Negative-continuum dielectronic recombination for heavy ions

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(Received 11 February 2003; published 28 May 2003)

The process of recombination of an electron with a bare heavy nucleus via the creation of a free-positron–bound-electron pair is considered. This process is denoted as ''negative-continuum dielectronic recombination'' because it results in the capture of an incident electron into a bound state accompanied by a transition of a negative-continuum electron into a bound state. The calculations are performed for a wide range of incident electron energies for $Z=82$ and 92.

DOI: 10.1103/PhysRevA.67.052711 PACS number(s): 34.80.Lx, 31.30.Jv

I. INTRODUCTION

In a collision between an electron and a bare heavy nucleus, the main reaction channel in a wide range of collision energies is the radiative recombination (RR) of the electron into a bound state of an H-like ion via the simultaneous emission of a photon. This process is well-studied both theoretically and experimentally [1–7]. However, at sufficiently high energies, alternative processes may occur. (In the following, electron energies are always defined as including the electron rest mass.) If the energy of the incident electron in the nuclear rest frame is larger than the ground-state energy of the corresponding He-like ion plus the positron rest energy, the incident electron can be captured into the $1s$ state with a simultaneous creation of a free-positron–$1s$-electron pair:

$$X^{Z+}+e^{-}\rightarrow X^{(Z-2)+}+e^{+}.$$

This process may be denoted as ''negative-continuum dielectronic recombination'' (NCDR), since it is similar to the usual dielectronic recombination (DR) for a few-electron atom (see Refs. [8,9,12], and references therein), except for the fact that the second electron is not an electron already bound to the ion but an electron from the negative continuum (''Dirac sea'') which is ''lifted'' into a bound state. This is illustrated in Figs. 1 and 2. Figure 1 indicates the usual DR for a heavy few-electron ion. The NCDR is conventionally shown in Fig. 2. In this process, we have a bare nucleus and an incoming electron in the initial state, and the He-like ion and an outgoing positron in the final state. In contrast to the DR process, NCDR is not a resonant process due to the continuum structure of the spectrum at electron energies $\varepsilon < -mc^2$.

With the increase of the energy ε_i of the incident electron above the threshold of $\varepsilon_i=E_{(1s)^2}+mc^2$ (where $E_{(1s)^2}$ denotes the ground-state energy of the heliumlike ion), the electrons can occupy excited states as well. When $\varepsilon_i > 2mc^2+\varepsilon_{1s}$, the creation of a free-electron–positron pair becomes also possible. In this paper, we consider NCDR into the ground state of a He-like heavy ion. Accurate calculations of this process in the framework of QED are presented for lead $(Z=82)$ and uranium $(Z=92)$.

It should be noted that NCDR is not a unique mechanism for electron-positron pair creation. A lot of previous calculations were devoted to electron-positron pair creation, in particular for collisions of heavy ions at the Coulomb barrier with supercritical fields involved (see, e.g., Refs. [10,11]). However, the processes investigated in these works considerably differ from NCDR, since in ion-ion collisions one has to deal with electrons and positrons in a two-center Coulomb field. A review on some investigations on electron-positron pair creation at relativistic energies can be found in Ref. [1].

The paper is organized as follows. In the following section, we give basic formulas for calculation of NCDR. Nu-

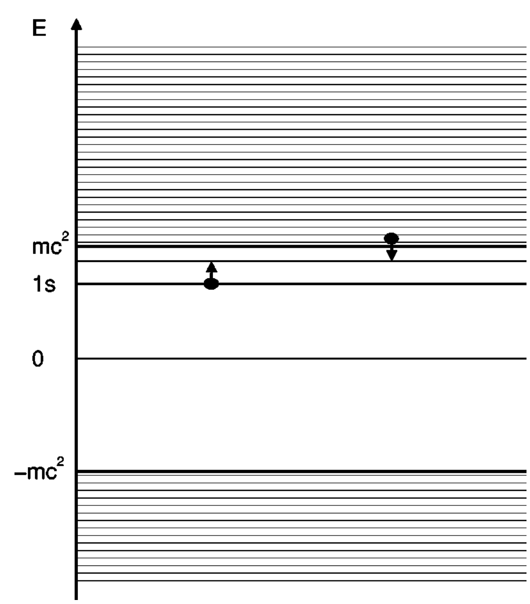

FIG. 1. A schematic representation of the dielectronic recombination.

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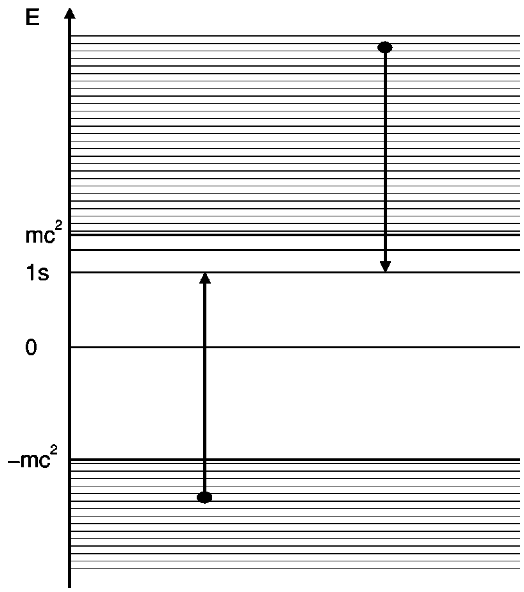

FIG. 2. A schematic representation of the negative-continuum dielectronic recombination into the $(1s)^2$ state.

merical results and a brief discussion are given in Sec. III.

Relativistic units ($\hbar = m_e = c = 1$) are used throughout the paper.

II. BASIC FORMULAS

The differential cross section of the process under consideration is given by [13]

$$\frac{d\sigma}{d\Omega_f} = \frac{(2\pi)^4}{v_i} \mathbf{p}_f^2 |\tau_{i\to f}|^2, \tag{1}$$

with the amplitude τ defined by the equation

$$2\pi i\,\delta(E_i - E_f)\,\tau_{i\to f} = \langle f|(S-\hat{I})|i\rangle. \tag{2}$$

Here, S is the scattering operator, $\hat{I}$ is the identity operator, v_i is the velocity of the incident electron, $\mathbf{p}_f$ is the momentum of the outgoing positron, and E_i and E_f are the total initial and final energies of the system, respectively. A systematic way to calculate the τ amplitude can be formulated within the two-time Green function approach [12,13]. This approach is the only one up to now which allows for a systematic QED treatment of transitions or scattering processes if bound states of few-electron atoms are involved. The S-matrix formalism [14,15], which also is sometimes employed in bound-state QED (cf. Ref. [16], and references therein), was developed for calculations of energy levels only.

To zeroth order of the perturbation theory, NCDR is given by the diagram shown in Fig. 3, where, according to the standard procedure (see, e.g., Refs. [17,18]), the outgoing positron with four-momentum p_f and polarization m_f is described as an incoming electron with four-momentum $-p_f$ and polarization $-m_f$. For the S-matrix element corresponding to this diagram, we obtain

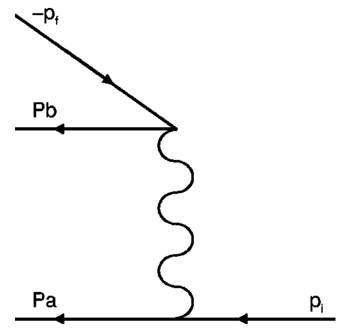

FIG. 3. Negative-continuum dielectronic recombination diagram. a and b are the $1s$ states with opposite angular momentum projections and P is the permutation operator.

$$\begin{aligned}\langle f|(S-\hat{I})|i\rangle &= 2\pi i\,\delta(\varepsilon_i - \varepsilon_f - \varepsilon_a - \varepsilon_b) \sum_P (-1)^P \\ &\quad \times \langle PaPb|I(\varepsilon_i - \varepsilon_{Pa})|(p_i,m_i),(-p_f,-m_f)\rangle,\end{aligned} \tag{3}$$

where

$$I(\omega) = \alpha(1-\boldsymbol{\alpha}_1\cdot\boldsymbol{\alpha}_2)\frac{\exp(i|\omega||\mathbf{r}_1-\mathbf{r}_2|)}{|\mathbf{r}_1-\mathbf{r}_2|}, \tag{4}$$

with the coordinate $\mathbf{r}_\nu$ and Dirac matrix $\boldsymbol{\alpha}_\nu$ referring to the electron $\nu=1,2$. Furthermore, $\varepsilon_i = p_i^0 \equiv \sqrt{\mathbf{p}_i^2+m^2}$ and $\varepsilon_f = p_f^0 \equiv \sqrt{\mathbf{p}_f^2+m^2}$, a and b indicate the $1s$ states with opposite angular momentum projections ($\varepsilon_a = \varepsilon_b = \varepsilon_{1s}$), and P is the permutation operator. The electron wave functions $|p_i,m_i\rangle$ and $|-p_f,-m_f\rangle$ are defined by the following integral equations:

$$\begin{aligned}|p_i,m_i\rangle &= \frac{u(p_i,m_i)}{\sqrt{\varepsilon_i(2\pi)^3}}\exp(i\mathbf{p}_i\cdot\mathbf{x}) \\ &\quad + [\varepsilon_i - H_0(1-i0)]^{-1}V_C|p_i,m_i\rangle,\end{aligned} \tag{5}$$

$$\begin{aligned}|-p_f,-m_f\rangle &= \frac{v(p_f,m_f)}{\sqrt{\varepsilon_f(2\pi)^3}}\exp(-i\mathbf{p}_f\cdot\mathbf{x}) \\ &\quad + [-\varepsilon_f - H_0(1-i0)]^{-1}V_C|-p_f,-m_f\rangle.\end{aligned} \tag{6}$$

Here u and v are the positive- and negative-energy spinors, correspondingly, normalized by the conditions $\overline{u}u=1$, $\overline{v}v=-1$; V_C is the Coulomb potential of the nucleus; and H_0 is the free Dirac Hamiltonian. Averaging over incident electron polarizations and summing over outgoing positron polarizations, we obtain the following formula for the differential cross section:

$$\frac{d\sigma}{d\Omega_f}=\frac{8\pi^4}{v_i}\mathbf{p}_f^2\sum_{m_i,m_f}\left|\sum_P(-1)^P \times\langle PaPb|I(\varepsilon_i-\varepsilon_{Pa})|(p_i,m_i),(-p_f,-m_f)\rangle\right|^2. \quad (7)$$

For the wave functions (5) and (6), one can derive partial-wave expansions over the states with defined angular momentum and its projection onto an axis (see Refs. [1,19]). Let us assume that in the ion-rest frame, the incident electron moves along the positive direction of the z axis. In this case, the wave function of the electron can be written in the following form:

$$|p_i,m_i\rangle=\frac{1}{\sqrt{4\pi}}\frac{1}{\sqrt{\varepsilon_i|\mathbf{p}_i|}}\sum_\kappa i^l\exp(i\Delta_\kappa)\sqrt{2l+1}C^{jm_i}_{l0,(1/2)m_i}\times\begin{pmatrix}g_{\varepsilon_i,\kappa}(r)\Omega_{\kappa m_i}(\hat{\mathbf{r}})\\ if_{\varepsilon_i,\kappa}(r)\Omega_{-\kappa m_i}(\hat{\mathbf{r}})\end{pmatrix}, \quad (8)$$

where $\kappa=(-1)^{j+l+1/2}(j+1/2)$ is the quantum number determined by the angular momentum and the parity of the state, $j=|\kappa|-1/2$, $l=|\kappa+1/2|-1/2$, $C^{JM}_{j_1m_1,j_2m_2}\equiv\langle j_1m_1,j_2m_2|JM\rangle$ is the Clebsch-Gordan coefficient, Δ_κ is the phase shift, and $\hat{\mathbf{r}}=\mathbf{r}/|\mathbf{r}|$. Since we perform summation over spin projections of the outgoing positron, we can use the following representation for its wave function [1]:

$$|-p_f,-m_f\rangle=\frac{1}{\sqrt{\varepsilon_f|\mathbf{p}_f|}}\sum_{\kappa,M_f}i^{l'}\exp(i\Delta_\kappa)\times C^{jM_f}_{l'm_{l'},(1/2)-m_f}Y^*_{l'm_{l'}}(-\hat{\mathbf{p}})\times\begin{pmatrix}g_{-\varepsilon_f,\kappa}(r)\Omega_{\kappa M_f}(\hat{\mathbf{r}})\\ if_{-\varepsilon_f,\kappa}(r)\Omega_{-\kappa M_f}(\hat{\mathbf{r}})\end{pmatrix}, \quad (9)$$

where $Y_{lm_l}(\hat{\mathbf{p}})$ is a spherical harmonic, and $l'=2j-l$.

Substituting Eqs. (8) and (9) into Eq. (7), we obtain the following formula for the differential cross section:

$$\frac{d\sigma}{d\Omega_f}=\frac{2\pi^3|\mathbf{p}_f|}{\varepsilon_f\mathbf{p}_i^2}\sum_{m_i,m_f}\left|\sum_{P,\kappa_i,\kappa_f,M_f}(-1)^P i^{l_i+l_f'}\exp(i\Delta_{\kappa_i}+i\Delta_{\kappa_f})\times\sqrt{2l_i+1}C^{j_i\,m_i}_{l_i\,0,\,(1/2)\,m_i}C^{j_f\,M_f}_{l_f'\,m_{l_f'},\,(1/2)\,-m_f}Y^*_{l_f',m_{l_f'}}(-\hat{\mathbf{p}}_f)\times\langle PaPb|I(\varepsilon_i-\varepsilon_{Pa})|(\varepsilon_i,\kappa_i,m_i)(-\varepsilon_f,\kappa_f,M_f)\rangle\right|^2, \quad (10)$$

where (ε,κ,m) is the electron wave function with energy ε, angular momentum and parity determined by κ, and angular momentum projection m. The above results were obtained in the Feynman gauge but are, of course, gauge invariant since they are based on the electron wave functions exact in (αZ).

III. NUMERICAL RESULTS AND DISCUSSION

Numerical calculations of expression (10) have been performed with the help of the RADIAL package [20]. This package can be applied for calculating both bound and continuum solutions of the Dirac equation, but only for positive energies. To calculate negative-continuum electron wave functions, we have used the fact that the radial components of the electron wave function, $g^{(e^-)}_{-\varepsilon,-\kappa}$ and $f^{(e^-)}_{-\varepsilon,-\kappa}$, can be expressed in terms of the radial components of the positron wave function $(V_C\to -V_C)$, $g^{(e^+)}_{\varepsilon,\kappa}$ and $f^{(e^+)}_{\varepsilon,\kappa}$, by the following equations: $g^{(e^-)}_{-\varepsilon,-\kappa}(r)=f^{(e^+)}_{\varepsilon,\kappa}(r)$ and $f^{(e^-)}_{-\varepsilon,-\kappa}(r)=g^{(e^+)}_{\varepsilon,\kappa}(r)$. The calculations have been performed using the homogeneously charged sphere model for the nuclear charge distribution. The integration over the angular variables in the one-photon-exchange matrix element in Eq. (10) has been performed analytically. The radial integrations have been accomplished numerically with the help of the Gauss-Legendre quadratures.

Before discussing our conclusions, we would like to mention that we are going to present our results in both the ion-rest frame and the electron-rest frame. The calculation formulas have the simplest form in the ion-rest frame which to the zeroth approximation coincides with that of the center-of-mass. However, experiments are performed with an electron cooler or with a gas-jet target, where the electron-rest frame is the one corresponding to the experimental conditions.

In Tables I and II, the results for the total cross section of the negative-continuum dielectronic recombination into the ground state of He-like lead and uranium are presented. In the first column of these tables, the kinetic energy T_{el} of the incident electron in the ion-rest frame is given. In the second column, the corresponding kinetic energy of the nucleus T_{nucl} in the electron-rest frame is displayed. In the third column, the values of the NCDR cross section are presented, in barns. For a comparison, in the fourth column, we list the values of the total cross section of radiative recombination into the 1s state. All the figures given are numerically exact in our

TABLE I. The total cross section of NCDR into the ground state of Pb^{80+} (initial charge state 82+) and the total cross section of RR into the ground state of Pb^{81+} for various incident electron energies.

T_{el} (keV)	T_{nucl} (MeV/u)	σ_{NCDR} (b)	σ_{RR} (b)
820	1494.8	4.48×10^{-30}	3.447
850	1549.5	1.55×10^{-8}	3.268
900	1640.6	9.14×10^{-7}	3.003
950	1731.7	3.21×10^{-6}	2.774
1000	1822.9	5.79×10^{-6}	2.573
1100	2005.2	9.46×10^{-6}	2.241
1200	2187.5	1.09×10^{-5}	1.977
1300	2369.8	1.10×10^{-5}	1.764
1400	2552.0	1.05×10^{-5}	1.588
1500	2734.3	9.84×10^{-6}	1.441
1600	2916.6	9.12×10^{-6}	1.317
1700	3098.9	8.46×10^{-6}	1.211
1800	3281.2	7.87×10^{-6}	1.119
1900	3463.5	7.35×10^{-6}	1.039
2000	3645.8	6.90×10^{-6}	0.969
2500	4557.2	5.27×10^{-6}	0.719
3000	5468.7	4.20×10^{-6}	0.566

zeroth-order approximation. The electron-electron interaction causes contributions of higher orders in $1/Z$ which are thought to be smaller by approximately this factor. Their consideration is beyond the scope of the present work.

The NCDR cross section increases rapidly above the threshold ($T_{el}=819$ keV for Pb^{80+} and $T_{el}=758$ keV for U^{90+}), has a flat maximum slightly above the energy needed

TABLE II. The total cross section of NCDR into the ground state of U^{90+} (initial charge state 92+) and the total cross section of RR into the ground state of U^{91+} for various incident electron energies.

T_{el} (keV)	T_{nucl} (MeV/u)	σ_{NCDR} (b)	σ_{RR} (b)
760	1385.4	1.67×10^{-23}	6.301
800	1458.3	9.40×10^{-8}	5.846
850	1549.5	2.41×10^{-6}	5.352
900	1640.6	7.75×10^{-6}	4.926
950	1731.7	1.38×10^{-5}	4.555
1000	1822.9	1.90×10^{-5}	4.229
1100	2005.2	2.53×10^{-5}	3.687
1200	2187.5	2.72×10^{-5}	3.255
1300	2369.8	2.67×10^{-5}	2.904
1400	2552.0	2.52×10^{-5}	2.615
1500	2734.3	2.34×10^{-5}	2.372
1600	2916.6	2.16×10^{-5}	2.167
1700	3098.9	2.00×10^{-5}	1.991
1800	3281.2	1.85×10^{-5}	1.839
1900	3463.5	1.72×10^{-5}	1.706
2000	3645.8	1.61×10^{-5}	1.590
2500	4557.2	1.20×10^{-5}	1.175
3000	5468.7	9.33×10^{-6}	0.923

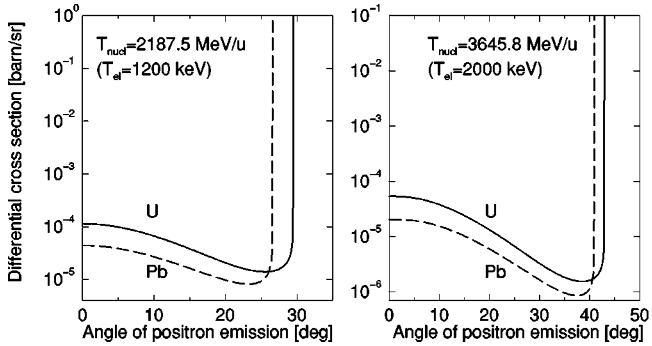

FIG. 4. The differential cross sections of NCDR in the electron-rest frame for the kinetic energies of the nucleus 2187.5 MeV/u and 3645.8 MeV/u. The singularity of the curves is discussed in the text.

to create a free electron-positron pair and then decreases slowly with the energy. In general, the NCDR cross sections are by about six orders of magnitude smaller than for the corresponding radiative recombination. In contrast to other pair production processes, the cross section does not steadily increase with the collision energy.

In Figs. 4 and 5, we plot the differential cross section of the negative-continuum dielectronic recombination as a function of the polar angle in the electron-rest frame and in the nucleus-rest frame, correspondingly, for two values of the collision energy. As one can see from Fig. 4, in the electron-rest frame there exists a maximal value of the polar angle, for which scattering is possible. This is a general feature of the kinematics of the process. If one of the two coordinate systems is moving with the velocity β_m with respect to the other, and in the moving coordinate system some particles with the velocity $\beta<\beta_m$ are scattered, then in the other coordinate system there exists a maximal value of the scattering angle given by (see, e.g., Refs. [1,21])

$$\sin(\theta_{max})=\frac{\beta\gamma}{\beta_m\gamma_m}, \tag{11}$$

where $\gamma=1/\sqrt{1-\beta^2}$ is the Lorenz factor. It can be shown that when the scattering angle reaches the maximum, the differential cross section becomes infinite. This is caused by the fact that the differential cross sections in the two frames are related by

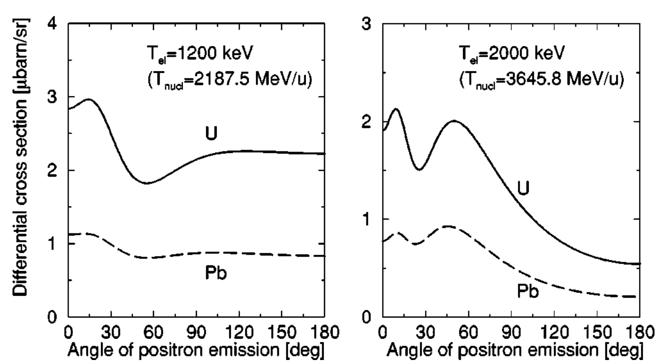

FIG. 5. The same as in Fig. 4, but for the nucleus-rest frame.

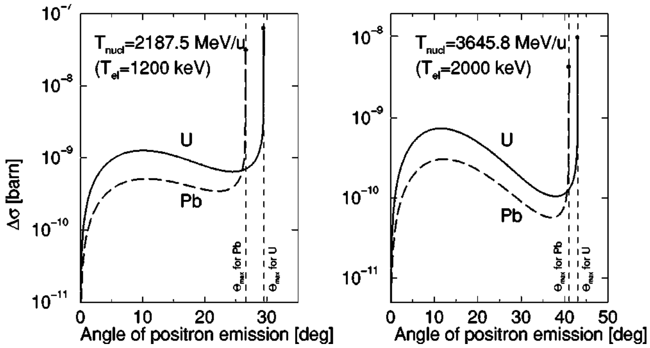

FIG. 6. The value $\Delta\sigma$ defined by Eq. (14) with $\Delta\theta = 1$ mrad, for the curves presented in Fig. 4. The bullets (●) indicate the finite end points of the curves.

$$\frac{d\sigma}{d\Omega} = \left|\frac{d\Omega'}{d\Omega}\right| \frac{d\sigma'}{d\Omega'}, \tag{12}$$

where the primed variables correspond to the moving frame. If the differential cross section is symmetric with respect to the z axis, the derivative in Eq. (12) can be calculated as

$$\left|\frac{d\Omega'}{d\Omega}\right| = \gamma_m^2 \frac{\left[\left(\frac{\beta_m}{\beta'} + \cos(\theta')\right)^2 + \frac{\sin^2(\theta')}{\gamma_m^2}\right]^{3/2}}{\left|1 + \frac{\beta_m}{\beta'}\cos(\theta')\right|}. \tag{13}$$

If $\beta_m/\beta' > 1$, the denominator in Eq. (13) becomes zero at $\cos(\theta') = -\beta'/\beta_m$. Nevertheless, the integral of the differential cross section over the angles in both frames converges and yields the same value that is the total cross section of NCDR. In order to show the integrability of the singularity of the differential cross section in the electron-rest frame, in Fig. 6, we plot the value $\Delta\sigma$ defined by

$$\Delta\sigma(\theta) = 2\pi \int_{\theta}^{\theta+\Delta\theta} \frac{d\sigma}{d\theta} \sin\theta \, d\theta, \tag{14}$$

where $\Delta\theta$ is chosen to be equal 1 mrad. Thus, the end point of the curve becomes finite as indicated in Fig. 6. For larger angles, the differential cross section is equal to zero.

Except for the maximal scattering angle $\theta_{\max}$, where the differential cross section becomes infinite because of the singularity of the angular transformation, the differential cross section has its maximum for forward scattering. Therefore, in the electron-rest frame, this direction is the best for experimental investigations. In Fig. 7, we present the differential cross section at the positron emission angle $\theta = 10°$ as a function of the kinetic energy of the incident nucleus.

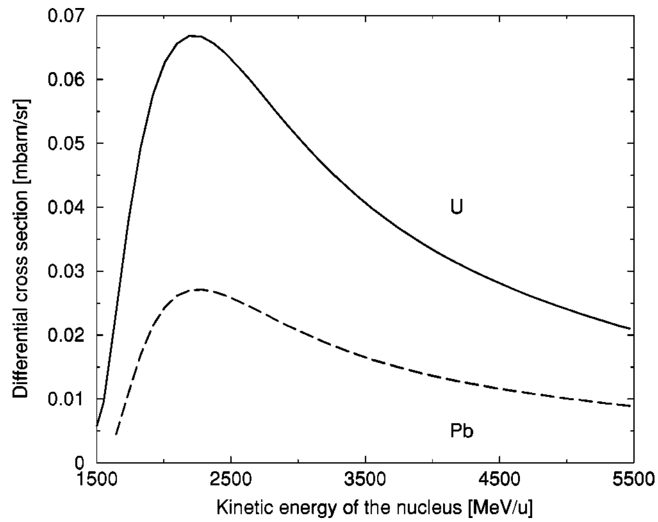

FIG. 7. The differential cross section for negative-continuum dielectronic recombination at the polar angle $\theta = 10°$ for the positron emission as a function of the kinetic energy of the nucleus in the electron-rest frame.

With collision energy increasing, excited states of the ion can also be involved into NCDR. When $\varepsilon_i > 2mc^2 + \varepsilon_{1s}$, the free-electron–positron-pair creation becomes possible as well. We have estimated NCDR for the case when the electrons are captured into the $(1s2s)_{0,1}$, $(1s2p_{1/2})_{0,1}$, or $(1s2p_{3/2})_{1,2}$ state. It has been found that at kinetic energies of the incident electron in nucleus-rest frame larger than 2000 keV, these channels give rise to an increase of the total NCDR cross section by 5–25%. In detail, these results will be published separately.

In summary, we have presented a new mechanism for positron creation in electron-heavy ion collisions at energies of around 1 MeV which is termed as negative-continuum dielectronic recombination, in analogy to the common dielectronic recombination. The signature of positron emission in a narrow angular range in the laboratory frame associated with projectiles that captured two electrons makes the new process clearly distinct from all other types of electron capture (e.g., radiative recombination). Thus, it will be easily observable at the presently planned accelerators at GSI [22]. Preparations for experiments aiming at the identification of this new process are currently being started at the existing GSI facilities.

ACKNOWLEDGMENTS

We would like to thank Professor G. Soff for helpful and encouraging discussions. This work was supported by the DFG (Grant No. 436 RUS 113/616), by RFBR (Grant No. 01-02-04011), by the Russian Ministry of Education and the Administration of Saint-Petersburg (Grant Nos. PD02-1.2-79 and E02-3.1-49), and by GSI. A. Klasnikov is also grateful to the Leonhard-Euler program of the DAAD.

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