in R/a_0 in my calculation, I recover the 5-eV result of Refs. 3 and 4.

Wichmann and Kroll[5] showed that $\rho(R,r)$ is proportional to a contour integral along the imaginary energy axis of the trace of the Green's function $\mathrm{Tr}G(\tilde{r},\tilde{r};z)$ for the Dirac equation. Expanding G in terms of the radial Green's functions G_k for "angular momentum" $k = \pm(j+\frac{1}{2})$, we define the VP density ρ_k for a given k, through the contour integral of $\mathrm{Tr}G_k$. The radial Dirac equation for G_k may be converted to an integral equation from which a power-series expansion of G_k in powers of $Z\alpha$ is obtained. In this way the Uehling term, $\rho_k^{\,1}$, and the third-order density, $\rho_k^{\,3}$, may be isolated. Since the $k = \pm 1$ ($S_{1/2}, P_{1/2}$) states are most sensitive to nuclear size, a natural approximation for $\rho(R,r)$ is

$$\rho(R,r) \cong \rho_{|k|=1}(R,r) + \sum_{|k|\geq 2} \rho_{|k|}(0,r); \tag{1}$$

i.e., the energy shift due to finite-size effects on VP is assumed to come mainly from the $|k|=1$ density. The accuracy of this approximation depends on how large the contribution from the $|k| \geq 2$ density is. The size of the $|k| \geq 2$ contribution to the total density can be estimated using the results of Ref. 5 for a point nucleus. The ratio, $Q_{k\geq 2}/Q_{k=1}$, of the VP charge accumulated at the origin for $|k| \geq 2$ and for $|k|=1$ gives a measure of the relative size of $\rho_{k\geq 2}$ to $\rho_{k=1}$. For order $\alpha(Z\alpha)^n$, $n \geq 5$, in Pb, Ref. 5 gives $Q_{k\geq 2}{}^{5+}/Q_{k=1}{}^{5+} \sim 0.008$ with $Q_{k=1}{}^{5+} = -6.83 \times 10^{-4}|e|$. From this we conclude that the $|k| \geq 2$ contribution to the density is less than 1% for these orders. For

TABLE I. Absolute energy shifts (in eV) due to VP orders $\alpha(Z\alpha)^n$ in Pb using nuclear models I and II described in text. The $|k| \geq 1$ are calculated from Eqs. (4) and (5).

Order, $\|k\|$	Model R (fm)	$5g_{9/2}$	$4f_{7/2}$	$3d_{5/2}$
$n=3, \|k\|=1$	I 5.5	43.39	79.24	151.9
	II 7.1	43.41	79.28	152.1
	I 0.6	45.16	85.10	177.0
	I 0.06	45.20	85.27	178.0
$n \geq 3, \|k\|=1$	I 5.5	48.51	88.36	168.3
	I 0.6	51.34	97.12	202.6
	I 0.06	51.39	97.42	204.3
$n \geq 5, \|k\|=1$	I 5.5	5.12	9.12	16.4
	I 0.06	6.19	12.15	26.3
$n \geq 3, \|k\|=1$	I 5.5	51.9 ± 0.1	94.8 ± 0.5	181.7 ± 2

third order, Ref. 5 gives the charge summed over k: $Q_{\mathrm{WK}}{}^3 = -4.487 \times 10^{-3} |e|$. To calculate what fraction of $Q_{\mathrm{WK}}{}^3$ comes from $|k|=1$, I calculated $\rho_{k=1}{}^3$ numerically using the integral equation for $G_{k=1}{}^3$ in which I set $m_e = 0$. The nuclear charge distribution used in the calculation was a shell of radius R. The $m_e = 0$ limit isolates the piece of $\rho_1{}^3$ which is only a function of r/R. It is precisely this piece that reduces to a δ function as $R \to 0$. (This assumes that the integral of $\rho_1{}^3$ over all space exists, which is the case here.) The third-order charge due to $|k|=1$ is then

$$Q_1{}^3 = \int_0^\infty dr\, 4\pi r^2 \rho_1{}^3(R, r, m_e = 0). \tag{2}$$

Note that $Q_1{}^3$ is in fact independent of R. This was checked numerically by calculating $Q_1{}^3$ for $R = 6.$, 0.6, 0.06 fm with the result in each case being $Q_1{}^3 = -4.177 \times 10^{-3} |e|$. Thus $Q_1{}^3/Q_{\mathrm{WK}}{}^3 = 0.93$; i.e., 7% of the third-order density comes from $|k| \geq 2$. Summarizing these relations,

$$Q_{k=1}{}^3 \cong 13.5 Q_{k\geq 2}{}^3 \cong 6.12 Q_{k=1}{}^{5+} \cong 770 Q_{k\geq 2}{}^{5+}. \tag{3}$$

For the case of a point nucleus, Blomqvist[6] has calculated the $5g$-$4f$ energy shift in Pb due to third-order VP to be $\Delta E^3(R=0) = -43$ eV. For a finite-size nucleus I calculated $\rho_1{}^3(R, r)$ numerically with $m_e \neq 0$ using two different models of the nuclear charge density: (I) a shell density, $\rho_{\mathrm{nuc}} = \delta(r-R)/(4\pi R^2)$ and (II) a uniform density, $\rho_{\mathrm{nuc}} = \theta(R-r)/(4\pi R^3/3)$. Tables I and II contain the results. The $R \to 0$ limit was examined by calculating the energy shifts for $R = 0.6$ and 0.06 fm. Extrapolating to $R=0$, we get $\Delta E_{k=1}{}^3 = -40$ eV for the $5g$-$4f$ transition. From Eq. (3) we estimate the $|k| \geq 2$ contribution to be $\Delta E_{k\geq 2}{}^3 = -3$ eV. Thus, $\Delta E_{k\geq 1}{}^3 = -43$ eV, in agreement with Ref. 6.

For the calculation of the finite-size effect, R was chosen in each model so that $[\langle r^2 \rangle_{\mathrm{nuc}}]^{1/2} = 5.5$ fm.[7] Dirac wave functions were used in the expectation values, although Schrödinger wave functions gave the same results to within 1–2%. (It should be noted that the uncertainty in the muon mass, ± 400 eV, alone generates a ± 2 eV uncertainty in the $5g$-$4f$ x ray.) Comparing the two model distributions in Table I, we see that the energy shifts are sensitive only to $\langle r^2 \rangle_{\mathrm{nuc}}$ for these high-angular-momentum states. The result from Table II is $\Delta E_1{}^3 = -36$ eV for $[\langle r^2 \rangle_{\mathrm{nuc}}]^{1/2} = 5.5$ fm. Thus the finite nuclear size caused a 10% decrease in magnitude of the third-order VP contribution for $|k|=1$. Since the $|k| \geq 2$ electrons are less sensitive to nuclear size, we estimate $-3\text{ eV} \leq \Delta E_{k\geq 2}{}^3(R) \lesssim 0.9 \times \Delta E_{k\geq 2}{}^3(0) \cong -2.7$ eV. Thus the total contribution to the $5g$-$4f$ x ray from third-order VP is $\Delta E^3 = -39$ eV as compared to the point-nucleus value of -43 eV.

To solve for the energy shift to all orders $\alpha(Z\alpha)^n$, $n \geq 3$, we construct the Green's function for the Dirac equation in the field of a finite-size nucleus and remove the Uehling term. Since the

TABLE II. The VP contribution to $5g_{9/2}$-$4f_{7/2}$ transition in Pb energy (in eV) for orders $\alpha(Z\alpha)^n$. The error in the contribution from $|k| \geq 2$ is less than 0.5 eV.

Order, $\|k\|$	$R_{\mathrm{rms}} = 5.5$ fm	$R=0$
$n=3, \|k\|=1$	-36	-40
$\|k\| \geq 2$	-3	-3
$n \geq 5, \|k\|=1$	-4	-6
$\|k\| \geq 2$	(<0.1)	(<0.1)
$n \geq 3, \|k\| \geq 1$	-43	-49

third-order calculation showed that the energy shift is sensitive only to $\langle r^2\rangle_{\rm nuc}$, a shell distribution (model I) is used with $R = 5.5$ fm. The shell distribution is most convenient since both the internal and external wave functions are simple. The Green's function is then constructed[5] with the regular and irregular solutions of the Dirac equation: For $r < R$ these are spherical Bessel functions and for $r > R$ they are Whittaker functions. Both types of functions are subject to rapid, high-precision, numerical computation.[8] The Uehling contribution is obtained from the integral equation for the radial Green's function and may be expressed in terms of elementary and exponential integral functions. The details of these and of all other calculations mentioned in this Letter will be given in a subsequent paper. The results of the calculations are listed in Tables I and II.

In the $R \to 0$ limit we get for orders $n \geq 3$, $\Delta E_{k=1}{}^{3+} = -46$ eV. From Eq. (3), the contribution of $|k| \geq 2$ to these orders is estimated to be -3 eV from third order and <0.1 eV from orders $n \geq 5$. The total shift for orders $n \geq 3$ is then $\Delta E^{3+}(R=0) = -49$ eV in agreement with Ref. 6. For finite radius we rewrite Eq. (1) as

$$\Delta E^{3+}(R) \cong \Delta E_{k=1}{}^{3+}(R) + \Delta E_{k\geq 2}{}^{3+}(0), \tag{4}$$

where the $|k| \geq 2$ term is estimated from $\Delta E_1{}^{3+}(0)$ using Eq. (3). The accuracy of Eq. (4) is then estimated by

$$\begin{aligned}\delta &= \Delta E_{k\geq 2}{}^{3+}(R) - \Delta E_{k\geq 2}{}^{3+}(0),\\ &\cong 0.074[\Delta E_1{}^3(R) - \Delta E_1{}^3(0)]\\ &\quad + 0.008[\Delta E_1{}^{5+}(R) - \Delta E_1{}^{5+}(0)],\end{aligned} \tag{5}$$

where Eq. (3) has again been used. For the $5g$-$4f$ transition, the error in the approximation in Eq. (4) is then estimated to be less than 0.5 eV with the result that $\Delta E^{3+}(R) = -43$ eV. Thus, the finite-nuclear-size effect on VP increases the energy of the x ray by 6 eV.

The VP densities $\rho_1{}^3$ and $\rho_1{}^{3+}$ calculated here with the energy contour along the imaginary axis satisfy gauge invariance. Therefore a good check on the numerical accuracy of these densities is provided by the evaluation of their integral over all space. It was found that for $r \lesssim 60$ fm the densities were negative, while for $r \gtrsim 60$ fm, they were positive; the densities were calculated out to $8\lambda\!\!\!^{-}_e$. The amount of charge contained in the region $r \lesssim 60$ fm was $\sim -4\times 10^{-3}|e|$, while the total charge out to $r = 8\lambda\!\!\!^{-}_e$ was $\sim -10^{-8}|e|$. Thus, better than five-place accuracy was achieved for these densities.

To study the accuracy of the $m_e = 0$ and lowest order in R/r approximations[4] in the calculation of $\Delta\rho = \rho(R,r) - \rho(0,r)$, for $r \geq R$, we note that $\Delta\rho$ is proportional to the energy contour integral of the difference, ΔG, between the Green's functions for the Dirac equations for a finite radius and point nucleus. The difference ΔG can be expressed as $\Delta G = f(R,z,m_e)W(r,z,m_e)$, where z is the energy, W involves products of Whittaker functions, and f depends on R through the ratio of internal and external wave functions evaluated at R. The approximation of neglecting the electron mass in comparison to $1/a_0$ is implemented by setting $m_e = 0$ in both f and W. The approximation based on $R/a_0 \ll 1$ is obtained by expanding $f(R,z,m_e) = 0$ in powers of R and retaining only the first term. I have made calculations with and without these approximations. The results for $|k| = 1$ are presented in Table III for the following three cases: (1) no approximation, (2) $m_e = 0$ only, and (3) both $m_e = 0$ and lowest order in R/r. The results for the third case are in good agreement with Refs. 3 and 4. Numerically, the comment in Ref. 3 that corrections to $\Delta\rho(m_e = 0)$ appear to $O((m_e r)^2)$ is supported by these results, and the functional form of $\Delta\rho(m_e = 0, O(R/r))$ is in good agreement with the analytic formula of Ref.

TABLE III. Perturbation of muonic levels (in eV) in Pb due to finite-nuclear-size effect on VP, $|k| = 1$, orders $(Z\alpha)^n$. $\Delta Q_{1,2}$ are given by Eq. (6) in units of $-|e|$.

Order	Model R (fm)	Approx.	$5g_{9/2}$	$4f_{7/2}$	$3d_{5/2}$	ΔQ_1	ΔQ_2
$n \geq 1$	I 5.5	None	-5.48	-20.53	-116.1	7.020×10^{-2}	1.60×10^{-4}
		$m_e = 0$	-6.03	-21.43	-117.7	7.018×10^{-2}	1.95×10^{-4}
		$m_e = 0, O(R/r)$	-5.79	-19.99	-102.6	4.481×10^{-2}	1.91×10^{-4}
$n = 1$	I 5.5	None	-2.60	-11.46	-80.02	6.598×10^{-2}	6.03×10^{-5}
	II 7.1	None	-2.60	-11.46	-79.38		

4. A simple comparison of $\Delta\rho$ in the various approximations is indicated by the values of the two integrals

$$\Delta Q_1 = \int_R^{30R} dr(4\pi r^2)\Delta\rho,$$
$$\Delta Q_2 = \int_{30R}^{\infty} dr(4\pi r^2)\Delta\rho, \qquad (6)$$

listed in Table III. The error committed in the $m_e = 0, O(R/r)$ approximation is seen to be 1 eV for the $5g$-$4f$ transition and 13 eV for the $4f$-$3d$ transition. To this error, the uncertainty in the $|k| = 1$ approximation, Eq. (5), must also be added. For such high-angular-momentum states, the accuracy of these approximations is nevertheless found to be quite adequate. The Uehling contribution was calculated in the two nuclear models and found to be the same for $[\langle r^2\rangle_{\rm nuc}]^{1/2} = 5.5$ fm. When this contribution is subtracted from results of order $n \geq 1$, the $n \geq 3$ energy shifts are in agreement with Table I, as they must be.

The problem of vacuum polarization in superheavy electronic atoms, $Z \sim 170$, has also been investigated and will be reported elsewhere.

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SEARCH FOR ^{7}Li BREAKUP IN ^{7}Li + ^{197}Au NEAR GRAZING INCIDENCE. J. L. Québert, B. Frois, L. Marquez, G. Sousbie, R. Ost, K. Bethge, and G. Gruber [Phys. Rev. Lett. 32, 1136 (1974)].

The formula in Ref. 5 should read

$$Q = (\epsilon_i - U_T)\left(\frac{bA}{aB} - 1\right) + \frac{2\epsilon_i}{1 + 1/\sin(\theta_i/2)}\left(1 - \frac{\rho}{R_T}\right)\frac{z_f Z_f}{z_i Z_i} - 1.$$

$Z_1{}^3$ DEPENDENCE OF K-SHELL IONIZATION CROSS SECTIONS AT 7.1 MeV/amu. N. Cue, V. Dutkiewicz, P. Sen, and H. Bakhru [Phys. Rev. Lett. 32, 1155 (1974)].

In the fifth line of the first paragraph, $Z_1 \geq 3$ should be replaced by $Z_1 \leq 3$. In the fourth from the last line on page 1155, $\xi_K v_1/\frac{1}{2}\theta_K v_{2K}$ should be replaced by $\xi_K = v_1/\frac{1}{2}\theta_K v_{2K}$.