# Direct reactions in relativistic atomic collisions and the influence of Coulomb boundary conditions

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It is shown that in a Born treatment of excitation, ionization, and pair production in relativistic atomic collisions, cross-section calculations are not affected by the presence or absence of explicitly imposed Coulomb boundary conditions. On the other hand, in relativistic single- or two-center coupled-channel calculations, the results are strongly affected. For $U^{92+}+U^{91+}$ collisions at 1 GeV/u, it is illustrated that in all calculations unperturbed atomic basis sets lead to long-range couplings along the trajectory while for basis states satisfying boundary conditions the couplings among states are localized around the distance of closest approach. The necessity of imposing Coulomb boundary conditions for relativistic direct reactions is emphasized.

## I. INTRODUCTION

For sufficiently high relativistic velocities, direct atomic reactions like excitation, ionization, and pair production are reasonably well described by the Born approximation. However, in cases where the collision velocity is comparable to the speed of the active electron, relativistic coupled-channel calculations constitute an appropriate method for simultaneously deriving cross sections both for direct reactions and for charge transfer.

In previous publications,[1-3] we have worked out and applied this approach for relativistic projectile and electron velocities. In Ref. 2 we gave a detailed description of the method that uses a two-center atomic expansion in terms of exact hydrogenic Dirac eigenstates. As an illustration, we have considered the collision of $U^{92+}$ projectiles with $U^{91+}$ target atoms at 500 MeV/u. In Ref. 3 we have augmented the basis sets by target and projectile pseudostates, thus simulating part of the continuum that is needed for a description of ionization.

The calculations in Refs. 1–3 are patterned in analogy to nonrelativistic coupled-channel calculations,[4] which have become a powerful tool for predicting atomic cross sections. This means that the basis states at both centers were taken to be *unperturbed* atomic eigenstates or pseudostates. In reality, even at asymptotically large projectile-target separations, the presence of one collision partner results in a distortion of the atomic states at the other collision partner. As has been discussed in Ref. 5 for nonrelativistic collisions, this effect is taken into account by a phase factor multiplying the atomic eigenfunctions. Since these phase factors depend on the internuclear separation, i.e., only on the time $t$ in an impact-parameter description, and *not* on the electronic coordinate, they can be simply absorbed in the time-dependent expansion coefficients. As a result, the asymptotic distortions of the basis wave functions by a remote charge, or in other words, the Coulomb boundary conditions, can be disregarded in nonrelativistic coupled-channel calculations.[5] The question arises whether this is also true for relativistic collisions.

There is a clue that this might not always be the case. In our relativistic coupled-channel calculations,[2] we discovered the existence of anomalous long-range couplings in excitation processes that are absent in nonrelativistic collisions. While in the latter case the coupling between states has the characteristic dipole behavior with an $R^{-2}$ dependence on the internuclear separation $R$, the leading coupling term for relativistic collisions decreases as $R^{-1}$, suggesting the influence of a monopole Coulomb contribution.

It is the purpose of this paper to investigate the role played by the Coulomb distortion in calculations for relativistic direct reactions. In Sec. II, we first establish the phase factor describing the asymptotic Coulomb distortion; subsequently, in Sec. III, we study its effect on Born calculations for direct reactions; and in Sec. IV, we discuss the effect of boundary conditions on single-center and two-center coupled-channel calculations. In Sec. V, the numerical results are presented and discussed, and in Sec. VI some conclusions are drawn. Atomic units are used unless explicitly stated otherwise.

## II. COULOMB BOUNDARY CONDITIONS

The target nucleus is considered as a classical point charge $Z_T$ fixed at the origin of the laboratory system, while the point charge $Z_P$ representing the projectile moves with a relativistic velocity $\mathbf{v}$ along a classical rectilinear trajectory $\mathbf{R}(t)=\mathbf{b}+\mathbf{v}t$, where $b$ is the impact parameter. We seek to construct the solution $\Psi(\mathbf{r}_T,t)$ of the exact time-dependent Dirac equation

$$i\frac{\partial}{\partial t}\Psi(\mathbf{r}_T,t)=\left[-ic\boldsymbol{\alpha}\cdot\boldsymbol{\nabla}_T-\frac{Z_T}{r_T}-S^2\frac{Z_P}{r_P'}+\gamma_4c^2\right]\Psi(\mathbf{r}_T,t), \quad (1)$$

 

where $(\mathbf{r}_T,t)$ and $(\mathbf{r}'_P,t')$ are the electronic space-time coordinates with respect to the target nucleus in the target frame and with respect to the projectile nucleus in the projectile frame. The Lorentz transformation into the projectile frame of an eigenfunction $\psi$ defined in the target frame is mediated by the spinor transformation[2,6]

$$\psi'(\mathbf{r}'_P,t')=S\psi(\mathbf{r}_T,t) , \tag{2}$$

with

$$S=\left[\frac{\gamma+1}{2}\right]^{1/2}(1-\delta\alpha_z)=S^{\dagger} , \tag{3}$$

where $\gamma=(1-\beta^2)^{-1/2}$, $\beta=v/c$, $\delta=[(\gamma-1)/(\gamma+1)]^{1/2}$, and $\alpha_x$, $\alpha_y$, $\alpha_z$, $\gamma_4$ are the $4\times4$ Dirac matrices.[6]

For asymptotically large internuclear separations, we may introduce the replacements

$$r_T\rightarrow R=(b^2+v^2t^2)^{1/2} \tag{4}$$

and

$$r'_P\rightarrow R'=(b^2+v^2t'^2)^{1/2} . \tag{5}$$

If in the asymptotic limit, $\Phi_T^{\infty}$ and $\Phi_P^{\infty}$ are the asymptotic wave functions for an electron bound to the target and to the projectile nucleus, respectively, the asymptotic Dirac equations to be satisfied are

$$i\frac{\partial}{\partial t}\Phi_T^{\infty}=\left[-ic\boldsymbol{\alpha}\cdot\boldsymbol{\nabla}_T-\frac{Z_T}{r_T}-S^2\frac{Z_p}{R'}+\gamma_4c^2\right]\Phi_T^{\infty} \tag{6}$$

and

$$i\frac{\partial}{\partial t}\Phi_P^{\infty}=\left[-ic\boldsymbol{\alpha}\cdot\boldsymbol{\nabla}_P-\frac{Z_T}{R}-S^2\frac{Z_P}{r'_P}+\gamma_4c^2\right]\Phi_P^{\infty} . \tag{7}$$

Introducing the Sommerfeld parameters $\nu_T=Z_T/v$ and $\nu_P=Z_P/v$, the solutions of Eqs. (6) and (7) can be written as

$$\Phi_T^{\infty}(\mathbf{r}_T,t)=e^{-i\nu_P\ln(R'-vt')}\psi_T(\mathbf{r}_T,t) \tag{8}$$

and

$$\Phi_P^{\infty}(\mathbf{r}_T,t)=e^{i\nu_T\ln(R-vt)}S^{-1}\psi'_P(\mathbf{r}'_P,t') . \tag{9}$$

Here $\psi_T$ is an unperturbed target wave function in the target frame, while $\psi'_P$ is an unperturbed projectile wave function in the projectile frame. In contrast to $\psi_T$ and $\psi'_P$, the functions $\Phi_T^{\infty}$ and $\Phi_P^{\infty}$ are said to satisfy Coulomb boundary conditions.

## III. BORN APPROXIMATION FOR EXCITATION, IONIZATION, AND PAIR PRODUCTION

Let us consider the excitation or ionization of a one-electron target atom by a relativistic projectile. In first-order perturbation theory, the amplitude for transitions between "boundary-corrected" states (8) is calculated by taking the appropriate matrix element of the transition operator $H-i\partial/\partial t$, where $H$ is the quantity in the large parentheses at the right-hand side of Eq. (1). The inclusion of the phase factors in Eq. (8) leads to the replacement

$$\frac{1}{r'_P}\rightarrow\frac{1}{r'_P}-\frac{1}{R'} . \tag{10}$$

As a result, we have a short-range perturbation and in the laboratory system obtain the transition amplitude

$$A_{fi}=i\int_{-\infty}^{\infty}dt\int d\mathbf{r}_T\psi_f^{\dagger}(\mathbf{r}_T,t)S^2\left[\frac{Z_P}{r'_P}-\frac{Z_P}{R'}\right]\psi_i(\mathbf{r}_T,t) , \tag{11}$$

where we have used the fact that the phase factors in Eq. (8) are state-independent and hence cancel one another for arbitrary initial and final target states. The term $Z_P/R'$ or any other potential depending on $R'$ alone would appear to contribute to the integral, since according to Eq. (5) and the relation $t'=\gamma(t-vz_T/c^2)$, the separation $R'$ depends on $\mathbf{r}_T$ and $t$. On the other hand, we may as well calculate $A_{fi}$ in the projectile system by replacing the $(\mathbf{r}_T,t)$ integration with an $(\mathbf{r}'_P,t')$ integration and by inserting the transformation (2) which is valid, provided the $\psi_{i,f}$ are *exact* eigenstates. Then the term $Z_P/R'$ does not depend on the space coordinate $\mathbf{r}'_P$ and hence gives a vanishing matrix element between orthogonal target states.

We therefore conclude that in first-order perturbation theory for target excitation or ionization, one obtains a result that is identical to (11) and reads

$$A_{fi}=i\int_{-\infty}^{\infty}dt\int d\mathbf{r}_T\psi_f^{\dagger}(\mathbf{r}_T,t)S^2\frac{Z_P}{r'_P}\psi_i(\mathbf{r}_T,t) . \tag{12}$$

This is just the expression usually written down for unperturbed target states, ignoring the Coulomb boundary conditions.[7,8] A corresponding expression is valid for pair production when the electron and positron states are target eigenstates and their orthogonality is hence ensured. For charge transfer, the phase factors as well as the additional interaction have to be included[9,7] because initial and final states are not orthogonal.

## IV. COUPLED-CHANNEL CALCULATIONS

We have shown that the inclusion of Coulomb boundary conditions in a first-order Born calculation does not change the transition amplitude (12) originally derived for unperturbed initial and final states. This observation relies on the fact that (a) the complete space-time integration occurring in (11) is Lorentz invariant and (b) the functions $\psi_{i,f}$ are exact eigenfunctions of the atomic Hamiltonian. These arguments are no longer valid for an expansion of the wave function in terms of a finite set of asymptotically distorted basis states, since it neither represents an eigenstate of the atomic Hamiltonian nor of the complete Hamiltonian.

We start with the discussion of a single-center expansion

$$\Psi(\mathbf{r}_T,t)=\sum_k a_k(t)e^{-i\nu_P\ln(R'-vt')}\psi_k(\mathbf{r}_T,t) \tag{13}$$

in terms of asymptotically Coulomb-distorted target states. The representation (13) is distinguished from the commonly adopted one[7,10] by the presence of the phase

factors $\exp[-i\nu_P \ln(R'-vt')]$. Since for *nonrelativistic* collisions $t' \to t$ and $R' \to R(t)$, the phase factors depend solely upon time, they can be absorbed[5] into the expansion coefficients $a_k(t)$, as has been pointed out in the Introduction. This is not so for *relativistic* collisions, owing to the Lorentz transformation of time as $t'=\gamma(t-vz_T/c^2)$. When inserting the expansion (13) into Eq. (1) and projecting upon the basis states of the form (8), we obtain the usual[7,10] coupled time-dependent equations for the expansion coefficients with the replacement (10). Similarly, as for the Born amplitude (11), the state-independent phase factors drop out. However, in contrast to the first-order case, the term $Z_P/R'$ cannot be removed in the laboratory system by simply transforming into the projectile system and by showing that they vanish there. The reason why such a procedure is not possible lies in the fact that time and space coordinates are not treated on an equal footing. The additional terms $Z_P/R'$ in the interaction have an important effect on the transition probabilities, as is confirmed numerically in Sec. V. Existing coupled-channel calculations using unperturbed basis states[10] therefore ought to be reconsidered.

While a description of the process in the target system represents the natural choice, which offers an unambiguous interpretation of the amplitudes, it is also possible, in principle, to describe target excitation and ionization in the *projectile frame*. In that case, the additional term $Z_P/R'$ has vanishing off-diagonal matrix elements and the phases drop out. Hence Coulomb boundary conditions are always satisfied whether or not they are explicitly included. This is paid for by the flaw that during the interaction time, the truncated expansion in terms of target-centered states cannot be transformed back to the laboratory system and hence cannot be interpreted in the coordinate frame in which the measurements are made. Calculations with sets of equivalent basis states in target and projectile frames are not expected to, and in fact do not, numerically lead to identical transition probabilities for target excitation. In order to ensure an unambiguous interpretation at all times and in order to avoid Lorentz-contracted basis states it is natural to choose the target frame with boundary-corrected basis sets (13) for representing the process.

In order to calculate charge transfer and to include its effect on excitation and ionization, it is necessary to attach basis states to both target and projectile nuclei. In our previous calculations,[1-3] we used unperturbed target and projectile wave functions. This is in accord with the usual procedure followed in nonrelativistic collisions.[4] We propose here the use of "boundary-corrected" wave functions of the type $\Phi_T^\infty$ and $\Phi_P^\infty$ defined in Eqs. (8) and (9) as basis states. Generalizing the expansion (13) and denoting target and projectile states by the labels $k$ and $k'$, respectively, we write

$$\Psi(\mathbf{r}_T,t)=\sum_k a_k(t)e^{-i\nu_P\ln(R'-vt')}\psi_k(\mathbf{r}_T,t) + \sum_{k'} a_{k'}(t)e^{i\nu_T\ln(R-vt)}S^{-1}\psi_{k'}(\mathbf{r}'_P,t') \,. \tag{14}$$

When we insert the boundary-corrected expansion (14) into Eq. (1) and project upon the basis states, we get the usual coupled time-dependent equations,[2] except for the replacement of the unperturbed basis states by the phase-distorted basis states appearing in Eq. (14), by the replacement (10), and by the substitution

$$\frac{1}{r_T} \to \frac{1}{r_T} - \frac{1}{R} \,. \tag{15}$$

We are now in a position to return to the long-range couplings acting in excitation processes induced by relativistic projectiles. These couplings have first been seen in two-center coupled-channel calculations,[1,2] but also would have appeared in single-center calculations[10] had the authors looked in detail at the time development. Let us expand the projectile-electron interaction

$$S^2\frac{1}{r'_P}=\gamma(1-\beta\alpha_z)\left[\frac{1}{R'_0}+\frac{bx_T+\gamma^2vtz_T}{(R'_0)^3}+\cdots\right], \tag{16}$$

in powers of the inverse nucleus-nucleus separation $R'_0=(b^2+\gamma^2v^2t^2)^{1/2}$ measured in the projectile frame. Here the leading off-diagonal matrix elements responsible for the long-range couplings arise from the term $-\gamma\beta\alpha_z/R'_0$. It is just this term that drops out when the replacement (10) is introduced and similarly expanded in powers of $1/R'_0$. Hence, if proper Coulomb boundary conditions are imposed upon the basis states, the long-range couplings are expected to disappear. This is borne out by numerical calculations discussed in Sec. V.

## V. RESULTS AND DISCUSSION

The range of the interaction within the process or, in other words, the effect of the boundary conditions on the theoretical description is best illustrated in the time evolution of the occupation probabilities of the various target shells for a given impact parameter $b$.

Let us first take a look at the Born approximation. The time-dependent occupation probabilities can be defined by performing the time integral in Eqs. (11) and (12) from $-\infty$ to $t$ and by subsequently taking the absolute square of the resulting amplitude. The final transition probability then is reached for $t \to \infty$.

Figure 1 shows the numerically calculated time evolution of the occupation probabilities of various excited target states populated from an initial $1s_{1/2}$ state in a $U^{92+}+U^{91+}$ collision at 1 GeV/u. The probabilities are calculated in the Born approximation at $b=0.01$ a.u., which is approximately equal to the $K$-shell radius $a_K$ of uranium and roughly corresponds to the impact-parameter region with maximum contribution to the cross section. The upper part of Fig. 1 is calculated from the space integral of Eq. (12) while the lower part is obtained from Eq. (11), which includes an additional $Z_P/R'$ term arising from boundary-corrected target states. As has been shown in Sec. III, the final transition probabilities are indeed the same in both cases, although the time development at intermediate stages is quite different. It is clearly seen that with unperturbed target states, the projectile acts over a longer part of the trajectory, while for

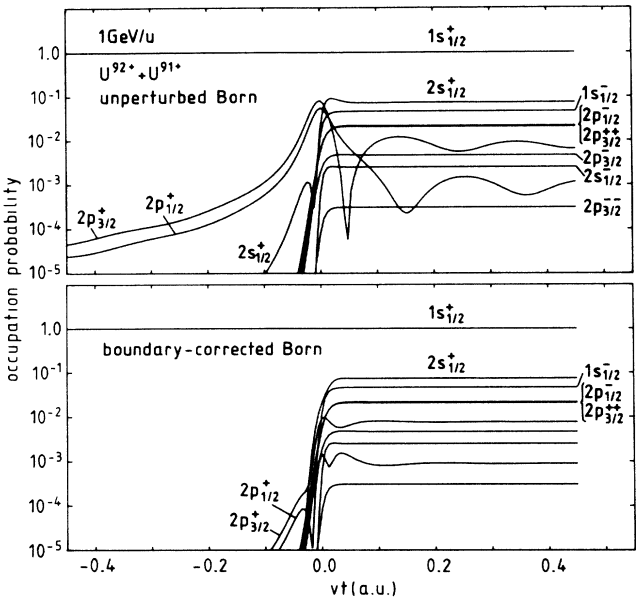


FIG. 1. Time evolution of the occupation probabilities of target states in $U^{92+}+U^{91+}$ ($1s_{1/2}$) collisions at 1 GeV/u laboratory energy. Calculations are performed in the Born approximation at an impact parameter $b=0.01$ a.u. The upper set of curves represents results obtained from unperturbed initial and final states, Eq. (12), while the lower set of curves corresponds to boundary-corrected states, Eq. (11). The absicssa plotted is the projection of the projectile-target separation on the beam direction. The projection of angular momentum is indicated by $+$, $-$, $++$, and $--$ for $m_j=+\frac{1}{2}$, $-\frac{1}{2}$, $+\frac{3}{2}$, and $-\frac{3}{2}$, respectively.

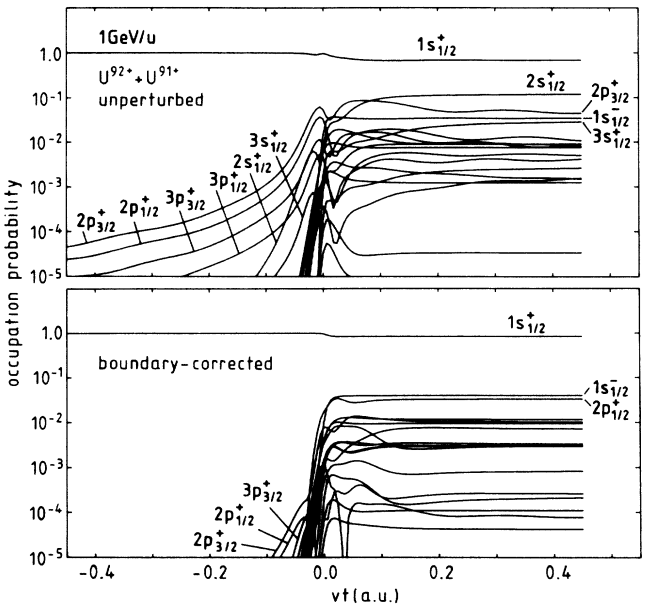


FIG. 2. Time evolution of the occupation probabilities of target states in $U^{92+}+U^{91+}$ ($1s_{1/2}$) collisions at 1 GeV/u laboratory energy. Calculations are performed with 18 hydrogenic basis states at both the target and projectile and for an impact parameter $b=0.01$ a.u. The upper set of curves represents results obtained from unperturbed basis states, while the lower set of curves corresponds to boundary-corrected basis states, Eq. (14). For the notation, see the caption of Fig. 1.

boundary-corrected target states the final occupation probability is determined within a short time span before and after the distance of closest approach is reached at $vt=0$.

While in a Born approximation there is only a unidirectional coupling between the initial and the final states, a more detailed treatment requires consideration of multiple couplings among all basis states. Following the procedure outlined in Ref. 2, we have treated the time-dependent two-center Dirac equations for the wave function (14) by solving the coupled equations for the occupation amplitudes $a_k(t)$ and $a_{k'}(t)$. The only approximation involved is the truncation of the basis set in Eq. (14). The matrix elements of the interactions (10) and (15) as well as the overlap matrix elements are evaluated by direct three-dimensional numerical integration. In contrast to earlier calculations[1-3] with unperturbed basis states, it is not possible now to take advantage of a symmetry[2] that relates matrix elements for the ingoing part to those of the outgoing part of the collision. This fact, together with the existence of the additional interaction term in Eqs. (10) and (15), leads to an increase in computing time.

In Fig. 2 we compare the time evolution during the collision of the occupation probabilities for the target shells (excitation) assuming again an impact parameter of 0.01 a.u. Similarly, as in Fig. 1, unperturbed basis states have been used in the upper part of the figure, while the lower part is obtained for boundary-corrected basis states (14). Here, the long-range couplings, that are visible for unperturbed basis states have disappeared.[11] The $2p_{3/2}(\frac{1}{2})$, $2p_{1/2}(\frac{1}{2})$, $3p_{3/2}(\frac{1}{2})$, and $3p_{1/2}(\frac{1}{2})$ (where the quantity in parentheses denotes the projection $m_j$ of angular momentum) states that are excited for unperturbed basis states already long before the distance of closest approach is reached, begin to be populated for boundary-corrected basis states only at about $vt=-10a_K$. Similarly, after the collision, the boundary-corrected basis states attain their asymptotic occupation probabilities at much smaller values of $vt$ than the unperturbed basis states. Moreover, the asymptotic values themselves are changed. This is different from the Born approximation discussed above. We verified that single-center calculations lead to exactly the same behavior.

The time evolution of the occupation probabilities of the *projectile states* (corresponding to charge transfer) is determined by the overlap of the atomic wave functions in target and projectile and hence is not qualitatively affected by the replacements (10) and (15). For the change in the cross sections see Table I. An example of this time evolution is given in Ref. 2 and is not repeated here.

While the two types of basis sets lead to different total excitation cross sections, one may ask whether the long-range or short-range couplings are reflected in the differential cross sections. However, this is not so, because for sufficiently large impact parameters $b$ the $z_T$ dependence of $t'$ in $R'=(b^2+v^2t'^2)^{1/2}\approx(b^2+\gamma^2v^2t^2)^{1/2}$ can be neglected, so that the term $1/R'$ in Eq. (10) does not contribute. As a result, the numerically calculated

TABLE I. Excitation and transfer cross sections (in barns) between target $1s_{1/2}(\frac{1}{2})$ and projectile $nl_j(m_j)$ states in $U^{92+}+U^{91+}$ collisions at 1.0 GeV/u laboratory energy. The 36-state close-coupling calculations with unperturbed or boundary-corrected basis states include target and projectile $K$, $L$, and $M$ shells. The numbers in square brackets give the power of 10 multiplying the preceding number.

| | Excitation | | | Transfer | |
|---|---|---|---|---|---|
| Final state | Unperturbed | Corrected | Born approximation | Unperturbed | Corrected |
| $1s_{1/2}(\frac{1}{2})$ | | | | 6.28[2] | 7.46[2] |
| $1s_{1/2}(-\frac{1}{2})$ | | | | 4.61[1] | 5.02[1] |
| $2s_{1/2}(\frac{1}{2})$ | 4.95[3] | 1.66[3] | 2.13[3] | 2.22[2] | 2.45[2] |
| $2s_{1/2}(-\frac{1}{2})$ | 3.94[2] | 1.14[2] | 4.60[1] | 1.21[1] | 1.28[1] |
| $2p_{1/2}(\frac{1}{2})$ | 3.12[3] | 6.48[2] | 4.23[2] | 8.80[1] | 7.26[1] |
| $2p_{1/2}(-\frac{1}{2})$ | 5.83[3] | 4.71[3] | 5.64[3] | 2.30[1] | 2.31[1] |
| $2p_{3/2}(\frac{3}{2})$ | 5.51[3] | 4.60[3] | 6.11[3] | 6.60[0] | 6.63[0] |
| $2p_{3/2}(\frac{1}{2})$ | 7.54[3] | 1.48[3] | 9.02[3] | 3.44[1] | 3.24[1] |
| $2p_{3/2}(-\frac{1}{2})$ | 1.16[3] | 1.01[3] | 1.36[3] | 1.09[1] | 4.75[0] |
| $2p_{3/2}(-\frac{3}{2})$ | 1.06[2] | 9.94[1] | 1.17[2] | 9.15[−1] | 4.92[−1] |

values $P(b)$ have almost the same impact-parameter dependence[2] in both cases.

In Table I we show excitation and transfer cross sections for $U^{92+}+U^{91+}$ collisions at 1 GeV/u, resulting from 36-state two-center coupled-channel calculations. Atomic states up to the $3p_{3/2}$ shell at both centers have been included. In all cases, the initial state is assumed to be $1s_{1/2}(\frac{1}{2})$. We see that for excitation, the inclusion of boundary corrections decreases the cross section by a factor of about 2 while for charge exchange the corrections are of the order of 10% or less in most cases. The Born cross section, which for excitation is also shown, does not have a systematic correlation to the coupled-channel cross sections with or without boundary conditions. In fact, at 1 GeV/u, the projectile energy may still be too low for the Born approximation to be applicable.

## VI. CONCLUSIONS

We show that in a Born treatment of excitation, ionization, and pair production in relativistic atomic collisions, it is irrelevant whether or not one explicitly imposes proper Coulomb boundary conditions, since they are satisfied in either case. While the transient time development of the occupation probabilities is different in both cases, the final populations and hence the transition probabilities are the same.

Similarly, for relativistic single-center and two-center coupled-channel calculations with *unperturbed basis states,* the coupling among states is long range and acts long before and long after the encounter takes place, while for *basis states satisfying Coulomb boundary conditions,* the couplings are localized around the distance of closest approach. However, in contrast to the Born approximation, which couples only two states in a unidirectional way, the multiple couplings occurring in a coupled-channel calculation eventually lead to transition probabilities and cross sections that are distinctly different for unperturbed and boundary-corrected basis states. This shows that it is mandatory for a description of direct reactions to take care of the long-range Coulomb interaction from the beginning. It is to be expected that this also improves the convergence behavior with respect to the number of basis states.

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