Calculation of the first Coulomb correction to the process of double ionization of an atomic *K*-shell in the annihilation of a positron with a bound electron

A. I. Mikhaĭlov and S. G. Porsev

B. P. Konstantinov Nuclear Physics Institute of the Russian Academy of Sciences, 188350 St. Petersburg, Russia

(Submitted 23 November 1993)
Zh. Eksp. Teor. Fiz. **105**, 828–833 (April 1994)

We study radiationless positron annihilation on an atom accompanied by double ionization of the atomic *K*-shell. We calculate the angular distribution of the ejected electrons and the total cross section, taking into account the first Coulomb correction. For heavy atoms and at relativistic energies, the total cross section is shown to be of the order of 10^{-29} cm^2.

1. The present study is a continuation of the work done on radiationless annihilation of positrons on atoms.[1] In such a process one of the atomic electrons annihilates with a positron, and another, absorbing the energy released in annihilation, is ejected from the atom. As a result the atom proves to be doubly ionized. In Ref. 1 we studied the double ionization of the *K*-shell in the annihilation of positrons to leading order in αZ, where α is the fine-structure constant and Z is the atomic number. We found that the cross section of such an ionization process is proportional to $r_e^2(\alpha Z)^8$, where r_e is the classical electron radius. The appearance of the factor $(\alpha Z)^8$ in the cross section of $(\alpha Z)^4$ in the amplitude is easy to understand. The process amplitude incorporates the product of the normalization factors of the wave functions of the *K*-electrons, which yields $(\alpha Z)^3$ Another αZ appears because a large momentum (of order the electron mass) is transferred to the nucleus via the Coulomb interaction between the electron or positron and the nucleus. Experimental study of radiationless annihilation is, apparently, possible only with high-Z atoms, where the cross section is of the order of 10^{-30}–10^{-28} cm^2 (see Ref. 1). The literature also has other estimates,[2,3] which attribute higher values to the cross section of this process. However, in Ref. 2 an incorrect (plane wave) approximation was used for the wave function of the ejected electron, in view of which the value of the cross section given in Ref. 2 cannot be correct. Shimizu, Mikoyama, and Nakayama[3] employ exact relativistic Coulomb wave functions in the form of partial-wave expansions, but their numerical calculation for lead coincides with the results of Ref. 2, which is strange. Unfortunately, Ref. 3 contains no complete relations for the amplitude and cross section: the answer is presented in the form of involved infinite series whose terms are double integrals and their products, which hinders comparison of these formulas with ours. On the contrary, in Ref. 1 the cross section is given by a simple formula, but the value calculated by this formula for $Z=82$ and the value of 500 keV for the positron's kinetic energy are smaller than the values found in Refs. 2 and 3 by a factor of 100. The reason for such a considerable discrepancy remains unclear. Of course, in the case of high-Z atoms αZ is not, strictly speaking, a small parameter, and a power expansion in this parameter is not justified, so we cannot claim a high accuracy for our formula. Nevertheless, an order-of-magnitude agreement could be expected. Obviously, the formula obtained in Ref. 1 requires refining. Here we calculate the first Coulomb correction to the cross section of the double ionization of the *K*-shell in the annihilation of positrons on the atom.

2. In the relativistic system of units ($\hbar=c=1$), the cross section of the process we are considered here is defined by the following formula:

$$d\sigma=\frac{\varepsilon}{k}|M|^2 2\pi\delta(2m+\varepsilon-E)\frac{d^3\mathbf{p}}{(2\pi)^3}. \tag{1}$$

Here ε and $\mathbf{k}$ ($k=|\mathbf{k}|$) are the positron energy and momentum, E and $\mathbf{p}$ are the energy and momentum of the ejected electron, and m is the electron mass. The energy of the bound electron is assumed equal to m, since we restrict our discussion to the first (of order αZ) Coulomb correction to the leading term. The transition amplitude M is expressed in terms of the amplitudes of one-photon annihilation and photoabsorption:

$$M=4\pi\alpha\int\frac{d\mathbf{f}}{(2\pi)^3}\frac{\langle\psi_{-k}|\hat{A}^\mu(-\mathbf{f})|\psi_b\rangle\langle\psi_p|\hat{A}_\mu(\mathbf{f})|\psi_a\rangle}{f^2-\omega^2-i0}$$
$$-(\psi_a\leftrightarrow\psi_b),\quad \omega=\varepsilon+m, \tag{2}$$

where ψ_{-k}, ψ_p, ψ_a, and ψ_b are the wave functions of the positron, the ejected electron, and the bound electrons, ω and $\mathbf{f}$ are the energy and momentum of a virtual photon, and $\hat{A}_\mu(\mathbf{f})$ is the electromagnetic-field operator (summation over μ is assumed). Here and in what follows $a^2=|\mathbf{a}|^2$. In momentum representation a matrix element of this operator is

$$\langle\mathbf{s}_1|\hat{A}_\mu(\mathbf{f})|\mathbf{s}\rangle=\gamma_\mu(2\pi)^3\delta(\mathbf{s}_1-\mathbf{s}-\mathbf{f}). \tag{3}$$

Since in the given process a large momentum (of order m) is transferred to the nucleus, the process takes place at a small distance from the nucleus (of order m^{-1}), where the nuclear field is only weakly screened by the atomic electrons. For this reason we use Coulomb wave functions for

 1063-7761/94/040441-04$10.00

all the particles participating in the processes. Following Ref. 4, we can show that for a K-electron the following is true:

$$\langle \mathbf{s}|\hat{A}_\mu(\mathbf{f})|\psi_a\rangle=\gamma_\mu N\left(-\frac{\partial}{\partial\eta}+\frac{\alpha Z}{2}\tilde{\nabla}_f\right)\left(-\frac{\partial}{\partial\eta}\right)\times\int_0^\infty \lambda^\sigma\langle\mathbf{s}|V_{\lambda+\eta}|\mathbf{f}\rangle u_a d\lambda, \qquad (4)$$

with $N=\eta^3/\pi$, $\eta=m\alpha Z$, $\sigma=\alpha^2/Z^2/2$, $\tilde{\nabla}_f=\boldsymbol{\alpha}\nabla_f$, $\boldsymbol{\alpha}$ the Dirac matrices, ∇_f the gradient in $\mathbf{f}$, and u_a the bispinor of the a-electron in the electron's rest frame of reference. Expansion in the small parameter σ can be performed after integration with respect to $d\mathbf{s}$. The matrix element in the integrand in (4),

$$\langle\mathbf{s}|V_\lambda|\mathbf{f}\rangle=\frac{4\pi}{(\mathbf{s}-\mathbf{f})^2+\lambda^2}, \qquad (5)$$

is the Fourier transform of the Yukawa potential

$$\langle\mathbf{r}|V_\lambda|\mathbf{r}_1\rangle=\frac{e^{-\lambda r}}{r}\delta(\mathbf{r}-\mathbf{r}_1).$$

The wave function of the ejected electron can be represented by a power series in αZ, the first two terms of which are the Furry-Sommerfeld—Maue function[5]

$$|\psi_p\rangle=N_p(|\varphi_p^0\rangle+\alpha Z|\varphi_p^1\rangle-\alpha^2Z^2G_E\hat{V}_0|\varphi_p^1\rangle+\cdots)u_p, \qquad (6)$$

where $N_p=\exp(\pi\xi/2)|\Gamma(1-i\xi)|$, with $\xi=\alpha ZE/p$, $p=|\mathbf{p}|$, and $\hat{V}_0=\gamma_0V_0$, with γ_0 a Dirac matrix and V_0 the Coulomb-field operator; u_p and G_E are the Dirac bispinor and Green's function of a free electron with the four-momentum $(E,\mathbf{p})$. In the momentum representation the operator V_0 is given by Eq. (5) with $\lambda=0$ and G_E by the following matrix:

$$\langle\mathbf{f}|G_E|\mathbf{s}\rangle=G_E(\mathbf{f})(2\pi)^3\delta(\mathbf{f}-\mathbf{s}),\qquad G_E(\mathbf{f})=\frac{\gamma\mathbf{f}-\gamma_0E-m}{f^2-p^2-i0}. \qquad (7)$$

The first two terms in (6) provide the same contribution of the order of αZ to the amplitude (2) and were allowed for in Ref. 1. To obtain the first Coulomb correction to the amplitude of the process we must retain in (6) the third term, which is proportional to $(\alpha Z)^2$. Note that the function (6) contains no expansion in the Coulomb parameter ξ and, therefore, is valid for all values of p. In the momentum representation $|\varphi_p^0\rangle$ and $|\varphi_p^1\rangle$ have the form[4]

$$\langle\mathbf{f}|\varphi_p^0\rangle=-\frac{\partial}{\partial\varepsilon}\langle\mathbf{f}|\Phi_p(i\varepsilon)\rangle|_{\varepsilon\to0}, \qquad (8)$$

$$\langle\mathbf{f}|\varphi_p^1\rangle=-\frac{\tilde{\nabla}_p}{2i\xi}\langle\mathbf{f}|\Phi_p(i\varepsilon)\rangle|_{\varepsilon\to0}, \qquad (9)$$

$$\langle\mathbf{f}|\Phi_p(i\varepsilon)\rangle=\frac{4\pi}{(\mathbf{f}-\mathbf{r})^2+\varepsilon^2}\left\{\frac{(\mathbf{f}-\mathbf{r})^2+\varepsilon^2}{(\mathbf{f}-\mathbf{r}+\mathbf{p})^2-(p+i\varepsilon)^2}\right\}^{i\xi}, \qquad (10)$$

where $\mathbf{r}=\mathbf{p}$, and the gradient ∇_p does not act on $\mathbf{r}$ or ξ. The function (6) is normalized in a way common to scattering problems: in the coordinate representation the function $\langle\mathbf{r}|\psi_p\rangle$ in the asymptotic region is the sum of a plane wave and an outgoing spherical wave. Since the Dirac-conjugate wave function must have the same normalization,[6] it can be constructed from (6) by the following rule:

$$\langle\psi_p|=|\psi_p\rangle^+\gamma_0,$$

where Hermitian conjugation refers only to the Dirac matrices and spinors and does not act on the imaginary parts of the function related to $i\varepsilon$ and $i\xi$. Then

$$\langle\psi_p|=N_p\bar{u}_p(\langle\varphi_p^0|+\alpha Z\langle\varphi_p^1|-\alpha^2Z^2\langle\varphi_p^1|\hat{V}_0G_0+\cdots), \qquad (11)$$

$$\bar{u}_p=u_p^+\gamma_0,\quad \langle\varphi_p^0|\mathbf{f}\rangle=\langle\mathbf{f}|\varphi_p^0\rangle,\quad \langle\varphi_p^1|\mathbf{f}\rangle=-\langle\mathbf{f}|\varphi_p^1\rangle. \qquad (12)$$

Employing Eqs. (7)–(12), we can write the photoelectric-effect amplitude as

$$\langle\psi_p|\hat{A}_\mu(\mathbf{f})|\psi_a\rangle=N_pN\bar{u}_pT(p)u_a, \qquad (13)$$

$$T(p)=4\pi\{T_0+\alpha ZT_1+\alpha^2Z^2T_2\}\left(\frac{a_1}{b_1}\right)^{i\xi}, \qquad (14)$$

$$T_0=\gamma_\mu\left\{(1-i\xi)\frac{2\eta-\alpha Z\tilde{q}_1}{a_1^2}+i\xi\frac{-2ip+2\eta-\alpha Z\tilde{f}}{a_1b_1}+\frac{\pi\alpha^2Z^2}{4a_1q_1}\right\}, \qquad (15)$$

$$T_1=-\frac{\tilde{c}_1}{a_1b_1}\gamma_\mu-\frac{\alpha Z}{2}\tilde{\Phi}_p\gamma_\mu\tilde{\nabla}_f, \qquad (16)$$

$$T_2=\tilde{\Phi}_p\gamma_0G_E(\mathbf{f})\gamma_\mu, \qquad (17)$$

$$\mathbf{q}_1=\mathbf{f}-\mathbf{p},\quad \mathbf{c}=\mathbf{q}_1-\frac{i\eta\mathbf{p}}{p},\qquad a_1=q_1^2+\eta^2,\quad b_1=f^2-(p+i\eta)^2, \qquad (18)$$

$$\tilde{\Phi}_p=\int_0^\infty\frac{\mathbf{c}_1}{a_1b_1}d\eta,\quad \tilde{a}=\alpha\mathbf{a}. \qquad (19)$$

The operator $\tilde{\nabla}_f$ in (16) acts only on the function $\tilde{\Phi}_p$. An expression for the annihilation amplitude $\langle\psi_{-k}|\hat{A}^\mu(-\mathbf{f})|\psi_b\rangle$ can be obtained from Eqs. (12)–(19) by replacing E, $\mathbf{p}$, $\mathbf{f}$, γ_μ, and u_a with $-\varepsilon$, $-\mathbf{k}$, $-\mathbf{f}$, γ^μ, and u_b, respectively. As result of this substitution, $\mathbf{q}_1$, $\mathbf{c}_1$, a_1, and b_1 become

$$\mathbf{q}_2=\mathbf{k}-\mathbf{f},\quad \mathbf{c}_2=\mathbf{q}_2+i\eta\mathbf{k}/k,\qquad a_2=q_2^2+\eta^2,\quad b_2=f^2-(k+i\eta)^2. \qquad (20)$$

After substituting (13) and the respective expression for the annihilation amplitude into (2) we get

$$M=4\pi\alpha N_pN_{-k}N^2U, \qquad (21)$$

$$U=\int\frac{d\mathbf{f}}{(2\pi)^3}\frac{1}{f^2-\omega^2-i0}\{\bar{u}_pT(p)u_a\bar{u}_{-k}T(-k)u_b-(u_a\leftrightarrow u_b)\}. \qquad (22)$$

Analysis of Eqs. (22), (14), and (15) shows that the quantities not containing αZ can appear in U only owing to the product of η/a_1^2 and η/a_2^2, since

$$\left.\frac{8\pi\eta}{(q^2+\eta^2)^2}\right|_{\eta\to 0}=(2\pi)^3\delta(\mathbf{q}). \tag{23}$$

However, the product of the two delta-functions $\delta(\mathbf{f}-\mathbf{p})$ and $\delta(\mathbf{k}-\mathbf{f})$ is zero because, as the energy-momentum conservation law implies, $\mathbf{k}$ is never equal to $\mathbf{p}$. For this reason the expansion of U in powers of αZ beings with terms proportional to αZ. As shown in Ref. 1, the leading term in this expansion is real, so that to calculate the cross section with a relative accuracy of the order of αZ it suffices to find only the real part of the Coulomb correction to the amplitude (knowing the imaginary part of the correction is imperative when calculating spin correlations, but we do not touch on these aspects here). All integrals with respect to $d\mathbf{f}$ can be expressed in terms of elementary functions, although the calculations are rather tedious. Using the qualities that follow from energy conservation,

$$p^2-\omega^2=\omega^2-k^2=2m\omega,$$

we can reduce integration with respect to $d\mathbf{f}$ to

$$U=\frac{2\pi\alpha Z}{m\omega^2q^2}(1-\pi\xi)\left[\gamma_\mu\times\gamma^\mu-\gamma_\mu\times\left(\gamma^\mu\tilde{q}\frac{\omega}{q^2}+\tilde{q}\gamma^\mu\frac{1}{4m}\right)+\left(\gamma_\mu\tilde{q}\frac{\omega}{q^2}-\tilde{q}\gamma_\mu\frac{1}{4m}\right)\times\gamma^\mu\right]+\frac{2\pi(\alpha Z)^2}{m\omega}\left\{\tilde{Q}\left(-\frac{1}{2}\gamma_\mu\tilde{\nabla}_k+\frac{\tilde{k}-E-\gamma_0 m}{k^2-p^2}\gamma_\mu\right)\times\gamma^\mu+\gamma_\mu\times\tilde{Q}\left(\frac{1}{2}\gamma^\mu\tilde{\nabla}_p-\frac{\tilde{p}-\varepsilon+\gamma_0 m}{p^2-k^2}\gamma^\mu\right)\right\}, \tag{24}$$

$$\mathbf{Q}=\mathrm{Re}\int_0^\infty\frac{(\mathbf{q}+i\lambda\mathbf{k}/k)d\lambda}{(q^2+\lambda^2)[p^2-(k+i\lambda)^2]}=-\mathrm{Re}\int_0^\infty\frac{(\mathbf{q}-i\lambda\mathbf{p}/p)d\lambda}{(q^2+\lambda^2)[k^2-(p+i\lambda)^2]}=\frac{\pi}{4\Delta}\left(\frac{\mathbf{q}}{q}-\frac{\mathbf{p}}{p}\right), \tag{25}$$

$$\mathbf{q}=\mathbf{k}-\mathbf{p},\quad \Delta=pq-\mathbf{pq}. \tag{26}$$

The differential operators ∇_k and ∇_p act in Eq. (24) on the vector function $\mathbf{Q}$. The terms separated by multiplication signs belong to different currents and are surrounded by the appropriate spinors. For instance, the term $\gamma_\mu\times\gamma^\mu$ should be interpreted as

$$\gamma_\mu\times\gamma^\mu=(\bar{u}_p\gamma_\mu u_a)(\bar{u}_{-k}\gamma^\mu u_b)-(\bar{u}_p\gamma_\mu u_b)(\bar{u}_{-k}\gamma^\mu u_a). \tag{27}$$

The other terms in (24) have a similar appearance. Let us now shift from bispinors and Dirac matrices to spinors (w) and Pauli matrices ($\boldsymbol{\sigma}$) (see Ref. 6):

$$u_p=\sqrt{\frac{E+m}{2E}}\begin{pmatrix}1\\ \boldsymbol{\sigma}\boldsymbol{\nu}_p\end{pmatrix}w_p,\quad u_{-k}=\sqrt{\frac{\varepsilon+m}{2\varepsilon}}\begin{pmatrix}\boldsymbol{\sigma}\boldsymbol{\nu}_k\\ 1\end{pmatrix}w_k, \tag{28}$$

$$u_{a,b}=\begin{pmatrix}1\\0\end{pmatrix}w_{a,b},\quad \boldsymbol{\nu}_p=\frac{\mathbf{p}}{E+m},\quad \boldsymbol{\nu}_k=\frac{\mathbf{k}}{\varepsilon+m}.$$

Under such a transformation the terms proportional to $\nabla\tilde{Q}$ (we put operator ∇ instead of ∇_k or ∇_p) are expressed in terms of the scalar product $\nabla\mathbf{Q}$ and the vector product $\nabla\mathbf{Q}$. Employing Eq. (25), we can easily show that $\nabla\mathbf{Q}=0$ and $\nabla\mathbf{Q}=0$. The final expression for U assumes the simple form

$$U=\frac{p}{\sqrt{2\varepsilon E}}\frac{\pi\alpha Z}{m\omega^2q^2}w_p^+(\boldsymbol{\sigma}[\mathbf{nx}])w_k^*, \tag{29}$$

$$\mathbf{n}=\frac{[\mathbf{kp}]}{|[\mathbf{kp}]|}, \tag{30}$$

$$\mathbf{x}=(\boldsymbol{\nu}_k-\boldsymbol{\nu}_p)(1-\pi\xi)+\frac{\pi\alpha Z}{4}\frac{\omega q^2}{m\Delta}\left\{\boldsymbol{\nu}_k\left(\frac{2m}{q}-\frac{\varepsilon}{p}\right)-\boldsymbol{\nu}_p\left(\frac{pE}{\omega^2}+\frac{6m}{q}\right)\right\}. \tag{31}$$

[The asterisk in Eq. (29) stands for complex conjugation.] Substituting Eqs. (21) and (29) into (1) and summing over polarizations, we arrive at the following formula for the electron angular distribution:

$$\frac{d\sigma}{d\Omega}=2r_e^2(\alpha Z)^8N_p^2N_{-k}^2\frac{p}{k}\frac{m^6}{\omega^4q^2}\left\{1-\frac{4m^2}{q^2}+\frac{\pi\eta}{p}\left(\frac{8mE}{q^2}-\frac{2p}{q}-1\right)\right\},$$

$$r_e^2=\left(\frac{\alpha}{m}\right)=7.94\times10^{-26}\ \mathrm{cm}^2,\quad N_p^2=\frac{2\pi\xi}{1-\exp(-2\pi\xi)}, \tag{32}$$

$$N_{-k}^2=\frac{2\pi\zeta}{\exp(2\pi\zeta)-1},\quad \xi=\frac{\alpha ZE}{p},\quad \zeta=\frac{\alpha Z\varepsilon}{k}.$$

We do not expand the normalization factors in powers of αZ because this would result in expanding in parameters $\pi\xi$ and $\pi\zeta$, which are not assumed small. Integrating (32) over the electron ejection angles, we find the total cross section of double ionization of the K-shell in the annihilation of positrons on an atom:

$$\sigma=4\pi r_e^2(\alpha Z)^8N_p^2N_{-k}^2\frac{m^6}{k^2\omega^4}\left\{\frac{pk}{2\omega^2}+\left(1-\frac{\pi\eta}{p}\right)\left(\ln\frac{p+k}{p-k}-\frac{pk^2}{\omega}\right)\right\}. \tag{33}$$

[In Ref. 1, Eq. (4) for the amplitude of the process lacks the factor $1/\sqrt{2}$, emerging from the spin wave function of K-electrons. For this reason the cross sections in Ref. 1 must be halved.]

Let us calculate the annihilation cross section for $Z=82$ and a positron energy ε equal to $2m$. Equation (33) yields $\sigma=0.75\times10^{-29}$ cm^2 if we allow for the correction and 0.9×10^{29} cm^2 if we do not, while in Refs. 2 and 3 the respective values (with and without the correction) are 2×10^{-27} cm^2 and 1.5×10^{-27} cm^2. Thus, allowing for the first Coulomb correction did not eliminate the discrepancy between the results of Ref. 1 and of Refs. 2 and 3.

[1] A. I. Mikhaĭlov and S. G. Porsev, J. Phys. B **25**, 1097 (1992).
[2] H. S. Massey and E. H. Burhop, Proc. Roy. Soc. London, Ser. A **167**, 53 (1938).
[3] S. Shimizu, T. Mikoyama, and Y. Nakayama, Phys. Rev. **173**, 173 (1968).
[4] V. G. Gorshkov, A. I. Mikhaĭlov, and V. S. Polikanov, Nucl. Phys. **55**, 273 (1964).
[5] V. G. Gorshkov, Zh. Eksp. Teor. Fiz. **41**, 977 (1961) [Sov. Phys. JETP **14**, 694 (1962)].
[6] A. I. Akhiezer and V. B. Berestetskiĭ, *Quantum Electrodynamics*, Nauka, Moscow (1969), p. 623 [in Russian]; an earlier edition of this book was translated at Wiley, New York, in 1965.

Translated by Eugene Yankovsky.
This article was translated in Russia. It is reproduced here the way it was submitted by the translator, except for stylistic changes by the Translation Editor.