Nuclear excitation in positron-K-electron annihilation

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We have calculated the cross section for nuclear excitation during positron-K-electron annihilation. The calculations allow for the effect of the nuclear Coulomb field and for relativistic effects. The results are compared to earlier predictions which were derived using the Born approximation, and to renormalized Born approximation predictions. Our calculated cross sections are well below the available experimental values.

I. INTRODUCTION

The first prediction of nuclear excitation during positron annihilation was made by Present and Chen[1] more than three decades ago. The first experimental evidence for the effect was found by Mukoyama and Shimizu,[2] who measured the cross section for excitation of the 1078 keV level of ^{115}In and obtained a value many orders of magnitude greater than the theoretical predictions. Other experimental investigations[3–6] have also found cross sections much greater than the theoretical predictions. A more recent detailed calculation made by Grechukhin and Soldatov[7] for ^{115}In also predicts a cross section which is much lower than the experimental result.

The general assumption has been that the mechanism was based on a direct resonant excitation of the nuclear level, but it was recently proposed that a radiative nonresonant mechanism[8] could be sufficiently strong to explain the experimental results. However, Ljubičić *et al.*[9] have shown that the magnitude of the radiative nonresonant process has been overestimated, and this has also been shown in a more detailed analysis made by Pisk *et al.*[10] These calculations, while reasonably comprehensive, employ the Born approximation and neglect the effect of the Coulomb field on the positron motion and allow only a partial influence on the K-electron motion. In an attempt to improve the accuracy of the theoretical calculations, we have made more general estimates which allow for both the effects of the nuclear Coulomb field and relativistic effects.

II. CALCULATION OF THE CROSS SECTIONS

The matrix element for nuclear excitation in positron K-electron annihilation can be found by multiple expansion of the photon propagator between the charge currents involved. For the leading multipole it is

$$S^{(i)}=-i4\pi^3\alpha/\omega'\delta(\epsilon_0+\epsilon-\omega')\sum_M N_{LM}^{(i)}A_{LM}^{(i)} , \qquad (1)$$

$$A_{LM}^{(i)}=\int d\mathbf{r}\,\Psi_p^\dagger(\mathbf{r})O_{LM}^{*(i)}\Psi_0(\mathbf{r}) . \qquad (2)$$

In Eq. (1) M is the magnetic quantum number, ϵ_0 and ϵ are, respectively, the total energies of the K electron and the positron, and ω' is the nuclear transition energy. $N_{LM}^{(i)}$ are the nuclear matrix elements for the 2^L transition of electric type $(i=e)$, or magnetic type $(i=m)$, and they describe the process of nuclear γ-ray emission.

In Eq. (2) the positron and K-electron wave functions are represented by Ψ_p and Ψ_0, respectively, and the multipole operators $O_{LM}^{(i)}$ expressed in the conventional gauge[11] are

$$O_{LM}^{(m)}=i\omega\sqrt{2/\pi}h_L^{(1)}\boldsymbol{\alpha}\mathbf{Y}_{L,L}^M \qquad (3)$$

for the 2^L-pole magnetic transition, and for the 2^L-pole electric transition as

$$O_{LM}^{(e)}=-\omega\sqrt{2/\pi}[i(L/L+1)^{1/2}h_L^{(1)}Y_{LM}+(2L+1/L+1)^{1/2}h_{L-1}^{(1)}\boldsymbol{\alpha}\mathbf{Y}_{L,L-1}^M] . \qquad (4)$$

In Eqs. (3) and (4) the h's are spherical Hankel functions and Y_L and $\mathbf{Y}_{L,l}$ are spherical and spherical vector functions. The $\boldsymbol{\alpha}$'s are Dirac matrices.

In calculating the cross section we assume the density of final states has the form of a Lorentz shaped function with a width Γ. For unorientated nuclei, and unpolarized electrons and positrons, the cross section is found to be

$$\sigma^{(i)}=2\pi^2\alpha g\frac{\Gamma_0\epsilon}{\Gamma p\omega}\frac{1}{2L+1}\sum_{\substack{M\\ \mu\nu}} | A_{LM}^{(i)} |^2 , \qquad (5)$$

with the energy constraints

$$| \epsilon+\epsilon_0-\omega) < \Gamma/2 . \qquad (6)$$

In Eq. (5) g is the statistical weight, and Γ_0 is the ground state transition width of the excited level which has a total width Γ. The momentum of the incident positron is represented by p, and μ,ν represent the spin labels of the K electron and positron.

To calculate the matrix elements A_{LM} we assume Dirac Coulomb-type wave functions for the K electron and positron.[12] The K-electron wave function is given by

$$\Psi_0=\begin{bmatrix} iG\Omega_{1/2\,0\mu} \\ F\Omega_{1/2\,1\mu}\end{bmatrix} \tag{7}$$

and the positron wave function is chosen to represent asymptotically a distorted plane wave with an outgoing spherical wave

$$\Psi_p^\dagger=4\pi\sum_{jlm} p_{jlm}^*(\hat{\mathbf{p}},\nu)(f_{jl'}\Omega^\dagger{}_{jl'm};\Omega_{jlm}^\dagger)\ ,$$
$$l'=l\pm 1, j=l\pm\tfrac{1}{2}\ , \tag{8}$$

where

$$p_{jlm}(\hat{\mathbf{p}},\nu)=(\Omega_{jlm}^\dagger \mathcal{X}_{-\nu})\ , \tag{9}$$

and $\mathcal{X}$ is a two-component spinor.

In Eqs. (7)—(9) the Ω_{jlm} are spherical spinors, and the radial functions G, F, g, and f are derived in the Appendix.

With the above representation we were able to separate the radial integrations from the angular terms in the matrix elements A_{LM}. After some angular momentum algebra we obtained the following results for the electric 2^L-pole transition:

$$\sum_{\substack{M\\ \mu\nu}} |A^{(e)}|^2=\frac{4}{\pi}\omega^2\frac{L}{L+1}[(L+1)|R_1+R_2+2R_3|^2_{L+(1/2),L+1}+L\,|R_1+R_2-R_3/L-(2+1/L)R_4|^2_{L-(1/2),L-1}]\ , \tag{10}$$

where the radial integrals are

$$\begin{aligned}(R_1)_{jl}&=\int_0^\infty dr\, r^2 f_{jl'}h_L^{(1)}G\ ,\\ (R_2)_{jl}&=\int_0^\infty dr\, r^2 g_{jl}h_L^{(1)}F\ ,\\ (R_3)_{jl}&\int_0^\infty dr\, r^2 f_{jl'}h_{L-1}^{(1)}F\ ,\\ (R_4)_{jl}&=\int_0^\infty dr\, r^2 g_{jl}h_{L-1}^{(1)}G\ .\end{aligned} \tag{11}$$

In the case of the magnetic 2^L-pole transition we obtained the following result:

$$\sum_{\substack{M\\ \mu\nu}} |A_{LM}^{(m)}|^2=\frac{4}{\pi}\omega^2[L\,|R_1'+R_2'|^2_{L+(1/2),L} +(L+1)|R_1'+R_2'|^2_{L-(1/2),L}]\ , \tag{12}$$

where the radial integrals are

$$\begin{aligned}(R_1')_{jl}&=\int_0^\infty dr\, r^2 f_{jl'}h_L^{(1)}F\ ,\\ (R_2')_{jl}&=\int_0^\infty dr\, r^2 g_{jl}h_L^{(1)}G\ .\end{aligned} \tag{13}$$

All the defined radial integrals are calculated in the Appendix.

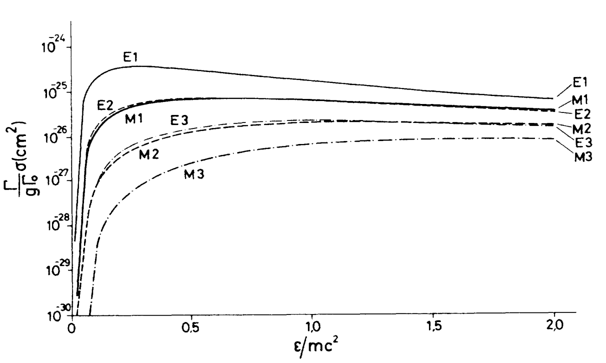

FIG. 1. The cross sections for the resonant nonradiative excitation for various multipoles, as a function of the incident positron energy. The atomic number $Z=50$ and nuclear energy level $\omega=1078$ keV are assumed.

III. RESULTS AND DISCUSSION

The calculated cross sections for resonant nonradiative excitation, for various multipoles, are shown as a function of the incident positron energy in Fig. 1. The Z dependence of the resonant nonradiative excitation is illustrated in Fig. 2. If we compute the radial integrals up to the leading term in the αZ expansion, the present results agree with the earlier estimates found using the Born approximation.

It is interesting to note that a reasonable correction can be made to the earlier calculations by renormalizing the Coulomb value of the positron wave function at the nucleus. The renormalized cross section σ_R can be written as

$$\sigma_R=\sigma_B F(Z,\epsilon)\ , \tag{14}$$

where σ_B is the cross section calculated using the Born approximation, Ref. 10, and $F(Z,\epsilon)$ is the Fermi factor[13]

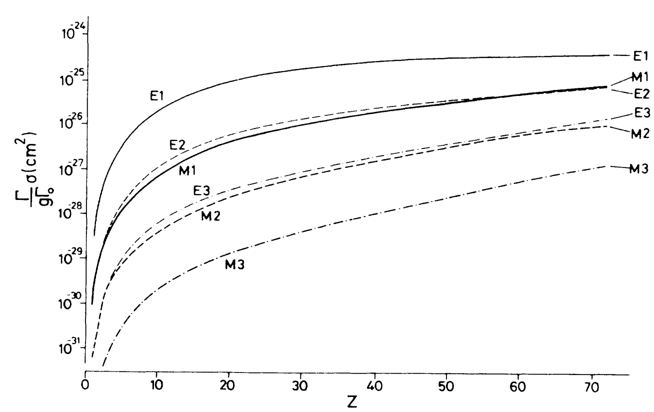

FIG. 2. The Z dependence of the resonant nonradiative excitation for various multipoles. The nuclear energy level $\omega=1078$ keV is assumed.

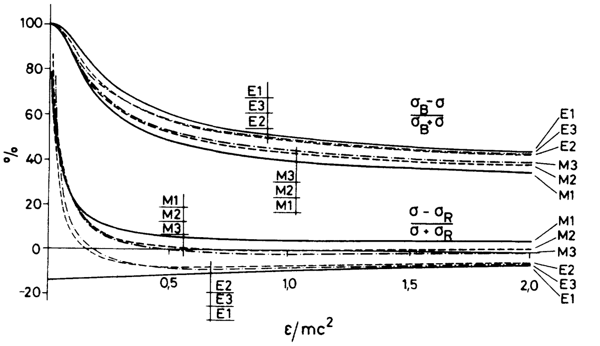

FIG. 3. The differences between the cross sections expressed in percentages for various multipoles, as a function of the incident positron energy. The atomic number $Z=50$ and nuclear energy level $\omega=1078$ keV are assumed. σ, σ_B, and σ_R are, respectively, the cross section calculated in this work, the cross section calculated using the Born approximation (Ref. 10), and the renormalized cross section given by Eq. (14).

$$F=2e^{-\pi\nu}(1+\gamma_1)\frac{|\Gamma(\gamma_1+i\nu)|^2}{|\Gamma(1+2\gamma_1)|^2}(2pR)^{2(\gamma_1-1)}, \quad (15)$$

where R represents the nuclear radius, and the other quantities are defined in the Appendix.

The differences between the cross sections calculated in this work and the Born approximation and the renormalized Born approximation values are shown in Fig. 3 as a function of positron energy, and in Fig. 4 as a function of Z. As one would expect, the renormalization procedure works best for larger positron energies and for lower Z values.

The nuclear Coulomb field is expected to have similar influences on the radiative, nonresonant process. This is illustrated in Fig. 5, where a comparison is made between the Born approximation (the momentum distribution of the K electron is taken into account) and renormalized Born approximation predictions.

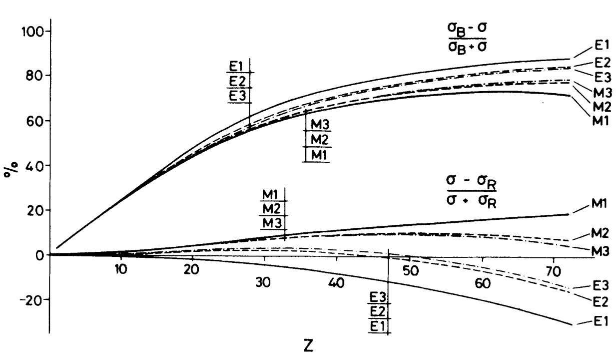

FIG. 4. The Z dependence of the cross section differences for various multipoles. The nuclear energy level $\omega=1078$ keV is assumed. The descriptions of σ, σ_B, and σ_R are the same as in Fig. 3.

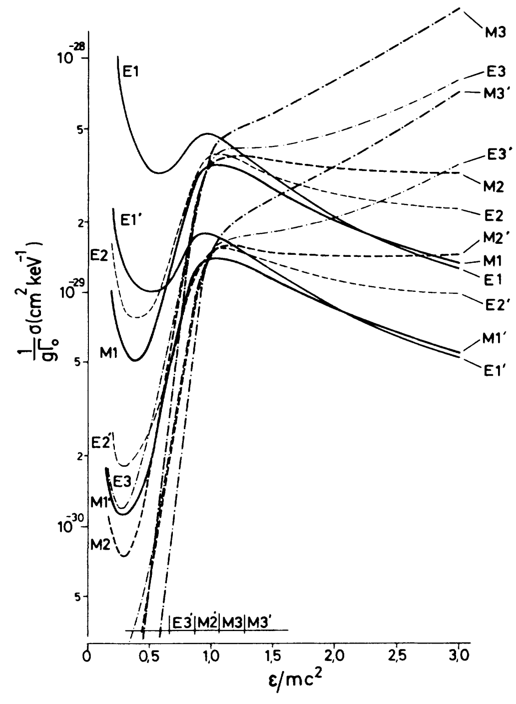

FIG. 5. The cross sections for the radiative nonresonant process as a function of the incident positron energy. The atomic number $Z=50$ and nuclear energy level $\omega=1078$ keV are assumed. The primed multipoles represent the renormalized cross sections, and multipoles without primes are the cross sections calculated in the Born approximation.

The present calculations are quite comprehensive and they further reduce the theoretical value for the excitation cross section, for the assumed mechanisms. Consequently, the experimental results are even much larger than the general range of our predictions, and it seems clear that much remains to be done if we are to have a quantitative understanding of the excitation of nuclear levels during positron annihilation.

APPENDIX

The radial parts of the wave functions used in Eqs. (7) and (8) are Dirac Coulomb-type wave functions.[12] The K-electron functions are given by

$$G=N[(1+\gamma_1)/2]^{1/2}(2\lambda r)^{\gamma_1-1}e^{-\lambda r},$$
$$F=N[(1-\gamma_1)/2]^{1/2}(2\lambda r)^{\gamma_1-1}e^{-\lambda r}, \quad (A1)$$

where

$$\lambda=m\alpha Z,\quad \gamma_1=(1-\alpha^2Z^2)^{1/2},$$

and the normalization constant is

$$N=[(2\lambda)^3/\Gamma(2\gamma_1+1)]^{1/2}.$$

The positron functions are given by

$$g_{jl} = -[(\epsilon+m)/2\epsilon]^{1/2} e^{i\gamma\pi/2-\nu\pi/2} \frac{\Gamma(\gamma-i\nu)}{\Gamma(2\gamma+1)} \times (2pr)^{\gamma-1} \{\ \}_- e^{-ipr} ,$$

$$f_{jl} = -[(\epsilon-m)/2\epsilon]^{1/2} e^{i\gamma\pi/2-\nu\pi/2} \frac{\Gamma(\gamma-i\nu)}{\Gamma(2\gamma+1)} \times (2pr)^{\gamma-1} \{\ \}_+ e^{-ipr} , \quad \text{(A2)}$$

with

$$\{\ \}_\pm = (\gamma-i\nu)F(\gamma+1-i\nu;2\gamma+1;2ipr) \pm (\kappa-i\nu')F(\gamma-i\nu;2\gamma+1;2ipr) ,$$

where

$$\kappa = \pm(j\pm\tfrac{1}{2}) \text{ for } j=l\pm\tfrac{1}{2} ,$$

$$\gamma=(\kappa^2-\alpha^2Z^2)^{1/2}, \quad \nu=\alpha Z\epsilon/p, \quad \nu'=\alpha Zm/p .$$

In the above equations α, Z, m, ϵ, and p are, respectively, the fine structure constant, atomic number, mass of the electron, positron energy, and positron momentum. Also, $F(a;b;x)$ represents the confluent hypergeometric function and $\Gamma(x)$ represents the gamma function.

Using these representations of the wave functions and multipole operators O_{LM} given by Eqs. (3) and (4), the radial integrals defined by Eqs. (11) and (13) can be expressed as a linear combination of the integrals

$$K_n(a,c) = \int_0^\infty dr\, r^2 (2pr)^{\gamma-1} (2\lambda r)^{\gamma_1-1} \times e^{-ipr} e^{-\lambda r} F(a;c;2ipr) h_n^{(1)}(\omega r) . \quad \text{(A3)}$$

To calculate the integral (A3) we used the following: (a) a series expansion for the spherical Hankel function[14]

$$h_n^{(1)}(x) = i^{-n-1} x^{-1} e^{ix} \sum_0^n (n+\tfrac{1}{2},k)(-2ix)^{-k} , \quad \text{(A4)}$$

where

$$(n+\tfrac{1}{2},k) = \frac{(n+k)!}{k!\Gamma(n-k+1)} ;$$

(b) the integral representation for the confluent hypergeometric function[14]

$$F(a;b;x) = \frac{\Gamma(b)}{\Gamma(a)\Gamma(b-a)} \int_0^1 dt\, e^{xt} t^{a-1} (1-t)^{b-a-1} , \quad \text{(A5)}$$

and for the hypergeometric function[14]

$$F(a;b;c;x) = \frac{\Gamma(c)}{\Gamma(b)\Gamma(c-b)} \int_0^1 dt\, t^{b-1} (1-t)^{c-b-1} \times (1-tx)^{-a} . \quad \text{(A6)}$$

By introducing expansion (A4) and representation (A5) into the integral (A3), one can perform r integration and obtain the result

$$K_n(a,c) = 2i^{-1} (2p)^{\gamma-1} (2\lambda)^{\gamma_1-1} \frac{\Gamma(c)}{\Gamma(a)\Gamma(c-a)} \times \sum_0^n [n,k] \frac{i^{k-\gamma-\gamma_1}}{(2i\omega)^{k+1}} \times \int_0^1 dt\, t^{a-1} (1-t)^{c-a-1} (u-2pt)^{k-\gamma-\gamma_1} , \quad \text{(A7)}$$

where $u=p-\omega-i\lambda$ and

$$[n,k] = \frac{(-n,k)(n+1,k)}{(1,k)} ,$$

where (a,b) are the Pochhammer's symbols:[14]

$$(a,b) = \frac{\Gamma(a+b)}{\Gamma(a)} .$$

The remaining integration in Eq. (A7) is recognized as a representation of the hypergeometric function given by Eq. (A6).

The final answer for the radial integrals is

$$\begin{aligned} R_1 &= (\epsilon-m)^{1/2}(1-\gamma_1)^{1/2} H \sum_0^L C_L^k [\ ]_+ , \\ R_2 &= i(\epsilon+m)^{1/2}(1+\gamma_1)^{1/2} H \sum_0^L C_L^k [\ ]_- , \\ R_3 &= i(\epsilon-m)^{1/2}(1-\gamma_1)^{1/2} H \sum_0^{L-1} C_{L-1}^k [\ ]_+ , \\ R_4 &= -(\epsilon+m)^{1/2}(1+\gamma_1)^{1/2} H \sum_0^{L-1} C_{L-1}^k [\ ]_- . \\ R_1' &= i(\epsilon-m)^{1/2}(1+\gamma_1)^{1/2} H \sum_0^L C_L^k [\ ]_+ , \\ R_2' &= -(\epsilon+m)^{1/2}(1-\gamma_1)^{1/2} H \sum_0^L C_L^k [\ ]_- . \end{aligned} \quad \text{(A8)}$$

In Eq. (A8) we introduced

$$H = -i^{-L+1-\gamma-\gamma_1} (2\lambda/\epsilon)^{1/2} e^{-\nu\pi/2} \frac{\Gamma(\gamma-i\nu)}{\Gamma(2\gamma+1)} \times \frac{\Gamma(\gamma+\gamma_1)}{[\Gamma(2\gamma_1+1)]^{1/2}} \frac{x^{\gamma} z^{\gamma}}{8p\lambda\omega} , \quad \text{(A9)}$$

$$C_l^k = \frac{(-l,k)(l+1,k)}{(1,k)(1-\gamma-\gamma_1,k)} (-1/y)^k ,$$

and

$$[\ ]_\pm = (\gamma-i\nu)F(\gamma+\gamma_1-k;\gamma+1-i\nu;2\gamma+1;x) \pm (\kappa-i\nu')F(\gamma+\gamma_1-k;\gamma-i\nu;2\gamma+1;x) , \quad \text{(A10)}$$

where

$$\begin{aligned} x &= 2p/u , \\ y &= 2\omega/u , \\ z &= 2\lambda/u . \end{aligned} \quad \text{(A11)}$$

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