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[5]This estimate is obtained by noting that charge is conserved in the induced density to about 5%, i.e., $[\int_0^\infty \rho_{vp}(r) r^2\, dr]/[\int_0^\infty |\rho_{vp}(r)| r^2\, dr] \approx 0.05$. We have conservatively increased this fraction by a factor of 2 when estimating the accuracy of the energy level shift.

Radiative Corrections of Order α^2 in Muonic Atoms of Heavy Nuclei*

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A part of the hitherto neglected radiative corrections of order α^2 is calculated. Its inclusion in the analysis virtually eliminates all the discrepancies between the measured and the calculated energies of the $5g$-$4f$ transitions in muonic atoms of heavy nuclei.

There appeared to be discrepancies between the measured[1,2] and the calculated[3-11] energies of the $5g$-$4f$ transitions in muonic atoms of heavy nuclei: Pb, Tl, and Hg. The measured energies are ~400 keV, while the calculated values are systematically higher by ~50 eV, or 2–3 standard deviations. The fractional discrepancies are roughly 1 part in 10^4, or $\sim\alpha^2$. Since $Z\alpha$ is not a small number for these nuclei, it is desirable, at least in principle, to keep the exact dependence on $Z\alpha$. The dominant correction of ~2 keV comes from the vacuum polarization diagram 1 of order α in Fig. 1. The self-energy diagram 2 of order α^2 has been completely neglected so far.

The order of magnitude of diagram 2 can be seen in the following way. Consider the electron screening diagram 3 and the atomic polarizability diagram 4 of the usual perturbation expansion:

$$H = H_\mu - Z\alpha/r_\mu + H_e - Z\alpha/r_e + \delta H, \qquad \delta H = H_\gamma, \tag{1}$$

where $H_\mu - Z\alpha/r_\mu$ and $H_e - Z\alpha/r_e$ represent the unperturbed muon and electron Hamiltonians, and H_γ represents the electromagnetic interaction between the muon and the electrons. Since the wave functions of the atomic electrons behave more like those in a nucleus of atomic number $Z-1$ rather than Z, a better first approximation is given by the alternative expansion

$$H = H_\mu - Z\alpha/r_\mu + H_e - Z\alpha/r_e + V_\mu(r_e) + \delta H, \qquad \delta H = H_\gamma - V_\mu(r_e), \tag{2}$$

where $V_\mu(r_e)$ represents the electrostatic potential created by the muon. (The fully self-consistent Hartree-Fock Hamiltonian is not necessary for the qualitative discussions given here, since the influence of the electrons on the muonic wave functions is very small.) The probability density of the $1s$ atomic electrons near the origin is roughly proportional to Z^3; therefore, the electron screening correction changes by an amount of the order of $-3/Z$ times the original correction. This change provides a simple estimate for

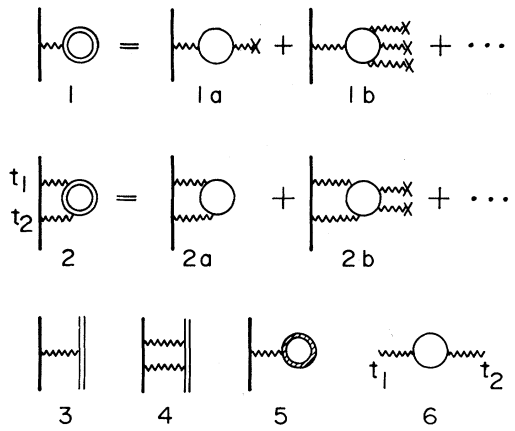

FIG. 1. Radiative corrections. The heavy lines represent the bound muonic states or the exact muon propagators in the Coulomb field of the nucleus. The double lines represent similar states or propagators of the electron. The hatched double line represents the exact electron propagator in the Coulomb field of the nucleus plus the static Coulomb field created by the muon. The single lines represent the free-electron propagators. The crosses represent the nucleus. The photon lines in diagram 2b can be permuted, and such permutations, not shown in the figure, are included in the calculation.

the size of the diagram 4. The new unperturbed Hamiltonian $H_e - Z\alpha/r_e + V_\mu(r_e)$ gives a better description for both the atomic electrons and all the virtual electrons and positrons. If the corrections of order α^2 are to be neglected, the expansion (2) should always be preferred over the expansion (1). The radiative correction of order α is then given by diagram 5. The difference between diagram 1 and diagram 5, $\sim -1/Z$ times diagram 1, or ~ -25 eV, provides a simple estimate for the size of diagram 2.

Since the apparent discrepancies are of the order of the above estimate, it is clearly necessary to compute the diagram 2. The expansion (2) is then of no more advantage, since additional counter-terms would appear. Diagrams 1 and 2, corresponding to the usual expansion (1), are diagrams of the noncovariant perturbation theory, with the origin of the spatial coordinates fixed on the nucleus. If the subtraction of infinite quantities is necessary, ambiguities could arise, and erroneous results could be obtained. Therefore, it is necessary to study the possible existence and the subtraction of divergent quantities for each of the diagrams 1 and 2 carefully.

Since the magnetic moment and the velocity of the muon in the orbits of interest are very small, it is sufficient to consider only the Coulomb interaction in the calculation of the higher-order diagram 2. If both photons of diagram 6, which describes the second-order vacuum-polarization correction to the photon propagator, represent instantaneous Coulomb interactions, the dependence of the diagram on t_1 and t_2 is given by $\delta(t_1 - t_2)$. Since $t_1 \neq t_2$ in diagram 2, diagram 2a is identically zero. The subtraction of the infinite photon self-energy function $\Pi(k)$ to yield the regularized $\Pi_R(k)$ is completely irrelevant here. The situation is totally different for diagram 1. Both diagrams 1 and 1a are divergent, and diagram 1a contains a large observable part. The noncovariant subtraction of the infinite quantity $\Pi(k)$, which is involved in the calculation of diagram 1b and higher diagrams by means of the subtraction of diagram 1a from diagram 1, must be carried out with great care.[3] The usual arguments for the existence of discrepancies are based on the term-by-term comparison of diagrams 1 and 2: Diagram 2b is scaled down from diagram 1b by a factor of $-1/Z$ to ~ 0.5 eV, a value of the wrong sign and much too small to explain the discrepancies. It is obviously wrong to estimate diagram 2a from the scaling of diagram 1a by $-1/Z$, or to compute diagram 2a by disconnecting one of the photon lines from the muon onto an external source. It is also wrong to do the same things for diagrams 1b and 2b, in view of the entirely different nature of the subtraction processes.

Although the logarithmic divergences in the photon-photon scattering tensor $J_{\mu\nu\sigma\lambda}(k_1, k_2, k_3, k_4)$ cancel after symmetrization, there still exists a constant term $J_{\mu\nu\sigma\lambda}(0,0,0,0) = \frac{2}{3}(\delta_{\mu\nu}\delta_{\sigma\lambda} + \delta_{\mu\sigma}\delta_{\nu\lambda} + \delta_{\mu\lambda}\delta_{\nu\sigma})$, which violates gauge invariance.[12] Consequently, erroneous results could still be obtained in the finite diagram 2. To circumvent this difficulty, the difference between diagram 2 and an identical diagram with the electron mass replaced by a much heavier mass, say, the muon mass, is calculated. The logarithmic divergences completely disappear in this difference, and the constant term cannot contribute. The calculation of this difference is, therefore, unambiguous.

The present work follows closely Wichmann and Kroll's calculation[3] of the vacuum-polarization diagram 1 to all orders in $Z\alpha$. Namely, the exact Green's function of the electron in an external Coulomb field is used to calculate the diagram. The starting point is the following expression for diagram 2:

$$\Delta E = \sum_{\substack{\mu,1,2 \\ (E_1<0,\, E_2<0)}} (E_0 - E_\mu + E_1 - E_2)^{-1} |\langle 0|H_\gamma|\mu,1,2\rangle|^2, \tag{3}$$

where the labels 0, μ, 1, and 2 refer to the initial muonic state and the intermediate muonic, positronic, and electronic states, respectively. Consider the Coulomb interaction. The angular part can be integrated to give

$$\Delta E = \sum_{E_\mu, j_\mu, l, l', k_1, k_2} \alpha^2 F(j_0, j_\mu, l, l', k_1, k_2) \int U_0^*(r_3) U_\mu(r_3) U_\mu^*(r_4) U_0(r_4) (r_<^l / r_>^{l+1})_{r_3, r_1} \times (r_<^{l'} / r_>^{l'+1})_{r_4, r_2} I(k_1, k_2, r_1, r_2)\, d^3r_1\, d^3r_2\, d^3r_3\, d^3r_4, \tag{4}$$

where the muonic states are normalized to $\int |U(r)|^2 d^3r = 1$, and in $(r_<^l / r_>^{l+1})_{r_i, r_j}$, $r_<$ is the smaller of

r_i and r_j; $r_>$, the larger. The angular integral is given by

$$F(j_0,j_\mu,l,l',k_1,k_2)=(2j_\mu+1)(2j_1+1)(2j_2+1)\begin{pmatrix} j_0 & l & j_\mu \\ -\frac{1}{2} & 0 & \frac{1}{2}\end{pmatrix}\begin{pmatrix} j_0 & l' & j_\mu \\ -\frac{1}{2} & 0 & \frac{1}{2}\end{pmatrix}\begin{pmatrix} j_1 & l & j_2 \\ -\frac{1}{2} & 0 & \frac{1}{2}\end{pmatrix}\begin{pmatrix} j_1 & l' & j_2 \\ -\frac{1}{2} & 0 & \frac{1}{2}\end{pmatrix}$$

$$\times\delta_p\sum_L(2L+1)\begin{pmatrix} L & j_1 & j_0 \\ l & j_\mu & j_2\end{pmatrix}\begin{pmatrix} L & j_1 & j_0 \\ l' & j_\mu & j_2\end{pmatrix}, \tag{5}$$

where $j=|k|-\frac{1}{2}$; the parity of the state is given by $(-1)^{j+1/2}$ or $(-1)^{j-1/2}$ according as $k>0$ or $k<0$; the factor $\delta_p=1$ if the parities $(-1)^l$ and $(-1)^{l'}$ are compatible with both pairs $(0,\mu)$ and $(1,2)$, $\delta_p=0$ otherwise. The remaining factor $I(k_1,k_2,r_1,r_2)$ can be expressed as a sum over all possible radial wave functions of the positron and the electron:

$$I(k_1,k_2,r_1,r_2)=\sum_{E_1<0,E_2>0}(E_0-E_\mu+E_1-E_2)^{-1}$$

$$\times\sum_{i,j=1}^{2}w_i(r_1,k_2,E_2)w_j^*(r_2,k_2,E_2)w_j(r_2,k_1,E_1)w_i^*(r_1,k_1,E_1), \tag{6}$$

where $w_i(r,k,E)$, $i=1,2$, denotes the large and the small components of the radial wave functions of the electron or the positron. The notations used here are the same as those in Wichmann and Kroll's original work,[3] except that the dependence on the quantum number k is made explicit, and the mass of the electron is set equal to 1.

The expression $I(k_1,k_2,r_1,r_2)$ can be transformed into a double contour integral:

$$I(k_1,k_2,r_1,r_2)=(2\pi i)^{-2}\int_L dz_1\int_R dz_2(E_0-E_\mu+z_1-z_2)^{-1}\,\mathrm{Tr}[K(r_1,r_2,k_2,z_2)K(r_2,r_1,k_1,z_1)]. \tag{7}$$

The Green's function $K(r_1,r_2,k,z)$ is defined by

$$K_{ij}(r_1,r_2,k,z)=\sum_E(z-E)^{-1}w_i(r_1,k,E)w_j^*(r_2,k,E), \tag{8}$$

where the sum is over all positive and negative energy states. The contours R and L are shown in Fig. 2. An explicit expression for the Green's function was obtained by Wichmann and Kroll in terms of two pieces of solutions of the Dirac equation, one being finite at the origin and the other bounded at infinity, joined together with a finite step discontinuity. The exact form, somewhat complicated, is given in the original paper.[3] The asymptotic behavior for large values of $|z|$ is given by

$$K(r_1,r_2,k,z)\to f\exp\{i|r_2-r_1|(z^2-1)^{1/2}\}\ \text{as}\ |z|\to\infty, \tag{9}$$

where f is a factor which approaches certain powers of z and $\ln z$.

In Wichmann and Kroll's work,[3] the polarization charge depends on the contour integral of $\mathrm{Tr}K(r,r,k,z)$. Since $r_1=r_2=r$ in their case, the exponential factor disappears, and the asymptotic behavior is given solely by the factor f. The difficult part of their work consists of expressing the Laplace transform of the induced charge density as contour integrals and separating the integrand into terms with different asymptotic properties. For those terms of the integrand which vanish at least as fast as z^{-2} for large $|z|$, the contour can be deformed and the only contributions come unambiguously from the integrals along the imaginary axis. For all other terms, the results are divergent or ambiguous, dependent upon the particular way the limiting process for the contour was performed. Such terms they eliminated and interpreted in terms of the charge renormalization.

These difficulties do not exist for the contour integral in Eq. (7). So long as $r_1\neq r_2$, there exists the exponential damping factor $\exp\{i|r_2-r_1|(z^2-1)^{1/2}\}$, where $\mathrm{Im}(z^2-1)^{1/2}\geq 0$ in the cut plane. The contour can always be deformed, and the only contributions come unambiguously from the integrals along the imaginary axes:

$$I(k_1,k_2,r_1,r_2)=-(2\pi)^{-2}\int_{-\infty}^{\infty}dy_1\int_{-\infty}^{\infty}dy_2[E_0-E_\mu+i(y_1-y_2)]^{-1}\,\mathrm{Tr}[K(r_1,r_2,k_2,iy_2)K(r_2,r_1,k_1,iy_1)]. \tag{10}$$

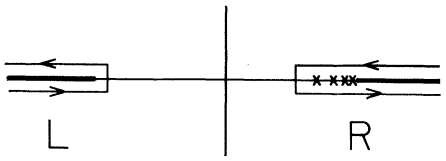

FIG. 2. Contours L and R in the complex z_1 and z_2 planes. The crosses represent the poles of the Green's functions; the heavy lines, the branch cuts.

TABLE I. Energy shifts.

Element	Particle	Transition	Shift (eV)
Pb	Muon	$5g$-$4f$	-35
Ba	Muon	$4f$-$3d$	-22
Pb	Kaon	$8j$-$7i$	-28
U	Kaon	$9k$-$8j$	-30

The difference[13] $I(k_1,k_2,r_1,r_2)-I(k_1,k_2,m_\mu r_1, m_\mu r_2)$, where m_μ is the muon mass in units of the electron mass, is then expanded in powers of $Z\alpha$. The leading term, independent of $Z\alpha$, is identically zero. The terms proportional to $Z\alpha$, as well as all other odd powers of $Z\alpha$, vanish upon integration, as they should. The $(Z\alpha)^2$ terms, corresponding to diagram 2b, and all higher terms are independent of the particular limiting process for the contours.

Only the $(Z\alpha)^2$ terms are evaluated numerically in this work. The neglect of the $(Z\alpha)^4$ and higher terms is expected to introduce an uncertainty of the order of $(Z\alpha)^2 \sim 36\%$. For this reason, the numerical accuracy of the $(Z\alpha)^2$ term has been carried out to about 20%, and the overall uncertainty is estimated to be about 40%. The results are given in Table I. It is clear that all the discrepancies concerning the $5g$-$4f$ transitions disappear.

The detailed algebraic and numerical works on the evaluation of the integral are complicated but straightforward, and will be published in a later paper. The evaluation of the $(Z\alpha)^4$ and higher terms is currently under way.

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