The probabilities of bound-free electron-positron pair creation are calculated for head-on collisions of bare uranium nuclei beyond the monopole approximation. The calculations are based on the numerical solving of the time-dependent Dirac equation in the target reference frame with multipole expansion of the projectile potential. In addition, the energy dependence of the pair-creation cross section is studied in the monopole approximation.

### 1 Introduction

Spontaneous electron-positron pair creation in the presence of supercritical Coulomb field is a fundamental effect of quantum electrodynamics, which was first predicted in references [1,2]. Low-energy heavy-ion collisions can provide a field of the required strength and therefore can serve as a tool for investigations of this phenomenon [3]. The crucial condition imposed on the colliding nuclei is that their total charge $Z_{\text{tot}} = Z_1 + Z_2$ should exceed the critical value, $Z_{\text{cr}} \approx 173$ (see Ref. [3] and references therein). However, the spontaneous contribution to the pair creation has to be distinguished from the dynamical one which occurs due to the time dependence of the potential of the moving nuclei. The pure spontaneous pair creation was investigated in references [4–6]. Analytical evaluation of the dynamical contribution for $\alpha Z_{1,2} \ll 1$ ($\alpha$ is the fine structure constant) was carried out in reference [7]. A rough estimate of this contribution for heavy ions was considered in references [8,9]. The nonperturbative consideration of pair creation with simultaneous inclusion of both contributions requires solving the time-dependent Dirac equation (TDDE). As applied to the pair-creation calculations, several techniques were utilized [10–14] for solving the TDDE in the monopole approximation. In this approximation, only the spherically symmetric part of the two-center potential is taken into account. Usually the monopole approximation is used in the center-of-mass (CM) reference frame, because it provides better description of the homonuclear quasi-molecule for small internuclear distances. However, for large internuclear distances the reference frame of one of the nuclei (target) is preferable.

The only way to test the validity of the monopole approximation is to go beyond it. In reference [15], calculations of pair creation with the full two-center potential were performed in the CM frame. Another way to go beyond the monopole approximation is to take into account the higher-order terms of the multipole expansion. This technique was used in references [16–19] for solving the two-center stationary Dirac equation and in references [20–22] for solving the TDDE as applied to calculations of ionization probabilities in heavy-ion collisions.

In the present paper, we consider the collision process in the target reference frame. The target potential is fully accounted, whereas the projectile potential is expanded in the multipole series truncated at some order. The TDDE is solved using the finite basis set of hydrogen-like wave functions. The basis functions are constructed from B-splines using the dual-kinetic-balance approach (DKB) [23]. The calculations of pair-creation probabilities
are performed for the collision of bare uranium nuclei at energy near the Coulomb barrier. In order to reduce the computation time, we consider only the bound-free pair creation since the bound-state contribution is expected to be the dominant one [11,13]. The obtained results are compared with the corresponding values calculated with the full two-center potential [15] and with the monopole-approximation potential in the CM frame [11,13]. We also evaluate the cross section of pair creation for the collision of bare uranium nuclei at different energies in the monopole approximation. These calculations are performed in the target as well as in the CM frames.

Throughout the paper \( \hbar = 1 \) is assumed.

2 Theory

In the present work, the nuclear collision process is treated semiclassically. Under this approximation, the colliding nuclei are regarded as the sources of an external time-dependent potential. Their motion is described classically with trajectories of the Rutherford type. The magnetic part of the potential is neglected due to the smallness of the relative collision velocity compared to the speed of light. The electron dynamics is described by the TDDE:

\[
i \frac{\partial}{\partial t} \psi(r,t) = H(t)\psi(r,t), \tag{1}
\]

where

\[
H(t) = c(\alpha \cdot p) + \beta m_e c^2 + V_{\text{tot}}(r,t). \tag{2}
\]

Here \( \alpha, \beta \) are the Dirac matrices, \( c \) is the speed of light, \( m_e \) denotes the electron mass, and \( V_{\text{tot}} \) is the total two-center potential of the colliding nuclei:

\[
V_{\text{tot}}(r,t) = V_T(|r - R_T(t)|) + V_P(|r - R_P(t)|), \tag{3}
\]

where vectors \( R_T \) and \( R_P \) denote the positions of the target and projectile nuclei, respectively, and

\[
V_{T,P}(r) = \int dr' \frac{\rho_{T,P}(r')}{|r - r'|}, \tag{4}
\]

are the corresponding nuclear potentials. For the nuclear charge distribution \( \rho(r) \) we utilize the model of the uniformly charged sphere.

Assuming the coordinate origin is on the internuclear axis, the multipole expansion of the two-center potential can be written as

\[
V_{\text{tot}}(r,t) = \sum_{L=0}^{\infty} \left( V_{T,L}^L(r,R_T(t)) + V_{P,L}^L(r,R_P(t)) \right) \times P_L(\cos \theta). \tag{5}
\]

Here \( P_L \) are the Legendre polynomials, \( \theta \) is the angle between vectors \( r \) and \( R = R_P - R_T \), and

\[
V_{T,P}^L(r,R_{T,P}) = \frac{2L + 1}{2} \int_0^\pi d(\cos \theta) V_{T,P}(r,R_{T,P}) \times P_L(\cos \theta). \tag{6}
\]

The expansion (5) depends on the position of the coordinate origin. In the target reference frame, \( R_T = 0 \) and \( R_P = R(t) \) is the internuclear distance. Then equation (5) gives

\[
V_{\text{tot}}(r,t) = V_T(r) + \sum_{L=0}^{\infty} V_{P,L}^L(r,R(t)) P_L(\cos \theta). \tag{7}
\]

Since the actual calculations are conducted within the finite basis set comprising only functions with the orbital angular momentum up to some value \( l_{\text{max}} \), the sums in (5) and (7) are effectively truncated at \( L_{\text{max}} = 2l_{\text{max}} \) as higher-order multipoles cannot couple any pair of the basis states.

In the monopole approximation, only the term with \( L = 0 \) is taken into account and equation (7) is reduced to

\[
V_{\text{tot}}(r,t) \simeq V_{\text{mon}}^T(r,R(t)) = V_T(r) + V_{P,0}^0(r,R(t)). \tag{8}
\]

In the CM frame, for two nuclei with equal masses the monopole approximation has the following form:

\[
V_{\text{tot}}(r,t) \simeq V_{\text{mon}}^{\text{CM}}(r,R(t)) = V_T^0(r,R(t)/2) + V_{P,0}^0(r,R(t)/2). \tag{9}
\]

The monopole potentials in different reference frames have different asymptotics for \( R \to \infty \): \( V_{\text{mon}}^T(r,R) \to V_T^T(r) \) and \( V_{\text{mon}}^{\text{CM}}(r,R) \to 0 \). Therefore only in the target frame the monopole Hamiltonian has well-defined bound states for large internuclear distances. However, the CM monopole potential is better in describing the two-center potential at small internuclear distances. The monopole approximation allows us to reduce the three-dimensional TDDE to the one-dimensional equation that drastically simplifies the numerical calculations. Adding the higher-order multipole terms, one should improve the approximation.

We note that the target reference frame is non-inertial. However, we neglect the corresponding correction to the Hamiltonian assuming that its influence is small enough.

To describe the process of pair creation, the formalism of quantum electrodynamics with the unstable vacuum is employed [3,24]. Let us introduce two sets of solutions of the TDDE (1): \( \{\psi_n^+(r,t)\} \) are the in-solutions and \( \{\psi_n^-(r,t)\} \) are the out-solutions. The sets differ by the boundary conditions imposed on the wave function at the initial \( t_{\text{in}} \) and final \( t_{\text{out}} \) time moments:

\[
\psi_n^+(r,t_{\text{in}}) = \phi_n(r), \tag{10}
\]

\[
\psi_n^-(r,t_{\text{out}}) = \phi_n(r). \tag{11}
\]
where \( \phi_n \) are the solutions of the stationary Dirac equation

\[
H_0 \phi_n = \varepsilon_n \phi_n, \quad (12)
\]
\[
H_0 = c(\alpha \cdot p) + \beta m_e c^2 + U(r). \quad (13)
\]

We assume that \( H(t_{in}) = H(t_{out}) = H_0 \) since \( R(t_{in}) = R(t_{out}) \) in our calculations. The sets \( \{\psi_n^{(+)}\} \) of in-solutions and \( \{\psi_n^{(-)}\} \) of out-solutions describe physical particles at times \( t_{in} \) and \( t_{out} \), correspondingly. We have chosen \( U(r) = V_T(r) \) for the calculations in the target frame and \( U(r) = V_{\text{mon}}^\text{CM}(r, t_{in}) \) for the calculations in the CM frame within the monopole approximation.

The amplitudes \( \psi_{mn} \) at the time moment \( t_{in} \) are time-independent [13], hence one can consider them at the time moment \( t_{in} \):

\[
a_{mn} = \int dr \psi_m^{(-)}(r, t_{in})\phi_n(r). \quad (15)
\]

The wave functions \( \psi_m^{(-)} \) at the time moment \( t_{in} \) are found using the numerical solution of the TDDE. The initial states \( \phi_n \), including the bound ones and the pseudostates from both (negative- and positive-energy) continuum spectra, are obtained by diagonalization of the \( H_0 \) matrix in a finite basis set. The basis functions are generated from the B-splines according to the DKB technique [23]. The time-dependent wave functions are decomposed over the obtained \( \phi_n \) states:

\[
\psi_k(r, t) = \sum_{k=1}^{N} c_{ki}(t)\phi_k(r)e^{-i\varepsilon_k t}, \quad (17)
\]

where \( N \) is the number of the states, \( \varepsilon_k \) are the eigenvalues of the \( H_0 \) matrix, and \( c_{ki} \) are the expansion coefficients.

At first, we studied the dependence of the probability of electron-positron pair-creation in collisions of bare uranium nuclei. To solve TDDE we used a time grid of exponential type with \( N_t = 4000 \) steps and a basis set consisting of \( n_b = 320 \) functions for each orbital angular momentum. Initial and final internuclear separations were chosen to be \( R_{\infty} = 12000 \) fm.

The system of equation (18) is solved employing the Crank-Nicolson scheme [25]:

\[
\bar{c}_i(t + \Delta t) = M(t + \Delta t; t)\bar{c}_i(t), \quad (20)
\]

where \( \Delta t \) is a sufficiently small time step, \( \bar{c}_i = \{c_{i1}, \ldots, c_{iN}\} \), and the matrix \( M \) is defined as

\[
M(t + \Delta t; t) = \left[ I + i\frac{\Delta t}{2} V \left( t + \frac{\Delta t}{2} \right) \right]^{-1} \cdot \left[ I - i\frac{\Delta t}{2} V \left( t + \frac{\Delta t}{2} \right) \right]. \quad (21)
\]

Using the described technique one can propagate all the bound states back in time from \( t_{out} \) to \( t_{in} \) and calculate the total bound-free pair-creation probability,

\[
P_b = \sum_{|\varepsilon_k| < m_e c^2} n_k, \quad (22)
\]

as well as the final electron population of each bound state. The pair-creation cross section can be found by integration over the impact parameter \( b \),

\[
\sigma_b = 2\pi \int_0^\infty db \; b \; P_b. \quad (23)
\]

### 3 Results

Employing the method described above, we performed the calculations of electron-positron pair-creation probabilities in collisions of bare uranium nuclei. To solve TDDE we used a time grid of exponential type with \( N_t = 4000 \) steps and a basis set consisting of \( n_b = 320 \) functions for each orbital angular momentum. Initial and final internuclear separations were chosen to be \( R_{\infty} = 12000 \) fm. At first, we studied the dependence of the probability on the impact parameter in the monopole approximation with the basis set including only functions of zero orbital momentum. The calculations were carried out in the target and CM reference frames. It is seen from Figure 1 that the probability decreases exponentially with the growth of the impact parameter. One can also notice that the CM values are systematically larger than the target ones. This can be explained by the fact that at small internuclear distances the CM monopole potential is stronger than the target one. Being closer to the full two-center potential, the CM monopole potential also gives better results compared to the target one. Taking into account higher-order multipoles makes the potential even stronger, which results in the probability increase and consequently in growth of the cross section. As it will be demonstrated below for head-on collisions, the discrepancy between CM and target calculations decreases in this case.
To obtain pair-creation cross sections we calculated the probabilities for impact parameters in the range 0–120 fm with the 3 fm step and performed integration according to equation (23). In Figure 2 we show the pair-creation cross sections obtained for various asymptotic collision velocities, which correspond to the collision energies in the range 2–10 MeV/u with 2 MeV/u step. The cross section calculated for the collision velocity near 0.1 relativistic unit (r.u.) is by about two orders of magnitude smaller than the value obtained by a rough estimate in reference [9]. Although our calculations were restricted to the monopole approximation, this comparison seems justified. As it will be shown below, for head-on collisions the inclusion of higher-order multipoles does not essentially change the pair-creation probability compared to the CM monopole results. Assuming the same dependence of the probability on the impact parameter, one can expect that the cross sections also will not alter significantly.

Next, we performed the calculations beyond the monopole approximation for the head-on collisions. For
Table 1. Probability of pair creation with electron captured into the ground state ($P_g$) and into any bound state ($P_b$) in U$^{92+}$–U$^{92+}$ head-on collisions at energy $E = 6.218$ MeV/u. Here $t_{\text{max}}$ is the maximal orbital momentum of the wave functions included in the basis set. For comparison, the results obtained in reference [13] with the CM monopole potential and the values of reference [15] calculated with the full two-center potential are also presented.

| $t_{\text{max}}$ | $P_g$ | $P_b$ |
|------------------|-------|-------|
| 0                | 5.73 · 10$^{-3}$ | 5.91 · 10$^{-3}$ |
| 1                | 9.23 · 10$^{-3}$ | 1.05 · 10$^{-2}$ |
| 2                | 1.05 · 10$^{-2}$ | 1.24 · 10$^{-2}$ |
| 3                | 1.10 · 10$^{-2}$ | 1.30 · 10$^{-2}$ |
| 4                | 1.11 · 10$^{-2}$ | 1.31 · 10$^{-2}$ |
| 5                | 1.09 · 10$^{-2}$ | 1.29 · 10$^{-2}$ |
| CM monopole [13] | 1.25 · 10$^{-2}$ |  |
| Two-center [15]  | 1.11 · 10$^{-2}$ | 1.32 · 10$^{-2}$ |

the direct comparison of our results with the data of references [13,15], the collision energy $E = 6.218$ MeV/u was used. Table 1 represents the pair-creation probabilities obtained according to expressions (14) and (22) with truncation of the time-dependent wave function decomposition (17) at different orbital momenta. The results of the full two-center calculation [15] and the value obtained within the monopole approximation in the CM frame [13] are also presented. Despite our approach being too rough to account properly for the process of pair creation with electron capture by the projectile, the obtained values are very close to ones of reference [15], where this process is embedded in the calculation technique. A possible explanation for this could be as follows: the electron-positron pairs are mainly created at small internuclear distances where the higher-order multipole terms of the projectile potential do not play a significant role.

It is worth noting that in our calculations we restricted the basis set to states with the total angular momentum projection on the internuclear axis $\mu$ equal to ±1/2 only. In the head-on collision, the time-dependent potential does not mix states with different $\mu$ values. Hence, the contributions of these states can be calculated independently. Moreover, the contributions of the states with opposite angular momentum projections are equal to each other. Thus, to get the probabilities we carried out the evaluation in the basis set with a certain sign of the angular momentum projection and then doubled the obtained value to account for the contribution of the opposite projection. As in reference [15], it is found that the contribution of states with the angular momentum projection larger than 1/2 is negligible.

4 Conclusion

In this paper we have evaluated the electron-positron pair-creation probabilities for the head-on collision of bare uranium nuclei at the energy $E = 6.218$ MeV/u beyond the monopole approximation. The calculations were performed using one-center basis set expansion in the target reference frame. The target potential was fully taken into account, while the potential of the projectile was approximated by few lowest-order terms of the multipole expansion with respect to the target nucleus. The results of the calculations are in reasonable agreement with the data obtained within the framework of the full two-center potential approach [15]. Further improvement of the accuracy by adding the higher-order terms is limited by computational resources.

We have also calculated the pair-creation cross section in the monopole approximation for collision energies in the range of 2–10 MeV/u. The calculations were carried out in the target as well as in the CM frames. The obtained values have the same order of magnitude in both frames.

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Author contribution statement

V.M.S. conceived the idea of the research and supervised the project. R.V.P., A.I.B., Y.S.K., and I.A.M performed the calculations and wrote the main manuscript text. I.I.T., X.M., G.P., and Th.S. contributed to the discussion of the calculations and the results.

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