Relativistic coupled-channel calculations including pseudostates

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The previously developed relativistic, two-center, coupled-channel treatment of atomic collisions between high-Z ions has been extended to include pseudostates. By augmenting the atomic basis sets by pseudostates, an approximate representation of the continuum is obtained as well as an improved description of quasimolecular states near the united-atom limit. The problems arising from approximate basis states, specifically in relativistic collisions, are discussed. Numerical calculations for $U^{92+}+U^{91+}$ at 500 MeV/u are performed with basis sets of up to 36 real and 16 continuum pseudostates. While the presently attainable basis sets are presumably still too small, one can get, nevertheless, reasonable estimates of the cross sections for ionization and K-vacancy production.

I. INTRODUCTION

In two previous publications[1,2] we have developed the theory of fully relativistic coupled-channel calculations for atomic collisions between high-Z projectiles and high-Z targets. Using a two-center atomic expansion in terms of exact hydrogenic Dirac eigenstates we have been able to give detailed predictions for single-electron excitation and charge-transfer cross sections between specific atomic states. As an example, we have considered the $U^{92+}+U^{91+}$ collision at 500 MeV/u.

The method is described in detail in Ref. 2 and shall be referred to as I. The essential ingredients are the following. The target nucleus and the projectile nucleus are considered as classical point charges, the target being fixed at the origin of the laboratory frame and the projectile moving with a relativistic velocity $\mathbf{v}$ along a classical rectilinear trajectory $\mathbf{R}(t)=\mathbf{b}+\mathbf{v}t$. The orbital motion of a single electron initially bound to the bare-target nucleus is described by a two-center time-dependent Dirac equation. The electromagnetic field generated by the moving projectile gives rise to excitation, ionization, or charge transfer. In I we have accounted for excitation and charge transfer by expanding the time-dependent electronic wave function throughout the collision in terms of exact bound eigenstates of the unperturbed target and projectile Hamiltonians. Solving the time-dependent Dirac equation within a truncated set of basis states is equivalent to numerically solving the coupled equations for the time-dependent expansion coefficients subject to appropriate initial conditions. For example, in our most detailed calculations[2] for $U^{92+}+U^{91+}$, we have coupled altogether 36 states, namely, $1s_{1/2}$, $2s_{1/2}$, $2p_{1/2}$, $2p_{3/2}$, $3s_{1/2}$, $3p_{1/2}$, and $3p_{3/2}$ states of target and projectile. By comparison with a preceding 20-state calculation[1] we found[2] that the expansion had almost converged within the space of bound basis states.

However, in order to describe ionization it is mandatory to include target and projectile continuum states. Ionization cross sections in relativistic collisions have mostly been calculated in first-order perturbation theory,[3–5] and only recently Becker *et al.*[6] used a finite-difference algorithm as a nonperturbative method to compute inner-shell excitation and ionization for $U^{92+}+U^{91+}$ collision at 1 GeV/u. Their exploratory computations were, however, confined to the impact parameter $b=0$ (which carries zero weight for the cross section). To supplement those results, Becker has also performed coupled-channel calculations[7] using a one-center atomic expansion in terms of target bound and discretized continuum states. In this method, the projectile merely acts as a moving source for an electromagnetic field. Molecular two-center effects during the collision and the possibility of charge transfer into bound or continuum states of the projectile are disregarded. Similarly, some relativistic single-center coupled-channel calculations have been performed by Mehler[8] who computed the impact-parameter dependence of ionization rates in $p+$Pb collisions.

The aim of the current work is to remove two of the interrelated difficulties still inherent in the two-center atomic-orbital (AO) expansion of I. One of them is the absence of final or intermediate continuum states mentioned above, and the other is the approximate representation of molecular states at small internuclear separations by a superposition of AO. While the first deficiency precludes the description of ionization, the second renders calculation unreliable whenever close collisions (i.e., small impact parameters) are important.

Of course, it would be desirable to include exact relativistic continuum states in the expansion. However, the overlap at infinite separations gives rise to serious problems, and, numerically, a discretization on a sufficiently dense energy grid entails presently unsurmountable problems. Nevertheless, as is known from nonrelativistic col-

lisions,[9] the flaws mentioned above may be largely removed by augmenting the AO expansion by appropriate "pseudostates" attached to target and projectile. Pseudostates are arbitrary basis functions chosen so as to improve the flexibility of the basis set in approximating the true two-center wave function throughout the collision. Not being eigenstates of the unperturbed atomic Hamiltonian but rather simulating some kind of wave packets, pseudostates, if properly chosen, have an overlap (a) with bound (highly excited) AO not explicitly included in the basis set, (b) with atomic or molecular continuum states, (c) with united-atom wave functions needed to improve the representation of molecular orbitals. Clearly, as in any basis optimization it requires many trial calculations and a great deal of experience to select a suitable set of pseudostates within the limits given by the available computer time. Through the years, this method has been forged into a powerful tool for describing excitation, ionization, and charge transfer in nonrelativistic collision.[9]

In relativistic collisions, two additional difficulties arise. (i) Certain pseudostates may have appreciable overlap with the negative-energy continuum. This is clearly undesirable as long as we wish to describe purely electronic processes. (ii) Approximate atomic eigenstates obtained by diagonalization within a finite set of exact eigenstates and pseudostates in the atomic rest frame lose their orthogonality property if viewed from a moving Lorentz frame. Both of these problems are inherent in the method and cannot entirely be removed. Nevertheless, we show that the introduction of pseudostates is a useful concept and in any case improves the results previously obtained with basis sets composed of exact eigenstates only.

We also show that cross sections calculated with a fixed truncated set of basis states depend on the Lorentz frame in which they are derived, but that only the target frame[1,2] represents a reasonable choice for computing excitation and transfer cross sections.

In Sec. II we discuss the particular difficulties associated with atomic pseudostates in relativistic close-coupling calculations. In Sec. III we present calculated results for the model system $U^{92+}+U^{91+}$ at 500 MeV/u. Finally, in Sec. IV we discuss the results and draw some conclusions. Atomic units are used unless explicitly stated otherwise.

II. TWO-CENTER EXPANSIONS FOR RELATIVISTIC COLLISIONS

The use of approximate wave functions such as pseudostates to describe relativistic collisions introduces two problems that are absent in nonrelativistic ion-atom encounters. One of them is the problem of negative-energy states arising from the Dirac theory for the relativistic electron motion, the other is the loss of the orthogonality property of approximate eigenfunctions when they are Lorentz transformed from the target frame in which they are constructed to a relativistically moving projectile frame or vice versa. To our knowledge, the latter problem has not been discussed before in the context of atomic collisions.

A. The problem of negative-energy components in pseudostates

As is well known,[10] the Dirac equation, while formally appearing as a single-particle equation, is fully interpretable only if considered as an equation for a field operator, with the consequence that many electron-many positron systems are represented at the same time. For the applications in atomic and molecular physics, however, we wish to confine ourselves to a system with a *fixed number of electrons.* Therefore, we want to avoid "negative-energy solutions" of the Dirac equation, that is, solutions with eigenenergies $E<-2mc^2$ (defining $E=0$ for a free electron at rest). While exact solution of the Dirac equation may immediately be classified by their eigenenergies and hence we may always choose the desired set of states, the situation is different for variational solutions. In this case, negative-energy solutions may always occur since the Dirac Hamiltonian, owing to its field-theoretical character, is not bounded from below. This effect, usually encountered when treating a many-electron system, is denoted as "variational collapse."[11] Closely related to this is the "Brown-Ravenhall disease"[12] which leads to negative-energy states arising from the electron-electron interaction. In spite of these problems, techniques have been developed over the years[11] to avoid negative-energy states and to perform reliable relativistic many-electron calculations for atoms and molecules. In fact, there seem to be many different recipes available leading to the desired results. The most important feature common to the majority of them appears to be that the ratio between upper and lower Dirac components has to be fixed to a reasonable value and is not left open to variation. The simplest illustration[13] is provided by a single-electron variational function of hydrogenic form. As long as the ratio between upper and lower components is subject to variation the energy surface is represented by a saddle providing no lower bound. If, however, this ratio is fixed to the hydrogenic value, the remaining variation of the exponent is constrained to the ridge along the saddle and thus leads to a stable variational minimum.

It is thus a reasonable procedure to augment the set of exact Dirac eigenstates as basis functions in a linear variational procedure by hydrogenic wave functions generated by effective charges Z^*. Specifically, for a collision problem, the time-dependent solution of the Dirac equation is expanded as[1,2]

$$\psi(t)=\sum_k a_k(t)\psi_k(\mathbf{r}_T,t)+\sum_{k'} a_{k'}(t)S^{-1}\psi_{k'}(\mathbf{r}'_P,t') \ , \qquad (1)$$

where ψ_k are basis functions attached to the target nucleus, while $\psi_{k'}$ are basis functions attached to the moving projectile and subsequently transformed to the target system with the aid of the spinor transformation S^{-1}, see Eqs. (2) and (3). Separately considering target and projectile states, we introduce the pseudostates as follows. (a) We first choose a subset of exact hydrogenic Dirac eigenstates corresponding to the actual charge Z of the target or projectile nucleus. These states are mutually orthogonal. (b) Next, we choose certain effective charges, both $Z^*<Z$ and $Z^*>Z$, and construct corresponding pseudo-

states defined as eigenstates belonging to the charge Z^* and characterized by a given nodal and angular momentum structure. (c) Subsequently, the atomic Dirac Hamiltonian is diagonalized within the basis set composed of the original exact eigenstates and the additional pseudostates. This leaves the exact eigenenergies E and corresponding eigenstates unchanged and leads to new eigenenergies E^* and associated eigenvectors. The resulting linear combination of states generated by different values of Z^* therefore represents a wave function that is Coulomb distorted by the *actual* nuclear charge Z. (d) If any unphysical eigenenergy $E^* < E_{\max}$ below the highest exact eigenenergy of the basis set appears the set is discarded. This rarely occurs, and if it does, inspection of the wave function shows that the lower Dirac components are dominant. (e) We reasonably choose the effective charges so that a few states represent the upper part of the discrete spectrum, and a few states the lower (positive-energy) continuum. Clearly, all states are orthogonal by construction.

The diagonalization of the target or projectile Dirac Hamiltonian is performed once and for all. As described above, one obtains new basis sets, separately for target or projectile, each of them composed of real bound states, pseudo-bound-states, and pseudo-continuum-states. Using these sets, the one-center and two-center matrix elements can be calculated numerically as described in I and, finally, the time-dependent coupled equations can be solved. Similarly, as for real bound states, one obtains occupation amplitudes and probabilities at $t \to +\infty$ for pseudo-bound- and pseudo-continuum-states at target and projectile. The occupation probability of pseudo-bound-states of the target (projectile) obviously represents excitation of (transfer into) higher excited states. Correspondingly, the occupation probability of pseudo- continuum-states of target and projectile represents target ionization and charge transfer into the continuum, respectively.

B. The problem of orthogonality loss for pseudostates

The relativistic motion of the projectile requires that matrix elements be transformed from the target system (with the electronic coordinates $\mathbf{r}_T, t$) to the projectile system (with the electronic coordinates $(\mathbf{r}'_P, t')$ and vice versa. The Lorentz transformation is mediated by the spinor transformation[2,10]

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

where

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

and $\gamma = (1 - v^2/c^2)^{-1/2}$, $\delta = [(\gamma-1)/(\gamma+1)]^{1/2}$, and α_z is the familiar Dirac matrix with the z axis chosen in the beam direction. The transformation given by Eqs. (2) and (3) is rigorously valid only for exact solutions of the Dirac equation involving invariant interactions of the type $\gamma_\mu A_\mu$ where γ_μ and A_μ are the Dirac γ matrices and the μ components of an external four potential, respectively. In other words, if we have *approximate* eigenfunctions such as pseudostates after diagonalization of the Dirac Hamiltonian, the boost operator S only represents an *approximate* Lorentz transformation.

This has consequences for the overlap matrix elements and hence the orthogonality properties. Let us consider the overlap $N_{i'k'}$ of two states

$$\psi'_{i'}(\mathbf{r}'_P, t') = \phi'_{i'}(\mathbf{r}'_P) \exp(-iE_{i'}t')$$

and

$$\psi'_{k'}(\mathbf{r}'_P, t') = \phi'_{k'}(\mathbf{r}'_P) \exp(-iE_{k'}t')$$

in the projectile system. By construction, in the projectile frame,

$$N_{i'k'} = \int \psi^\dagger_{i'}(\mathbf{r}'_P, t')\psi_{k'}(\mathbf{r}'_P, t') d^3r'_P = \delta_{i',k'} . \tag{4}$$

However, in the target frame

$$\begin{aligned} N_{i'k'} &= \int \psi^\dagger_{i'}(\mathbf{r}'_P, t') S^{-2} \psi'_{k'}(\mathbf{r}'_P, t') d^3r_T \\ &= \int \phi'^\dagger_{i'}(\mathbf{r}'_P, t') S^{-2} \phi'_{k'}(\mathbf{r}'_P) \\ &\quad \times \exp[-i\gamma(E_{i'} - E_{k'})(v/c^2) z_T] d^3r_T \\ &\quad \times \exp[-i\gamma(E_{i'} - E_{k'})t] . \end{aligned} \tag{5}$$

Here the explicit Lorentz transformation of the time coordinate t' has been used. By exploiting the transformation properties of the Dirac equation we can convince ourselves that the orthogonality expressed by Eq. (4) is also true in the target frame, provided $\psi_{i'}$ and $\psi_{k'}$ are exact eigenstates. This apparently trivial statement is confirmed by numerical calculations. However, it would be naive to assume that a similar equivalence also holds for pseudostates. This cannot be expected since pseudostates are not eigenstates of the Dirac equation whose transformation properties are needed to show that $N_{i',k'}$ in the form of Eq. (5) is diagonal as well. Indeed, numerical calculations reveal that this is not the case, so that

$$\begin{aligned} &N_{i'k'} = \delta_{i',k'} \quad \text{if } i', k' \text{ are real states} \\ &N_{i'k'} \neq \delta_{i',k'} \quad \text{if one or both of } i', k' \text{ is a pseudostate} . \end{aligned} \tag{6}$$

Note that in nonrelativistic collisions the exponential factors occurring in Eq. (5) reduce to translation factors. Since the space part of these factors is state independent, it cancels for initial and final states and hence does not destroy the orthogonality even for pseudostates.

A relation analogous to Eq. (6) holds for the Hamiltonian matrix. If the Hamiltonian has been diagonalized in the projectile frame only the submatrix spanned by real states is diagonal also in the target frame and vice versa.

The loss of the diagonal property of overlap and Hamiltonian matrices under Lorentz transformations poses serious problems to the calculation and interpretation within a framework of coupled channels involving pseudostates. Suppose the basis set in the projectile system includes pseudostates. Then, no matter whether the projectile Hamiltonian is diagonalized in the projectile or in the target frame, an observer in the target frame will al-

ways find that for $t \to \infty$ the coupling matrix $H'_P - i(\partial/\partial t')$ in the projectile frame is nondiagonal and hence the occupation amplitudes keep oscillating among the various projectile basis states. Such a behavior is physically meaningless. Diagonalizing the coupling matrix rather than the projectile Hamiltonian in the target frame does not help either since the eigenvalues of this matrix are almost degenerate (with eigenvalues $\simeq 0$) and hence a classification of states is not possible.

These difficulties seem to be unavoidable if basis states are used that are not eigenstates of the target or projectile Hamiltonian. For example, discretized continuum states are expected to give rise to similar problems.

In order to handle these problems in a reasonable manner we have taken the following approaches.

(i) Pseudostates are attached only to the target, not to the projectile. A complete description of the collision in the target frame then encounters no difficulties. This approach is adequate for a treatment of target ionization. In comparison to the single-center calculation by Becker[7] it has the advantage of including charge transfer into bound states of the projectile.

(ii) Similarly, pseudostates are attached to the projectile, not to the target, and the process is described in the projectile system. This allows for charge transfer to the continuum but excludes target ionization.

(iii) Pseudostates are attached to both target and projectile and each set is diagonalized in its own frame. Subsequently, overlap terms (deviations from diagonal structure of the Hamiltonian and the overlap matrix) arising from Lorentz transformation into the other frame are disregarded. This approximation has the advantage of being symmetric between target and projectile. It hence *approximately* includes both target ionization and charge transfer to the continuum.

C. The problem of the frame-dependence of cross sections

Exact cross sections for relativistic collisions are invariant under Lorentz transformation. This means that coupled-channel calculations with a complete set of infinitely many basis functions would yield the same cross sections in the target and in the projectile frame. For nonrelativistic collisions this is also true if a truncated finite set of basis functions is used. The question arises whether this frame independence of cross sections calculated with a truncated basis set is still valid for relativistic collisions.

It is easy to see that this not the case. For the simplicity of the argument consider a single-center expansion in terms of target basis functions. In the target system, Eq. (1) reduces to

$$\psi(\mathbf{r}_T,t)=\sum_{k(\le N)} a_k(t)\phi_k(\mathbf{r}_T)\exp(-iE_k t)\ , \tag{7}$$

where the time dependence is exhibited explicitly. It is assumed here that a finite number N of basis states leads to a sufficiently good approximation for excitation (or ionization) cross sections when the expansion (7) is inserted into the time-dependent Dirac equation[2] describing the process.

We now may view the same process of target excitation from the projectile frame. The corresponding expansion then reads

$$\psi(\mathbf{r}'_P,t')=\sum_{k'(\le N')} a_{k'}(t')S^{-1}\phi_{k'}(\mathbf{r}'_P) \times \exp\left[-i\gamma E_{k'}\left[t'+\frac{v}{c^2}z'_P\right]\right]\ , \tag{8}$$

where S^{-1} defined by Eq. (2) just rearranges the spinor components and the set of $\phi_{k'}(\mathbf{r}'_P)$ is again a set of target-centered basis functions, simply displaced by a Lorentz transformation from the target frame to the projectile frame. However, the original time oscillation in the target frame gives rise to an additional space oscillation in the projectile frame. Therefore, if N is large enough to yield a good approximation to the cross section in the target frame, N' must be considerably larger than N in order to compensate for these space oscillations and to give a similarly adequate representation of the target in the projectile frame. If the same expansion $N=N'$ is used in both Lorentz frames, it is clear that cross sections calculated by the coupled-channel method are different in the target and in the projectile system. This frame dependence is connected with the Lorentz transformation of the time oscillation and hence disappears in the nonrelativistic limit. This has been verified in numerical calculations.

It is obvious from the discussion given above that target excitation and ionization are best described in the target frame, as has been done in Refs. 1 and 2. The same is true for charge transfer which is mainly determined by (a) the coupling within the target, and (b) the subsequent single-step transfer from the target to the projectile. The latter is a first-order process and, in the same way as the first-order excitation, is, fortuitously, independent of the Lorentz frame.

III. RESULTS AND DISCUSSION

In this section, we present some results of pseudostate calculations for the system $U^{92+}+U^{91+}$ at 500 MeV/u. This collision system has served already as a model case in earlier publications in this series, so that we can best study the effect of augmenting the two-center basis by pseudostates. A discussion of the collision of $Xe^{54+}+Ag$ will also be given.

Similarly, as in I, the accuracy of the numerical calculations has been subject to several tests. We have examined the convergence of the matrix elements and of the time integration with respect to the number of mesh points chosen. We also compared with cases where a partially analytic solution is possible. Furthermore, for each calculation we verify that the unitarity requirement is satisfied to an accuracy of better than 10^{-4}. Finally, as a very stringent test, we find that for all cases examined, detailed balancing for target excitation and charge transfer is valid within an accuracy of 10^{-2} to 10^{-3}.

In Table I, we display four different sets of basis states that have been used with the target, or with the projectile, or with both of them, corresponding to the ap-

TABLE I. Basis sets for pseudostate calculations. The notation $(N_{\text{real}},N_{\text{pseudo}}|$ for the target or $|N_{\text{real}},N_{\text{pseudo}})$ for the projectile specifies the numbers N_{real} and N_{pseudo} of exact hydrogenic eigenstates of U^{91+} and of pseudostates, respectively. Each pseudo-basis-state is characterized by its effective charge Z and its angular momentum and nodal structure.

(10,10|		(10,12|		(10,16|		(18,8|	
Z	States	Z	States	Z	States	Z	States
92	$1s_{1/2}$	92	$1s_{1/2}$	92	$1s_{1/2}$	92	$1s_{1/2}$
92	$2s_{1/2}$	92	$2s_{1/2}$	92	$2s_{1/2}$	92	$2s_{1/2}$
92	$2p_{1/2}$	92	$2p_{1/2}$	92	$2p_{1/2}$	92	$2p_{1/2}$
92	$2p_{3/2}$	92	$2p_{3/2}$	92	$2p_{3/2}$	92	$2p_{3/2}$
						92	$3s_{1/2}$
						92	$3p_{1/2}$
						92	$3p_{3/2}$
100	$1s_{1/2}$	70	$1s_{1/2}$	60	$1s_{1/2}$	110	$1s_{1/2}$
100	$2s_{1/2}$	110	$1s_{1/2}$	100	$1s_{1/2}$	130	$2s_{1/2}$
70	$2p_{1/2}$	70	$2s_{1/2}$	60	$2s_{1/2}$	90	$2p_{1/2}$
100	$2p_{1/2}$	70	$2p_{1/2}$	80	$2p_{1/2}$	120	$2p_{1/2}$
110	$2p_{1/2}$	100	$2p_{1/2}$	100	$2p_{1/2}$		
		110	$2p_{1/2}$	120	$2p_{1/2}$		
				135	$2p_{3/2}$		

proaches (i) to (iii) of Sec. II B. Each set $(N_{\text{real}},N_{\text{pseudo}}|$ is characterized by the numbers N_{real} of "real" states, that is, of exact eigenstates of the target or projectile Dirac Hamiltonian and, in addition, by the number of pseudostates. For the (nonorthogonal) pseudo-basis-states we list the effective charges Z and the classification of the basis states. The pseudo-basis-states have been chosen such that after diagonalization of the atomic Hamiltonian the lowest pseudo-bound-state lies above the highest real state considered, and furthermore, such that pseudo-continuum-states occur at reasonable energies. (We found that pseudo-continuum-states with too high energies have little effect on the cross sections.) Clearly, as in any pseudostate treatment, the choice of the basis states is somewhat arbitrary.

In Table II we show the angular momentum classification and eigenenergies of the pseudostates after diagonalization. In the first three sets we have four pseudo-bound-states supplementing the ten real bound states, while the number of pseudo-continuum-states is increasing from 6 to 12. In the last set, (18,8 |, no further bound states are needed, so that the eight pseudostates all lie in the continuum.

The basis sets of Tables I and II are used in our calculations in different combinations, as shown in Tables III and IV. For each combination of target and projectile basis sets, we have performed a complete coupled-channel calculation as described in Sec. II and in Ref. 2. Since simultaneously we follow the time evolution originating from all possible initial conditions, we obtain a large number of state-to-state cross sections for excitation, ionization, and charge transfer. Here ionization is interpreted as excitation of a pseudo-continuum-state either in the target or in the projectile ("charge transfer to the continuum"). We do not present all of the data here and rather confine ourselves, in Tables III and IV, to the initial $1s_{1/2}$ state and, moreover, to cross sections summed over magnetic substates.

TABLE II. Angular momenta and energies $E-mc^2$ (in atomic units) associated with the pseudostates within the basis sets $(N_{\text{real}},N_{\text{pseudo}}|$ presented in Table I after diagonalization of the Hamiltonian. The energies of the real states are, of course, unchanged and not listed.

(10,10|		(10,12|		(10,16|		(18,8|	
State	$E-mc^2$	State	$E-mc^2$	State	$E-mc^2$	State	$E-mc^2$
$p_{1/2}$	−529.8	$p_{1/2}$	−529.8	$s_{1/2}$	−534.6		
$s_{1/2}$	−177.4	$s_{1/2}$	−506.4	$p_{1/2}$	−511.0		
$p_{1/2}$	333.3	$p_{1/2}$	333.3	$p_{3/2}$	435.2	$p_{1/2}$	102.4
$p_{1/2}$	7352	$s_{1/2}$	1482	$p_{1/2}$	692.9	$s_{1/2}$	6933
$s_{1/2}$	8861	$p_{1/2}$	7352	$s_{1/2}$	764.6	$p_{1/2}$	7013
		$s_{1/2}$	24 560	$p_{1/2}$	11 680	$s_{1/2}$	25 250
				$s_{1/2}$	16 780		

TABLE III. Excitation cross sections in barns per electron for $U^{92+}U^{91+}(1s_{1/2})$ at 500 MeV/u. The numbers in square brackets denote the power of 10 multiplying the preceding numbers. The basis sets for final and initial states are characterized by the notation defined in Table I.

Final \ Basis	1 (10|10)	2 (10,12|10)	3 (10,16|10)	4 (10|10,12)	5 (10|10,16)	6 (10,10|10,10)	7 (18|18)	8 (18,8|18,8)
$2s_{1/2}$	4.38[3]	3.50[3]	2.81[3]	4.48[3]	3.70[3]	4.21[3]	3.95[3]	4.58[3]
$2p_{1/2}$	5.19[3]	5.64[3]	5.57[3]	4.72[3]	4.54[3]	5.48[3]	5.45[3]	5.83[3]
$2p_{3/2}$	7.68[3]	7.02[3]	7.10[3]	6.98[3]	6.48[3]	6.61[3]	7.87[3]	6.76[3]
$n=2$ shell	1.77[4]	1.62[4]	1.56[4]	1.60[4]	1.48[4]	1.63[4]	1.73[4]	1.72[4]
$3s_{1/2}$							7.81[2]	7.81[2]
$3p_{1/2}$							4.07[2]	8.45[2]
$3p_{3/2}$							7.89[2]	8.78[2]
$n=3$ shell							1.98[3]	2.50[3]
Pseudo-bound-states		1.55[3]	2.89[3]			1.98[3]		
Target continuum		3.48[3]	1.16[4]			2.37[3]		2.63[3]
Projectile continuum				6.44[3]	7.44[3]	5.30[3]		7.33[3]
K-vacancy production	2.37[4]	2.72[4]	3.56[4]	3.02[4]	3.00[4]	3.48[4]	2.56[4]	3.79[4]

TABLE IV. Charge-transfer cross sections per electron for $U^{92+}+U^{91+}(1s_{1/2})$ at 500 MeV/u. The numbers in square brackets denote the power of 10 multiplying the preceding number. The basis sets for final and initial states are characterized by the notation defined in Table I.

Final \ Basis	1 (10|10)	2 (10,12|10)	3 (10,16|10)	4 (10|10,12)	5 (10|10,16)	6 (10,10|10,10)	7 (18|18)	8 (18,8|18,8)
$1s_{1/2}$	4.18[3]	4.24[3]	3.92[3]	4.43[3]	4.28[3]	4.64[3]	4.12[3]	4.47[3]
$2s_{1/2}$	1.12[3]	1.05[3]	9.98[2]	1.36[3]	1.53[3]	1.55[3]	1.06[3]	1.78[3]
$2p_{1/2}$	4.19[2]	3.46[2]	3.05[2]	4.35[2]	3.98[2]	4.01[2]	3.91[2]	5.35[2]
$2p_{3/2}$	2.37[2]	2.99[2]	2.63[2]	2.75[2]	2.92[2]	3.11[2]	2.31[2]	3.52[2]
$n=2$ shell	1.78[3]	1.69[3]	1.57[3]	2.07[3]	2.22[3]	2.27[3]	1.68[3]	2.67[3]
$3s_{1/2}$							3.33[2]	6.32[2]
$3p_{1/2}$							9.89[1]	3.66[2]
$3p_{3/2}$							7.14[1]	8.55[1]
$n=3$ shell							5.03[2]	1.08[3]
Real states	5.96[3]	5.93[3]	5.49[3]	6.50[3]	6.50[3]	6.91[3]	6.31[3]	8.22[3]
Pseudo-bound-states				1.22[3]	1.22[3]	1.96[3]		
Total bound state	5.96[3]	5.93[3]	5.49[3]	7.71[3]	7.71[3]	8.87[3]	6.31[3]	8.22[3]
Pseudo-continuum-states				6.44[3]	7.44[3]	5.30[3]		7.33[3]

Let us consider Table III for excitation and ionization. Columns 2 and 8 summarize the calculations with the bases of 20 and 36 exact atomic eigenstates of Refs. 1 and 2, respectively. In columns 3 and 4, following method (i) of Sec. II B, we have augmented only the target basis by pseudostates. Correspondingly, in columns 5 and 6 we have augmented the projectile basis by pseudo states. Finally, in columns 7 and 9, we have chosen method (iii) of Sec. II B and supplemented both target and projectile bases with pseudostates at the expense of ignoring small overlap terms among projectile pseudostates. Table IV displays the corresponding data for charge exchange and is organized in the same manner.

In the lower part of Table III we collect ionization data. By construction, there is only target ionization in columns 3 and 4, only charge transfer to the continuum (taken from Table IV) in columns 5 and 6, and both target and projectile ionization in columns 7 and 9. We have also included K-vacancy production which comes about by excitation, charge transfer and ionization. In a fully analogous fashion, Table IV contains cross sections for charge transfer into various final states.

Inspection of Tables III and IV shows that the cross sections for final bound states are not drastically altered by the inclusion of pseudostates. Most changes are on the 10% level. Quantitatively, the addition of target pseudostates tends to decrease the excitation cross sections because some of the probability flux is diverted into the additional states. On the other hand, the addition of projectile pseudostates tends to increase the capture rates because the rearrangement channel attracts more probability flux which subsequently is redistributed among the projectile states. The latter observation is particularly evident when comparing the 52-state calculation of column 9 with 36-state calculation of column 8 in Table IV; however, in this case also, excitation is enhanced by adding continuum pseudostates.

Regarding ionization, only the sets of columns 7 and 9 allow for both target ionization and charge transfer into the continuum. If one adds both terms, one obtains K-shell ionization cross sections (per K electron) of 7.7×10^3 b and 1.0×10^4 b, respectively. A similar number is derived if target ionization of column 3 and charge transfer to the continuum from column 5 are added. Summing the corresponding numbers from columns 4 and 6, however, yields almost twice this value. From our calculations, we therefore estimate an ionization cross section of $(1-2)\times10^4$ b per K electron. While the ionization data still contain considerable ambiguity, the cross section per electron for K-vacancy production can be more reliably estimated and compared with experimental data. From Table III we get $\sigma_K\sim(3-3.8)\times10^4$ b. This is in approximate accordance with the cross section of $(3-3.5)\times10^4$ b per electron in U+U collisions at 422 MeV/u measured by Anholt *et al.*[3] Of course, the existence of filled target shells reduces the theoretical number given above while the change of the energy from 500 to 422 MeV/u increases it.

We have also performed calculations for $Xe^{54+}+Ag$. However, the technique of pseudostates becomes very difficult for a complex target atom with many filled shells. In order to remove the overlap of pseudostates with occupied electronic levels one would have to include a large number of target shells explicitly. This is generally not feasible within an acceptable computing time. Nevertheless, we can conclude from our tentative calculations that excitation and charge-transfer cross sections are altered only on the 10% level by including pseudostates in the basis set.

IV. CONCLUDING REMARKS

Within our series of papers[1,2] on two-center coupled-channel calculations we have extended the formalism to augment the atomic basis sets by the inclusion of pseudostates. We have found that in comparison to nonrelativistic or to relativistic single-center calculations additional problems arise owing to the loss of orthogonality of approximate eigenstates of a Dirac Hamiltonian under Lorentz transformations. This problem is not specific to pseudostates but will also arise in connection with other approximate states like discretized continuum states. On the other hand, what one might expect to be a problem, namely, the occurrence of spurious negative-energy solutions, can be coped with on a practical level.

In our calculations, we have either avoided the nonorthogonality problem by attaching pseudostates to only one of the collision partners or we have ignored it by discarding the small overlap terms while at the same time retaining the symmetry between target and projectile.

It is furthermore shown that relativistic cross sections (unlike nonrelativistic ones) calculated within a coupled-channel approach that uses a fixed number of basis states depend on the choice of the Lorentz frame. One can easily see that only the target frame is appropriate if the number of channels is to be kept at a minimum.

The numerical calculations for $U^{92+}+U^{91+}$ at 500 MeV/u have been extended up to basis sets composed of 52 states, including 36 real and 16 continuum pseudostates. The results show that excitation and capture cross sections are changed only on the 10% level in most cases. While the basis sets are presumably still too small to ensure convergence one can, nevertheless, estimate cross sections for ionization and K-shell vacancy production. The results for K-vacancy production appear to be in reasonable accord with experimental data.

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