Charge Transfer from the Negative-Energy Continuum: Alternative Mechanism for Pair Production in Relativistic Atomic Collisions

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As an alternative mechanism for bound-free electron-positron pair production, the transfer of a negative-energy electron in the Coulomb field of one of the collision partners to a bound state of the other is considered, supplementing the usually adopted view that an electron is excited from a negative-energy state to a bound state of the same atom. Under simplifying assumptions, analytic expressions for the differential and total cross sections can be derived, which explicitly exhibit the dependencies on the nuclear charges and show a surprisingly strong increase with the collision energy.

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The production of free electron-positron pairs in relativistic high-Z ion-atom collisions can be viewed to result from the collision between photons representing the transient electromagnetic field of the passing ions. This process [1] is described by quantum electrodynamics [2] or, approximately, by the equivalent-photon method [3]. Alternatively, one may regard free pair production as the excitation of a target electron from a negative to a positive Coulomb continuum state by the perturbing action of the passing projectile (or vice versa). This picture also allows for bound-free pair production, in which the electron is created in a *bound* state of the projectile [4,5], thus decreasing its detectable charge, a process that has recently been identified experimentally [6,7] and is schematically illustrated by the mechanism (a) of Fig. 1.

Until now, theoretical treatments, by distorted-wave perturbation theory as well as by nonperturbative single-center coupled-channel calculations [8], have exclusively considered process (a). In the present Letter, we describe an alternative mechanism (b), in which the electron is transferred from a negative-energy state of the target to a bound state of the projectile.

Whereas the Dirac equation for the complete two-center system has a single continuum in any inertial frame, the continua of the two subsystems, if described in one of them, are different. That is, a negative-energy state in one of the subsystems requires for its representation in the other subsystem a complete set of eigenstates, including bound and positive-energy wave functions. In this sense, it is meaningful to associate different "mechanisms" with the alternatives (a) and (b). While (a) is a single-center process like excitation or ionization with the passing ion merely generating the transient field, process (b) is the charge transfer from the negative-energy continuum with both ions acting as carriers of eigenstates. We here present a first systematic calculation of this alternative process.

For this purpose, the Born or Oppenheimer-Brinkman-Kramers (OBK) approximation known from capture theory [1] should be a reasonable starting point for the problem at hand. This approximation (which is *postprior* symmetric) yields the correct parametric dependencies of the cross section although its magnitude is usually too large. Adopting natural units ($\hbar = m = c = 1$) and the impact parameter (**b**) formulation, we may write the transition amplitude [9] in the *post* form as

$$A_{f,\mathbf{p}}(\mathbf{b}) = i\alpha Z_T \int dt \int d^3 r_T \varphi_f'^{\dagger}(\mathbf{r}_P') \, e^{iE_f t'} \times \frac{S^{-1}}{r_T} \varphi_{\mathbf{p}}(\mathbf{r}_T) \, e^{iE_p t}. \quad (1)$$

Here $\alpha = e^2 = 1/137.036$ is the fine structure constant, Z_T and Z_P are the charge numbers of target and projectile,

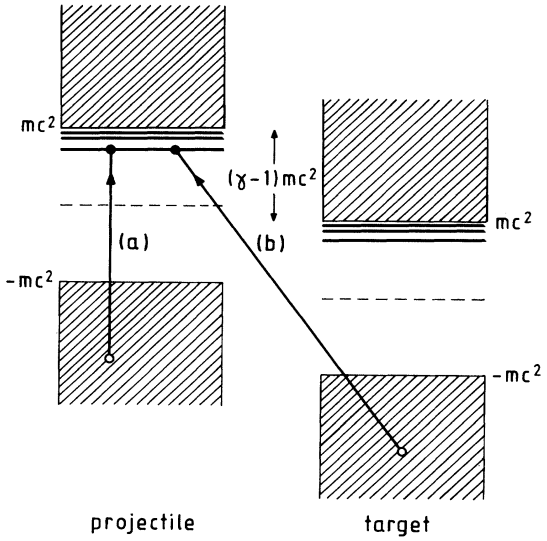

FIG. 1. Schematic energy diagram illustrating the two mechanisms for pair production: (a) excitation type or single-center process; (b) transfer type or two-center process. In the figure, the spectrum of the moving projectile in its rest frame is shifted upwards by the kinetic energy of an electron attached to it. Conversely, if one is interested in transfer from the projectile to the target, the *target* spectrum has to be shifted upwards by the same amount with respect to the projectile.

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and $\mathbf{r}_T, t$ and $\mathbf{r}'_P, t'$ are the space and time coordinates of the electron in the target and in the projectile frame, respectively. The initial wave function $\varphi_{\mathbf{p}}$ denotes a negative-energy electron in the Coulomb field of the target nucleus corresponding to positron momentum $\mathbf{p}$ and energy $E_p > 0$, while the final wave function ψ'_f with energy E_f represents a bound electron in the projectile field, transformed to the target frame by the matrix $S^{-1} = [(\gamma + 1)/2]^{1/2}(1 + \delta\alpha_z)$, where $\gamma = (1 - v^2)^{-1/2}$, v is the projectile velocity, $\delta = [(\gamma - 1)/(\gamma + 1)]^{1/2}$, and α_z is the component of the Dirac matrix in the beam direction.

By rewriting $S^{-1}r_T^{-1} = S^{-2}r_T^{-1}S$ in Eq. (1), and by performing the space-time integration in the *projectile* system, one may reinterpret the amplitude (1) as caused by the usual Liénard-Wiechert potential $S^{-2}r_T^{-1}$ of the target moving with respect to the projectile, however, acting on a negative-energy state not of the projectile as in Fig. 1(a), but of the target as in Fig. 1(b).

The energy-differential cross section is obtained by integrating the transition probability over the impact parameter plane and over the emission angle Ω_p of the positron and by summing over the spin projections s and μ_f in the initial and final states, so that

$$\frac{d\sigma}{dE_p} = \frac{p\,E_p}{(2\pi)^3}\int d\Omega_p \sum_{s,\mu_f}\int d^2b\,|A_{f,\mathbf{p}}(\mathbf{b})|^2. \quad (2)$$

By introducing the Fourier transforms $\tilde{\varphi}_f^{\mu_f}(\mathbf{q})$ of $\varphi_f^{\mu_f}(\mathbf{r}')$ and $\tilde{g}_{\mathbf{p}}^s(\mathbf{k})$ of $\varphi_{\mathbf{p}}^s(\mathbf{r})/r$ into Eq. (2), expressing the space-time coordinates of the projectile system by those in the target system, and by integrating over space and time, we obtain [1]

$$A_{f,\mathbf{p}}(\mathbf{b}) = i\frac{2\pi\alpha Z_T}{v\gamma}\int d^2k_b\,\tilde{\varphi}_f^{\mu_f\dagger}(-\mathbf{k}_b, -k_-) \times S^{-1}\,\tilde{g}_{\mathbf{p}}^s(\mathbf{k}_b, k_+)e^{i\mathbf{k}_b\cdot\mathbf{b}}, \quad (3)$$

where the vectors $\mathbf{q}$ and $\mathbf{k}$ are decomposed into their transverse components $\mp\mathbf{k}_b$ and longitudinal parts $-k_-$ and k_+. The latter quantities are given by

$$k_- = (E_p/\gamma + E_f)/v \approx (E_p/\gamma + 1)/v\,,$$
$$k_+ = (E_p + E_f/\gamma)/v \approx (E_p + 1/\gamma)/v\,, \quad (4)$$

connected by the relation

$$k_+^2 - k_-^2 = p^2 + \alpha^2 Z_P^2\,. \quad (5)$$

It is important to note that in the momentum transfers (4) for the two-center transition considered here, only one of the initial and final energies is Lorentz transformed, while in the minimum momentum transfer $q_0 = (E_p + E_f)/v$ known from the excitation-type transition within a single inertial frame, both energies are treated in the same way. This replacement has a drastic influence on the γ dependence of the cross section.

In order to study the dominant dependence of the cross section on Z_T, Z_P, and γ, it is useful to adopt a simplified analytical treatment, while deferring a more rigorous evaluation to a later publication. We assume $\alpha Z_T \ll 1$ and $\alpha Z_P \ll 1$, knowing from experience that the approximate applicability often extends beyond this range of validity.

Considering the most important case of transfer into the K shell of a bare projectile, we adopt a Darwin wave function for the bound state in the projectile and a Sommerfeld-Maue wave function for the continuum state in the target [1]. Moreover, in the latter case, we disregard the derivative term, which yields an αZ_T correction to the leading charge dependence and decreases as E_p^{-1}. With these simplifications, the Fourier transforms can be given in a closed form. The resulting density matrices

$$P_f(\mathbf{q}) = \sum_{\mu_f}\tilde{\varphi}_f^{\mu_f}(\mathbf{q})\,\tilde{\varphi}_f^{\mu_f\dagger}(\mathbf{q})\,,$$
$$P_{E_p}(\mathbf{k}) = \int d\Omega_p \sum_s \tilde{g}_{\mathbf{p}}^s(\mathbf{k})\,\tilde{g}_{\mathbf{p}}^{s\dagger}(\mathbf{k}) \quad (6)$$

are diagonal in the momenta, because of the b integration in Eq. (2), which now can be written as

$$\frac{d\sigma}{dE_p} = 2\pi\frac{(\alpha Z_T)^2}{v^2\gamma^2}\,p\,E_p\int d^2k_b\,\mathrm{Tr}\{S^{-1}P_f S^{-1}P_{E_p}\}. \quad (7)$$

Following the procedure of [1], we may evaluate the trace occurring in Eq. (7) to obtain the result as a one-dimensional integral evaluated numerically to derive the cross sections of Figs. 2 and 3. In order to give a more explicit form, we make use of the fact that the integrand of Eq. (7) contains the strongly peaked momentum distribution of the bound electron state and a

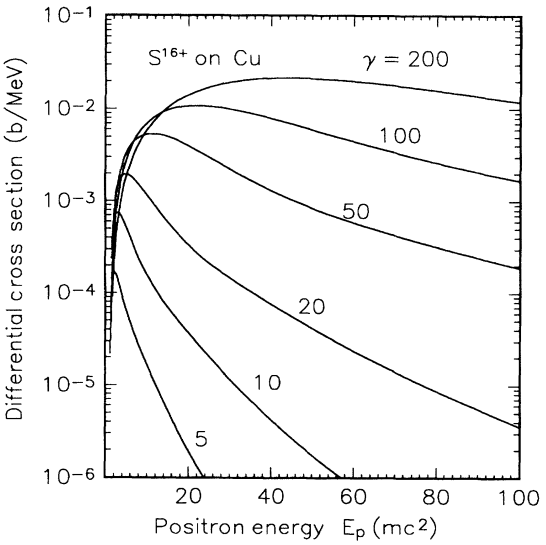

FIG. 2. Energy-differential cross sections [Eq. (7)] for charge transfer from the negative-energy continuum of a Cu target into the $1s_{1/2}$ state of a S^{16+} projectile.

similarly peaked positron density matrix. Therefore some slowly varying functions can be taken out of the integral, so that the differential cross section in natural units is obtained in the simple analytical form

$$\frac{d\sigma}{dE_p} = \frac{64(\gamma+1)}{5v^2\gamma^2}(\alpha Z_T)^2(\alpha Z_P)^5 \frac{2\pi\eta_T}{e^{2\pi\eta_T}-1} \frac{p(E_p+1)}{(k_-^2+\alpha^2Z_P^2)^5} \times \left\{ \delta_p^2 + \delta^2 - \delta(1+\delta_p^2)k_- + \tfrac{5}{16}(1+\delta_p^2\delta^2)k_-^2 + \delta_p\left[\delta - (\tfrac{5}{9}+\tfrac{4}{9}\delta^2)k_- + \tfrac{5}{16}\delta k_-^2\right]\frac{k_+^2+p^2}{k_+p} + \delta_p\left[\tfrac{5}{6}\delta - (\tfrac{1}{2}+\tfrac{1}{3}\delta^2)k_- + \tfrac{5}{16}\delta k_-^2\right]\frac{(k_-^2+\alpha^2Z_P^2)^2}{k_+^2p^2}\ln\left|\frac{k_+-p}{k_++p}\right| \right\}. \quad (8)$$

Here $v_p = (1 - 1/E_p^2)^{1/2}$ is the positron velocity in the target frame, $\eta_T = \alpha Z_T/v_p$, $p = (E_p^2 - 1)^{1/2}$, and $\delta_p = [(E_p - 1)/(E_p + 1)]^{1/2}$. The denominator $(k_-^2 + \alpha^2 Z_P^2)^5$ has the same structure as in the corresponding simple formula for charge transfer [10] and is crucial for the dependence on the Lorentz factor γ, in particular, when the positron energy E_p is large. Then, with increasing γ, the denominator becomes smaller, so that the decrease as $1/\gamma$ of the prefactor is more than compensated. The reason is the following: While for transfer between bound states the overlap in momentum space decreases with the collision energy, leading to an asymptotic $1/\gamma$ dependence, the transfer from a (negative-energy) continuum state to a bound state is not subject to such a constraint. As the projectile energy increases, higher and higher positron momenta in the target will contribute to the momentum overlap with the bound projectile state.

Figure 2 shows positron spectra calculated from Eq. (7) for collisions of S^{16+} ions with copper targets. The results of Eq. (8) agree with those of Eq. (7) within about 10%. One observes that for large values of γ the differential cross section decreases very slowly as a function of the positron energy, a fact that can be attributed to the denominator discussed above. This behavior is distinctly different from that of the excitation-type mechanism [4,5]; see Fig 1(a).

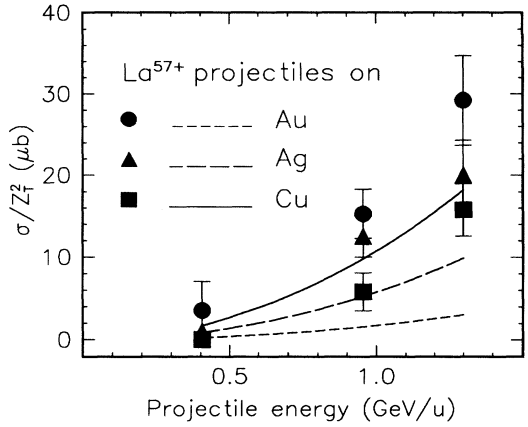

FIG. 3. Reduced cross sections σ/Z_T^2 as a function of the collision energy for collisions of La^{57+} projectiles with Cu, Ag, and Au targets. Experiment [7]: squares: Cu; triangles: Ag; circles: Au. Theory [Eq. (7)]: solid line: Cu; long-dashed line: Ag; short-dashed line: Au.

If we furthermore assume $\gamma \gg 1$ and observe that $E_p \gg 1$ contributes most, in this case, we can integrate Eq. (8) from a reasonable value, say, $E_p = 2$ to infinity to obtain the total cross section

$$\sigma_{\text{appr}} = \frac{32\pi}{35}(\alpha Z_T)^2(\alpha Z_P)^5 \frac{\alpha Z_T}{e^{2\pi\alpha Z_T}-1} \times \frac{16+2\gamma+\frac{1}{9}\gamma^2}{(1+2/\gamma)^9}. \quad (9)$$

This is to be compared with the estimate of Bertulani and Baur [3]

$$\sigma_{\text{BB}} = \frac{33\pi}{10}(\alpha Z_T)^2(\alpha Z_P)^5 \frac{\alpha Z_P}{e^{2\pi\alpha Z_P}-1}\left[\ln 0.34\gamma - \tfrac{5}{3}\right]$$

for the excitation-type pair production based on similar simplifications.

In Fig. 3, we compare experimental [7] and theoretical total cross sections for collisions of La^{57+} projectiles with Cu, Ag, and Au targets. This comparison merely serves to show that the process proposed here may compete in magnitude with the process (a) of Fig. 1. However, in contrast to the experimental data, the theoretical reduced cross sections σ/Z_T^2 decrease with increasing charge number. This is due to the factor $\alpha Z_T/[\exp(2\pi\alpha Z_T) - 1]$ arising from the Coulomb repulsion between the positron and the target nucleus, which decreases the matrix element (1) at small values of r_T. Perturbation theory for the excitation-type process (a) yields a constant reduced cross section. It is worth mentioning that calculations for 0.956 GeV/u [11] using exact bound-state and exact Coulomb-Dirac continuum wave functions with the dominant partial waves $|\kappa| \leq 2$ lead to cross sections that exceed the present estimates by about 30% for $Z_T = 29$, by 50% for $Z_T = 47$, and by a factor of 2.8 for $Z_T = 79$ showing that the approximation $\alpha Z_T \ll 1$ is no longer valid in the last case. While in these calculations the Z_T dependence is too weak, the Z_P dependence [11] agrees well with the data [7].

The γ dependence of the total cross section is exhibited in Fig. 4 for S^{16+} projectiles impinging on Cu, Ag, and Au targets. Similarly, as in Fig. 3, it is assumed here that our approximate wave functions still reflect the leading charge dependence. The solid curves are calculated from

the simple formula (9), which yields within about 10% the same results for $\gamma \geq 10$ as a numerical evaluation of Eq. (7) using Darwin or exact bound-state Dirac wave functions. In contrast, the dashed curve depicts the behavior of the approximate equation (10); see [3], which relies on similar assumptions. The logarithmic γ dependence is characteristic for the excitation-type behavior, found both in ionization [1] and in the single-center treatment of free or bound-free pair production [4,5,12]. Of course, unitarity requirements will limit the steady increase of the cross section with γ. Other reaction channels will open up and take flux out of bound-free pair production.

The basic view underlying the present approach is the following: In a rigorous treatment, the negative-energy continuum is a two-center continuum, which contains portions that are difficult to represent by the complete set of single-center eigenstates [13]. Given the incompleteness, in practice, of a single-center expansion, the negative-energy continuum of the second center (in practice also incomplete, so that overcompleteness is avoided) is needed to supplement an important part of the basis space. In this way, the description is rendered more symmetric between the collision partners.

In summary, we propose a novel mechanism for bound-free pair production, namely, charge transfer from the negative-energy continuum of the target into a bound state of the projectile. (A similar mechanism will apply to free pair production.) This process may become identifiable in the future if the momentum transfer can be measured by the use of recoil-ion momentum spectroscopy. While the mechanism deserves a more detailed investigation, we show in an initial simplified treatment: (i) For high values of γ, the positron spectra extend to very high energies, which still provide appreciable momentum overlap with the moving bound-state wave function. (ii) Because of this, the total cross sections increase much more rapidly with γ than for the usual excitation-type mechanism. While the detailed behavior and the magnitude of the total cross sections will certainly be modified in a more accurate theory, we believe that the main parametric dependencies will survive.

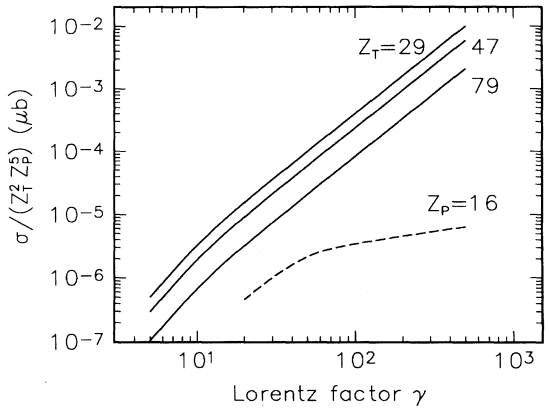

FIG. 4. Reduced cross sections $\sigma/(Z_T^2 Z_P^5)$ for bound-free pair production by S^{16+} projectiles as a function of γ with target charges $Z_T = 29$, 47, and 79. Solid lines (not depending on the projectile charge): present results for charge transfer from the negative-energy continuum, Eq. (9); dashed line (not depending on the target charge): excitation-type mechanism, Eq. (10); see [3].

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