THE RELATIONSHIP BETWEEN THE FORCE CONSTANT AND THE ELECTRIC FIELD GRADIENTS

It has been shown[30] that the Hellman-Feynman theorem leads to the following relationship

$$\Delta_A = k/Z_A - q_A = (4\pi/3)\rho(A) - \int \partial\rho/\partial X_A \cos\theta_A/r^2 A d\tau .$$

Here k is the force constant, q_A is the electric field gradient at nucleus A, $\rho(A)$ is the electron density at nucleus A and X_A is the nuclear position coordinate. We find from our computed values of q_A and $\rho(A)$ at $R=3.0a_0$ that $\Delta_{\rm Li}=+0.063a_0^{-3}$ and $\Delta_{\rm H}=+0.0043a_0^{-3}$.

It can be shown[30] that $\Delta_A=0$ if the charge distribution around A is spherical and if it follows the motion of A. Inspection of the LiH wave function shows that these conditions are not met and that small value of $\Delta_{\rm H}$ is due to a fortuitous cancellation of $\rho(A)$ and $\int(\partial\rho/\partial X_A)\times(\cos\theta_A/r^2)d\tau$. When q_A is negative as for lithium, the cancellation clearly cannot occur.

[30] L. Salem, J. Chem. Phys. 38, 1227 (1963).

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Single-Quantum Annihilation of Positrons*

W. R. Johnson, D. J. Buss, and C. O. Carroll
University of Notre Dame, Notre Dame, Indiana
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Calculations of the cross section for single-quantum annihilation of positrons by K-shell electrons in the Coulomb field of a nucleus are presented. Numerical results are given for nuclear charges $Z=73$, 74, 78, 79, 82, and 90 and for energies from threshold to 1.75 MeV. For $Z=82$ the numerical results agree well but not in detail with previous results of Jaeger and Hulme, and show that the Born approximation is too large by a factor of nearly 2.

I. INTRODUCTION

THERE has been some recent experimental interest in the process of single-quantum annihilation of positrons.[1] In a one-photon process recoil momentum must be taken up by a nucleus, so that annihilation is more probable in the K shell than in outer atomic shells. The K-shell annihilation cross section is known numerically for lead, $Z=82$, from the computation of Jaeger and Hulme[2]; and analytically for arbitrary Z from the Born approximation.[3]

The Born-approximation formula, Eq. (20), shows that the cross section is proportional to Z^5; annihilation is therefore more probable for heavy elements than for light. For elements with Z greater than 70 the Born parameter αZ is greater than $\frac{1}{2}$ and the Born approximation is certainly not reliable.

Because of the need for accurate cross sections for elements other than lead it was decided to formulate the problem in such a way that a detailed numerical analysis would be simple.

In Sec. II we explain how the single-photon cross section is reduced to a sum of partial-wave cross sections corresponding to an angular momentum decomposition of the incident positron wave function. The radial integrals occurring in the partial-wave cross sections are reduced to sums of hypergeometric functions in Sec. III. The results of the numerical analysis, together with a discussion of various limiting cases, are presented in Sec. IV.

The numerical results are in precise agreement with the Born approximation as $Z\to 0$, and agree approximately, but not in detail, with the results of Jaeger and Hulme for $Z=82$.

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[2] J. C. Jaeger and H. R. Hulme, Proc. Cambridge Phil. Soc. 32, 158 (1936).

[3] H. J. Bhabha and H. R. Hulme, Proc. Roy. Soc. (London) A146, 723 (1934).

II. REDUCTION OF THE CROSS SECTION

The cross section for single-quantum annihilation is given by

$$\sigma = \frac{\alpha}{4\pi}\frac{W\omega}{p}\int d\Omega_{\mathbf{k}} \sum_{\zeta,\epsilon,\mu} |M|^2 , \tag{1}$$

where the matrix element M is

$$M = -i\int d^3r (v_\zeta^\dagger(\mathbf{r})\boldsymbol{\alpha}\cdot\hat{\epsilon}u_\mu(\mathbf{r}))e^{-i\mathbf{k}\cdot\mathbf{r}} . \tag{2}$$

In the above we denote the energy-momentum vectors of the positron and photon by $(\mathbf{p},iW)$ and $(\mathbf{k},i\omega)$; and the photon polarization vector by $\hat{\epsilon}$. The electron binding energy is given by $m\gamma_1$, where m is the electron mass and $\gamma_1=(1-\alpha^2Z^2)^{1/2}$. We use $v_\zeta(\mathbf{r})$ and $u_\mu(\mathbf{r})$ for the Coulomb field Dirac wave functions of a positron with spin ζ, and a K shell electron with magnetic quantum number μ, respectively.

The K-shell Coulomb wave function is given by[4]

$$u_\mu(\mathbf{r})=\begin{pmatrix} ig_{-1}(\lambda r)\Omega_{-1\mu}(\hat{r}) \\ f_{-1}(\lambda r)\Omega_{1\mu}(\hat{r})\end{pmatrix},\quad \mu=\pm\tfrac{1}{2}. \tag{3}$$

The radial functions g_{-1} and f_{-1} are

$$g_{-1}(\lambda r)=N[(1+\gamma_1)/2]^{1/2}(2\lambda r)^{\gamma_1-1}e^{-\lambda r}, \tag{4}$$
$$f_{-1}(\lambda r)=N[(1-\gamma_1)/2]^{1/2}(2\lambda r)^{\gamma_1-1}e^{-\lambda r},$$

where $\lambda=m\alpha Z$, and $N=[(2\lambda)^3/\Gamma(2\gamma_1+1)]^{1/2}$. The angular dependence in Eq. (3) is expressed by spherical spinors[5]

$$\Omega_{\kappa\mu}(\hat{r})=\textstyle\sum_\lambda C(l,\tfrac{1}{2},j;\mu-\lambda,\lambda)\chi_\lambda Y_{l,\mu-\lambda}(\hat{r}), \tag{5}$$

in which χ_λ are Pauli spinors, $C(l_1,l_2l;m_1,m_2)$ are Clebsch-Gordan coefficients, $Y_{lm}(\hat{r})$ are spherical harmonics, and in which $\kappa=\mp(j+\frac{1}{2})$ for $j=l\pm\frac{1}{2}$.

The positron Coulomb wave function, which is chosen to represent asymptotically a distorted plane wave with an outgoing spherical wave, is

$$v_\zeta^\dagger(\mathbf{r})=4\pi\sum_{\kappa_1,m_1}P_{\kappa_1m_1}{}^*(\hat{p},\hat{\zeta})(f_{\kappa_1}(pr)\Omega_{-\kappa_1m_1}{}^\dagger(\hat{r}),\; ig_{\kappa_1}(pr)\Omega_{\kappa_1m_1}{}^\dagger(\hat{r})), \tag{6}$$

$$P_{\kappa m}(\hat{p},\hat{\zeta})=(\Omega_{\kappa m}{}^\dagger(\hat{p})\chi_{-\zeta}).$$

In Eq. (6) the radial functions f_κ and g_κ are

$$g_\kappa(pr)=-\left(\frac{W+m}{2W}\right)^{1/2}e^{i\gamma\pi/2-\nu\pi/2}\times\frac{\Gamma(\gamma-i\nu)}{\Gamma(2\gamma+1)}(2pr)^{\gamma-1}\{\ \}_-e^{-ipr},$$
$$f_\kappa(pr)=i\left(\frac{W-m}{2W}\right)^{1/2}e^{i\gamma\pi/2-\nu\pi/2}\times\frac{\Gamma(\gamma-i\nu)}{\Gamma(2\gamma+1)}(2pr)^{\gamma-1}\{\ \}_+e^{-ipr}, \tag{7}$$

with

$$\{\ \}_\pm=(\gamma-i\nu)F(\gamma+1-i\nu;2\gamma+1;2ipr)\pm(\kappa-i\nu')F(\gamma-i\nu;2\gamma+1;2ipr), \tag{8}$$
$$\gamma=(k^2-\alpha^2Z^2)^{1/2},\; k=|\kappa|,\; \nu=\alpha ZW/p,\quad \nu'=\alpha Zm/p.$$

With the aid of the above representations for the electron and positron wave functions one is able to reduce the matrix element in Eq. (2) to products of radial integrals and angular coefficients obtained by integrating products of three spherical harmonics. One obtains

$$M=-(4\pi)^2i\sum_{\kappa_1m_1lm}P_{\kappa_1m_1}{}^*(\hat{p},\hat{k})Y_{lm}(\hat{k})\epsilon_{m+m_1-\mu}{}^*\times\{A_{\kappa_1m_1lm\mu}I_{\kappa_1l}-B_{\kappa_1m_1lm\mu}J_{\kappa_1l}\}. \tag{9}$$

The summation indices l and m are associated with the angular decomposition of the photon wave function. The radial integrals I and J occurring in Eq. (9) are given by

$$I_{\kappa_1l}=i^{-l}\int_0^\infty dr\,r^2f_{-1}(\lambda r)f_{\kappa_1}(pr)j_l(kr),$$
$$J_{\kappa_1l}=i^{-l}\int_0^\infty dr\,r^2g_{-1}(\lambda r)g_{\kappa_1}(pr)j_l(kr). \tag{10}$$

The angular coupling coefficients are

$$A_{\kappa_1m_1lm\mu}=(3/4\pi)^{1/2}(2[1][l])C(l,1,l_1';0,0)\times\textstyle\sum_f[f]W(l,1,j_1,\tfrac{1}{2};l_1'f)W(1,\tfrac{1}{2},f,1;\tfrac{1}{2},\tfrac{1}{2})\times(-1)^mC(l,f,j_1;-m,m_1+m)\times C(\tfrac{1}{2},1,f;\mu,m_1+m-\mu), \tag{11}$$
$$B_{\kappa_1m_1lm\mu}=(3/4\pi)^{1/2}\delta_{l_1l}(-1)^mC(l,\tfrac{1}{2},j_1;-m,m_1+m)\times C(\tfrac{1}{2},1,\tfrac{1}{2};\mu,m_1+m-\mu).$$

In Eqs. (11) $[j]=(2j+1)^{1/2}$, $l_1'=2j_1-l_1$, and $W(a,b,c,d;e,f)$ is a Racah coefficient.

Squaring the matrix element M, summing over μ, ζ, $\hat{\epsilon}$, and integrating over photon angles one obtains with some algebra a remarkably simple expression for the cross section:

$$\sigma=16\pi\alpha\frac{W\omega}{p}\sum_{k=1}^\infty k\{|J_{k,k}|^2+|J_{-k,k-1}|^2$$
$$+[1/(2k-1)][(kI_{k,k}+(k-1)I_{k,k-2})J_{k,k}{}^*+\text{c.c.}]+[1/(2k+1)][(kI_{-k,k-1}+(k+1)I_{-k,k+1})J_{-k,k-1}{}^*+\text{c.c.}]$$
$$+[1/(2k-1)^2][(2k^2-1)|I_{k,k}|^2+2k(k-1)|I_{k,k-2}|^2-(k-1)(I_{k,k}I_{k,k-2}{}^*+\text{c.c.})]$$
$$+[1/(2k+1)^2][2k(k+1)|I_{-k,k+1}|^2+(2k^2-1)|I_{-k,k-1}|^2+(k+1)(I_{-k,k-1}I_{-k,k+1}{}^*+\text{c.c.})]\}. \tag{12}$$

The summation index k in Eq. (12) is related to the positron angular momentum by $k=j_1+\frac{1}{2}$. As the positron energy increases one thus expects more and more terms in the sum to contribute. This decomposition is therefore most suitable for studying low-energy annihilation processes.

[4] M. E. Rose, *Relativistic Electron Theory* (John Wiley & Sons, Inc., New York, 1961), p. 177.
[5] M. E. Rose, *Elementary Theory of Angular Momentum* (John Wiley & Sons, Inc., New York, 1957), Chap. III.

III. ANALYSIS OF THE RADIAL INTEGRALS

The evaluation of the radial integrals occurring in Eq. (11) requires the integral

$$K=\int_0^\infty dr\, r^2(2\lambda r)^{\gamma_1-1}(2pr)^{\gamma-1}e^{-\lambda r-ipr}j_l(kr)F(a;b;2ipr). \tag{13}$$

A technique similar to that used by Jaeger and Hulme[6] in the study of internal conversion coefficients is used here. We introduce an integral representation for the confluent hypergeometric function and use the asymptotic series for the spherical Bessel function to find

$$K=\frac{\Gamma(b)}{\Gamma(b-a)\Gamma(a)}\int_0^1 du\, u^{a-1}(1-u)^{b-a-1}\Bigg[i^l\sum_{m=0}^{l}\frac{(-l,m)(l+1,m)}{(1,m)}i^{m+1}\int_0^\infty dr\, r^2(2\lambda r)^{\gamma_1-1}(2pr)^{\gamma-1}(2kr)^{-m-1}$$
$$\times\exp(-\lambda r-ipr-ikr+2ipru)+i^{-l}(k\to -k)\Bigg]. \tag{14}$$

The r integral is written as a gamma function and the remaining parametric integral is expressed as a hypergeometric function. The radial integrals $I_{\kappa l}$ then reduce to

$$I_{\kappa l}=F_I\frac{\Gamma(\gamma-i\nu)\Gamma(\gamma+\gamma_1)}{\Gamma(2\gamma+1)}x^\gamma\sum_{m=0}^{l}\frac{(-l,m)(l+1,m)}{(1,m)(1-\gamma_1-\gamma,m)}\frac{1}{y^m}$$
$$\times\Bigg\{[(\gamma-i\nu)F(\gamma_1+\gamma-m,\gamma+1-i\nu;2\gamma+1;x)+(\kappa-i\nu')F(\gamma_1+\gamma-m,\gamma-i\nu;2\gamma+1;x)]$$
$$+e^{i\pi(\gamma_1+\gamma-l-1)}\left(\frac{p+k-i\lambda}{p+k+i\lambda}\right)^{\gamma+\gamma_1-m}[(\gamma-i\nu)F^*(\gamma_1+\gamma-m,\gamma-i\nu;2\gamma+1;x)$$
$$+(\kappa-i\nu')F^*(\gamma_1+\gamma-m,\gamma+1-i\nu;2\gamma+1;x)]\Bigg\}. \tag{15}$$

The integrals $J_{\kappa l}$ are obtained from Eq. (15) by replacing F_I by iF_J and changing $(\kappa-i\nu')$ to $-(\kappa-i\nu')$. In Eq. (15)

$$F_I=-N[(1-\gamma_1)/2]^{1/2}[(W-m)/2W]^{1/2}e^{-i\pi\gamma_1/2-\nu\pi/2}z^{\gamma_1-1}y/8pk^2,$$
$$F_J=-N[(1+\gamma_1)/2]^{1/2}[(W+m)/2W]^{1/2}e^{-i\pi\gamma_1/2-\nu\pi/2}z^{\gamma_1-1}y/8pk^2, \tag{16}$$

and

$$x=2p/(p+k-i\lambda),\quad y=2k/(p+k-i\lambda),\quad z=2\lambda/(p+k-i\lambda).$$

To avoid repetitive evaluation of the hypergeometric functions we have generated only $F(\gamma_1+\gamma-k-1,\gamma-i\nu;2\gamma+1;x)$ and $F(\gamma_1+\gamma-k-1,\gamma+1-i\nu;2\gamma+1;x)$ from the series, and determined the other F's relevant to a given value of k by use of the contiguous relations

$$dF(d+1,a;b;x)=(d-a)F(d,a;b;x)+aF(d,a+1;b;x),$$
$$d(1-x)F(d+1,a+1;b;x)=(b-a-1)F(d,a;b;x)+(d+1+a-b)F(d,a+1;b;x). \tag{17}$$

This procedure materially reduces the computing time necessary.

IV. NUMERICAL RESULTS AND CONCLUSIONS

The sum in Eq. (12) was evaluated on the Univac 1107 computer at Notre Dame for various values of charge, and as a function of energy from threshold to 1.75 MeV. The accuracy of the computation was maintained at better than 0.1% throughout the range of charge and energy. Results of the calculation are shown in Fig. 1 and in Table I.[7]

[6] J. C. Jaeger and H. R. Hulme, Proc. Roy. Soc. (London) **A138**, 708 (1935).

[7] A FORTRAN IV program to compute the cross section for arbitrary Z and W is available upon request from the Notre Dame Computing Center.

An interesting check on the formalism occurs for the fictitious case of a plane-wave positron incident on a Sommerfeld-Maue bound-state electron. The radial integrals for this case are

$$J_{l,l}=J_{-l-1,l}=N_1(2m/p)Q_l'(1/\beta),$$
$$I_{l,l}=I_{l+2,l}=N_1(lQ_l(1/\beta)-(m/p)Q_l'(1/\beta)), \tag{18}$$
$$I_{-l+1,l}=I_{-l-1,l}=N_1(-(l+1)Q_l(1/\beta)+(m/p)Q_l'(1/\beta)),$$

with

$$N_1=i(\lambda^{5/2}/2mp^2k)[(W-m)/2W]^{1/2}.$$

TABLE I. Annihilation cross sections $\sigma(W,Z)$ in barns for the energies and charge numbers shown.

W/m	47	73	74	78	79	82	90
1.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
1.0625	0.0114	0.0194	0.0193	0.0188	0.0186	0.0180	0.0155
1.1250	0.0298	0.123	0.127	0.143	0.146	0.157	0.180
1.1875	0.0401	0.235	0.246	0.292	0.304	0.341	0.441
1.2500	0.0450	0.315	0.333	0.408	0.429	0.492	0.682
1.3125	0.0472	0.365	0.387	0.485	0.511	0.597	0.862
1.3750	0.0478	0.392	0.417	0.530	0.561	0.661	0.983
1.4375	0.0477	0.404	0.431	0.552	0.586	0.696	1.057
1.5000	0.0472	0.407	0.435	0.560	0.595	0.710	1.095
1.5625	0.0466	0.403	0.413	0.558	0.594	0.711	1.109
1.6250	0.0458	0.396	0.424	0.550	0.585	0.703	1.106
1.6875	0.0450	0.387	0.414	0.538	0.573	0.690	1.091
1.7500	0.0442	0.376	0.403	0.524	0.559	0.673	1.069
1.8125	0.0435	0.366	0.391	0.509	0.543	0.655	1.043
1.8750	0.0428	0.355	0.380	0.494	0.527	0.636	1.015
1.9375	0.0421	0.344	0.368	0.479	0.511	0.616	0.985
2.0000	0.0415	0.334	0.357	0.465	0.495	0.597	0.955
2.0625	0.0409	0.325	0.347	0.451	0.480	0.579	0.926
2.1250	0.0403	0.315	0.337	0.438	0.466	0.562	0.898
2.1875	0.0397	0.307	0.328	0.425	0.453	0.545	0.870
2.2500	0.0392	0.299	0.319	0.413	0.440	0.529	0.844
2.3125	0.0387	0.291	0.311	0.402	0.428	0.514	0.819
2.3750	0.0382	0.284	0.303	0.391	0.416	0.500	0.795
2.4375	0.0378	0.277	0.296	0.381	0.405	0.487	0.773
2.5000	0.0373	0.271	0.289	0.372	0.395	0.474	0.751
2.5625	0.0369	0.264	0.282	0.363	0.386	0.462	0.731
2.6250	0.0364	0.259	0.276	0.354	0.376	0.451	0.712
2.6875	0.0360	0.253	0.270	0.346	0.368	0.440	0.693
2.7500	0.0356	0.248	0.264	0.338	0.360	0.430	0.676
2.8125	0.0352	0.243	0.259	0.331	0.352	0.420	0.660
2.8750	0.0348	0.238	0.254	0.324	0.344	0.411	0.644
2.9375	0.0344	0.234	0.249	0.318	0.337	0.402	0.629
3.0000	0.0340	0.229	0.244	0.311	0.330	0.393	0.615
3.0625	0.0336	0.225	0.239	0.305	0.324	0.385	0.601
3.1250	0.0332	0.221	0.235	0.299	0.317	0.377	0.588
3.1875	0.0328	0.217	0.231	0.293	0.311	0.370	0.575
3.2500	0.0324	0.213	0.227	0.288	0.305	0.363	0.563
3.3125	0.0320	0.209	0.223	0.283	0.300	0.356	0.551
3.3750	0.0317	0.206	0.219	0.277	0.294	0.349	0.540
3.4375	0.0313	0.202	0.215	0.272	0.289	0.342	0.529
3.5000	0.0309	0.199	0.211	0.268	0.283	0.336	0.519

In Eqs. (18) $Q_l(1/\beta)$ is a Legendre function of the second kind and $\beta=p/W$. The sum in Eq. (12) can be carried out analytically to give

$$\sigma=\frac{4\pi r_0^2\alpha^4Z^5}{[\eta^2-1]^{1/2}(\eta+1)^2}(\eta^2-\tfrac{1}{3}\eta+\tfrac{4}{3}), \tag{19}$$

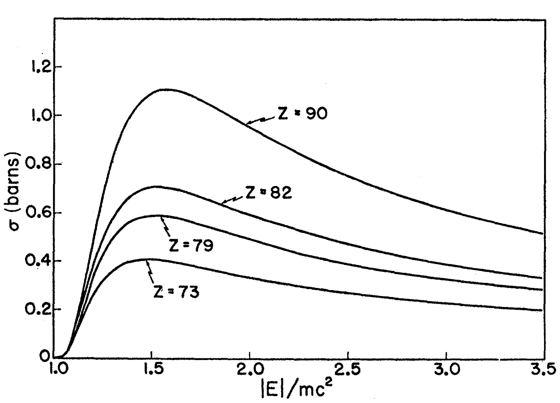

FIG. 1. Total cross section for single-photon annihilation for various elements.

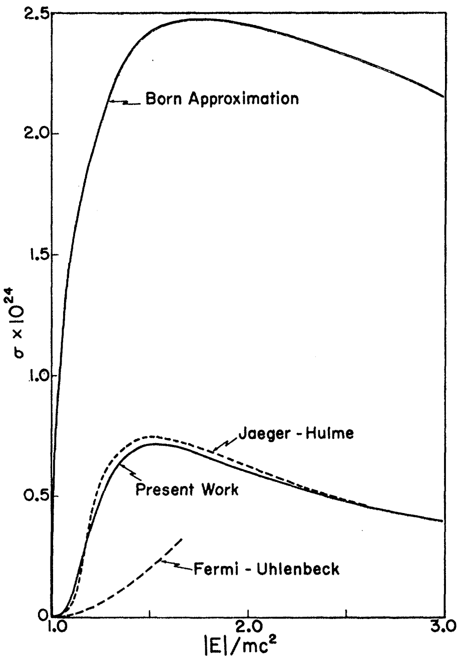

FIG. 2. Comparison of the present work with previous calculations for $Z=82$.

with $\eta=W/m$, and $r_0=\alpha/m=$ electron radius. This formula, which can of course be obtained by standard means, serves to check the procedure used here.

A further check is provided by requiring that the Born approximation be obtained as $Z\rightarrow 0$. Quadratically extrapolating the numerical results for $Z=1$, 5, and 13 to $Z=0$ one recovers the Born-approximation result

$$\sigma=\frac{4\pi r_0^2\alpha^4Z^5}{(\eta^2-1)^{1/2}(\eta+1)^2}\Big[\eta^2+\tfrac{2}{3}\eta+\tfrac{4}{3}-\frac{\eta+2}{(\eta^2-1)^{1/2}}\ln(\eta+(\eta^2-1)^{1/2})\Big], \tag{20}$$

accurately to three significant figures.

As mentioned in the Introduction the numerical results for lead agree well, but not precisely, with the earlier results of Jaeger and Hulme. Figure 2 gives the Jaeger-Hulme result, and the Born result, as well as earlier results of Fermi and Uhlenbeck[8] for comparison purposes.

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[8] E. Fermi and G. E. Uhlenbeck, Phys. Rev. 44, 510 (1933).