COMMENTS AND ADDENDA

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Comments on Screening and Shell-Ratio Effects in Single-Quantum Pair Annihilation*

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We show that atomic-electron screening and subshell-ratio effects in single-quantum pair annihilation, reported by Broda and Johnson and by Sheth and Swamy, have a simple origin observed also in pair production and atomic photoelectric effect. In all three processes, the characteristic distances are small on an atomic scale, but large on a nuclear scale; wave functions have a point-Coulomb shape, but not the point-Coulomb normalization. Atomic-electron screening effects cause appreciable modifications of the total pair-annihilation cross section for positron energies below $1.5m_ec^2$ in heavy elements ($Z>47$). For low-Z elements, screening effects are always important. The n^3 rule of Bethe for subshell ratios is good only for low-Z elements (where n is the principal quantum number); we find that the subshell ratio between the K and L_I single-quantum pair-annihilation cross sections is well predicted by the square of the ratio of the K and L_I bound-electron wave-function normalizations.

The single-quantum annihilation of a positron with an atomic electron, proposed and calculated nonrelativistically in 1933 by Fermi and Uhlenbeck, [1] is most probable for a K-shell electron. (Energy-momentum conservation does not allow annihilation with a free electron.) Exact relativistic point-Coulomb calculations for the K-electron cross section in a partial-wave formulation have been performed by Jaeger and Hulme[2] for lead and more recently by Johnson, Buss, and Carroll (JBC)[3] for several heavy elements ($Z=47-90$) and positron energies below 2 MeV. These calculations show that Born-approximation[4] results for heavy elements are too large by a factor of nearly 2 and the nonrelativistic results[1] are too small. The books of Heitler[5] and of Roy and Reed[6] provide a summary of the theory to 1967. Recently, Sheth and Swamy[7] have calculated relativistically the L_I-subshell cross sections in a point-Coulomb potential and confirm the earlier predictions of Bethe[8] that higher-shell contributions should be about 16% of the K shell. The use of a point-Coulomb model relies on the expectation, based on form-factor estimates, [8] that atomic-electron screening effects are small. However, Broda and Johnson (BJ)[9] have performed the lengthy relativistic calculations of single-quantum pair-annihilation K- and L-shell cross sections in a screened potential, for elements $Z=47-90$ and positron energies $E_+=1.25$, 1.50, and $1.75m_ec^2$, and find that the atomic-electron screening is not small for low positron energies and tends to increase the cross section. This is the same screening behavior found in low-energy atomic-pair production. [10] We wish to point out that the screening and subshell-ratio effects in single-quantum pair annihilation have a simple origin which we also observed in atomic-pair production[10] and the atomic photoelectric effect. [11]

For qualitative purposes, the simplest Born approximation, replacing the positron wave function by a plane wave, can be used to estimate the important regions of configuration space for the single-quantum pair-annihilation matrix element. [8] The matrix-element integral, [12]

$$M_{fi} \propto \int e^{i\vec{q}\cdot\vec{r}}\psi_{\text{bound}}d^3r \ ,$$

is cutoff at large distances by the exponentially decaying bound-electron wave function ψ_{bound} and the oscillating momentum transfer factor $e^{i\vec{q}\cdot\vec{r}}$, where $\vec{q}=\vec{p}_+-\vec{k}$ is the momentum transfer to the atom with $\vec{p}_+$ and $\vec{k}$, the momentum of incident positron and the momentum of emitted photon, respectively. For single-quantum pair annihilation, the momen-

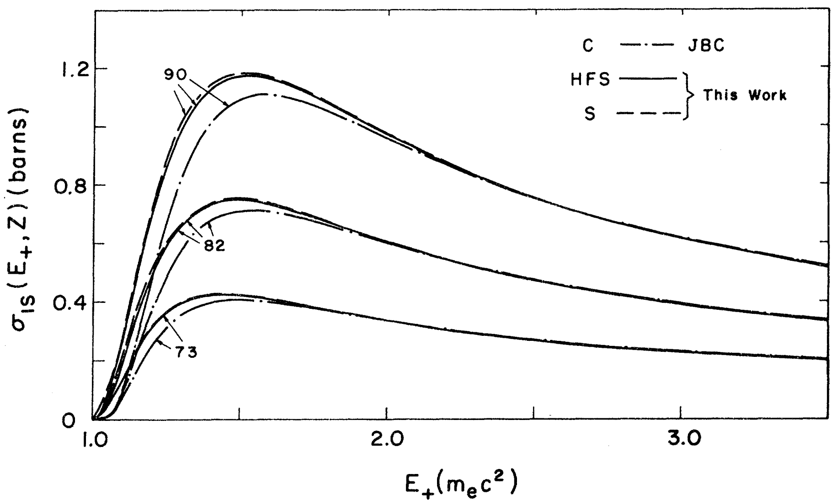

FIG. 1. Comparisons of K-shell single-quantum pair-annihilation cross sections σ_{1s} for positron energies $E_+ = 1.0$–$3.5 m_ec^2$. The numbers attached to the curves give the atomic number of the target element. The symbol s refers to results for a relativistic-Hartree-Fock-Slater bound state and without exchange for the positron, as assumed by Broda and Johnson (Ref. 9). Symbols C and HFS refer to results which assumed that both bound and continuum states see the same point-Coulomb or relativistic-Hartree-Fock-Slater potentials, respectively.

tum transfer cutoff always acts first, because irrespective of photon energy the minimum momentum transfer[12] $q_{\min} \approx 1$. This leads to a cutoff at the order of electron-Compton-wavelength distances. (Since all volume elements of d^3r for which $r \lesssim 1/q$ give comparable contributions, the contribution from the region of the nuclear volume is negligible.) By contrast, in the atomic photoeffect such distances dominate only for photon energies well above threshold[11] and in pair production they only dominate close to threshold.[10] At electron-Compton-wavelength distances an electron sees a point-Coulomb potential corresponding to the nuclear charge Z. The electron wave function has a hydrogenlike shape; the only effect of atomic-electron screening, as described by a central potential $V(r)$ deviating from the point-Coulomb form, is to modify the normalization.[13] For bound states, this change in normalization is greater in low-Z elements and much larger for higher shells—1–25% for the K shell and 10–90% for the L shell over the range of $Z = 2$–100. For high-Z elements the very-low-energy continuum-state normalization are also sensitive to screening, while at higher energies the continuum normalization is unaffected by screening.

We have recently examined[13] in greater detail the shapes of electron wave functions near, but outside, the atomic nucleus. This leads us to a simple quantitative prediction of the effect of atomic-electron screening on single-quantum pair-annihilation cross sections, which we propose to describe here for the entire energy range of the point-Coulomb calculations of JBC.[3] Our observation was that a screened continuum electron or positron wave function of shifted energy $\delta E_\pm = \pm(\epsilon_s - \epsilon_c)$, + for positron and − for electron, at small distances is even closer in shape to a point-Coulomb wave function than is a screened wave function of the same energy, i.e., $\delta E_\pm = 0$. Here $\delta E = E_s - E_c$ (the subscripts s and c stand for screened and point-Coulomb potentials, respectively) and ϵ is the binding energy of the bound state. An analytic calculation[13] indicated that the deviation from the point-Coulomb shape at small distances is approximately

$$\frac{\alpha^2 Z^{4/3} r^2}{2l+3} \quad \text{for} \quad \delta E_\pm = 0$$

and

$$\frac{\alpha^2 Z^{2/3} r^2}{4(2l+3)} \quad \text{for} \quad \delta E_\pm = \pm(\epsilon_s - \epsilon_c)\,,$$

for lth partial waves. This was verified in numeri-

TABLE I. Values of $\epsilon_c - \epsilon_s$ and Ξ^2, where ϵ is the binding energy of bound K states and Ξ is the ratio of screened to point-Coulomb bound-K-state normalizations. Symbols c, s, HFS, and HFN refer to the point-Coulomb, screened, the Hartree-Fock-Slater, and the Hartree-Fock-Slater without exchange potentials, respectively.

Z	47	73	74	78	79	82	90
ϵ_{HFS}(keV)	25.490	67.588	69.715	78.656	81.004	88.351	110.250
$\epsilon_c - \epsilon_{HFS}$ (m_ec^2)	0.0108	0.0214	0.0219	0.0240	0.0244	0.0259	0.0310
$\epsilon_c - \epsilon_{HFN}$ (m_ec^2)	0.0120	0.0235	0.0240	0.0261	0.0268	0.0285	0.0340
Ξ^2_{HFS}	0.9801	0.9852	0.9853	0.9858	0.9859	0.9861	0.9867

TABLE II. Comparisons of K-shell single-quantum pair-annihilation cross sections. Symbols c, s, and EST refer to the point-Coulomb potential, the screened potential Broda and Johnson used (Ref. 9), and the energy-shift screening theory, respectively, $\Delta_{EST} \equiv [\sigma_{EST} - \sigma_s(BJ)]/\sigma_s(BJ)$.

E_+ (m_ec^2)	Z	σ_c(JBC)	σ_s(BJ) (b/atom)	σ_{EST}	Δ_{EST} (%)
1.25	47	0.0450	0.0477	0.0470	−1.5
	73	0.315	0.369	0.366	−0.8
	82	0.492	0.605	0.605	0.0
	90	0.682	0.879	0.895	1.8
1.50	47	0.0472	0.0481	0.0475	−1.2
	73	0.407	0.427	0.423	−0.9
	82	0.710	0.755	0.750	−0.7
	90	1.095	1.182	1.180	−0.2
1.75	47	0.0442	0.0446	0.0441	−1.1
	73	0.376	0.385	0.381	−1.0
	82	0.673	0.693	0.687	−0.9
	90	1.069	1.107	1.102	−0.5

cal calculations. Since in single-quantum pair annihilation for a given emitted photon energy k, if the bound-state energy is shifted $\delta E_B = \epsilon_c - \epsilon_s$ because of screening, the incident positron must also have an energy shift $\delta E_+ = -\delta E_B$; we predict that a point-Coulomb single-quantum pair-annihilation cross section with a specified positron energy E_{+c} and photon energy k differs only by a normalization factor from the screened cross section corresponding to the same photon energy k but positron energy $E_{+s} = E_{+c} + \epsilon_s - \epsilon_c$. We further noted a simple behavior of the continuum-state normalization. For low-κ partial waves, except at very low energies, $\tilde{N}_s \equiv (p_s E_s)^{1/2} N_s$ is equal to $\tilde{N}_c \equiv (p_c E_c)^{1/2} \times N_c$ for the case with energy shift, where N_s and N_c are the normalization of the continuum wave functions of screened and point-Coulomb potentials, respectively. At high energies, even for high-κ partial waves, $\tilde{N}_s$ is equal to $\tilde{N}_c$ with or without energy shift. For single-quantum pair annihilation, the low-κ partial waves dominate the cross section for low positron energies. Consequently, since for a cross section the square of the matrix element is multiplied[9] by the kinematic factor E/p, we are led to predict the relation

$$\sigma_s(E_{+s}) = \Xi^2 \frac{p_{+c}^2}{p_{+s}^2} \sigma_c(E_{+c})$$

between screened and point-Coulomb single-quantum pair-annihilation total cross sections resulting in photons of the same energy k, where Ξ is the ratio of screened to point-Coulomb bound-state normalization and $E_{+s} = E_{+c} + \epsilon_s - \epsilon_c$. Values of $\epsilon_c - \epsilon_s$ and Ξ^2 for the Hartree–Fock–Slater potential are given in Table I.

With this energy-shift screening theory (EST) we have converted all the point-Coulomb K-shell single-quantum pair-annihilation results of JBC[3] for incident positron energies in the range 1.0–3.5m_ec^2 and elements of $Z = 47-90$. Samples of results are shown in Fig. 1. From these data we then made comparisons with the exact numerical calculations of Broda and Johnson (BJ)[9] to test the

TABLE III. K-shell single-quantum pair-annihilation cross sections in the Hartree–Fock–Slater potential obtained with energy-shift screening theory from the JBC (Ref. 3) point-Coulomb results.

$E_+(m_ec^2)$ \ Z	47	74	82	90
		σ_{HFS} (b)		
1.0625	0.0176	0.0688	0.0886	0.114
1.1250	0.0343	0.200	0.282	0.383
1.1875	0.0430	0.312	0.465	0.662
1.2500	0.0467	0.384	0.594	0.875
1.3125	0.0483	0.426	0.678	1.021
1.3750	0.0484	0.446	0.723	1.109
1.4375	0.0481	0.452	0.743	1.155
1.5000	0.0474	0.451	0.746	1.171
1.5625	0.0466	0.443	0.738	1.169
1.6250	0.0457	0.433	0.724	1.152
1.6875	0.0448	0.421	0.706	1.127
1.7500	0.0440	0.408	0.685	1.098
1.8750	0.0425	0.382	0.643	1.033
2.0000	0.0412	0.359	0.602	0.967
2.2500	0.0388	0.319	0.530	0.849
2.5000	0.0368	0.288	0.474	0.752
2.7500	0.0351	0.263	0.429	0.677
3.0000	0.0335	0.243	0.392	0.614
3.2500	0.0319	0.226	0.361	0.561
3.5000	0.0304	0.209	0.333	0.516

TABLE IV. Subshell ratios σ_{1s}/σ_{2s} for the K-shell and the L_I-subshell single-quantum pair-annihilation cross sections in the point-Coulomb potential. (N_{1s} and N_{2s} are the K- and L_I-bound-electron wave-function normalizations.)

$E_+(m_ec^2)$ \ Z	47	73	90
		σ_{1s}/σ_{2s}	
1.0625	7.13	6.47	5.96
1.1250	7.10	6.47	6.00
1.2500	7.14	6.43	5.93
1.3750	7.24	6.43	5.92
1.5000	7.38	6.46	5.92
2.0000	7.55	6.68	6.01
3.0000	7.73	6.94	6.34
		N_{1s}^2/N_{2s}^2	
	7.20	6.17	5.35

validity of the energy-shift screening theory. The agreement is very good as shown in Table II. For L_I subshell, our predictions also agree quite well with the exact results of BJ. (The point-Coulomb L_I-subshell results were taken from the results of Sheth and Swamy. [7]) From this conversion of the point-Coulomb results of JBC, we present a tabulation, Table III, of the single-quantum pair-annihilation K-shell cross section for positron energies $1.0-3.5 m_e c^2$ and target elements of $Z = 47$, 74, 82, and 90. We can see from Fig. 1 and Table II that the screening effect is not important for positron energies $E_+ > 1.5 m_e c^2$ and $Z = 47-90$. For low positron energies and elements of $Z \gtrsim 47$, the atomic-electron screening increases the K-shell single-quantum pair-annihilation cross section, while for higher positron energies it tends to decrease the cross section. The turning point is $E_+ \approx 1.57$, 2.19, and $2.62 m_e c^2$ for $Z = 47$, 74, and 90, respectively. For low-Z elements the atomic-electron screening decreases the cross section. Although the existing data allow us to test the energy-shift screening theory for K-shell and L_I-subshell annihilations, we expect that it should also be good for higher subshells.

Another consequence of the dominance of electron-Compton-wavelength distances in single-quantum pair annihilation is that cross sections from bound states of the same orbital angular momentum but different principal quantum number n are related, for example, the n^3 rule predicted by Bethe. [8] This follows[13] because the dependence on binding energy ϵ (i.e., n) only enters starting from the r^2 term of a wave-function expansion for small r. Thus at small distances, dependence on n enters only through the wave-function normalization. The agreement in shape between wave functions of different subshells in the same potential is not as close as between point-Coulomb and screened wave functions for the same subshell. This agreement is the origin of the observed nearly energy-independent ratios of cross sections in a given potential, as shown in Table IV, where the point-Coulomb L_I-subshell results were taken from the results of Sheth and Swamy. [7] The n^3 rule is good only for low-Z but not for high-Z elements, where further n dependence enters the normalizations. However, we indeed find that

$$\frac{\sigma_{1s}}{\sigma_{2s}} \approx \frac{N_{1s}^2}{N_{2s}^2},$$

where N_{1s} and N_{2s} are the K- and L_I-bound-electron wave-function normalizations. The deviations from this prediction reflect the fact that agreement of wave-function shapes is only fair.

Single-quantum pair annihilation has so far received little attention. The cross section is small compared to two-quanta pair annihilation and amounts in heavy elements (in which it is largest) to less than 20% of the two-quanta annihilation (based on the Born approximation). [4,8] The first successful experiment on single-quantum pair annihilation was reported by Sodickson *et al.* [14]; subsequent results are due to Langhoff *et al.* and Mazaki *et al.* [15] The experimental errors are still too large to test the details of the theory.

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