Production or annihilation of positrons with bound electrons

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We have investigated the recently reported discrepancy between theory and a new experiment [Palathingal *et al.*, Phys. Rev. A **51**, 2122 (1995)] for single-quantum annihilation of positrons with bound electrons. Fully relativistic calculations of total cross sections for the production and the annihilation of positrons involving an electron bound in the K or L shells of atoms have been performed in screened atomic potentials, for a number of elements ranging from germanium ($Z=32$) to thorium ($Z=90$) and for positron kinetic energies up to 4 MeV above threshold. Very good agreement with earlier calculations, that had been performed over a more restricted range of elements and energies, is obtained, also confirming that the Z and shell dependence previously seen continues at higher energies. The results presented here extend theory to energies where recent experiments have been performed, at forward angle, which were assumed to characterize the Z and shell dependence of the corresponding total cross sections. Our new theoretical predictions are not consistent with the strong dependence of the K- and L-shell bound-pair-annihilation cross sections on the nuclear charge of the target reported in those experiments. An explanation of these discrepancies is proposed, namely, that it is not correct to assume the same ratios for total cross sections as for forward distributions. This is demonstrated using existing data for the related photoeffect process, and it is seen that such forward data are indeed consistent with the pair-annihilation experiments.

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The first observations of the positron [1] were readily understood as the production of a free positron-electron pair [2]. The resulting positron usually annihilates with an electron, producing two photons, each with energy equal to the rest mass of the electron. Annihilation of positrons by electrons deeply bound in the atom was originally proposed to explain harder radiation, at energies nearly equal to twice the rest mass of the electron, in cosmic ray showers [3]. The cross section for the proposed process was first evaluated by Fermi and Uhlenbeck [4]. Since that time, interest in the process (or its inverse, bound-pair production) has recurred on a tridecenial basis. Each burst of activity has reflected remarkable advances in the techniques used to address this and other problems. While the initial calculations of Fermi and Uhlenbeck [4] were performed within a nonrelativistic framework, within a few years full S-matrix calculations were available [5]. This increasing sophistication of theory mirrored that for the photoelectric effect, as the single-quantum annihilation of pairs may be conceptualized as a radiative recombination process.

Unfortunately, one thing the early calculations of the annihilation process made clear was that it was far too weak to be detected at the time. (The bound-pair-production process is still less likely to be observed in neutral atoms, where the dominant inner shells are filled.) Nearly thirty years later the single-quantum annihilation of positrons by bound electrons was finally unambiguously observed by Sodickson and coworkers [6]. Their result for lead was in agreement with the S-matrix calculation of Jaeger and Hulme [5], and the dependence of the cross section on the nuclear charge of the target agreed with the predictions of the Born approximation [7]. The latter point was perhaps surprising as the Born approximation cross section had been shown to be far too large for lead (as it also is in the related process of photoeffect for high Z). A number of the experiments that followed explored the cross section for other elements and energies and its Z dependence at other energies [8–11]. Corresponding extensions of S-matrix theory were made to other elements and energies [12], to the angular distribution of the annihilation radiation [13], to the L_1 subshell [14] and to calculations for the K and L shells in screened atomic potentials [15]. Because of the relationship of bound-pair annihilation and production to photoeffect, certain aspects of the process, such as the high-energy limit, the ratio of the cross sections in the L_1 and K shells, and the effects of screening, were readily understood in terms of simpler theories initially applied to photoeffect [16,17].

More recently, interest has turned to bound-pair production. This inverse process to single-quantum annihilation is only appreciable for highly charged ions, where vacancies in the dominant inner shells occur. This process is expected to be a limiting factor in beam lifetime at the next generation of heavy-ion colliders [18], currently under construction in the hopes of investigating features in highly relativistic ion-ion collisions, such as quark-gluon plasmas. An ion that changes its state in this way will no longer be accelerated with the ion beam as designed. Two classes of techniques to calculate bound-pair production in ion-ion collisions have mainly been used. One class is nonperturbative and involves the numerical evaluation of the time-dependent Dirac equation [19–21]. The other class is perturbative and includes such approaches as the use of cross sections for bound-pair production by real photons together with the method of virtual quanta [22]. Recent studies have indicated that the nonperturbative part of the total cross section should be fairly small [23], except at small impact parameter.

It is useful then to study the creation or annihilation of bound pairs by photons in order to better understand the details of the analogous process in ion-ion collisions. Recently, experiments were performed by Palathingal *et al.* [24], finding a stronger dependence on Z of the cross section for the related process of bound-pair annihilation than had been calculated or observed at lower energies. It is the purpose of this paper (1) to extend S-matrix calculations of this process to higher energies in order to address these new results, and (2) to offer a possible explanation of the apparent discrepancy between experiment and theory.

The methods used for the calculations of the present work depart somewhat from earlier S-matrix calculations of single-quantum pair annihilation. Here the total cross section for bound-pair production is obtained from the forward-scattering amplitude for elastic photon-atom (Rayleigh) scattering via the optical theorem,

$$\sigma^{\rm BPP}=\frac{4\pi c}{\omega}{\rm Im}A^{\rm EF}(\omega), \tag{1}$$

where $\sigma^{\rm BPP}$ is the bound-pair-production cross section. $A^{\rm EF}$ is the emission-first amplitude for Rayleigh scattering; its relationship to the matrix element for bound-pair production or annihilation is immediately apparent upon examination:

$$A^{\rm EF}=\sum_n \frac{\langle i|\alpha\epsilon e^{i\mathbf{k}\cdot\mathbf{r}}|n\rangle\langle n|\alpha\epsilon^* e^{-i\mathbf{k}\cdot\mathbf{r}}|i\rangle}{E_i-E_n-\hbar\omega}. \tag{2}$$

The scattering state $|i\rangle$ is obtained by direct integration of the Dirac equation in a screened atomic potential. The sum over intermediate states $|n\rangle$ is not performed explicitly but is replaced by the solution of an inhomogeneous equation in the same atomic potential (using the method of Brown, Peierls, and Woodward [25], also utilized by Dalgarno and Lewis [26] in electron scattering processes). We make use of a computer code developed previously to calculate Rayleigh scattering [27]. This code has been extensively tested and is found to agree with experiment for a wide range of energies and elements [28]. A scheme for interpolating partial waves in slowly convergent series has made it possible to perform calculations with this code for higher energies than those [12–15,22] that had originally been considered. Our approach here has the advantage of utilizing a well understood, robust code; however, it only obtains the total cross sections for these processes, not the angular distribution.

In Fig. 1 total cross sections for annihilation of positrons with electrons bound in the K or L shell of a range of elements are given for the extremes of the range of the positron energies considered here. These cross sections are obtained through detailed balance from the bound-pair-production cross sections produced by the code, using the relationship (which may be obtained by considering the different densities of final states and incident fluxes in the two processes)

$$\frac{\sigma^{\rm BPA}}{\sigma^{\rm BPP}}=\frac{(\hbar\omega)^2}{(\hbar\omega-mc^2+E_b)^2-(mc^2)^2}, \tag{3}$$

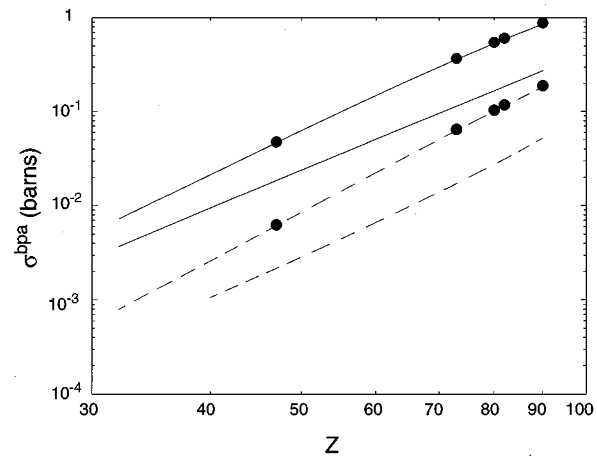

FIG. 1. The cross section for positron annihilation with bound electrons is shown as a function of atomic number. The solid curves are for the K shell where the top (bottom) curve is for positron kinetic energies of 128 (4066) keV. The dashed curves are for the L shell at the same energies. The results of Broda and Johnson [15] at 128 keV are also shown (circles).

where E_b is the electron binding energy. The data of Broda and Johnson [15], obtained in similar screened atomic potentials, are also shown for the low-energy cases where they are available. The agreement between the calculations is very good, confirming the equivalence of the different methods used [29]. This figure also serves to illustrate that the cross section does scale fairly well as Z^ν. However, the value of ν is clearly somewhat dependent on the scattering shell and on the positron energy.

Figure 2 contains the results obtained for the exponent ν of the Z dependence of the K-shell total cross section. The present theoretical results are given by the solid curve, shown together with the available experimental data. The

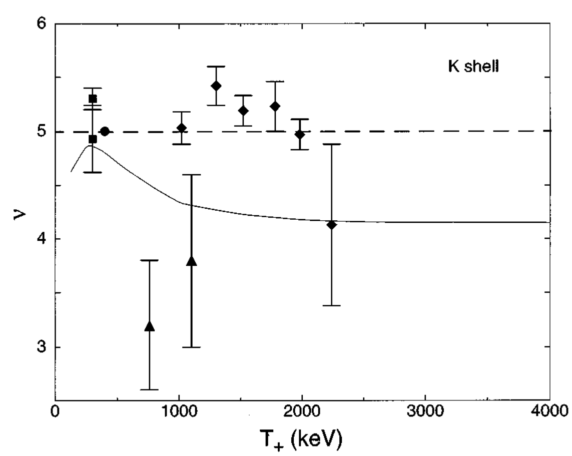

FIG. 2. The exponent in the charge dependence of the total cross section is given for annihilation of a positron by electrons bound in the K shell as a function of positron kinetic energy (solid curve). The other data are the reported experimental results of Sodickson *et al.* [6] (circle), Weigmann, Hansen, and Flammersfeld [9] (triangles), Mazaki, Nishi, and Shimizu [10] (squares), and Palathingal *et al.* [24] (diamonds). The dashed line $\nu=5$ is the Born approximation prediction of Bhabha and Hulme [7].

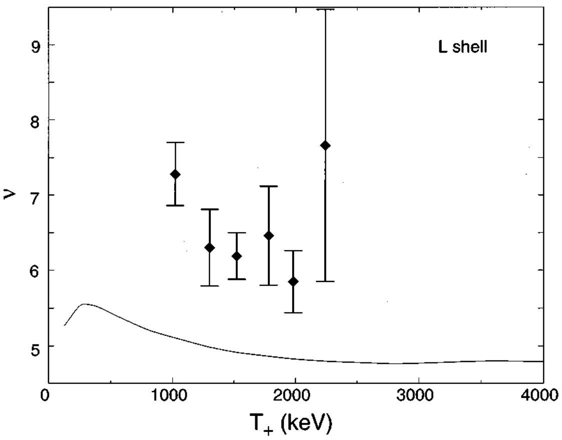

FIG. 3. The exponent in the charge dependence of the total cross section is given for annihilation of a positron by electrons bound in the L shell as a function of positron kinetic energy (solid curve). The other data are the reported experimental results of Palathingal *et al.* [24] (diamonds).

experimental data vary between groups of experimenters, possibly reflecting the very different techniques chosen to obtain total cross sections from data at fixed angle. The result in the Born approximation [7], proceeding from relativistic Coulombic wave functions, gives the fixed value 5 for this exponent at all positron energies. Figure 3 presents the corresponding results for the L shell. The only available experimental data are from the recent experiment of Palathingal and co-workers [24]. Their data, as for the K shell, lie far above theory, suggesting in both cases a much stronger dependence of the cross section on nuclear charge. We note the theoretical L-shell predictions lie above K-shell predictions. This may be understood by realizing that, at the relativistic Born approximation level, $1s$ and $2s$ cross sections go as Z^5, but $2p$ cross sections go as Z^7.

In Fig. 4 we present comparisons between theory and experiment for the ratios of the L-shell to K-shell cross sections for gadolinium $(Z=64)$, for halfnium $(Z=72)$, for lead $(Z=82)$, and for thorium $(Z=90)$. The agreement is reasonable, particularly at the lower Z. The ratio found here is similar to that obtained from the total photoeffect cross sections of Scofield [30]. In fact, a more detailed breakdown of this ratio by subshell is similar to what may be expected from photoeffect.

How can we understand the discrepancies between theoretical predictions and results reported from recent experiments [24]? Palathingal *et al.* [24] used thin targets and detected photons emitted in the forward direction. They assumed that the charge dependence of these forward measurements should be the same as for the total cross section. (This assumption was based on an analysis of Johnson's [13] low-energy data.) We argue that this assumption is incorrect and can explain the discrepancy between experimental data and theoretical calculations of total cross sections. Single-quantum annihilation is analogous to photoeffect from s states, where the forward cross section vanishes at low Z and "fills in" at high energies for high Z targets. This "filling in" of the forward cross section is due to additional factors of Z in its charge dependence relative to the total cross section [31–33,37], eventually characterized by Z^2 in the high-energy limit. This may be seen, for example, in the numerical K-shell data of Hultberg, Nagel, and Olsson [34]. These observations also apply in the case of bound-pair annihilation or production. In fact, as may be seen from Figs. 2 and 3, the forward-angle data of the recent measurements are consistent with this interpretation, showing extra Z dependence (approximately one extra power at these energies) in comparison to the total cross-section predictions. The same argument

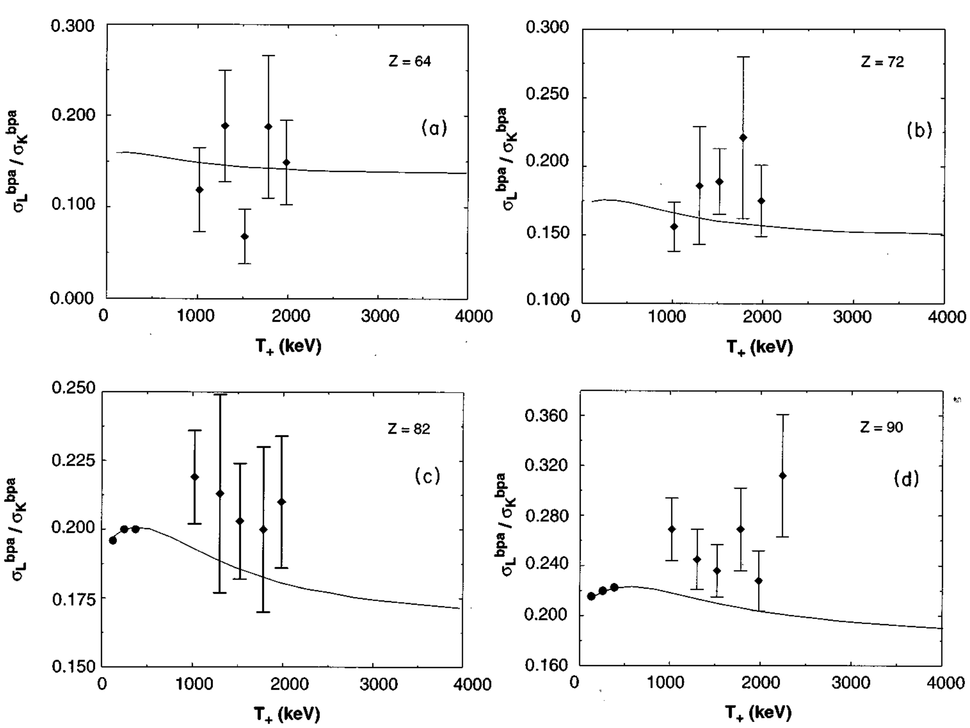

FIG. 4. The ratio of the L-shell to the K-shell total cross sections for positron annihilation by (a) gadolinium $(Z=64)$, (b) halfnium $(Z=72)$, (c) lead $(Z=82)$, and (d) thorium $(Z=90)$. The results of the present work are denoted by the solid curves. The calculations of Broda and Johnson [15] are shown where available (circles). The experimental data as reported by Palathingal *et al.* [24] are also shown.

does not apply to the p electrons in the L shell. Indeed, the Born approximation predicts an isotropic distribution for photoionization from the $2p$ states [35]. Tseng *et al.* [36] have demonstrated that this is not true, particularly for high Z. However, the L-shell data for pair annihilation of Broda and Johnson [15] show that, at the relatively low positron kinetic energy of 128 keV, the p states account for 1/3 of the forward and for 1/4 of the total L-shell cross section for lead. The experimental data of Fig. 4 are suggestive of a ratio of forward to total L to K ratios, which is increasing with Z.

In summary, we have extended the range of available theoretical total cross section data for the single-quantum annihilation of positrons into the range of recent experiments. The results that are obtained at low energy agree reasonably well with earlier calculations of this process [12–15,22], both in numerical values at low energies and in predicting the Z dependence and the L to K ratios. The greater Z dependence of the cross sections reported in recent experiments [24] is not found in our total-cross-section calculations. We suggest that this is likely due to the greater Z dependence of the forward cross section relative to the total cross section. This feature has been observed in the related photoeffect process. It would be of interest to perform measurements at other angles, so that total cross sections could be obtained to test this interpretation.

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