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Pair production and electron capture in relativistic heavy-ion collisions

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Results are presented for simulations of electron-positron pair production in relativistic heavy-ion collisions leading to electron capture and positron ejection. We apply a two-center relativistic continuum distorted-wave model to represent the electron or positron dynamics during the collision process. The results are compared with experimental cross-section data for La^{57+} and Au^{79+} impact on gold, silver, and copper targets. The theory is in good agreement with experiment for La^{57+} impact, verifying the result that the process increases in importance with both collision energy and target atomic number, and improves upon previous simulations of this process.

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Early theoretical work on the production of an e^--e^+ pair through heavy-ion collisions considered only the creation of the electron and positron in the continuum. However *capture by pair production* (CPP), in which the electron is formed in a bound state of one or other ion, becomes a significant process at highly relativistic energies. Remarkably, this process was sufficiently important to enable the synthesis of atomic antihydrogen using the low-energy antiproton ring at CERN. A beam of fast antiprotons impacting on a xenon gas target [1] led to pair production with positron capture. Theory predicted [2,3] that cross sections for CPP would increase with energy, and indeed this has been verified experimentally [4–6] . In fact, this process eventually becomes the dominant mechanism for charge exchange in highly relativistic atomic collisions [6,7]. As well as being an interesting area of study in its own right, this process has important applications in the physics of heavy-ion colliders such as the large-hadron collider and the relativistic heavy-ion collider [8]. The process of CPP will lead to depletion of the charge state of the beam, and hence a loss in luminosity of the collider. For typical operating conditions of such facilities, these losses might amount to 50% [8] or more.

Although the process is strongly coupled at high energy, simulations based on relativistic coupled-channel calculations [9,10] have indicated that leading-order perturbation theory is adequate for total cross-section estimates for energies (E) up to 150 GeV/u [6]. Nonetheless in the energy range $E\sim 1$ GeV/u, where reliable experimental data exist, theory and experiment have been in least agreement. It is this region which we address in this paper.

It is now some 13 years since Becker and co-workers [11–13] obtained the first estimates of cross sections for pair creation with simultaneous capture of the electron into the K shell of one of the colliding ions. However with the exception of Deco and Rivarola, who gave a two-center description of the continuum positron [14], two somewhat artificial modes of reaction have been distinguished and treated separately when modeling this process: excitation from the negative-energy continuum of an ion to one of its bound states [2,12,15] or transfer to a bound state of the other ion [16,17]. Such approaches, while suited to circumstances in which one ion is much more highly charged than the other, lack symmetry, and make a distinction between two separate modes of CPP. They lead to different formulas within first-order perturbation theory [16], and hence different projectile charge (Z_P), target charge (Z_T), and E dependencies. As a result, theoretical estimates of the asymptotic ($E\rightarrow\infty$) energy dependence of the total cross sections are not in agreement, with estimates of [2,3] $\sigma_{\mathrm{CPP}}\sim\ln(E)$, and more recently [16] $\sigma_{\mathrm{CPP}}\sim E^2$. The former is based on the positron-electron pair being created around the same ion, the latter assuming that the pair is divided between the two ions. Of course both pathways will interfere and contribute to the process, thus pointing to the necessity of a two-center treatment for the positron and electron. Moreover it was shown [14] that a two-center description is essential to obtain the correct positron emission spectrum and accurate total cross sections for CPP. However, leading-order perturbation theory (the first Born approximation) does give reasonably good estimates for the cross section in the high-energy region ($E\sim 150$ GeV/u) [6] for collisions of heavy ions, and has been a reliable model for fast collisions of light ions with low-Z targets in the process of antihydrogen formation involving CPP by antiprotons [1,18].

Experimental results for highly relativistic heavy ions on a variety of targets [8] support the simple scaling law derived from the virtual-photon method (Born approximation) which included multiple scattering from the projectile ion [2] alone, $\sigma_{\mathrm{CPP}}\sim Z_T^2$, for a given energy. At lower energies this is not the case [5,19,20]: the Z_T dependence is more complex, showing an enhancement in excess of the Z_T^2 scaling. In this paper we propose a refinement of the Born approximation to take into account higher-order scattering processes. In particular, we tackle the question of the two-center nature of the continuum positron and the polarization of the captured electron. We find that both these effects are vital, and lead to theoretical results which are in accord with experiment. We discuss the physical explanation for scaled cross-section enhancement, and provide numerical estimates which agree well with experiment in qualitative and quantitative terms.

Through crossing symmetries the leading-order matrix element for the pair production process, in which the electron is captured by the projectile P,

$$P+T\rightarrow(P,e^-)+T+e^+, \tag{1}$$

is the same as that for the related reaction, $e^-+P+T\rightarrow(P,e^-)+T$, which is mathematically equivalent to the time-reversed ionization process

$$(P,e^-)+T\rightarrow e^-+P+T. \tag{2}$$

In each crossing symmetry the equivalence relies on the electron-positron interaction being much weaker than their interactions with the highly charged ions: a reasonable assumption. Let $\boldsymbol{r}_P,t$ and $\boldsymbol{r}'_T,t'$ be the space and time coordinates of the electron in the projectile and target frames, respectively. The nuclei follow straight-line paths with relative velocity $\boldsymbol{v}$. The Hamiltonian, in the projectile frame of reference and in atomic units, is given by:

$$H=-ic\boldsymbol{\alpha}\cdot\boldsymbol{\nabla}_{\mathbf{r}_P}+\beta c^2+V_P(\boldsymbol{r}_P)+S^2V'_T(\boldsymbol{r}'_T) \tag{3}$$

where $\boldsymbol{\alpha}$ and β are Dirac matrices, and S is the operator which transforms the wave function from the projectile frame to the target frame, namely,

$$S=(\tfrac{1}{2}+\tfrac{1}{2}\gamma)^{1/2}(\mathbf{1}-x\boldsymbol{\alpha}\cdot\hat{\boldsymbol{v}}), \tag{4}$$

where $x=v\gamma c^{-1}(\gamma+1)^{-1}, \gamma=(1-v^2/c^2)^{-1/2}$, and $\mathbf{1}$ represents the unit matrix. For a given impact parameter $\boldsymbol{b}$, the transition amplitude can be written in the form [21]

$$A(\boldsymbol{b})=-i\int_{-\infty}^{\infty}dt\int d\boldsymbol{r}_P\,\chi_f^\dagger(H-i\partial_t)\chi_i, \tag{5}$$

where χ_i and χ_f are the initial and final states.

The undistorted bound-state is approximated by a semirelativistic $(Z_T\ll c)$ wave function,

$$\Phi_i=\Phi_{0i}+\Phi_{1i}, \tag{6}$$

where

$$\Phi_{0i}=Z_P^{3/2}\pi^{-1/2}e^{-Z_Pr_P-ic^2t-iE_{si}t}\boldsymbol{\omega}_i \tag{7}$$

and

$$\Phi_{1i}=(2ic)^{-1}\boldsymbol{\alpha}\cdot\boldsymbol{\nabla}_{\mathbf{r}_P}\Phi_{0i}, \tag{8}$$

with E_{si} the nonrelativistic eigenenergy, and the electron spin along the beam axis defined as ''up'' by $\boldsymbol{\omega}_i^T=(1\ 0\ 0\ 0)$ and ''down'' by $\boldsymbol{\omega}_i^T=(0\ 1\ 0\ 0)$.

The continuum function is given by

$$\Phi_f=\Phi_{0f}+\Phi_{1f}, \tag{9}$$

where

$$\Phi_{0f}=(2\pi)^{-3/2}N^*(\omega_P)\,{}_1F_1[-i\omega_P;1;-i\gamma_e(v_er_P+\boldsymbol{v}_e\cdot\boldsymbol{r}_P)]e^{-i\gamma_ec^2t+i\gamma_e\boldsymbol{v}_e\cdot\mathbf{r}_P}S_{\boldsymbol{v}_e}^{-1}\boldsymbol{\omega}_f. \tag{10}$$

The spinor correction term is given by

$$\Phi_{1f}=(2\pi)^{-3/2}(2i\gamma_ec)^{-1}N^*(\omega_P)\boldsymbol{\alpha}\cdot\boldsymbol{\nabla}_{r_p1}F_1[-i\omega_P;1;-i\gamma_e(v_er_P+\boldsymbol{v}_e\cdot\mathbf{r}_P)]e^{-i\gamma_ec^2t+i\gamma_e\boldsymbol{v}_e\cdot\mathbf{r}_P}S_{\boldsymbol{v}_e}^{-1}\boldsymbol{\omega}_f, \tag{11}$$

with $\omega_P=Z_P/v_e$, where $\boldsymbol{v}_e$ is the electron velocity. $N(\zeta)=\exp(\pi\zeta/2)\Gamma(1-i\zeta)$ and,

$$S_{\boldsymbol{v}_e}=(\tfrac{1}{2}+\tfrac{1}{2}\gamma_e)^{1/2}(\mathbf{1}-x_e\boldsymbol{\alpha}\cdot\hat{\boldsymbol{v}}_e), \tag{12}$$

where $x_e=v_e\gamma_ec^{-1}(\gamma_e+1)^{-1}$ and $\gamma_e=(1-v_e^2/c^2)^{-1/2}$. These functions are appropriate when $Z_{P,T}\ll c$.

The initial distortion factor $\boldsymbol{L}'_i$ is a matrix given by

$$\boldsymbol{L}'_i=\boldsymbol{L}'_{0i}+\boldsymbol{L}'_{1i}, \tag{13}$$

where

$$\boldsymbol{L}'_{0i}=\exp(-i\nu_T\ln[\gamma vr'_T+\gamma\boldsymbol{v}\cdot\boldsymbol{r}'_T])\mathbf{1} \tag{14}$$

and

$$\boldsymbol{L}'_{1i}=S^{-1}(2i\gamma c)^{-1}\boldsymbol{\alpha}\cdot\boldsymbol{\nabla}_{r'_T}\boldsymbol{L}_{0i}S, \tag{15}$$

with $\nu_T=Z_T/v$.

Similarly, the distortion factor on the final-state [14] is given by:

$$\boldsymbol{L}'_f=\boldsymbol{L}'_{0f}+\boldsymbol{L}'_{1f}, \tag{16}$$

where

$$\boldsymbol{L}'_{0f}=N^*(\omega'_T)\,{}_1F_1(-i\omega'_T;1;-i\gamma'_e(v'_er'_T+\boldsymbol{v}'_e\cdot\boldsymbol{r}'_T))\mathbf{1} \tag{17}$$

and

$$\boldsymbol{L}'_{1f}=S^{-1}(2i\gamma'_ec)^{-1}\boldsymbol{\alpha}\cdot\boldsymbol{\nabla}_{r'_T}\boldsymbol{L}'_{0f}S. \tag{18}$$

Retaining terms of first order in Z/c, we have relativistic continuum distorted wave eikonal initial state (RCDWEIS) wave functions [21,15]:

$$\chi_i=\boldsymbol{L}'_{0i}\Phi_{0i}+\boldsymbol{L}'_{1i}\Phi_{0i}+\boldsymbol{L}'_{0i}\Phi_{1i}, \tag{19}$$

$$\chi_f=\boldsymbol{L}'_{0f}\Phi_{0f}+\boldsymbol{L}'_{1f}\Phi_{0f}+\boldsymbol{L}'_{0f}\Phi_{1f}. \tag{20}$$

We first compare our results for the Relativistic Distorted-Wave Born (RDWB) approximation [14], where the two-center positron wave function is used but the initial state distortion is omitted, and the Relativistic first-order Born (R1B), projectile centered approximation, in which the initial and final state distortions are neglected. The Born approximation, which assumes that the positron is in the continuum of only one of the ions, is ambiguous. The Born approximation of Bertulani and Baur [2] takes the positron wave function as projectile centered, while the Born approximation of Eichler [16] takes the scattering center at the target nucleus. As the Born approximation of Eichler is analogous to the OBK theory of electron capture, we henceforth refer to it as OBK. These two models (R1B and OBK) can be viewed as approximations of wave function (20) in which $\omega'_T=0$ and

$\omega_P = 0$, respectively. By retaining both scattering center contributions the interference effects are taken into account. In comparing RDWB and R1B, it is known that *these* two-center interference effects reduce the cross section for CPP in the relativistic domain [14]. This suppression of CPP is the converse of the two-center enhancement (capture to the continuum) that arises in ion-atom ionization [21], and is analogous to the effect of the Fermi function for $\beta^{\pm}$ decay [22].

The triply differential cross section, with respect to the electron momentum $(\boldsymbol{p}_e)$, is defined as:

$$\sigma(\boldsymbol{p}_e) = (d\sigma_{\rm CPP}/d\boldsymbol{p}_e) = \int d\boldsymbol{b} |A(\boldsymbol{b})|^2. \tag{21}$$

Using the Fourier transform method [21], we define

$$T(\boldsymbol{\eta}) = \gamma v \int d\boldsymbol{b} \exp(-i\,\boldsymbol{\eta}\cdot\boldsymbol{b}) A(\boldsymbol{b}), \tag{22}$$

where $T(\boldsymbol{\eta})$ is a product of single-center integrals. The total cross section is obtained from the integral over the ejectile momentum (or velocity), and takes the form

$$\sigma_{\rm CPP} = \sum_{\rm spins} \frac{1}{2\pi(\gamma v)^2} \int_0^c dv_e \gamma_e^5 v_e^2 \int_0^{\pi} d\theta \sin\theta \int d\boldsymbol{\eta} |T(\boldsymbol{\eta})|^2 \tag{23}$$

where we sum over all the spin states of the electron and positron pair.

In order to compute CPP cross sections [Eq. (1)] we note that a positron with energy ϵ_+ and momentum $\mathbf{p}_+$ traveling forward in time in the final state, is equivalent to an electron with energy $-\epsilon_+$ and momentum $-\mathbf{p}_+$ in the initial state. Thus we must take

$$\begin{aligned} v_e &\to -v_+ \qquad v_e' \to -v_+', \\ \epsilon_f &\to -\epsilon_+ \qquad \epsilon_f' \to -\epsilon_+'. \end{aligned} \tag{24}$$

The experiments of Belkacem *et al.* [5,19,20] were for fully stripped lanthanum ions (La^{57+}) striking thin foils of copper ($Z_T = 29$), silver ($Z_T = 47$), and gold ($Z_T = 79$). The collision energies were $E = 0.405$, 0.956, and 1.300 GeV/u. The two graphs presented compare the scaled total cross sections ($\sigma_{\rm CPP}/Z_T^2$) given by theory and experiment. Consider Fig. 1, which compares R1B and RDWB with the measured values. Of course, the scaled R1B curve is independent of Z_T, and it clearly shows the increase in importance of CPP with increasing collision energy. Considering the RDWB model, however, we see a progressive reduction in the scaled cross section as Z_T increases. This is in agreement with the findings of Deco and Rivarola [14], who reported a decrease in the size of the singly differential cross sections by an order of magnitude. Their model is similar to our RDWB approximation, but using only the scalar part of the final-state distortion factor [Eq. (17)]. While this model shows Z_T dependence for the scaled cross section, the trends and absolute values are incorrect. It predicts a suppression of the scaled cross section rather than an enhancement as Z_T increases.

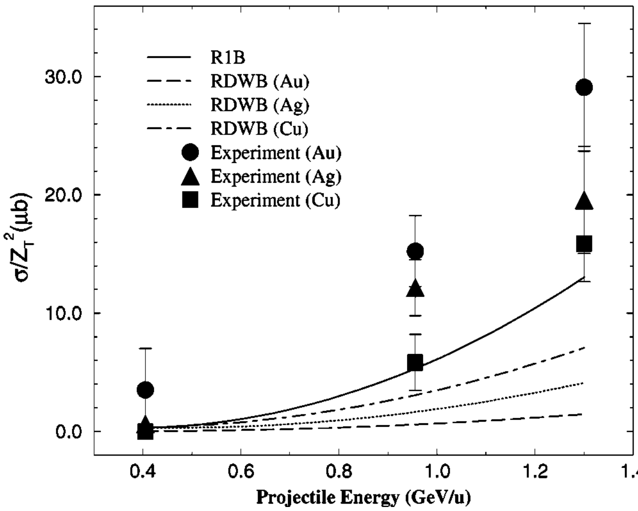

FIG. 1. Scaled cross sections $\sigma_{\rm CPP}/Z_T^2$, in mb, for pair production with electron capture by fully stripped Lanthanum ions (La^{57+}) striking thin foils of copper ($Z_T = 29$), silver ($Z_T = 47$), and gold ($Z_T = 79$). Comparison with RDWB theory for capture to the 1s state.

Thus the RDWB theory data for Gold gives the lowest scaled cross section, while experiment shows that it should be the highest. This same incorrect trend is obtained in the target-centered Born approximation (OBK) [16], as can be seen in Fig. 2. These results were also calculated using semirelativistic wave functions (6) and (9).

In contrast (Fig. 3) the equivalent results for RCDWEIS show an observed enhancement with increasing Z_T. However, the theoretical data lie below the experiment for the more energetic collisions. In comparing with experiment we have only presented simulations for the dominant channel, that is, capture to the 1s ground state. At very high energies capture to excited states is thought to contribute ~30% to the total capture cross section [6,23]. This would partly ex-

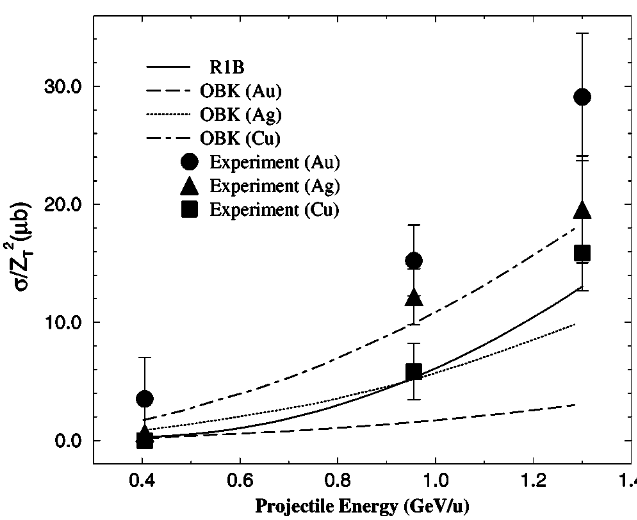

FIG. 2. Scaled cross sections $\sigma_{\rm CPP}/Z_T^2$, in mb, for pair production with electron capture by fully stripped Lanthanum ions (La^{57+}) striking thin foils of copper ($Z_T = 29$), silver ($Z_T = 47$), and gold ($Z_T = 79$). Comparison with OBK theory for capture to the 1s state.

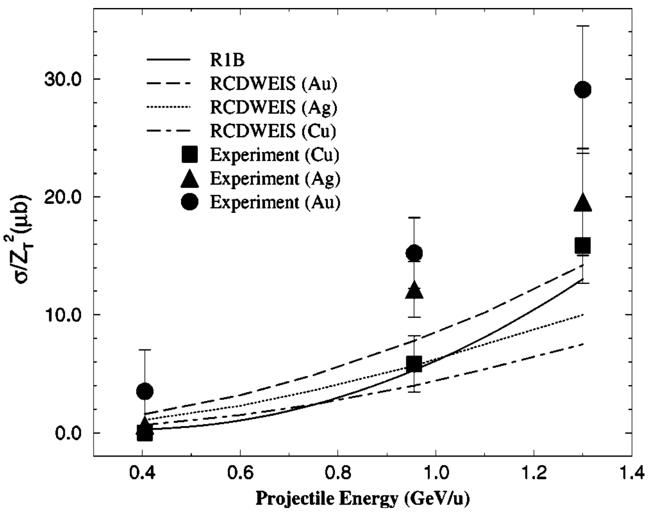

FIG. 3. Scaled cross sections $\sigma_{\mathrm{CPP}}/Z_T^2$, in mb, for pair production with electron capture by fully stripped Lanthanum ions (La^{57+}) striking thin foils of copper ($Z_T=29$), silver ($Z_T=47$), and gold ($Z_T=79$). Comparison with RCDWEIS theory for capture to the $1s$ state.

plain the differences between our results and the experimental data. Nonetheless, given the approximate nature of the semirelativistic wave functions used, the theoretical results are very encouraging, in that, for the first time, the correct ordering of the total cross sections with respect to nuclear charge is obtained. It is expected that the implementation of full Coulomb-Dirac wave functions within the overall context of this model will lead to an increase in total cross sections similar to that observed by Ionescu and Eichler [17] in their fuller calculations using Dirac wave functions within the OBK approximation. Thus the present underestimation of the cross sections at higher energy and charge [12,16] may well be revised in a treatment employing fully relativistic wavefunctions (see Fig. 3).

Other experimental results are available for the impact of faster and more highly charged beams: 10.8-GeV/u Au^{79+} [8] and 0.956 GeV/u U^{92+} [4] for the same targets. The gold beam results (Table I) indicate that the Z_T^2 dependence is established at the higher energies, as predicted by the simple projectile-centered Born approximation [11]. Even at this higher energy our theoretical results (Table I) show an enhancement in excess of Z_T^2. The experiment is in much better accord with the flat scaled cross section data given by the

TABLE I. Total cross sections σ_{CPP}, in b, for electron capture from pair production for 10.8-GeV/nucleon Au^{79+} impact on gold, silver, and copper foils.

Z_T	Experiment [8]	CDWEIS theory	Becker *et al.* [11]
79	8.8 ± 1.5	15.85	10.1
47	4.4 ± 0.73	3.44	3.6
29	1.77 ± 0.31	0.74	1.36

Born approximation [11]. For U^{92+} the high value of Z/c means that the semirelativistic approximations used for the wave functions are not valid.

The validity of the semirelativistic continuum-distorted wave approach has been questioned [24] on the grounds that the approximate wave functions might produce unphysical transitions [25]. However Glass *et al.* [26,27] considered symmetric-eikonal wave functions with prior interaction, and showed that the spurious spin-flip contribution to the amplitude vanishes when full cognizance is taken of the two-center spinor nature of the noncommuting operators. This is the procedure used in this paper, which thus avoids unphysical effects.

In summary, we have proposed and tested a distorted-wave model which improves on approximations used previously to describe CPP. We confirm that, as previously shown [14], the inclusion of distortions from both ions on the positron continuum state leads to a reduction in the cross sections. However, including distortion of the bound electron leads to an increase in the total cross sections and a more accurate fit to the experimental data for fully stripped relativistic Lanthanum ions. This demonstrates once more the necessity of a two-center treatment for an accurate theoretical description of this reaction. However, our cross-section predictions for faster and more highly charged gold ions do not accord with the experimental data, which show a Z_T^2 dependence.While the refinements introduced in our model are significant theoretical improvements, clearly there still exist several unresolved important differences between theory and experiment.

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