Positron interactions with high-Z atoms at relativistic energies

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We consider the interaction of a positron with a bound electron of a high-Z atom. In particular, we present relativistic calculations of the cross sections for knockout and/or positronium formation in a thorium target, as well as an internal process in a hypothetical Z = 164 "atom." Both plane-wave and distorted-wave Born approximations are discussed. We find peaks in the final sum energy of the electron-positron pairs due to the momentum distribution of the atomic electron. However, these peaks are too low in energy and are too broad compared with peaks claimed in e⁺e⁻ scattering or with the anomalous positron peaks in heavy-ion experiments.

I. INTRODUCTION

Among the most exciting recent developments in nuclear physics is the experimental evidence for anomalous positron peaks, later found to be coincident with electrons in heavy-ion collisions close to the Coulomb barrier.¹ The positrons and electrons appear to emerge with equal kinetic energies of several hundred keV. There have been numerous attempts to explain these peaks,²,³ but so far none with any success.

In a related experiment, Erb and collaborators found an electron-positron coincidence peak in the final state when positrons are scattered from thorium, but no peak when a tantalum target was used.⁴ If these peaks are real (Ref. 4 states that they might be due to Compton scattering in the detectors) then it is interesting that the singles (electron or positron) peaks are at about 850 keV, which are the energies seen in the heavy-ion collision experiments.⁵

The final electron and positron kinetic energies in both cases are large enough so that processes associated with the bulk (i.e., solid-state) structure of the target can be ruled out, but atomic or nuclear phenomena cannot. The presence of an electron coincident with the positron in the final state suggests, but does not imply, an atomic process. However, the interaction of high-energy positrons with heavy atoms has not been a topic of great interest to date, perhaps because monochromatic beams have not been available and new phenomena are not obviously present.

In this paper we consider conventional atomic processes in which an incident positron knocks out a deeply bound electron (K or L shell) from a heavy atom. We have in mind here the secondary interaction of positrons produced in a heavy-ion collision with other atoms in the target or the primary interactions of the positrons in the experiment of Erb et al. It is not implausible that such a mechanism could produce equal-energy electron-positron pairs at a particular total energy. The Coulomb attraction between the outgoing electron and positron tends to correlate their momenta, the extreme limit being a bound state of positronium (subsequently dissociated by its passage through the target). Peaking in the total energy arises from the momentum content of the bound-state wave function. For example, the K-shell wave function is largest at zero momentum, implying that the knockout or positronium cross section will peak at a particular incident positron (and hence total) energy. Of course, the effects of phase-space factors, being off-mass shell, and distortion of the initial and final states by the atomic potential will modify this peak. Our calculations in this paper are aimed at determining whether the locations, strengths, and widths of these peaks are at all compatible with the experiments we have cited above.

There have also been speculations that long-lived compound nuclei might be formed in heavy-ion collisions just above the Coulomb barrier.⁶ With this in mind, we have also considered the interaction of a positron emitted from such a system (by an unspecified mechanism) with the bound electrons. Considerations similar to those described above lead to a similar expectation of peaking in the "internal" knockout and positronium probabilities.

Our presentation is organized as follows. Section II describes nonrelativistic and relativistic plane-wave Born-approximation calculations of both the knockout and positronium formation processes induced by a mildly relativistic positron incident on a heavy atom. Section III extends the calculation to the distorted-wave Born approximation to include the effects of the atomic potential on the initial and final states. Section IV discusses internal scattering of a positron from the bound electrons of a hypothetical Z = 164 compound nucleus. We then draw together these three sets of results in Sec. V and discuss their relations to experimental data, before we summarize and conclude in Sec. VI.

II. PLANE-WAVE APPROXIMATION

Our plane-wave calculation is very similar to that for free Bhabha scattering,⁶,⁷ except that the electron is bound in the initial state. This means a fixed energy but arbitrary momentum, and the cross section will be proportional to the square of the bound-state wave function at the relevant momentum transfer. We first present a nonrelativistic plane-wave calculation to illustrate the relevant physics.
A. Nonrelativistic calculation

The initial state consists of a bound electron with wave function $\psi_B$, and an incident positron plane wave,

$$\psi_{\text{initial}} = \psi_B(r_-) e^{i p_+ \cdot r_+},$$

where $p_+$ is the three-momentum of the incident positron and $r_-$ is the position of the electron (positron). The final state can be written as the product of two plane waves and the relative wave function between the final positron and electron $\psi_e$,

$$\psi_{\text{final}} = e^{i p_+ \cdot r_+} e^{-i p_- \cdot r_-} \psi_e(r_+ - r_-).$$

Here $p_+$ ($p_-$) is the momentum of the outgoing positron (electron). The first Born approximation to the knockout amplitude is therefore

$$M = \iint \int d^3 r_+ d^3 r_- e^{-i p_+ \cdot r_+} e^{-i p_- \cdot r_-} \psi_e^*(r_+ - r_-)$$

$$\times \frac{-e^2}{|r_+ - r_-|} e^{i p_+ \cdot r_+} \psi_B(r_-).$$

For small relative momenta of the electron and positron, $\psi_e$ varies on a length scale ($\lambda$) much greater than those of the other terms (fm) in the amplitude, while for large relative momenta $\psi_e \approx 1$. Thus we can safely put $\psi_e(r) = \psi_e(0)$ and move it outside of the integral. After some straightforward manipulations and inserting the phase-space factors, we arrive at the differential cross section

$$\frac{d^3 \sigma}{d \Omega_+d \Omega_-dE_+} = \frac{\alpha^2}{2\pi^2} \frac{E_i}{p_i} (p_+ + p_- - E_+ - E_-)^{-(2j_B + 1)}$$

$$\times |\psi_e(0)|^2 |\psi_B(p_B)|^2.$$

(1)

Here $\Omega_+ (\pm)$ and $E_+(\pm)$ are the solid angles and energies for the final positron and electron, $p_B = p_+ + p_- - p_i$, and $j_B$ is the angular momentum of the bound state. For a 1S electron, the bound wave function $\psi_B$ peaks at zero momentum, so that the cross section will peak for nonzero momenta of the final-state pair, depending strongly upon the momentum of the incident positron. Correlations due to the final-state Coulomb attraction between the electron and positron can be accounted for by the nonrelativistic Gamow factor,

$$|\psi_e(0)|^2 \equiv f(|p_+ - p_-|) = \frac{2\pi \eta}{1 - e^{-2\pi \eta}},$$

$$\eta = \frac{m \alpha}{|p_+ - p_-|}$$

(2)

since it is important only for small relative momenta.

We can integrate Eq. (1) over the solid angles to obtain the total cross section,

$$\frac{d\sigma}{dE_+} = \frac{\alpha^2}{\pi^2} \frac{E_i}{p_i} p_+ + p_- E_+ + E_- \int_{-1}^{1} d\cos\theta_+ \int_{-1}^{1} d\cos\theta_- \int_{0}^{2\pi} d\phi - \frac{1}{(p_i - p_+)^2} |\psi_e(0)|^2 |\psi_B(p_B)|^2,$$

(3)

where

$$p_B^2 = p_+^2 + p_-^2 + 2p_+ p_- (\cos \theta_+ \cos \theta_- + \sin \theta_+ \sin \theta_- \cos \phi_-) = p_i^2 - 2p_i (p_+ \cos \theta_+ + p_- \cos \theta_-),$$

and $\theta_\pm (\phi_\pm)$ is the polar (azimuthal) angles of the final positron and electron.

The cross sections for positronium formation are very similar to Eqs. (1) and (3), except that in the phase-space factor they are modified and $\psi_e$ is the 1S positronium wave function. Thus

$$\left[ \frac{d\sigma}{d\Omega_+} \right]_{\text{Ps}} = (2\pi \eta)^{1/2} \frac{1}{p_+ + E_+} |\psi_{\text{Ps}}(0)|^2 \left[ \frac{d\sigma}{d\Omega_+ d\Omega_- dE_+} \right]_{\text{ko}} |E_+ = E_- , \theta_+ = \theta_- , \phi_+ = 0|.$$

Here $E_+$ is one half of the positronium energy, and we use the nonrelativistic positronium wave function $|\psi_{\text{Ps}}(0)\rangle^2 = m^3 \alpha^3 / 8\pi$.

B. Relativistic calculation

The relativistic plane-wave calculation follows the same spirit as the nonrelativistic one. We must calculate the matrix element for the sum of two Feynman diagrams; scattering and annihilation (Fig. 1). The resulting cross section for knockout is given by (see Appendix A)

$$\frac{d^3 \sigma}{d \Omega_+ d \Omega_- dE_+} = \frac{\alpha^2}{2\pi^2} \frac{p_+ + p_-}{p_i} (2j_B + 1) |\mathcal{M}_B|^2,$$

(4)

$$|\mathcal{M}_B|^2 = \left[ \left( k_\perp \cdot k_\perp \right) (B_\perp \cdot k_i) + (k_\perp \cdot k_i) (k_\perp \cdot B_\perp) - m^2 (k_\perp \cdot B_\perp) - mB_s (k_\perp \cdot k_i) + 2m^2 B_s \right] \frac{1}{(k_i - k_\perp)^4}$$

$$+ \left( k_\perp \cdot k_i (B_\perp \cdot k_\perp) + (k_\perp \cdot k_i) (k_\perp \cdot B_\perp) + m^2 (k_\perp \cdot B_\perp) + mB_s (k_\perp \cdot k_\perp) + 2m^2 B_s \right] \frac{1}{(k_\perp + k_\perp)^4}$$

$$+ [2(k_\perp \cdot k_i) (B_\perp \cdot k_\perp) - mB_s (k_\perp \cdot k_i - k_\perp \cdot k_\perp - k_\perp \cdot k_\perp)$$

$$- m^2 (k_\perp \cdot B_\perp - k_\perp \cdot B_\perp - k_\perp \cdot k_\perp) + 2m^2 B_s] \frac{1}{(k_i - k_\perp)^2 (k_\perp + k_\perp)^2}.$$
tron wave functions is therefore in order.

We approach the problem using the relativistic distorted-wave Born approximation, which consists of evaluating the graphs in Fig. 1, but replacing the lepton plane-wave states by distorted waves. In this case, the electron and positron spinors, as well as the photon propagator, are expanded in partial waves, and the amplitudes are calculated explicitly before adding and squaring to give the cross section. The differential cross section for electron-positron knockout is given by

$$\frac{d^3\sigma}{dE_+d\Omega_+d\Omega_-} = \frac{1}{(2\pi)^5} \frac{E_i}{p_i} (p_+ E_+ p_- E_-)$$

$$\times f(\mid p_+ - p_- \mid )$$

$$\times \frac{1}{2} \sum_{S,P,Q,M_Q} \mid \mathcal{M}(S,P,Q,M_Q;\kappa_B) \mid^2 , (6)$$

where $f(\mid p_+ - p_- \mid )$ is a correlation function describing the final-state interaction of the emerging leptons. In the case of positronium formation, the differential cross section is

$$\frac{d\sigma}{d\Omega_+} |_{PS} = \frac{1}{(2\pi)^2} \frac{E_i}{2p_i} \frac{p_+ E_+}{2} \mid \psi_{PS}(0) \mid^2$$

$$\times \frac{1}{2} \sum_{S,P,Q,M_Q} \mid \mathcal{M}(S,P,Q,M_Q;\kappa_B) \mid^2 |_{p_+ = p_-} , (7)$$

where $E_+ = (E_i + E_B)/2$, and the positronium wave function has been evaluated at the origin. We can integrate the cross sections over the solid angles $\Omega_+$ and $\Omega_-$ to obtain the total knockout cross section. The outline of the calculation of the matrix elements $\mathcal{M}$ and the final cross section formulas are given in Appendix B.

As a test of our distorted-wave calculation, we examined the convergence of the cross section as a function of the number of partial waves. The convergence of the total cross section with the partial-wave sum is quite rapid; four partial waves in the photon propagator and eight in the lepton wave functions were sufficient for convergence to 10% accuracy. We also find that the cross section with the distortions omitted is in good agreement with the plane-wave results of the previous section. However, the convergence of the angle-differential cross section with partial waves is quite slow. Cross terms between different partial waves are important here and so the contributions of higher partial waves are amplified when they interfere with lower partial waves. Because of practical limits on the number of partial waves we can include in our calculations, we will not present results for angle-differential cross sections in this paper.

### III. DISTORTED-WAVE CALCULATION

Since the potential energy at the K shell of thorium ($Z = 90$) is about 200 keV, we expect a significant Coulomb distortion of the incident and outgoing particles in the scattering process. Indeed, a naive treatment of this distortion using the appropriate Gamow factors shows that the cross section will be dramatically different in the distorted case. A relativistic treatment taking into account the Coulomb distortion of the electron and positron wave functions is therefore in order.

$$B = (B_0, \text{sgn}(\kappa_B) F_B(p_B) G_B(p_B) \hat{p}_B),$$

$$B_0 = \frac{[G_B^2(p_B) + F_B^2(p_B)]}{2}, \quad B_s = \frac{[G_B^2(p_B) - F_B^2(p_B)]}{2}.$$

$B$ labels the bound-state quantum numbers, $k$, $k_+$, and $k_-$ are the four-momenta of the initial positron and final-state positron and electron, respectively [$k = (E, p)$]. $G_B$ and $F_B$ are the radial parts of the upper and lower components of the bound-state electron in momentum space, as given in Appendix A.

To study positronium formation, the cross section is modified by the phase-space restriction $p_+ = p_-$. The result is

$$\frac{d\sigma}{d\Omega_+} = \alpha^2 \frac{p_+}{p_i |E_+|} (2j_B + 1) \mid \mathcal{M}(p_+ = p_-) \mid^2 \mid \psi_{PS}(0) \mid^2 . (5)$$

Note the different kinematic prefactors from the knockout cross section. The extra factor of $\alpha^2$ in the positronium wave function severely reduces the magnitude of the cross section compared to the simple knockout.

### IV. INTERNAL SCATTERING WHEN $Z = 164$

Reinhardt et al. have proposed that a compound nucleus might be formed during heavy-ion collisions at energies just above the Coulomb barrier. Such a compound nucleus would have an "atomic" charge so large that the electric fields around it would be very high. In fact, for
supercritical systems \((Z \geq 173)\), it is expected that the vacuum will break down spontaneously, producing electron-positron pairs.\(^5\) We discuss in this section the scattering of a positron produced close to a hypothetical \(Z = 164\) compound nucleus with one of its bound-state electrons.

The first-order diagrams we need to evaluate are the same as those in Fig. 1, except that now a Coulomb distorted propagator

\[
S_p(\mathbf{R}, \mathbf{r}_1) = \pi \sum_{\kappa, \mu} \psi_{\kappa, \mu}^{(+)}(\mathbf{R}) \psi_{\kappa, \mu}^{(-)}(\mathbf{r}_1)
\]

(8)

is used for the incident positron, instead of a distorted-wave spinor. In Eq. (8), the propagator is formed from the Coulomb distorted positron wave functions \(\psi_{\kappa, \mu}^{(\pm)}\), with outgoing waves boundary conditions. We have specified that the positron propagates from coordinate \(\mathbf{R} \approx 0\) (close to the nucleus) to \(\mathbf{r}_1\), but not the physical process that produces the positron. Then the contribution from higher partial waves in the sum in Eq. (8) is small, and we can approximate the propagator by its \(S\)-wave component only,

\[
\psi_{\ell \mu}^{(+)}(\mathbf{r}_1) = \left[ \frac{E_i + m}{\pi} \right]^{1/2} \sqrt{\frac{\mathbf{p}_1 \cdot \mathbf{e}}{\mathbf{p}_1 \cdot \mathbf{r}_1}} \times \left\{ \begin{array}{l}
-i \mathbf{J} \mathbf{r}_1 | (1 \frac{1}{2}, -\mu) \\
\mathcal{G}(\mathbf{r}_1) | (0 \frac{1}{2}, -\mu)
\end{array} \right.
\]

where

\[
\mathcal{G}(\mathbf{r}_1) = i \mathcal{R} \rightarrow \mathbf{p}_1 \mathbf{r}_1 \hbar \delta(\mathbf{p}_1 \cdot \mathbf{r}_1) \rightarrow e^{i(p_1 r_1 + \delta)}
\]

at asymptotically large \(r_1\). Here \(\mathcal{R}\) and \(\mathcal{J}\) are the regular and irregular solutions, respectively, of the Dirac equation with a Lenz-Jensen potential (defined in Appendix B) and \(p_i = (E_i^2 - m^2)^{1/2}\).

The absolute cross section of internal scattering depends on the particular process that creates the positron. However, we are interested only in the ratio of the internal scattering cross section to the cross section of a positron being emitted without interacting with the electrons. To study a simple example, we assume that the coupling between the positron and its source has the form \(g \psi_{\pm} \gamma_0 \psi_{\pm}\), where \(\psi_{\pm}\) is the wave function of the emitted positron and \(\psi_{\pm}\) is arbitrary and will factor out when we take the ratio. The rest of the calculation is now very similar to that in Sec. III, except that for such a high-Z system, the bound-state wave functions would be drawn very close to the nucleus, and we can no longer use the hydrogen atom wave functions for the bound state electrons. We instead integrate the Dirac equation with a smeared nuclear charge and obtain the bound-state wave functions numerically. The rate of positron internal scattering is

\[
\frac{d \Gamma}{dE_+} = \frac{p_i^2}{2} \left| \frac{d \sigma}{dE_+} \right|_{\text{ext}},
\]

(9)

where \(\Gamma = R_i / R_f\) is the ratio of the rates of internal scattering events to free positron emission. \(\left| d \sigma / dE_+ \right|_{\text{ext}}\) is the differential cross section for scattering using the formula for external scattering, Eq. (B8), but with the positron propagator replacing the incident wave function.

V. RESULTS

If thick targets are used (such as the one of Erb et al.), \(\approx 50\) mg/cm\(^2\), electrons and positrons undergo multiple scattering in the target sufficient to destroy any angular information, so that we need consider only the total cross sections for knockout. The plane-wave calculation is straightforward, with good convergence in the angular integrals using 48-point Gauss-Legendre quadrature (needed for convergence at high \(E\)). The distorted-wave calculation was performed on the National Science Foundation-San Diego Supercomputer Center (NSF/SDSC) Cray X-MP computer and convergence was good, as discussed in Sec. III. The calculation took about 5 central-processing-unit (CPU) minutes per point in the \(E_+ - E_-\) plane.

In Figs. 2(a) and 2(b) we show the total cross section for knockout of a 1S electron in \(^{232}\)Th without and with distortion. Both cases are Bhabha-like, with a large cross

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FIG. 2. Angle-integrated knockout cross section (barn/MeV) for positron scattering from the 1S electron of a thorium atom. The final electron (\(E_-\)) and positron energy (\(E_+\)) are in MeV. The plane-wave (a) and distorted-wave (b) results are shown.
section at high-positron and low-electron energies. There
is a broad hump at low energies reflecting the momentum
distribution of the bound-state electrons. This is shown
clearly in Fig. 3, where the distorted-wave cross section is
plotted along the $E_+ = E_-$ diagonal. Comparing the
plane-wave and distorted-wave results, we find that the
distortion pushes the peak to higher energy, although
only by about 50 keV. This peak in the sum energy is too
low and too broad compared to those seen in either the
Gesellschaft für Schwerionenforschung (GSI)
or Erb's experiments. Knockout from higher shells gives
narrower sum peaks, but at even lower energies (see
Table I). We found no peaks in the difference spectrum,
as angle integration destroys the final-state Coulomb
correlation.

In Fig. 4 we show the cross section for positron formation from a 1S electron of $^{90}\text{Th}$ as a function of the
final positron energy (half of the positronium energy).
Again comparing with the plane-wave results, we find
that distortion suppresses the cross section, as well as
pushing the peak to a higher energy. The sum peak is
quite narrow, though again at too low an energy when
compared with experiments. Results for higher shells are
qualitatively similar (Table I). A comparison of Figs. 3
and 4 shows that positronium formation is suppressed by
a factor of $10^6$ relative to knockout.

The internal scattering cross section for 1S knockout and
positronium formation in a $Z = 164$ compound nuclu
are shown in Fig. 5. The sum peaks move up to
0.88 and 1.25 MeV, respectively, but are very broad.

### Table I. Location and widths of peaks in the cross section
for external positron scattering from thorium. Widths are given
at half maximum.

<table>
<thead>
<tr>
<th>Electron states</th>
<th>Knockout (MeV)</th>
<th>Positronium (MeV)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1S</td>
<td>$0.61^{+0.06}_{-0.18}$</td>
<td>$0.58^{+0.04}_{-0.10}$</td>
</tr>
<tr>
<td>2S</td>
<td>$0.54^{+0.03}_{-0.02}$</td>
<td>$0.53^{+0.01}_{-0.02}$</td>
</tr>
<tr>
<td>2P(_{1/2})</td>
<td>$0.54^{+0.04}_{-0.02}$</td>
<td>$0.54^{+0.02}_{-0.03}$</td>
</tr>
</tbody>
</table>

**Figure 3.** The cross section in Fig. 2(b) along the $E_+ = E_-$ diagonal.

**Figure 4.** Positronium formation cross section with 1S thorium
electrons, as a function of half of the positronium energy.

**Figure 5.** Ratio of the rates of internal positron scattering and
free positron emission in a hypothetical $Z = 164$ "atom," for (a)
knockout and (b) positronium formation.
TABLE II. Location and widths of peaks in the cross section for internal positron scattering in a Z = 164 atom. Widths are given at half maximum.

<table>
<thead>
<tr>
<th>Electron states</th>
<th>Knockout (MeV)</th>
<th>Positronium (MeV)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1S</td>
<td>0.88 ± 0.18</td>
<td>1.25 ± 0.40</td>
</tr>
<tr>
<td>2S</td>
<td>0.77 ± 0.14</td>
<td>1.25 ± 0.20</td>
</tr>
<tr>
<td>2P_{1/2}</td>
<td>0.87 ± 0.22</td>
<td>1.00 ± 0.30</td>
</tr>
<tr>
<td>2P_{3/2}</td>
<td>0.61 ± 0.11</td>
<td>0.66 ± 0.32</td>
</tr>
<tr>
<td>3S</td>
<td>0.61 ± 0.05</td>
<td>0.61 ± 0.16</td>
</tr>
</tbody>
</table>

(≈0.5–1.0 MeV); these can both be understood as consequences of a more deeply bound electron with a broader momentum distribution. Results from higher shells are again qualitatively similar (Table II).

VI. SUMMARY AND CONCLUSION

We have shown that positron knockout of a bound-state electron in a high-Z atom gives rise to peak structures in the final sum energy of the electron-positron pair. For external scattering by a thorium target, we found that the peaks corresponding to the knockout from inner shells are all at relatively low energies, E_{sum} ≤ 1.2 MeV. Distortion of the lepton waves moves the peaks to slightly higher energies relative to a plane-wave calculation, but at the same time suppresses the cross section. The knockout cross sections show no peak structures in the difference energy spectrum, and positronium formation cross section is suppressed by a factor of ≈α^3 compared to knockout. Internal scattering of a positron in a Z = 164 atom also shows peaks in the final sum energy. These peaks are at much higher energies (E_{sum} = 1.7–2.5 MeV) than those for thorium, though their widths are also much larger. In conclusion, the atomic processes we have considered in this paper do not seem to be directly responsible for either the Erb's peak or the GSI peaks.

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APPENDIX A: PLANE-WAVE-CALCULATION DETAILS

In this appendix we derive the plane-wave amplitude for the knockout of a bound electron by an incident positron. We will follow the conventions of Bjorken and Drell. The transition-matrix element is given by the difference of the direct and annihilation terms,

\[ M_B = e^2 \left\{ \bar{u}(k_i) \gamma_\mu v(k_+) \frac{1}{(k_+ - k_i)^2} \bar{u}(k_-) \gamma_\mu u_B(k_B) - \bar{u}(k_-) \gamma_\mu v(k_+) \frac{1}{(k_+ + k_B)^2} \bar{u}(k_i) \gamma_\mu u_B(k_B) \right\}. \]

The only difference between this matrix element and that of Bhabha scattering is that the initial electron is in a bound state

\[ u_B = \begin{pmatrix} G_B \\ -\text{sgn}(k_B) \sigma \cdot \hat{p}_B \end{pmatrix} \frac{\mathcal{U}_M}{\mathcal{U}_d} \frac{1}{\sqrt{2}}. \]

with \( \sigma \) the Pauli spin matrices and \( \mathcal{U} \) a spin-angular harmonic. \( G_B \) and \( F_B \) are the radial parts of the upper and lower components of the wave function in momentum space. For scattering from electrons in the inner shells of thorium (Z = 90), we use hydrogen wave functions. For example, for the 1S state,

\[ G_B(p_B) = C_1 \frac{4\pi}{p_B} \frac{\Gamma(\gamma + 1)}{(a^2 + p_B^2)^{\gamma/2}} \times \sin \left( (\gamma + 1) \tan^{-1} \left( \frac{p_B}{a} \right) \right) \]

and

\[ F_B(p_B) = C_2 \frac{4\pi}{p_B} \frac{\Gamma(\gamma + 1)}{\sqrt{2}} \frac{1}{(a^2 + p_B^2)^{\gamma/2}} \cos \left( (\gamma + 1) \tan^{-1} \left( \frac{p_B}{a} \right) \right), \]

where \( B_r \) and \( B_z \) are defined in Eq. (4). We can therefore calculate the square of the matrix element (summed over final spins and initial electron spins, averaged over initial positron spins), using standard trace techniques. The result is given in Eq. (4).

APPENDIX B: DISTORTED-WAVE CALCULATION DETAILS

In this appendix we derive the distorted-wave amplitude for the knockout of a bound electron by an incident
positron. The transition amplitude is given by the difference of the direct and annihilation terms,

\[
T_d = \int d^4x \int d^4y \left[ \bar{u}^{(-)}_{\gamma \mu}(x) (\gamma^\mu - i e) u_B(x) \right] i D_{\mu \nu}(x, y) \left[ \bar{v}^{(-)}_{\gamma \nu}(y) (\gamma^\nu - i e) v_k^{(-)}(y) \right]
\]

\[
T_a = \int d^4x \int d^4y \left[ \bar{u}^{(-)}_{\gamma \mu}(x) (\gamma^\mu - i e) v_k^{(-)}(x) \right] i D_{\mu \nu}(x, y) \left[ \bar{v}^{(-)}_{\gamma \nu}(y) (\gamma^\nu - i e) u_B(y) \right]
\]

where

\[
iD_{\mu \nu}(x, y) = \int \frac{d^4q}{(2\pi)^4} e^{-iq \cdot (x - y)} \frac{-ig_{\mu \nu}}{q^2 + i\epsilon}
\]

is the photon propagator, \(u\) and \(v\) are distorted wave spinors related by charge conjugation,

\[
v^{(+)\dagger}_{ks}(x) = i \gamma^2 u^{(+)\dagger}_{ks}(x)
\]

and displaying the appropriate boundary conditions. In the presence of the strong Coulomb generated by the heavy nucleus, the Dirac spinors do not satisfy the free Dirac equation and therefore no longer carry a simple plane-wave dependence. The spinors, however, still carry a simple harmonic time dependence, which enables us to perform both time integrals, as well as the integral involving the photon propagator, in a straightforward way. The transition amplitude can thus be written as

\[
T = -2\pi \delta(E_e + E_B - E_+ - E_-) \mathcal{M}
\]

where \(\mathcal{M} = M_d - M_a\), with

\[
M_d = \left[ \frac{e^2}{4\pi} \left( \int d^3x \int d^3y \left[ \bar{u}^{(-)}_{\gamma \mu}(x) (\gamma^\mu - i e) u_B(x) \right] \right) \right]^{1/2}
\]

\[
\times \left[ \bar{v}^{(-)}_{\gamma \nu}(y) (\gamma^\nu - i e) v_k^{(-)}(y) \right]
\]

\[
M_a = \left[ \frac{e^2}{4\pi} \left( \int d^3x \int d^3y \left[ \bar{u}^{(-)}_{\gamma \mu}(x) (\gamma^\mu - i e) u_B(x) \right] \right) \right]^{1/2}
\]

\[
\times \left[ \bar{v}^{(-)}_{\gamma \nu}(y) (\gamma^\nu - i e) u_B(y) \right]
\]

\[
\times \frac{e^2}{4\pi} \left( \int d^3x \int d^3y \left[ \bar{u}^{(-)}_{\gamma \mu}(x) (\gamma^\mu - i e) u_B(x) \right] \right) \left[ \bar{v}^{(-)}_{\gamma \nu}(y) (\gamma^\nu - i e) v_k^{(-)}(y) \right]
\]

The electron spinors can then be written as

\[
u^{(+)\dagger}_{ps}(x) = \left[ \frac{E + m}{2E} \right]^{1/2} \sum_{\kappa, M, m_s} 4\pi \delta(-1)^{\kappa - M} (\gamma^\mu)_{\gamma\mu} \left\{ Y_{\kappa m_s}^{(\pm)} \left( \hat{\mu} \right) \frac{e^{iB_{\gamma\mu}(\hat{\mu}) \gamma^\mu - \kappa M}}{p \times} \right\}
\]

In the preceding expressions, \(E = (p^2 + m^2)^{1/2}\) is the energy of the lepton and the spinors have been normalized to one particle per unit volume. The radial components of the Dirac spinors are real functions of \(x\) satisfying the first-order coupled differential equations

\[
\begin{align*}
\left( \frac{d}{dx} + \frac{\kappa}{x} \right) G_{E_s}(x) &= \left[ E + m - V(x) \right] F_{E_s}(x), \\
\left( \frac{d}{dx} - \frac{\kappa}{x} \right) F_{E_s}(x) &= -\left[ E + m - V(x) \right] G_{E_s}(x)
\end{align*}
\]

with boundary conditions to be specified below, and with a relative minus sign between the electron-nucleus and positron-nucleus potentials.

The preceding system of differential equations can be

\( \text{easily manipulated into a one dimensional Schrödinger-type equation. We write the lower component of the wave function in terms of the upper,} \)

\[
F_{E_s}(x) = \frac{1}{\left[ E + m - V(x) \right]} \left( \frac{d}{dx} + \frac{\kappa}{x} \right) G_{E_s}(x)
\]

substitute it into the second equation, and introduce \(\phi_{ik}(x)\) through the definition

\[
G_{E_s}(x) = \sqrt{E + m - V(x)} \phi_{ik}(x)
\]

to obtain

\[
\left( \frac{d^2}{dx^2} + \frac{k^2}{x^2} - \frac{l(l+1)}{x^2} - U(x) \right) \phi_{ik}(x) = 0
\]
together with the boundary conditions
\[ \phi_{\text{H}}(x = 0) = 0, \]
\[ \phi_{\text{H}}(x) - \sin \left( kx - \frac{\pi}{2} + \delta_1(k) \right) \quad \text{as} \quad x \to \infty. \]
The effective potential \( U(x) \) is given by
\[
U(x) = 2EV(x) - V^2(x) - \frac{\kappa}{E + m - V(x)} \frac{dV}{dx} + \frac{1}{4(E + m - V)^2} \left( \frac{dV}{dx} \right)^2 + \frac{1}{2(E + m - V)} \frac{d^2V}{dx^2}.
\]
We use the Lenz-Jensen approximation to the Thomas-Fermi potential,
\[
V(r) = -\frac{Ze^2}{r}e^{-\gamma(1 + y + b_3y^2 + b_4y^3 + b_4y^4)},
\]
with \( b_2 = 0.3344, \quad b_3 = 0.0485, \quad b_4 = 2.647 \times 10^{-3}, \)
and \( y = 0.20166Z^{1/2}(r \text{ in MeV}^{-1}, V \text{ in MeV}). \)
After expanding the photon propagator in spherical harmonics, with coefficients given in terms of spherical Bessel functions,
\[
e^{i|\mathbf{x} - \mathbf{y}|} = 4\pi \sum_{\lambda, \mu} j_{\lambda}(x_\gamma) \hat{h}_{\lambda}^{\mu}(x_\gamma Y_{\lambda\mu}(\mathbf{x})Y_{\lambda\mu}^*(\mathbf{y}),
\]
where \( x_\gamma = \max\{|x|, |y|\} \) and \( x_\gamma = \min\{|x|, |y|\}. \)
We can evaluate analytically the angular part of the scattering amplitude. A typical matrix element encountered in the evaluation of the direct amplitude has the form
\[
B = \sum_m (-1)^m \langle \kappa_\text{-}m_\text{-} | \langle (Y_{\lambda} \sigma_{\gamma})_m | \kappa_B m_B \rangle \langle (Y_{\lambda} \sigma_{\gamma})_{-m} | \kappa_\text{+} m_\text{+} \rangle
\]
\[
= \sum_m (-1)^m \langle j_B m_B ; j m_\text{-} | j_\text{+} m_\text{-} ; j_\text{+} m_\text{+} \rangle \langle j_B m_B | \kappa_B \rangle \langle \kappa_\text{+} m_\text{+} \rangle \langle j_B m_B | j_\text{+} m_\text{-} | j_\text{+} m_\text{+} ; j_\text{+} m_\text{+} \rangle
\]
\[
\times \langle \kappa_\text{+} | (Y_{\lambda} \sigma_{\gamma})_m | \kappa_B \rangle \langle \kappa_\text{+} | (Y_{\lambda} \sigma_{\gamma})_{-m} | \kappa_\text{+} \rangle,
\]
where the reduced matrix element is given by
\[
R_{\lambda, \mu}^{\kappa_\text{+}, \kappa_\text{-}} \equiv \langle \kappa_\text{+} | (Y_{\lambda} \sigma_{\gamma})_{-m} | \kappa_\text{-} \rangle = \frac{i^2 \hat{j}_\text{+} \hat{j}_\text{-}}{4\pi} \langle l_\text{+} 0 | \lambda 0 | l_\text{-} 0 \rangle \left( \begin{array}{c c c}
\lambda & \frac{1}{2} & \frac{1}{2} \\
\frac{1}{2} & \frac{1}{2} & \nu \\
\frac{1}{2} & \frac{1}{2} & \frac{1}{2}
\end{array} \right)
\]
and \( \hat{j}_\text{+} \equiv \sqrt{2j_\text{+} + 1}. \) Similar expressions appear in the evaluation of the annihilation term.

We simplify the calculation of the scattering cross section by changing from the \( jj \) to the \( LS \) coupling scheme. We combine the above two Clebsch-Gordan (CG) coefficients together with the CG coefficients appearing in the definition of the Dirac distorted spinors, \( (B_2) \), and employ all the necessary Dirac algebra to obtain
\[
\mathcal{M}(m_B, m_j, m_\lambda, m_\lambda_+) = \sum_{S, M_S, P, M_P, Q, M_Q} \left( \frac{e^2}{4\pi} \right) \kappa, \lambda, J, L, M_L \\langle (\frac{1}{2} m_\lambda; \frac{1}{2} m_\lambda; | S M_S \rangle \langle \frac{1}{2} m_\lambda; j_B m_B | P M_P \rangle \langle S M_S; P, -M_P | Q M_Q \rangle \mathcal{M}(SPQM_Q; \kappa_B),
\]
where
\[
\mathcal{M}(S, P, Q, M_Q; \kappa_B) = \left( \frac{e^2}{4\pi} \right) \sum_{\kappa, \lambda, J, L, M_L} (-1)^\Theta_{\kappa, \lambda, J} A_{\lambda_+ m_\lambda}^{\lambda_+ m_\lambda} (-P_\lambda) A_{\lambda_+ m_\lambda}^{\lambda_+ m_\lambda} (P_\lambda) A_{\lambda_+ m_\lambda}^{\lambda_+ m_\lambda} (P_\lambda) \times \langle l_\text{+} - m_\lambda; l_\text{+} m_\lambda; | L M_L \rangle \langle L M_L; l_\text{+}, -m_\lambda; Q, -M_Q \rangle,
\]
and we have defined
\[
\kappa \equiv \left[ \kappa, \lambda, J, \lambda_+ \right], \quad M \equiv \left[ m_B, m_\lambda, m_\lambda_+ \right],
\]
\[
\Theta \equiv \lambda + S + P + \kappa_B
\]
\[
\mathcal{C}_{LSIPQP} = (2j_\text{+} + 1)(2j_\text{-} + 1)(2J + 1) \left( \begin{array}{c c c}
\hat{j}_\text{+} & \hat{j}_\text{-} & \hat{L} \hat{S} \\
\mathcal{C}_{LSIP} & J & P \end{array} \right)
\]
\[
R_{J, \lambda} = [I_{J, \lambda}(t) + J_{J, \lambda}(t) + K_{J, \lambda}(s) + L_{J, \lambda}(s)],
\]

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\[ A_{lm}(p) = 4\pi i \left\{ \frac{E + m}{2E\Omega} \right\}^{1/2} e^{i\delta_{m_i}(\hat{P})} \frac{Y_{lm}(\hat{P})}{p} , \]

\[ I_{\lambda\lambda}(t) = \delta_{\lambda\lambda} R_{\lambda\lambda,0}^{*} R_{\lambda\lambda,0} \int_{0}^{\infty} dx \int_{0}^{\infty} dy \, W_{\lambda}(x,y;t)(G_{-\lambda} F_{-\lambda} + F_{-\lambda} G_{-\lambda})(x)(G_{+\lambda} F_{+\lambda} + F_{+\lambda} G_{+\lambda})(y) , \]

\[ J_{\lambda\lambda}(t) = \sum_{j} \delta_{j,j} \int_{0}^{\infty} dx \int_{0}^{\infty} dy \, W_{\lambda}(x,y;t)[(R_{\lambda\lambda,0}^{*} R_{\lambda\lambda,0} - R_{\lambda\lambda,0}^{*} R_{\lambda\lambda,0}) F_{-\lambda}^*(x) \times (R_{\lambda\lambda,0}^{*} R_{\lambda\lambda,0} - R_{\lambda\lambda,0}^{*} R_{\lambda\lambda,0}) F_{+\lambda}^*(y)] , \]

\[ K_{\lambda\lambda}(s) = \frac{\delta_{j,j}}{2\lambda + 1} R_{\lambda\lambda,0}^{*} R_{\lambda\lambda,0} \int_{0}^{\infty} dx \int_{0}^{\infty} dy \, W_{\lambda}(x,y;s)(G_{-\lambda} + G_{+\lambda})(x)(G_{\lambda} F_{\lambda} + F_{\lambda} G_{\lambda})(y) , \]

\[ L_{\lambda\lambda}(s) = \frac{1}{2j + 1} \int_{0}^{\infty} dx \int_{0}^{\infty} dy \, W_{\lambda}(x,y;s)[(R_{\lambda\lambda,0}^{*} R_{\lambda\lambda,0} - R_{\lambda\lambda,0}^{*} R_{\lambda\lambda,0}) G_{-\lambda} \times (R_{\lambda\lambda,0}^{*} R_{\lambda\lambda,0} - R_{\lambda\lambda,0}^{*} R_{\lambda\lambda,0}) G_{+\lambda} F_{\lambda} + F_{\lambda} G_{\lambda})(y) , \]

\[ \delta_{\lambda} \equiv \begin{pmatrix} j_{+} & j_{+} & \lambda \\ j_{-} & j_{-} & J \end{pmatrix} , \quad W_{\lambda}(x,x';t) = 4\pi t j_{\lambda}(tx_{<}) h_{\lambda}^{(+)}(tx_{>}) . \]

Cross sections for the different unpolarized processes of interest can now be simply written in terms of \( M(S,P,Q,M_{Q}\kappa_{B}) \). The knockout cross section is

\[ \frac{d\sigma}{dE_{+}d\Omega_{+}d\Omega_{-}} = \frac{1}{(2\pi)^{5}} \left| \frac{E_{i}}{p_{i}} \right| \left( \frac{p_{+}E_{+}E_{-}}{2p_{i}} \right)^{1/2} \sum_{Q,M_{Q}} \left| M(S,P,Q,M_{Q}\kappa_{B}) \right|^{2} , \tag{B6} \]

where \( f(\mid p_{+} - p_{-} \mid) \) is a correlation function describing the final-state interaction of the emerging leptons, and \( p_{i} = (E_{i}^{2} - m_{i}^{2})^{1/2} \). In the case of positronium formation, the differential cross section is

\[ \frac{d\sigma}{d\Omega_{p_{+}}} = \frac{1}{(2\pi)^{2}} \left| \frac{E_{i}}{p_{i}} \right| \left| \frac{p_{+}E_{+}^{2}}{2} \right| \sum_{Q,M_{Q}} \left| M(S,P,Q,M_{Q}\kappa_{B}) \right|^{2} , \tag{B7} \]

where \( E_{+} = (E_{i} + E_{+})/2 \) and the positronium wave function has been evaluated at the origin.

We can integrate Eq. (B6) over the solid angles to obtain the angle-integrated knockout cross sections. We first expand the correlation function in spherical harmonics,

\[ f(\mid p_{+} - p_{-} \mid) = \sum_{l,m} \frac{4\pi}{2l+1} f_{l}(k_{+},k_{-}) Y_{lm}(\hat{P}_{+}) Y_{lm}^{*}(\hat{P}_{-}) , \]

with the coefficients given by the orthogonality of the Legendre polynomials:

\[ \frac{f_{l}(k_{+},k_{-})}{2l+1} = \frac{1}{2l+1} \int_{-1}^{1} dz \, P_{l}(z)f((p_{+}^{2} + p_{-}^{2} - 2p_{+}p_{-}z)^{1/2}) . \]

We then do the angular integration using the relation

\[ \int d\Omega_{p_{+}} Y_{lm_{1}}^{*}(\hat{P}_{+}) Y_{lm_{2}}(\hat{P}_{+}) Y_{lm_{3}}(\hat{P}_{+}) = \frac{\delta_{l_{1}l_{3}}}{\sqrt{4\pi l_{1}}} \langle l_{1}m_{1};l_{2}m_{2} \mid l_{1}m_{1} \rangle \langle l_{3}0;l_{2}0 \mid l_{1}0 \rangle . \]

The final result for the knockout angle-integrated cross section is

\[ \frac{d\sigma}{dE_{+}} = \frac{2\alpha^{2}}{p_{i}^{2}} \left( \frac{E_{i} + m}{p_{i}} \right) \left( \frac{E_{+} + m}{p_{+}} \right) \left( \frac{E_{-} + m}{p_{-}} \right) \left| M_{ko} \right|^{2} , \tag{B8} \]

with

\[ \left| M_{ko} \right|^{2} = \sum_{S,P,Q} (2Q + 1) \sum_{|k_{+}|,|k_{-}|,J} \delta_{L_{1}L_{2}} \delta_{l_{1}l_{3}} (-1)^{l_{1}} \phi(l_{1},l_{-}) C_{S,LSPQ}^{\lambda_{1}J_{1}} R_{\lambda_{1},L_{1}}^{*} \hat{P}_{+}^{l_{1}} \hat{P}_{-}^{l_{1}} \]

\[ \times (-1)^{l} \phi^{*}(l_{-},l_{+}) C_{S,LSPQ}^{\lambda_{2}J_{2}} R_{\lambda_{2},L_{2}}^{*} \hat{P}_{+}^{l_{+}} \hat{P}_{-}^{l_{+}} \]

\[ \times \frac{f_{l}(k_{+},k_{-})}{2l+1} \frac{l_{-}^{l_{-}l_{+}l_{+}l_{-}}}{l_{+}^{l_{+}l_{+}l_{+}l_{+}}} \langle l_{+}0;l_{-}0 \mid l_{0} \rangle \langle l_{-}0;l_{+}0 \mid l_{0} \rangle . \tag{B9} \]
where
\[ \phi_{l_-, l_+} = \psi_{l_+ - l_-} e^{i[b_{l_-}] (p_{l_-}) - b_{l_+} (p_{l_+})} . \]

In practice, we use the Gamow form of the correlation, Eq. (2).

The positronium formation cross section can also be written in a form that conveniently displays its angular dependence,

\[ \frac{d\sigma}{d\Omega_{Pl}} = \frac{1}{(2\pi)^2} \left| \frac{E_i}{p_i} \right| \left| \frac{p_i + E_+}{2} \right| \left| \psi_{Pl}(0) \right|^2 \frac{1}{2} \left| M_{Pl} \right|^2, \]

where
\[ \left| M_{Pl} \right|^2 = \sum_{s, r, q} (-1)^q \frac{2Q + 1}{4\pi} \sum_{k, j, j', l, l', \ell, r, R} (-1)^{k+j} \phi_{l_-, l_+}^{*} C_{kLSQP}^{R_{j}j_{s}k \ell_{-} \ell_{+}j_{-} \ell_{+}} \langle l_0 0 \mid L0 \rangle \]
\[ \times (-1)^{k} \phi_{l_-, l_+}^{*} C_{k'L'SPQ}^{R_{j'}j' \ell_{-} \ell_{+}j' \ell_{+}} \langle l'_0 0 \mid L'0 \rangle \]
\[ \times \left[ \langle l_0 0 | R0 \rangle \langle L0 0 | R0 \rangle \frac{L L' R \ell \ell' \ell'}{4\pi} \right], \]

with
\[ \phi_{l_-, l_+} = (i)^{l_+ - l_-} e^{i[b_{l_-}] (p_{l_-}) - b_{l_+} (p_{l_+}) - b_{l} (p_l)} . \]

Here \( \theta \) is the angle between the outgoing positronium and the incident positron. Angle integration over \( \theta \) is done simply by taking only the \( R = 0 \) term in Eq. (B11).

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5The existence of these peaks has not been established without doubt. Some recent experiments have yielded contradictory results. See, for example, R. Peckhaus, W. Elze, T. Happ, and T. Dresel (unpublished); K. Maier et al. (unpublished); M. Sakai et al., Institute for Nuclear Study (Tokyo) Report No. INS-Rep-632, 1987 (unpublished).