still indicative of the Yb^{3+} occupying a position at $x \approx 0.6$ since it is not hard to move the nearest neighbor to positions that begin to approximate the above ratios.

In summary the fits obtained for the crystal-field split levels of the $^2F_{7/2}$ and $^2F_{5/2}$ states of Yb^{3+} and for the g values of the ground doublet of the $^2F_{7/2}$ state indicate that Yb^{3+} is located at ≈ 0.6 Å from an oxygen plane. While there are several inequivalent positions in the lattice that are 0.6 Å from an oxygen plane the interstitial sites (i.e., those not normally occupied by Li or Nb) are improbable as possible sites for the Yb^{3+} ion since the internal strains would be far too large to accommodate a Yb^{3+} ion at these sites. We believe that the results indicate that Yb^{3+} is most likely substitutional on the Li site but the possibility that it is substitutional on the Nb site with a subsequent relaxation of its position by 0.3 Å cannot be rigorously excluded. Also optical and electron-spin-resonance data is reported for Cr^{3+} and Nd^{3+} in $LiNbO_3$[14] and $LiTaO_3$.

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Higher-Shell Contributions and Polarization Correlations in Single-Quantum Annihilation of Positrons

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It is shown that contribution to the single-quantum annihilation cross section from the $2s_{1/2}$ bound electrons cannot be ignored. Calculations of the cross sections have also been made by applying the Biedenharn-Swamy symmetric model, and the region of validity of this model is estimated. Polarization correlations are studied using Dirac-Coulomb wave functions.

I. INTRODUCTION

EXPERIMENTAL and theoretical studies of single-quantum annihilation of positrons with bound electrons have gained momentum in the past few years.[1] The experimental work reported till now refers to measurement of the cross section as a function of positron kinetic energy and the Z value of the atoms in the solid. After the first nonrelativistic estimate of this cross section by Fermi and Uhlenbeck[2] and the approximate relativistic calculations made several years ago,[3] more refined work has recently been carried out.[4] While Fermi and Bethe take into account the annihilation of positrons with K- and L-shell electrons, Johnson's cross sections are based on ignoring all but the K-shell annihilation.

It has long been known that polarization correlations exist in other electron-photon interactions as a result of their carrying a spin angular momentum. For instance, in the case of bremsstrahlung with polarized electrons, an electron which is longitudinally polarized has a high probability of radiating in the forward direction a circularly polarized high-energy photon with the same helicity.[5] Similarly, there is a preferential ejection of photoelectrons in the plane defined by the momentum and polarization vectors of linearly polarized photons.[6] While electrons are polarized in Coulomb scattering,[7]

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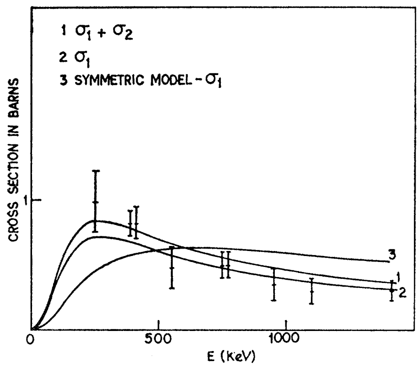

FIG. 1. Comparison of total cross sections for $Z=82$ with and without the $2s_{1/2}$ contribution. Symmetric-model cross section is also shown for comparison.

this effect is much less for positrons which are essentially repelled by the nuclear field, and annihilation methods may be of use in detecting positron polarization. Unfortunately, the cross section for single-quantum annihilation is so small compared to double-quantum annihilation that experimental interest centers only around the observation of the annihilation. McVoy[8] calculated polarization correlations in single-quantum annihilation (total cross sections), using the Born approximation. This is more applicable to light Z atoms, where the annihilation is less likely to take place. Johnson[9] has recently shown the existence of azimuthal asymmetry in the angular distribution of photons resulting from transversely polarized positrons.

A difficulty in relativistic calculations other than the Born approximation is the complexity of the radial parts of the wave functions that are eigenfunctions of the Dirac Hamiltonian, even in the case of the unscreened Coulomb potential for which the Dirac equation possesses exact solutions. In this respect, a simplification—for the Coulomb potential at any rate—exists in the symmetric model.[10] In this paper, we (a) show that the contribution of the higher-shell electrons to the total cross section is not negligible, (b) establish the range of validity of the symmetric model for this problem, and (c) demonstrate the existence of polarization correlations using more realistic wave functions than plane waves.

II. THEORY

We use the notation of Ref. 4 and omit all the detail that can be found in this paper. Since we are also concerned with polarization effects, it is convenient to write the total cross section as a function of ζ (spin of the positron in its rest frame) and ϵ (spin of the photon), and attach a subscript to differentiate annihilation with the $1s_{1/2}$ and $2s_{1/2}$ bound electrons:

$$\sigma(\zeta,\epsilon)=\sigma_1(\zeta,\epsilon)+\sigma_2(\zeta,\epsilon). \quad (1)$$

When we are interested only in the cross section irrespective of polarization effects, there would be an averaging over ζ and summing over ϵ. We shall use the notation $\sigma=\sigma_1+\sigma_2$ when such summation and averaging have been carried out. In this work, we have studied the effect of including the next higher spin-orbit coupled state of the bound electron (L_I), and part of the reason for this stems from the consideration that the symmetric model arranges particles in shells defined by the Dirac quantum number κ, and inclusion of the $2s_{1/2}$ state closes the lowest $\kappa=-1$ subshell. The derivation of the cross section parallels the one given in R4 and the angular parts of the differential cross section are common to both. We only need, therefore, to furnish the appropriate wave functions and radial integrals, which we do in Appendix A. The formula for σ_2 is equivalent to Eq. (12) of R4, with the radial integral given in (A5) of Appendix A. For the symmetric model, similarly, we have to specify the relevant wave functions and appropriate radial integrals occurring in the matrix element, and these are given in Appendix B. This model has been used to compare only σ_1.

Using helicity eigenstates, McVoy[8] estimated polarization-correlation effects and showed that for high enough energies the outgoing photon emerges with the same helicity as the ingoing positron. When the positron is not in field-free space, a unique physical meaning cannot be assigned to the direction of its spin,[11] except in its own rest frame.[12] It can be shown,[13] however, that one can define a polarization vector operator $\mathbf{O}$ such that v_ζ can be regarded as an eigenstate of the z component of the vector with eigenvalue $+1$ (up) and -1 (down), corresponding to $\zeta=+\frac{1}{2}$ and $-\frac{1}{2}$, respectively. We choose the z axis in the direction of the outgoing photon. We now start with a given ζ, say, $+\frac{1}{2}$, and ask for the probability that, for a given positron energy, the outgoing photon is either left circularly polarized $(\sigma_{\frac{1}{2}L})$ or right circularly polarized $(\sigma_{\frac{1}{2}R})$. In specifying left and right circular polarization, we conform to the usual conventions.[8] Equal mixtures of up and down spin positrons in the incident beam correspond to unpolarized incident wave, and this leads to the Johnson cross sections. We now define an asymmetry parameter

$$\delta=(\sigma_{\frac{1}{2}R}-\sigma_{\frac{1}{2}L})/(\sigma_{\frac{1}{2}R}+\sigma_{\frac{1}{2}L}), \qquad \sigma_{\frac{1}{2}R}\equiv\sigma(\tfrac{1}{2},R) \quad (2)$$

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and note in passing that Lenard's theorem is applicable here. A nonzero δ means the existence of polarization correlation, and $\delta=1$ means complete polarization.

III. RESULTS AND DISCUSSION

The cross sections σ and σ_1 in barns for lead as a function of the positron kinetic energy E (in keV) are shown in Fig. 1. Table I gives the cross sections for selected Z values. The symmetric-model estimates are also shown in Fig. 1 for comparison. In Fig. 2, the asymmetry parameter δ, calculated for K-shell annihilation cross sections, is shown as a function of positron energy for different charge numbers. The experimental values of Langhoff[1] for K-shell annihilation are compared with the appropriate theoretical estimates in Fig. 1. The $2s_{1/2}$ contribution appears to be roughly 16% of the K-shell cross section, and this is in general agreement with the earlier predictions of Fermi[2] and Bethe,[3] who had considered the entire L shell. For too large energies, the higher shells may not contribute much, as the positron is now energetic enough to go very near the nucleus. In Fig. 3, we plot $\log\sigma$ versus $\log Z$ in order to extract a Z dependence of the cross section at 1100 keV. The graphs of $\log\sigma$ versus $\log Z$ and $\log\sigma_1$ versus $\log Z$ at 1100 keV happen to be parallel straight lines, and the slope of these indicates that the cross section varies as $Z^{4.4}$, agreeing better with the experimental results of Langhoff[1] than the Born-approximation law of Z^5. The annihilation is predominant in the K shell and, as such, screening correction is inappreciable, and the energies involved clearly rule out solid-state effects like positron-phonon interactions. The annihilation being dependent on the density of bound electrons, this process may be of interest in the matter of the valence-band states, just as a study of the angular correlations in the γ rays of two-photon decay leads to information about the Fermi surface. The symmetric-model estimates agree with experiment in the energy region $0.45<E<1$. While we have not plotted the other cross sections, our results show that a criterion for the validity of this model can

TABLE I. Annihilation cross sections, $\sigma=\sigma_1+\sigma_2$, in barns, for the energies and charge numbers shown.

W/m	47	73	78	82	90
1.0000	0.0000	0.0000	0.0000	0.0000	0.0000
1.0625	0.0130	0.0224	0.0218	0.0209	0.0181
1.1250	0.0340	0.1420	0.166	0.182	0.210
1.1875	0.0457	0.272	0.339	0.396	0.515
1.2500	0.0513	0.364	0.473	0.572	0.797
1.3125	0.0537	0.422	0.562	0.694	1.007
1.3750	0.0544	0.453	0.615	0.769	1.149
1.4375	0.0542	0.467	0.640	0.809	1.236
1.5000	0.0536	0.470	0.649	0.825	1.280
1.5625	0.0529	0.465	0.647	0.826	1.296
1.6250	0.0520	0.457	0.637	0.817	1.293
1.6875	0.0510	0.446	0.623	0.801	1.274
1.7500	0.0501	0.434	0.606	0.781	1.249
1.8125	0.0493	0.422	0.589	0.760	1.218
1.8750	0.0485	0.409	0.571	0.738	1.185
1.9375	0.0477	0.396	0.553	0.714	1.149
2.0000	0.0470	0.384	0.537	0.692	1.114
2.0625	0.0463	0.373	0.520	0.670	1.079
2.1250	0.0456	0.362	0.505	0.650	1.046
2.1875	0.0449	0.352	0.490	0.630	1.013
2.2500	0.0443	0.343	0.476	0.611	0.982
2.4000	0.0429	0.322	0.442	0.571	0.913
2.5500	0.0416	0.304	0.417	0.536	0.855
2.7000	0.0406	0.289	0.395	0.505	0.799
2.8500	0.0393	0.273	0.375	0.478	0.753
3.0000	0.0384	0.262	0.357	0.452	0.712
3.1500	0.0370	0.249	0.340	0.431	0.675
3.3000	0.0363	0.240	0.325	0.411	0.641
3.4500	0.0355	0.232	0.312	0.394	0.616
3.6000	0.0339	0.225	0.298	0.375	0.582

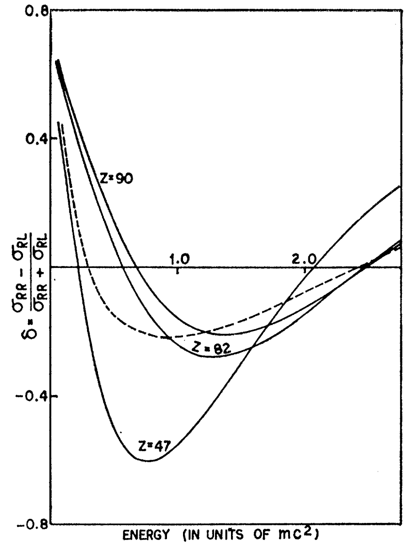

FIG. 2. Asymmetry δ as a function of the kinetic energy E of the positron, in units of mc^2. The dashed curve is on the basis of the symmetric model for $Z=82$.

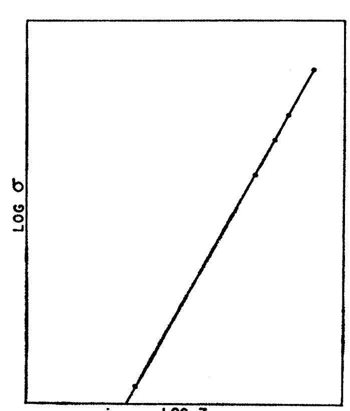

FIG. 3. Log σ versus log Z on an arbitrary scale. The slope is 4.4.

be formed as

$$0.07 < (\alpha Z)^4/\beta < 0.09. \tag{3}$$

Here β is the relativistic velocity parameter. This is understandable because the symmetric model differs from the exact Dirac-Coulomb Hamiltonian by $(\alpha Z)^2/\kappa$, where κ is the Dirac quantum number.

In Fig. 2, the asymmetry parameter δ is plotted as a function of the dimensionless parameter $\epsilon = E/mc^2$ for different Z values. We see that the symmetric model agrees with the exact Dirac-Coulomb curves in qualitative behavior. For high Z values, as the graph shows, the approach to complete polarization commences around 2 MeV, which is higher than the Born-approximation estimate, as can be expected; moreover, the rise is less rapid because of the long range of the Coulomb interaction. As we go to lighter elements, however, the approach of δ to 1 resembles the Born-approximation result. There exists, furthermore, an energy region wherein the asymmetry is such that $\sigma_{\frac{1}{2}L}$ dominates over $\sigma_{\frac{1}{2}R}$, and all this only goes to show that polarization correlations do exist in the annihilation process also.

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APPENDIX A

We shall use the notation of R4 throughout, with the choice $\hbar = c = m = 1$. The radial parts of the $2s_{1/2}$ bound-electron wave functions are given by

$$f_{-1} = N(1-w_1)^{1/2}(a_0 + a_1 r) r^{\gamma_1 - 1} \exp(-\lambda_1 r), \tag{A1}$$

$$ig_{-1} = -N(1+w_1)^{1/2}(c_0 + c_1 r) r^{\gamma_1 - 1} \exp(-\lambda_1 r), \tag{A2}$$

where

$$w_1 = [\tfrac{1}{2}(1+\gamma_1)]^{1/2}, \qquad \lambda_1 = \alpha Z/2w_1, \tag{A3}$$

N is the normalization factor, and

$$\begin{aligned} a_0 &= 2(w_1+1), \\ c_0 &= a_0 - 2, \\ a_1 &= c_1 = -\lambda_1[(4w_1+2)/(2\gamma_1+1)]. \end{aligned} \tag{A4}$$

$I_{\kappa l}^{(\gamma_1, \lambda)}$ in Eq. (15) of R4 goes over into a sum of the two terms

$$I_{\kappa l}(\gamma_1 + 1, \lambda_1) + I_{\kappa l}(\gamma_1, \lambda_1), \tag{A5}$$

with a similar replacement for $J_{\kappa l}$.

APPENDIX B

For the symmetric model, the following changes have to be made in the different wave functions: in Eq. (3) of R4, the changes

$$g_{-1} = [2(1+\epsilon_1) k_b^3]^{1/2} \exp(-k_b r), \tag{B1}$$

$$f_{-1} = -[2(1-\epsilon_1) k_b^3]^{1/2} \exp(-k_b r), \tag{B2}$$

where

$$k_b = \alpha Z \epsilon_1 \qquad \epsilon_1 \equiv [1 + (\alpha Z)^2]^{-1/2}; \tag{B3}$$

in Eqs. (6)–(8) of R4, the changes

$$f_{\kappa 1}(pr) = B(E-1)^{1/2}(\phi_2 + \phi_1), \tag{B4}$$

$$ig_{\kappa 1}(pr) = B(E+1)^{1/2}(\phi_2 - \phi_1), \tag{B5}$$

where

$$B \equiv \left(\frac{i}{(2E)^{1/2}}\right) \frac{\Gamma(k_1 + i\nu)}{\Gamma(2k_1+1)} \exp[(\pi/2)(ik_1 - \nu)],$$

$$\phi_1 = (k_1 - i\nu)(2pr)^{k_1 - 1} e^{-ipr} {}_1F_1(k_1 + i\gamma, 2k_1 + 1; 2ipr), \tag{B6}$$

$$\begin{aligned} \phi_2 = {} & [(k_1^2 + \lambda^2)^{1/2} \exp[-\pi i(k_1 - l_1)] - i(\lambda/p)] \\ & \times (2pr)^{k_1 - 1} e^{-ipr} {}_1F_1(k_1 + 1 + i\nu, 2k_1 + 1; 2ipr). \end{aligned} \tag{B7}$$

Integral K [Eq. (13) of R4] is evaluated to be

$$\begin{aligned} & e^{\pi i/4} \pi^{1/2} 2^{k_1 - l - 2} \frac{\Gamma(l + k_1 + 2)}{\Gamma(l + \frac{3}{2})} \left\{ \frac{k_1^{l + (1/2)} p^{k_1 - 1}}{[k_b + i(k+p)]^{k_1 + l + 2}} \right. \\ & \times F\left[k_1 + l + 2, a, l+1; b, 2l+2; \right. \\ & \left. \left. \times \frac{2ip}{k_b + i(k+p)}, \frac{2ik}{k_b + i(k+p)} \right] \right\}, \end{aligned} \tag{B8}$$

where, in the generalized hypergeometric function of two variables,[14] the simplification is that the parameters are integers.

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