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Coupled channel analysis of electron-positron pair production in relativistic heavy ion collisions*

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Abstract. The production of electron-positron pairs by electromagnetic fields in relativistic heavy ion collisions is studied nonperturbatively within a coupled-channel formalism. For the description of the electron field an expansion in atomic wave functions around the target nucleus is employed. The positive and negative continua are discretized by means of time-dependent relativistic wave packets. For the system $U^{92+}+U^{92+}$ at $E_{\text{lab}}=10$ GeV/nucleon and $b=386$ fm and with a limited set of angular momenta we calculate probabilities for free pair production and production with inner-shell capture, which are by about two orders of magnitude larger than those obtained in first order perturbation theory. This indicates a drastic failure of the perturbation theory of first order for high-Z heavy ion collisions.

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1. Introduction

Theoretical predictions of the total cross section for the production of electron-positron pairs in collisions of fast charged particles started with the work of Landau and Lifschitz [1], who described the electron-positron production in the Born approximation. Common to all the former work was the use of free Dirac spinors for the electron and positron (for references see e.g. Heitler [2]). With the development of colliders for relativistic heavy ions new interest came up for more elaborate work on electron-positron pair creation. For example, the equivalent photon method (Weizsäcker-Williams method) has been applied by several authors in the extremely relativistic regime [3–6]. Similar results for pair production were obtained with the semi-classical approximation in first or second order perturbation theory [7–10]. Becker et al. [7] chose exact Coulomb-Dirac wave functions around the target nucleus which require a multipole expansion of the electromagnetic potentials. Deco and Grün [10] took the perturbation of the target states by the projectile into account employing distorted wave functions for the electron and positron.

A first 3-dimensional, fully nonperturbative treatment of lepton-pair production has been carried out by Strayer et al. [11] solving the time-dependent Dirac equation with a basis spline expansion [12]. They found results for μ-pair production with capture into the $1s_{1/2}$ ground state of the target ion which are by several orders of magnitude larger than the predictions of the first order perturbation theory [13]. Although their treatment lacks by a not completely consistent procedure for projection on the continuum, their work can be regarded as the first computational indication for the nonperturbative character of lepton-pair production in relativistic heavy ion collisions.

In this paper, we present another nonperturbative approach to the pair creation which is based on the solution of coupled equations for the time-dependent coefficients used for an expansion of the electron-positron field in basis functions. Such a treatment has already been applied to the problem of charge exchange, excitation and ionisation in relativistic heavy ion collisions [14–16]. A very similar calculation for pair production has been carried out by Rumrich et al. [17] with slightly different basis functions and a different method for the evaluation of the necessary matrix elements.

In Sect. 2 we present the method for the calculation of the probabilities for pair creation. In Sect. 3 we apply the method to the collision of U^{92+} on U^{92+} at an energy of $E_{\text{lab}}=10$ GeV/nucleon for an impact parameter $b=386$ fm. The procedure is based on an expansion of the potentials and wave functions in multipoles. In connection with this expansion the calculation had to be restricted to a limited number of angular momenta of the wave functions up to $p_{3/2}$ in order that the program was manageable on the computer. However, in the considered collision angular momenta up to 21/2 contribute in first order perturbation theory to the pair creation. Therefore, our resulting probabilities will be interpreted as a demonstration for the failure of perturbation theory

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Dedicated to Professor Wilhelm Hanle on the occasion of his 90th birthday and can not be taken as values directly comparable with experiment. Natural units are applied throughout the paper ($\hbar = m = c = 1$).

2. The method

The semiclassical approximation is used. The projectile moves on a straight line with constant velocity and the target is fixed at the center of the coordinate system. The field operator $\hat{\Psi}$ of the electron-positron field is expanded in terms of time-dependent single-particle wave functions ψ_i.

$$\hat{\Psi} = \sum_{E_i > E_F} \hat{b}_i \psi_i(\mathbf{r}, t) + \sum_{E_i < E_F} \hat{d}_i^+ \psi_i(\mathbf{r}, t). \tag{1}$$

The annihilation operators $\hat{b}_i$ and the creation operators $\hat{d}_i^+$ are time-independent. E_F is the Fermi energy which is $E_F = -mc^2$ in our case. The basis functions ψ_i obey the time-dependent Dirac equation

$$H_D \psi_i(\mathbf{r}, t) = i \frac{\partial}{\partial t} \psi_i(\mathbf{r}, t). \tag{2}$$

The Dirac Hamiltonian H_D is given by

$$H_D = H_0 + V_P(t), \tag{3}$$

$$H_0 = \boldsymbol{\alpha}\mathbf{p} + \beta - Z_T e^2/r, \tag{3a}$$

$$V_P = -Z_P e^2 \gamma (1 - v_P \alpha_Z)/r', \tag{3b}$$

$$r' = ((x-b)^2 + y^2 + \gamma^2 (z - v_P t)^2)^{1/2}, \tag{3c}$$

$$\gamma = (1 - v_P^2)^{-1/2}. \tag{3d}$$

Here, H_0 is the target Hamiltonian, V_P the interaction between electron and projectile, b the impact parameter and v_P the velocity of the projectile. In order to solve (2), the wave functions ψ_i are expanded into functions which solve the Dirac equation with the target Hamiltonian H_0 (see (3a)):

$$\psi_i = \sum_j a_{ji} \phi_j \exp(-iE_j t). \tag{4}$$

Insertion of this expansion into the time-dependent Dirac equation (2) and projection to a particular basis state labeled j yields the coupled channel equations for the expansion coefficients:

$$i \dot{a}_{ji} = \sum_k < \phi_j | V_P(t) | \phi_k > \exp(i(E_j - E_k)t) a_{ki}. \tag{5}$$

The initial conditions are

$$a_{ji}(t = -\infty) = \delta_{ij}. \tag{6}$$

The time evolution of the single-particle amplitudes a_{ji} is completely determined by the set (5) of coupled differential equations. As shown by Reinhardt et al. [18], it suffices to known the single-particle amplitudes in order to determine the probabilities to create a particle in a electron or positron state, if the electron-electron interaction is neglected (see also [19]).

By following the usual practice we obtain the probability for an electron in an unperturbed state i with $E_i > E_F$:

$$P_i(t \to \infty) = \sum_{E_k < E_F} |a_{ik}(t \to \infty)|^2 \tag{7}$$

and the probability for a positron in an unperturbed state i with $E_i < E_F$:

$$P_i(t \to \infty) = \sum_{E_k > E_F} |a_{ik}(t \to \infty)|^2. \tag{8}$$

Unperturbed state means here the target states described by the wave functions ϕ_i. It should be pointed out that the expressions (7) and (8) are the inclusive probabilities to find a single electron or positron in a certain state i independent of the creation of further electron-positron pairs which can be excited from the initial vacuum state with other energies.

In a further step of the analysis, we want to extract the probability of a correlated production of a single electron-positron pair. Since in the numerical realization both continua are discretized by means of wave packets, the basis set is approximated by a finite set of normalized single-particle functions. Hence, it is completely equivalent to the formalism of second quantization to describe the time evolution of the initial vacuum state with a finite Slater determinant. Let us construct the Slater determinant by the subset of time-dependent single-particle states ψ_i, that initially ($t \to -\infty$) describe the fully occupied negative continuum. Since we neglect the electron-electron interaction, the single-particle functions evolve independently in time according to the time-dependent single-particle Dirac equation (2). For $t \to \infty$ we can calculate the amplitude by projecting with the Slater determinant of the observed excited state, built up by the unperturbed target wave functions ϕ_j. E.g., if we were interested in the amplitude to create a single electron-positron pair, the negative-energy continuum state p in the original Slater determinant related to the positron has to be replaced by the positive-energy state e of the electron. The corresponding amplitude can then be calculated for N discretized states of the negative continuum in form of a Slater determinant of single-particle amplitudes $\langle \phi_i | \psi_j \rangle = a_{ij}$:

$$A_{p \to e} = \begin{vmatrix} \langle \phi_1 | \psi_1 \rangle & \dots & \langle \phi_e | \psi_1 \rangle & \dots & \langle \phi_N | \psi_1 \rangle \\ \vdots & & \vdots & & \vdots \\ \langle \phi_1 | \psi_N \rangle & \dots & \langle \phi_e | \psi_N \rangle & \dots & \langle \phi_N | \psi_N \rangle \end{vmatrix}_{t \to \infty} = \begin{vmatrix} a_{11} & \dots & a_{e1} & \dots & a_{N1} \\ \vdots & & \vdots & & \vdots \\ a_{1N} & \dots & a_{eN} & \dots & a_{NN} \end{vmatrix}_{t \to \infty} \tag{9}$$

The column $\langle \phi_e | \psi_j \rangle = a_{ej}$ ($j = 1, \dots, N$) is inserted at the position p. In an analogous manner, probabilities for the production of two electron-positron pairs and other excited states can be easily calculated.

A detailed description of the coupled-channel code used has been given in a paper of Momberger et al. [16], where the ionization and excitation of inner-shell electrons were considered. In addition, in the present paper the negative continuum has to be taken into account. The continua are represented by a finite set of orthonormal wave packets of the form (Weyl packets):

$$\phi_{Ej}(\mathbf{r}, t) = \frac{1}{\sqrt{\Delta E_j}} \int_{E_j - \frac{\Delta E_j}{2}}^{E_j + \frac{\Delta E_j}{2}} \mathrm{d}E\, \phi_E(\mathbf{r}) \exp(i(E_j - E)t). \qquad (10)$$

The functions ϕ_E in the integrand are exact Coulomb-Dirac eigenfunctions of H_0. The wave packets are time-dependent, located at the target for $t=0$ and, for example, travel outwards with momentum $p_j = (E_j^2 - 1)^{1/2}$ for $t > 0$ and $E_j > 1$. For the bound states we take exact Coulomb-Dirac wave functions at the target.

3. Results and comparison with first order perturbation calculations

This formalism was applied to the collision system $U^{92+} + U^{92+}$ at $E_{\mathrm{lab}} = 10$ GeV/nucleon. We present results for an impact parameter $b = 386$ fm. This is a reasonable choice since this impact parameter yields approximately the maximum contribution to the total cross section in first order perturbation theory. For the basis set we employed 5 bound states ($1s_{1/2}$, $2s_{1/2}$, $2p_{1/2}$, $2p_{3/2}$, $3s_{1/2}$) and wave packets at 20 energies for both continua ($E_j = 1.3, \ldots, 7.3$; $-1.3, \ldots, -6.1$; $\Delta E = 0.6$) for each of the three angular momenta $s_{1/2}$, $p_{1/2}$, $p_{3/2}$ ($\kappa = -1, +1, -2$). The number of coupled coefficients is 172 for this basis set including all magnetic substates. The restriction in the angular momentum summation is presently the most important shortcoming of our calculations, because we can conclude from first order perturbation theory that this basis set is too small in order to obtain sufficient convergence. We estimate that the summation should be extended up to about $|\kappa| = 10$ (corresponding to 20 angular momenta). However, coupled channel calculations with so large basis sets are presently not feasible for us.

The coupled channel equations have to be solved for each of the initially occupied states of the negative continuum, which are 72 single-particle wave functions in our basis system (including all magnetic substates). For the case of pair creation with simultaneous K-shell capture the time-reversal symmetry of the coefficients can be employed and hence only one integration in time has to be performed by starting with the $1s_{1/2}$ bound state.

In Fig. 1 we show results for the differential probability to observe a positron of energy E_{e+} as a function of this energy. The histogram-like curves show the total probability and its decomposition into contributions from pair creaction of free pairs and with simultaneous capture. Also the total probability for the correlated production of a single pair is indicated. The continuous lines below the histograms are the results of a calculation in first order perturbation theory, where the same angular momentum quantum numbers of the continuum are taken into account as in the coupled-channel calculation. The astounding result is that couplings of higher order increase the positron spectrum by more than one order of magnitude. The direct pair production is increased by one order of magnitude and the capture from vacuum by roughly two orders of magnitude. The production of a single electron-positron pair during the collision is dominant to about 90%, i.e. the production of many pairs can not explain the large probabilities.

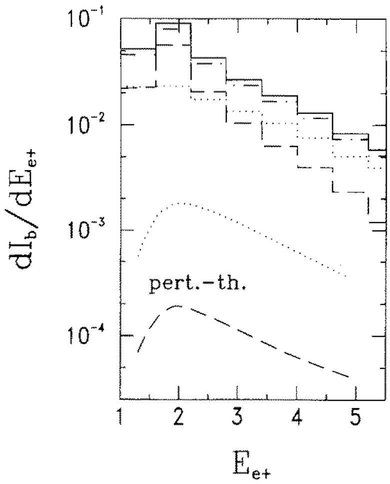

Fig. 1. Differential probability for observation of a positron of energy E_{e+} in the collision $U^{92+} + U^{92+}$ at $E_{\mathrm{lab}} = 10$ GeV/nucleon and impact parameter $b = 386$ fm. The histrogram-like curves show the coupled-channel results, the continuous curves below are the results of the first order perturbation theory. The solid curve gives the total positron spectrum and the dotted-dashed curve the contribution from the production of a single electron-positron pair during the collision. The dotted curves show the probabilities for the production of free pairs and the dashed curves those for the production of pairs with simultaneous inner-shell capture. The energy E_{e+} is measured in units of $mc^2 = 511$ keV

The results of our calculations have been subjected to several tests. A very useful test for consistency can be drawn from the time reversal symmetry, which results in

$$|a_{ij}(\infty)|^2 = |a_{ji}(\infty)|^2. \qquad (11)$$

We tested the time reversal symmetry in the case of the total $1s$-capture probability. The following equation has to be fulfilled exactly:

$$\sum_{E_j < -1} |a_{1s, E_j}(\infty)|^2 = \sum_{E_j < -1} |a_{E_j, 1s}(\infty)|^2. \qquad (12)$$

The agreement between both sides of the equation was found to be better than 1%, which is sufficiently accurate for our purpose. As a further test we required, that for $Z_P \to 1$ the solutions of the coupled channel equations should approach those of the first order perturbation theory, since then $Z_P\,\alpha$ is small. As an example, in Fig. 2 we show the time evolution of the transition from a state described by a wave packet with negative energy $E_j = -3.7$ and $\kappa = -1(s_{1/2})$ to the bound $1s_{1/2}$ state. This transition is described by four amplitudes if we consider

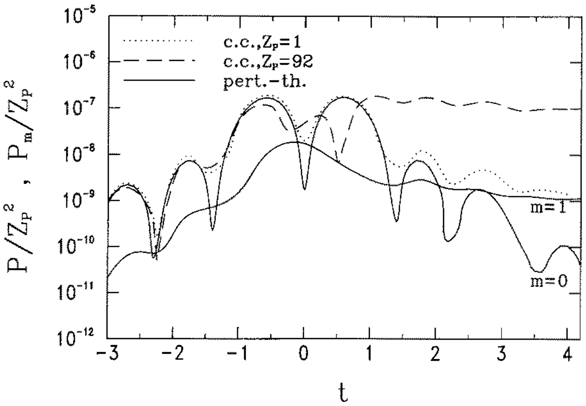

Fig. 2. Comparison of probabilities divided by Z_P^2 and obtained in first order perturbation theory and by coupled-channel calculation for a transition from a state of the negative continuum with $E_j=-3.7$ and $\kappa=-1$ $(s_{1/2})$ to the bound $1s_{1/2}$ state of U^{91+} for $Z_P=1$ and $Z_P=92$. The solid curves are the probabilities P_m for $m=0$ and 1 defined in (13) and calculated with the perturbation theory. The dotted curve is the coupled-channel result of $P=P_{m=0}+P_{m=1}$ for $Z_{P=1}$, the dashed curve for $Z_P=92$. The unit of time is $\hbar/mc^2=1.288\cdot10^{-21}$ s

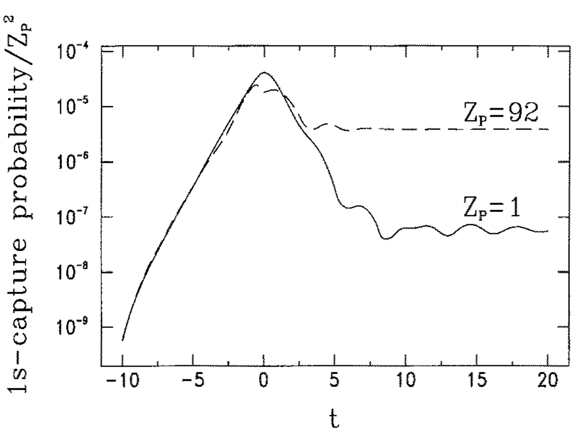

Fig. 3. Total probability for pair production with the capture of the electron into a $1s_{1/2}$ state as a function of time for $Z_P=1$ and $Z_P=92$. The result for $Z_P=1$ is equivalent to the first order perturbation theory. The probability for $Z_P=92$ is divided by Z_P^2. The unit of time is $\hbar/mc^2=1.288\cdot10^{-21}$ s

the magnetic quantum numbers $\pm 1/2$ of the initial and final states. We get two probabilities depending on the difference m of these magnetic quantum numbers:

$$P_{m=0}=|a_{1/2,1/2}|^2+|a_{-1/2,-1/2}|^2=2|a_{1/2,1/2}|^2, \qquad (13a)$$

$$P_{m=1}=|a_{1/2,-1/2}|^2+|a_{-1/2,1/2}|^2=2|a_{1/2,-1/2}|^2. \qquad (13b)$$

The solid curves in Fig. 2 show the results of the first order perturbation theory which are obtained by time-integration of the corresponding coupling matrix elements from $-\infty$ to t. The curves demonstrate that strong oscillations arise from the $m=0$ component which has a very symmetric structure with respect to $t=0$ as a function of time. The dotted curve shows the result of the coupled channel code for $Z_P=1$. Obviously, the agreement between both calculations is very good. The dashed curve is the coupled channel result for $Z_P=92$ which has been divided by Z_P^2. Since the first order perturbation theory scales with Z_P^2, the solid lines are also valid for $Z_P=92$. We find the result that the capture probability for this specific wave packet is increased by two orders of magnitude.

In Fig. 3 we plotted the total K-shell capture probability divided by Z_P^2 as a function of time for $Z_P=1$ and $Z_P=92$ in order to demonstrate the effect of couplings of higher order. The difference by two orders of magnitude is obvious.

In order to study the probability for pair production with K-shell capture in more detail we have carried out calculations starting the integration in time with the $1s_{1/2}$ state and employing time reversal symmetry. In these calculations the enhancement effects were analyzed by switching on or off different types of matrix elements. The minimal set of matrix elements we used consists of all couplings between the initial $1s_{1/2}$ state and the states of the positive and negative continuum and preserves unitarity. Already this coupling scheme yields an enhanced occupation of the negative continuum by more than one order of magnitude compared with the result of the perturbation theory as shown in Fig. 4. Also this

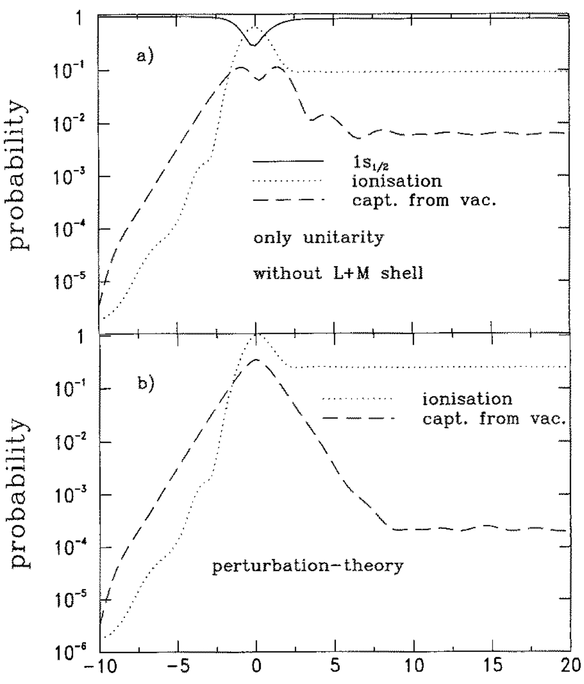

Fig. 4. a Time evolution of the initial $1s_{1/2}$ state in a $U^{92+}+U^{92+}$ collision at $E_{lab}=10$ GeV/nucleon in a minimal coupling scheme, describing ionisation and pair production with K-shell capture and preserving unitarity. No other bound states or continuum-continuum couplings are included. The solid curve gives the probability of the initial $1s_{1/2}$ state, the dotted and dashed curves the probabilities for ionisation and pair production with K-shell capture. **b** Probabilities for ionisation and pair production with K-shell capture as a function of time calculated in first order perturbation theory. The unit of time is $\hbar/mc^2=1.288\cdot10^{-21}$ s

figure shows that the probabilities for ionisation and pair production are strongly peaked around the point of closest approach of the colliding ions and that both probabilities have comparable values there. As a consequence the requirement of unitarity becomes most important, even if the final probabilities are small. Due to the structure of the probabilities around $t=0$ also the direct interaction between both continua becomes important. Switching on all the further types of couplings, we find an enhancement of the pair production probability with K-shell capture of two orders of magnitude compared with the probability obtained by perturbation theory. This effect demonstrates that the enhancement effect arises to its full amount only in a complete coupling scheme with continuum-continuum couplings where all higher order effects are included.

As a further possible explanation for the enhancement one might think of intermediate states having strong couplings both to the initial and final states, that lead to enhanced population of the negative continuum at larger times $t>0$. However, we could not find clear hints in our calculations for this argument.

4. Conclusions

In this paper we have nonperturbatively calculated probabilities for pair creation in relativistic collisions of U^{92+} on U^{92+} with a basis set limited in angular momenta up to $p_{3/2}$. For this set we have shown that the coupled equations yield much larger probabilities than the first order perturbation theory. The failure of the first order perturbation theory can be understood by the solid curve in Fig. 3 which has to be multiplied by the factor 92^2 for the $U^{92+}+U^{92+}$ collision in order to obtain the unscaled probability as function of time. Whereas the perturbative probability is small for $t\rightarrow\infty$, it shows a steep rise at the point of closest approach of the U^{92+} ions ($t=0$), where the probability has a value of the order of 0.5. These large probabilities have as consequence, that the first order perturbation theory becomes invalid for large projectile charges, since in the perturbative calculation unitarity is violated, even if the final probabilities are quite small.

The probabilities calculated in this paper clearly demonstrate the effects of the higher-order couplings. But they do not represent an answer to values for pair creation comparable with experiment, since we were strongly limited in angular momentum. Therefore, future work has to concentrate on calculations with a larger range of angular momenta than we used up to now. Then also a reliable nonperturbative calculation of cross sections can be made.

The results of this paper might be of considerable practical importance for the construction and management of colliding beam accelerators. Larger cross sections for lepton pair creation have to be expected than previously assumed. Because of the present computational difficulties we think that this field is progressing further when the proposed experiment [20] at CERN will deliver first measured cross sections of electron-positron pair creation with and without capture.

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