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Positron creation probabilities in low-energy heavy-ion collisions*

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Abstract. The previously developed technique for calculation of ionization probabilities in low-energy heavy-ion collisions [A.I. Bondarev et al., Phys. Scr. **T156**, 014054 (2013)] is extended to evaluation of positron creation probabilities. The differential probabilities are evaluated by two alternative methods. The first one uses hydrogenic continuum wave functions, while the second one uses discretized continuum wave functions corresponding to a finite basis expansion. These methods are applied to the calculation of the differential positron creation probabilities in the $U^{91+}(1s)$-U^{92+} collision. The results obtained by both methods are found in good agreement.

1 Introduction

Collisions of highly charged ions allow to study relativistic and quantum electrodynamic effects in atomic processes. Of particular interest is the collision of two heavy ions provided that the total charge of the colliding nuclei exceeds the critical value $Z_c = 173$. The investigation of processes accompanying such a collision gives a unique opportunity for testing quantum electrodynamics in the supercritical Coulomb field [1].

In our recent paper [2], we presented a technique for calculation of ionization probabilities in low-energy heavy-ion collisions. In this work, the method is extended to evaluation of positron creation probabilities. The calculations were performed for the uranium-uranium collision, which had been studied before a lot (see, e.g., Refs. [3–9]; review [10], and references therein). Two alternative ways of extracting the differential positron creation probabilities are discussed and compared.

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

2 Theory

2.1 Time-dependent Dirac equation

We consider the collision of a hydrogenlike ion with a bare nucleus. Within the semiclassical approximation, we treat the nuclei as sources of an external time-dependent potential. Thus the three-particle problem of an electron and nuclei is reduced to the problem of a relativistic electron in a two-center time-dependent potential. Since the collision is low-energy, we neglect the magnetic part of the interaction. The electron dynamics is described by the time-dependent Dirac equation,

$$i\frac{\partial\Psi(\boldsymbol{r},t)}{\partial t} = \hat{H}(t)\Psi(\boldsymbol{r},t), \quad \hat{H}(t) = \boldsymbol{\alpha}\cdot\boldsymbol{p}+\beta+V(\boldsymbol{r},t), \quad (1)$$

where $\boldsymbol{\alpha}$ and β are the Dirac matrices. The time dependence enters the potential $V(\boldsymbol{r},t)$ through the internuclear distance $\boldsymbol{R}(t)$,

$$V(\boldsymbol{r},t) = V_{\rm T}(r) + V_{\rm P}(|\boldsymbol{r}-\boldsymbol{R}(t)|). \quad (2)$$

Here we assume that the target (a hydrogen-like ion) is fixed at the origin, while the projectile (a bare nucleus) moves along the classical Rutherford trajectory $\boldsymbol{R}(t)$. In fact, this reference frame is a non-inertial one, but in the monopole approximation used in the calculations, the effect of noninertiality does not contribute to the results.

In order to solve equation (1), we apply the following two-step procedure. At first the stationary Dirac equation is solved employing the dual kinetic balance approach with the basis functions constructed from B-splines [11]:

$$H_0\phi_k(\boldsymbol{r}) = \varepsilon_k\phi_k(\boldsymbol{r}). \quad (3)$$

Here H_0 is the matrix representation of the time-independent Hamiltonian $\hat{H}_0 = \boldsymbol{\alpha}\cdot\boldsymbol{p}+\beta+V_{\rm T}(r)$ in the finite B-spline basis set. Along this line, sets of eigenenergies $\{\varepsilon_k\}$ and eigenstates $\{\phi_k(\boldsymbol{r})\}$, $k = 1,\ldots,N$ of H_0 are obtained, and their overall number N depends on the size of the B-spline basis set.

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Then the time-dependent wave function $\Psi(\boldsymbol{r},t)$ is approximated by its expansion $\widetilde{\Psi}(\boldsymbol{r},t)$ over the finite basis set $\{\phi_k(\boldsymbol{r})\}$,

$$\Psi(\boldsymbol{r},t) \simeq \widetilde{\Psi}(\boldsymbol{r},t) = \sum_k C_k(t) e^{-i\varepsilon_k t}\phi_k(\boldsymbol{r}). \quad (4)$$

Substituting equation (4) in equation (1), one derives the system of coupled channel equations on the expansion coefficients $C_j(t)$

$$i\frac{dC_j(t)}{dt} = \sum_k C_k(t) e^{i(\varepsilon_j-\varepsilon_k)t} V_{jk}(t), \quad (5)$$

$$V_{jk}(t) = \langle\phi_j|V_{\mathrm{P}}(t)|\phi_k\rangle. \quad (6)$$

It should be noted that since the basis set $\{\phi_k(\boldsymbol{r})\}$ is orthonormal, the overlapping matrix $S_{jk} = \langle\phi_j|\phi_k\rangle$ is reduced to the identity matrix $I_{jk} = \delta_{jk}$. The initial conditions for the system of equations (5) correspond to the initial electron state. For instance, for the initial ground state they can be written as

$$C_k(t\to-\infty) = \delta_{1s,k}. \quad (7)$$

It is also worth noting that the atomiclike basis set is centered at the target and does not allow for the proper description of charge transfer processes.

To evaluate the matrix elements of the projectile potential $V_{jk}(t)$, it is convenient to re-expand this potential to the position of the target, where the basis functions are centered. For the Coulomb potential of a point nucleus or a homogeneously charged sphere, it can be done analytically [12–14]. The calculation in the so-called monopole approximation takes into account only the spherically symmetric part of the re-expanded potential with respect to the origin.

The system of equations (5) can be rewritten in the matrix form,

$$i\frac{d\boldsymbol{C}(t)}{dt} = M(t)\boldsymbol{C}(t), \quad M_{jk}(t) = e^{i(\varepsilon_j-\varepsilon_k)t}V_{jk}(t), \quad (8)$$

where $\boldsymbol{C}(t)$ is the vector incorporating the expansion coefficients $C_k(t)$.

To solve equation (8), we use the Crank-Nicolson method [15]. Within this method, one derives

$$\boldsymbol{C}(t+\Delta t) \simeq U(t+\Delta t,t)\boldsymbol{C}(t), \quad (9)$$

with the unitary propagator

$$U(t+\Delta t,t) = \left[I + i\frac{\Delta t}{2}M(t+\Delta t/2)\right]^{-1} \times \left[I - i\frac{\Delta t}{2}M(t+\Delta t/2)\right], \quad (10)$$

which, hence, preserves the norm of the wave function.

So to determine the coefficients $\boldsymbol{C}(t+\Delta t)$ at each time step, we have to solve the following system of linear equations:

$$\left[I + i\frac{\Delta t}{2}M(t+\Delta t/2)\right]\boldsymbol{C}(t+\Delta t) = \left[I - i\frac{\Delta t}{2}M(t+\Delta t/2)\right]\boldsymbol{C}(t). \quad (11)$$

2.2 Transition amplitudes and probabilities

The transition amplitude to the stationary state $\Psi_\varepsilon(\boldsymbol{r},t) = \psi_\varepsilon(\boldsymbol{r})e^{-i\varepsilon t}$ of the unperturbed Hamiltonian $\hat{H}_0$ with the energy ε belonging to the negative-energy Dirac continuum can be calculated as a projection of the wave packet $\widetilde{\Psi}(\boldsymbol{r},t)$ onto this state at the limit $t\to\infty$,

$$T_\varepsilon(t) = \left\langle\Psi_\varepsilon(t)\middle|\widetilde{\Psi}(t)\right\rangle. \quad (12)$$

Here we assume that wave functions $\psi_\varepsilon(\boldsymbol{r})$ are normalized on the energy scale,

$$\langle\psi_\varepsilon|\psi_{\varepsilon'}\rangle = \delta(\varepsilon-\varepsilon'). \quad (13)$$

The radial part of the final state Dirac wave function $\psi_\varepsilon(\boldsymbol{r})$ is obtained numerically using the RADIAL package [16].

The function $\Psi_\varepsilon(\boldsymbol{r},t)$ satisfies the time-dependent equation (1) at the limit $t\to\infty$, when $\hat{H}(t)\to\hat{H}_0$, while the function $\widetilde{\Psi}(\boldsymbol{r},t)$ satisfies a similar equation, but with the matrix representation H_0 of the time-independent Hamiltonian $\hat{H}_0$ in the finite basis set. This leads to a time-dependence of their scalar product $T_\varepsilon(t)$ even at the limit $t\to\infty$. To overcome this, we can approximate $\Psi_\varepsilon(\boldsymbol{r},t)$ at $t=0$ by the function $\widetilde{\psi}_\varepsilon(\boldsymbol{r})$ which is a linear combination of the eigenfunctions $\phi_k(\boldsymbol{r})$ of the time-independent Hamiltonian matrix H_0,

$$\Psi_\varepsilon(\boldsymbol{r},t=0) = \psi_\varepsilon(\boldsymbol{r}) \simeq \widetilde{\psi}_\varepsilon(\boldsymbol{r}) = \sum_k \langle\phi_k|\psi_\varepsilon\rangle\phi_k(\boldsymbol{r}). \quad (14)$$

Then the time-dependent wave function $\widetilde{\Psi}_\varepsilon(\boldsymbol{r},t)$ takes the form

$$\widetilde{\Psi}_\varepsilon(\boldsymbol{r},t) = \sum_k \langle\phi_k|\psi_\varepsilon\rangle\phi_k(\boldsymbol{r})e^{-i\varepsilon_k t}. \quad (15)$$

This function satisfies the unperturbed time-dependent equation

$$i\frac{\partial\widetilde{\Psi}_\varepsilon(\boldsymbol{r},t)}{\partial t} = H_0\widetilde{\Psi}_\varepsilon(\boldsymbol{r},t), \quad (16)$$

where H_0 is the time-independent Hamiltonian matrix. It should be noted that the wave function $\widetilde{\Psi}_\varepsilon(\boldsymbol{r},t)$ formally does not correspond to a stationary state.

Thus instead of equation (12) for the transition amplitude $T_\varepsilon(t)$ we come to the following expression:

$$\widetilde{T}_\varepsilon(t) = \left\langle\widetilde{\Psi}_\varepsilon(t)\middle|\widetilde{\Psi}(t)\right\rangle, \quad (17)$$

which has a well defined limit at the asymptotic time $t \to \infty$.

It is also worth noting that since the wave function $\widetilde{\Psi}(t)$ is also the solution of the time-dependent equation (16) at the limit $t \to \infty$, one can use some relations which hold for solutions of equation (1). For instance, one can prove that the following expression is completely equivalent to formula (17):

$$\widetilde{T}_\varepsilon(t) = -i \int_{-\infty}^{t} dt' \left\langle \widetilde{\Psi}_\varepsilon(t') \right| V(t') \left| \widetilde{\Psi}(t') \right\rangle. \qquad (18)$$

The transition probability corresponding to emission of a positron with the energy ε is defined by

$$\frac{dP}{d\varepsilon} = \left| \widetilde{T}_\varepsilon(t \to \infty) \right|^2. \qquad (19)$$

Substituting equations (4), (15) and (17) in equation (19), and using the orthonormality of the basis functions $\phi_k(\boldsymbol{r})$, we finally get

$$\frac{dP}{d\varepsilon} = \left| \sum_k C_k(t) \left\langle \psi_\varepsilon \middle| \phi_k \right\rangle \right|^2, \quad t \to \infty. \qquad (20)$$

So all dependence of the differential probability (20) on the hydrogenic continuum wave function $\psi_\varepsilon(\boldsymbol{r})$ left in the expansion coefficient $\langle \psi_\varepsilon | \phi_k \rangle$ of $\psi_\varepsilon(\boldsymbol{r})$ over the basis set $\{\phi_k(\boldsymbol{r})\}$. Equation (20) was used for the calculation referred as the first method.

The second method of evaluation of the differential positron emission probability uses the discretized continuum wave functions corresponding to the finite basis expansion $\phi_k(\boldsymbol{r})$, $\varepsilon_k < 0$ solely. In contrast to the first method, it does not utilize the hydrogenic continuum wave functions $\psi_\varepsilon(\boldsymbol{r})$ at all.

The projection of the wave packet $\widetilde{\Psi}(\boldsymbol{r}, t)$ at the asymptotic time $t \to \infty$ onto the negative-energy eigenstates $\phi_k(\boldsymbol{r})$ of H_0 gives the probability dP/dk, where k is a discrete eigenfunction index. This probability does not take into account the density of continuum states. Multiplying it by the density $dk/d\varepsilon$, we get the differential probability $dP/d\varepsilon$. Making use the Stieltjes method, which has been widely used before for various calculations [17–20], one obtains the following approximate expression for the differential probability:

$$\frac{dP}{d\varepsilon}\left(\frac{\varepsilon_{k+1} + \varepsilon_k}{2}\right) = \frac{1}{2}\frac{P_{k+1} + P_k}{\varepsilon_{k+1} - \varepsilon_k}, \quad P_k = |C_k(t \to \infty)|^2, \qquad (21)$$

which becomes exact in an infinite basis set.

Since the monopole approximation is used in the calculations, the results are independent on the positron emission angle.

2.3 Influence of the negative-energy Dirac continuum

In this subsection, the second quantization formalism used for the proper account for the negative-energy Dirac continuum is introduced. Such a description is not the main goal of the article, however, it helps to compare a part of our results with ones previously published.

We thus are also able to calculate the total positron creation probabilities in the collision of two bare uranium nuclei U^{92+}-U^{92+}. Using methods of Section 2.1 to solve the time-dependent Dirac equation, which now is formulated in the center of mass frame, we obtain the expansion coefficients $C_k(t)$ at the asymptotic time $t \to \infty$. Within the second quantization technique exhaustively developed by the Frankfurt group (see, e.g., Ref. [3]), the probability of formation of a hole in a negative-energy state k (creation of a positron in this state) reads

$$N_k = 2 \sum_{i:\, \varepsilon_i > 0} \left| C_k^{(i)}(t \to \infty) \right|^2, \quad \varepsilon_k < 0, \qquad (22)$$

where the upper index i of the expansion coefficient $C_k^{(i)}$ means the initial condition $C_k^{(i)}(t \to -\infty) = \delta_{i,k}$. The factor 2 in equation (22) refers to a summation over projections of the total angular momentum $j = 1/2$. We would like to note that according to equation (22) all the positive-energy basis states should be propagated in time in order to calculate the total positron creation probability,

$$P_{e^+} = \sum_{k:\, \varepsilon_k < 0} N_k. \qquad (23)$$

Moreover, in accordance with the law of conservation of electric charge, the total electron creation probability equals to the total positron creation probability.

Table 1. The total positron creation probabilities P_{e^+} for U^{92+}-U^{92+} collision at center-of-mass kinetic energy 740 MeV for different impact parameters b.

b, fm	P_{e^+}, this work	P_{e^+}, Ref. [4]
0	1.29×10^{-2}	1.26×10^{-2}
5	1.08×10^{-2}	1.06×10^{-2}
10	7.26×10^{-3}	7.15×10^{-3}
15	4.51×10^{-3}	4.47×10^{-3}
20	2.75×10^{-3}	2.73×10^{-3}
25	1.69×10^{-3}	1.68×10^{-3}
30	1.04×10^{-3}	1.04×10^{-3}
40	4.12×10^{-4}	4.11×10^{-4}

3 Results and discussion

First, let us present the results for the total positron creation probabilities P_{e^+} in the U^{92+}-U^{92+} collision. In Table 1, the comparison of our results calculated according to equations (22) and (23) with the data of reference [4] is given. The calculation was performed in the monopole approximation with respect to the center of mass at kinetic energy 740 MeV for the $s_{1/2}$ and $p_{1/2}$ angular momentum channels. Since spherically symmetric (monopole) potential does not mix these channels, they give independent contributions to the total positron creation yield.

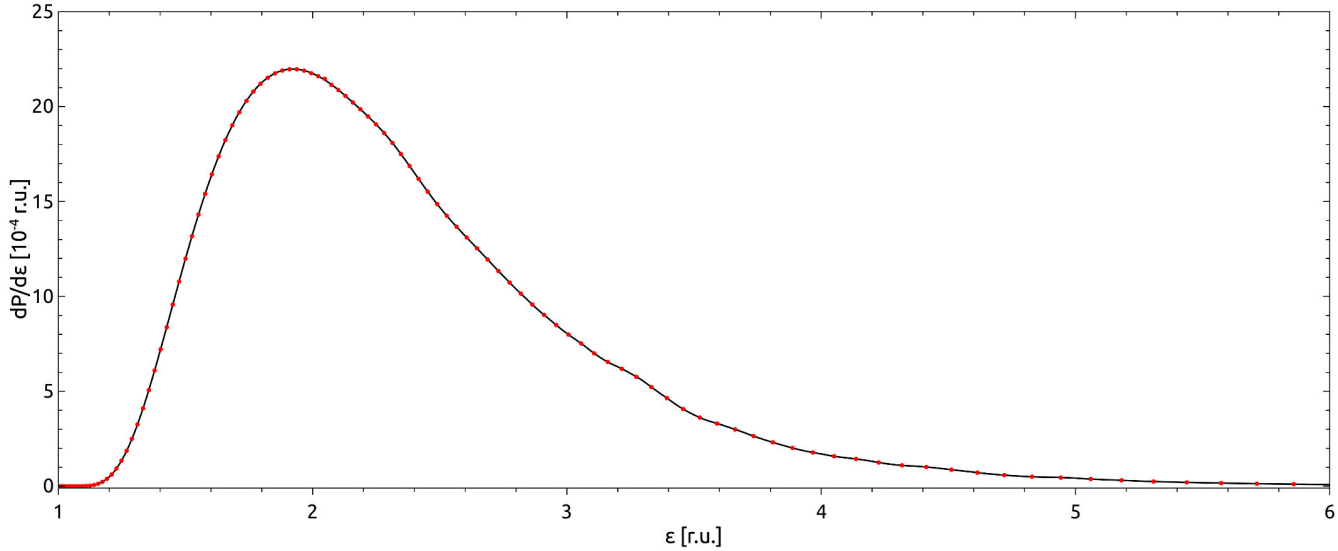

Fig. 1. The differential positron creation probability in the $U^{91+}(1s)$-U^{92+} collision for zero impact parameter and at center-of-mass kinetic energy 740 MeV. The calculation was performed in the monopole approximation with respect to the target. The black line and red dots represent the results calculated according to formulae (20) and (21) correspondingly.

The same as in reference [4] nuclear charge distribution was used for the clarity of the comparison.

The results of the present calculations being in good agreement with the ones from reference [4] are systematically larger. This can be explained by the size of the basis set used in the calculations. Our basis set contained 400 states for each angular momentum channel, while the results of reference [4] were obtained with about 50 basis states. We also found that in agreement with the data of reference [4] the main contribution to the total positron creation probabilities P_{e^+} is given by a pair creation with an electron captured into a bound state.

Now let us proceed with presenting the results for the process of $U^{91+}(1s)$-U^{92+} collision obtained within the theory given in Sections 2.1 and 2.2. We thus neglected that the negative-energy continuum states are occupied by electrons, and calculated the differential transition probability of the electron initially bound in the $1s$ state of the target to a negative-energy state. In the approximation we used, this probability can be referred as a positron creation probability. It should be also noted that within the second quantization formalism, this quantity can be considered as a positron creation probability in the U^{92+}-U^{92+} collision with capture of the created electron in the $1s$ state of the target.

In Figure 1, the results calculated according to formulae (20) and (21) are plotted. The calculation was performed in the monopole approximation with respect to the target for the zeroth impact parameter, which gives the largest positron creation yield, at the same center-of-mass kinetic energy 740 MeV, which corresponds to 6.218 MeV/u in the target reference frame. The calculation according to formula (20) can be performed for an arbitrary energy ε (here a step of 0.01 r.u. was taken), while energies ε_k used in the calculation according to formula (21) are defined by the solution of equation (3).

The total contribution of the negative-energy Dirac continuum, which is the area under the curve at Figure 1, equals to 3.16×10^{-3}. As one can see from the figure, the results of both methods (Eqs. (20) and (21)) are in good agreement.

4 Conclusion

The total probabilities of electron-positron pair creation were evaluated for the U^{92+}-U^{92+} collision in the monopole approximation using two dominant channels ($s_{1/2}$ and $p_{1/2}$). The results were found in good agreement with the data of the Frankfurt group [4].

Two alternative methods of extracting the differential probabilities were compared. The first one uses hydrogenic continuum wave functions, while the second one uses discretized continuum wave functions corresponding to a finite basis expansion and Stieltjes technique. These methods were applied for evaluation of the positron creation probabilities in the $U^{91+}(1s)$-U^{92+} collision, and the corresponding results were found consistent with each other. Our calculations in the monopole approximation can provide only the energy distribution of created particles. In order to study the angular distribution, one should go beyond this approximation. The corresponding calculations will be presented in a forthcoming paper.

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