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Single and double charge transfer in $Be^{4+}+He$ collisions: A molecular (Feshbach) approach

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In recent articles, we pointed out the fundamental difference between the molecular treatment of processes involving a multicharged ion and hydrogen or helium atoms, which is the (formal) autoionizing character of the molecular channels, and we reported a (new) implementation of the Feshbach method to calculate the molecular energies and couplings. In the present work we use the wave functions calculated with this Feshbach method for the $BeHe^{4+}$ quasimolecule, introduce a common translation factor in the formalism, and calculate the single and double charge-exchange cross sections in $Be^{4+}+He(1s^2)$ collisions for impact energies 0.2–20 keV/amu. The mechanisms of the processes are discussed in detail.

I. INTRODUCTION

The study of charge-transfer collisions between slow bare ions and neutral species has become a subject of increasing interest, because of the role played by these collisions in the behavior of high-temperature plasmas, the development of short-wavelength lasers, and in the loss of multicharged species in the interstellar medium.

In a recent paper,[1] we pointed out a fundamental difference between the molecular treatment of processes involving hydrogen as a neutral target, and of those involving heavier neutral ions, like helium.[2] Basically, the difference is that in the latter processes, the relevant molecular channels, as defined in the Born-Oppenheimer approximation, have energies that lie above the ionization threshold of the system and above those of an infinite number of bound electronic states. Fortunately, when treating the collision process, the fact that one has to deal with autoionizing rather than stable electronic wave functions is a formal problem, except at very low impact energies, i.e., it can be ignored, much in the way as one usually ignores the finite lifetime of the molecular channels with respect to photon emission. On the other hand, a considerable modification of the usual techniques of quantum chemistry has to be effected in order to calculate the energies and dynamical couplings corresponding to those autoionizing and infinitely excited molecular states. For the special case of Li^{3+} + He collisions, we have reported implementation of stabilization[3] and Feshbach-type[1] techniques to calculate energies and couplings which were then used in another work[4] to calculate the single charge-exchange cross section and to compare our *ab initio* data with the experimental data and with the results of the pseudopotential approach of Opradolce *et al.*[5]

In a separate publication,[6] we have explained the fact that Li^{3+} + He collisions are, in a sense, also exceptionally simple, meaning that passage to other collisional systems such as $X^{n+}+He$ with $n\geq 3$ can lead to two-electron autoionizing $X^{(n-2)+}$ species through charge-exchange processes such as originally considered by Lichten,[7] and which have recently received a great deal of attention.[2,8–15] The practical interest of these collision processes lies in the fact that a large number of autoionizing states of ions, which are otherwise difficult to obtain, become accessible and can be studied.[10] From the more technical, strictly quantum chemical viewpoint, the appearance of open exit channels such as $X^{(n-2)+}+He^{2+}$ is very important because, not only are correlation diagrams considerably more complicated than in Ref. 1, but pseudopotential effective one-electron approaches are inapplicable, and an *ab initio* treatment seems the only alternative.[6] In Ref. 6 we have reported the application of Feshbach-type techniques to the calculation of energies and couplings of $BeHe^{4+}$, as the simplest case that presents the features of formally autoionizing molecular channels some of which remains so at infinite internuclear separation. We studied in detail the correlation diagram, which involves a whole Rydberg series embedded in the ionization continuum, and two diabatic states whose energies cross those of the series members and penetrate in the second ionization continuum.

In the present work we employ the wave functions calculated in Ref. 6 with our Feshbach method to evaluate single and double charge-transfer cross sections in Be^{4+} + He collisions, since these data are of practical interest because of the presence of beryllium ions as impurities,[16] originating from limiter and first-wall material[17,18] in tokamak plasmas, and because no measurements of the cross sections have been performed so far, possibly due to the toxic nature of Be compounds.

According to the analysis carried out in Ref. 6, single and double charge exchange in Be^{4+} + He collisions occur through transitions caused by radial couplings which are so origin dependent that it is indispensible to introduce translation factors in the theory. In the present work we introduce the common translation factor[19] (CTF) of Errea *et al.*,[20] which has been successfully employed in several calculations[4,20,21] for processes with similar characteristics to those studied here. The modified couplings are displayed in Sec. II. In Sec. III we present our calculated single and double charge-exchange cross sections, and discuss the corresponding mechanisms in detail. Atomic units are used unless otherwise specified.

II. INCLUSION OF THE COMMON TRANSLATION FACTOR

The common translation factor approach substitutes[19] the usual molecular expansion of the electronic wave function representing the colliding system by the ansatz

$$\Psi(\mathbf{r}_1,\mathbf{r}_2,t)=e^{i[U(\mathbf{r}_1,t)+U(\mathbf{r}_2,t)]}\times\sum_j a_j(t)\chi_j(\mathbf{r}_1,\mathbf{r}_2,R)\exp\left[-i\int_0^t E_j dt'\right] , \qquad (1)$$

where χ_j are molecular wave functions defined in the Born-Oppenheimer approximation, E_j their energies, and U the exponential factor of the CTF, for which we have taken the simple form introduced by Errea *et al.*:[20]

$$U(\mathbf{r}_j,t)=f(\mathbf{r}_j,R)\mathbf{v}\cdot\mathbf{r}_j-\tfrac{1}{2}f^2(\mathbf{r}_j,R)\mathbf{v}\cdot\mathbf{r}_j , \qquad (2)$$

$$f(\mathbf{r}_j,R)=\frac{R^2}{R^3+\beta^3}[\mathbf{r}_j\cdot\hat{\mathbf{R}}+(p-p_0)R]-(p-p_0) , \qquad (3)$$

where R is the internuclear distance, and the origin of electronic coordinates is situated at a distance pR from the Li nucleus. It is easy to show[20] that (i) the coupling matrix elements in the basis of modified molecular wave functions,

$$\Phi_j(\mathbf{r}_1,\mathbf{r}_2,t)=e^{i[U(\mathbf{r}_1,t)+U(\mathbf{r}_2,t)]}\chi_j(\mathbf{r}_1,\mathbf{r}_2,R) , \qquad (4)$$

can be calculated analytically, provided that χ_j is written as a sum of configurations built from atomic Gaussian-type orbitals (GTO's), and (ii) that these couplings are independent of the choice of the origin of electronic coordinates, i.e., of the value of p in Eq. (3).

The meaning of the parameters β and p_0 introduced in our definition (2) and (3) of the CTF has been explained in detail[20,4] and will not be repeated here. A study carried out by Riera and co-workers at our laboratory[22] has shown that, for reactions whose mechanisms involve transitions at not too small R, a choice $1<\beta<5$ yields optimal results. In the present case, we have chosen $\beta=1.5$ which, as we shall see, has the advantage that the resulting modified energies and couplings are practically independent of the choice of the other parameter p_0, whose optimization is more sensitive[22] than β to the reaction's characteristics, to the nuclear trajectory, and to the impact energy of the collision.

As mentioned by Errea *et al.*,[4] an additional advantage of the CTF approach is that inclusion of an exponential factor as in Eq. (4) does not mix the Feshbach P and Q subspaces, and preserves the basic asymptotic behavior of the corresponding wave functions as r_1 or $r_2\rightarrow\infty$. On the other hand, the close connection between the molecular method and the introduction (through the CTF) of a local effective velocity field for the electrons becomes a liability at high impact energies, and yields results that fail to reproduce the rapid fall of charge-exchange cross sections beyond their maximum.[23,24] Hence, our calculations will not be extended to this energy region.

Substitution of expansion (1) in the impact parameter equation

$$i\frac{\partial}{\partial t}\Psi=H\Psi , \qquad (5)$$

with $\mathbf{R}=b\hat{\mathbf{X}}+vt\hat{\mathbf{Z}}$, with b the impact parameter, yields the system of coupled linear differential equations for the expansion coefficients

$$i\frac{da_j}{dt}=\sum_{\substack{j,k\\(k\neq j)}} M_{jk}a_k\exp\left[-i\int_0^t(E_k-E_j)dt'\right] , \qquad (6)$$

where the coupling matrix elements are given by

$$M_{jk}=\left\langle\chi_j\left|-i\frac{\partial}{\partial t}+\sum_{l=1}^{2}\left[-i(\nabla_l U)\cdot\nabla_l-\frac{i}{2}(\nabla_l^2U)+\tfrac{1}{2}(\nabla_l U)^2+\frac{\partial U}{\partial t}\right]\right|\chi_k\right\rangle . \qquad (7)$$

Finally, the partial cross sections are given by integration over all impact parameters:

$$\sigma_j=2\pi\int_0^\infty |a_j(+\infty)|^2 b\,db . \qquad (8)$$

III. RESULTS AND DISCUSSION

Our implementation[1,6] of the Feshbach method yields, for the molecular channels involved in the treatment of single and double charge-exchange Be^{4+} + He collisions, the results displayed in Figs. 1 (electronic energies), 2 (radial couplings modified by the CTF), and 3 (rotational coupling modified by the CTF). In these figures, we have diabatized (i) the (in principle infinite) series of pseudocrossings between, on one hand a molecular Rydberg series[6] of states with character $2s\sigma nl\sigma$ and $2p\sigma nl\sigma$, and on the other hand two diabatic states whose energies penetrate, at very small R, in the second ionization continuum, and (ii) all other sharp avoided crossings that are also traversed diabatically during the collision in the impact-energy range ($E>100$ eV/amu) considered here, since the corresponding needlelike peaks in the radial couplings, and laddertype structures in the rotational ones, hinder the integration of the system (6).

As mentioned in the previous section, the dynamical couplings are seen in Figs. 2 and 3 to be independent of the parameter p_0 of our CTF [Eq. (3)] in the region $R>2$ a.u., where all transitions significantly contributing to the cross section (8) take place. Comparison with the unmodified molecular data (without translation factors) of Ref. 6 shows that, for $R<2.5$ a.u., the variation of the present couplings with respect to the parameter p_0 is much smaller than that of the unmodified couplings with p, i.e., with the position of the origin of electronic coordinates.

To integrate the system of coupled differential equations (6), the program PAMPA (Ref. 25) was conveniently modified[20,21] to include the new coupling terms in Eq. (7). The cross sections for the processes

$$Be^{4+}+He(1s^2)\rightarrow Be^{3+}(2s,2p)+He^{+}(1s)\ , \tag{9}$$

$$Be^{4+}+He(1s^2)\rightarrow Be^{2+}(2s^2,2s\,2p,2p^2)+He^{2+}\ , \tag{10}$$

were calculated, employing expansion (1), with the CTF of Eqs. (2) and (3), and the wave functions of the 1, 3, 4, and $5\,^1\Sigma$ states and the lowest autoionizing $^1\Pi$ state, whose energies and couplings were displayed in Figs. 1, 2, and 3.

At infinite internuclear separation the entrance channel is represented by the $3\,^1\Sigma$ wave function and transitions to $1\,^1\Sigma$ and $2\,^1\Sigma$ states correspond to single charge-exchange yielding $Be^{3+}(n=2)+He^{+}(1s)$ and transitions to $4\,^1\Sigma$, $5\,^1\Sigma$, and $6\,^1\Sigma$ states correspond to double charge ex-

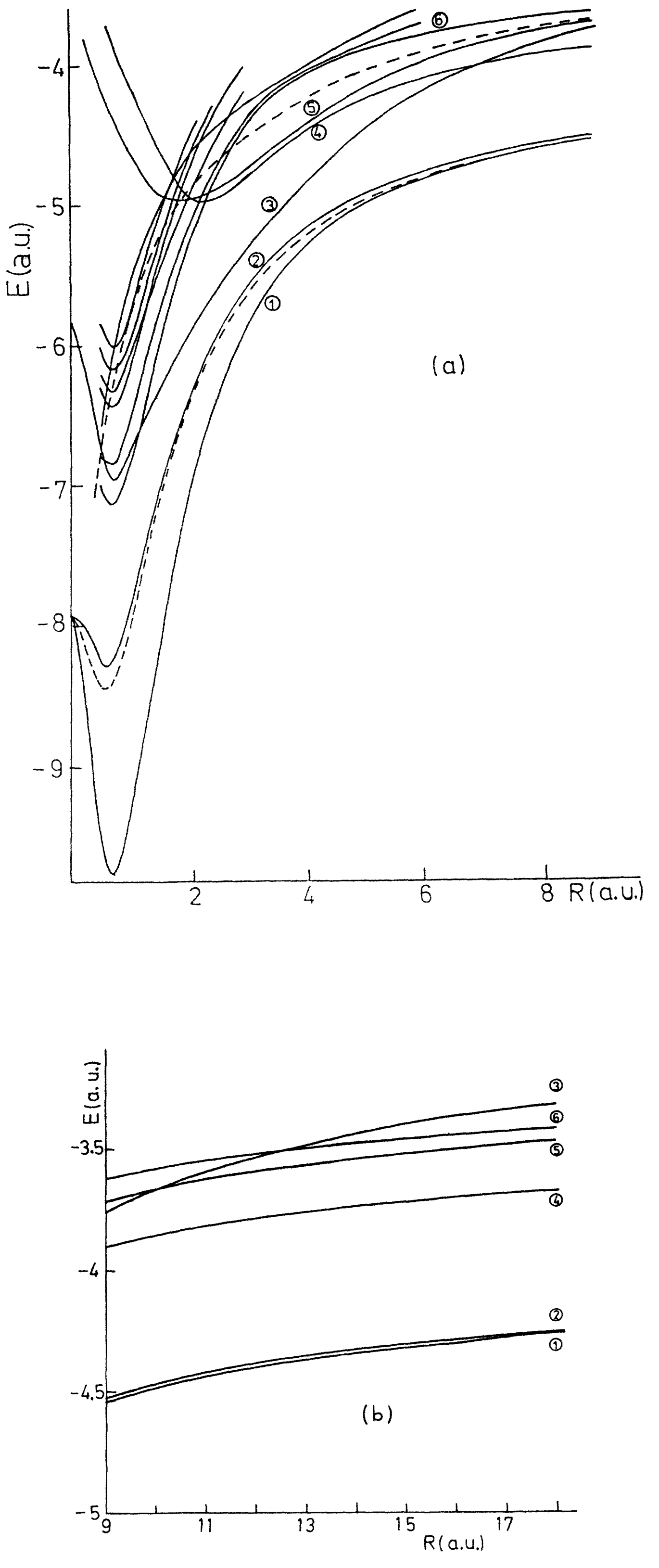

FIG. 1. Quantitative correlation diagram for the (formally autoionizing) states of the quasimolecule $BeHe^{4+}$. ——, $^1\Sigma$; — — —, $^1\Pi$. The symbols $1\,^1\Sigma$, $1\,^1\Pi$ refer to the lowest states which lie above the first ionization limit. (a) Energy values for $0<R<9.0$ a.u. (b) For $9<R<18$ a.u.

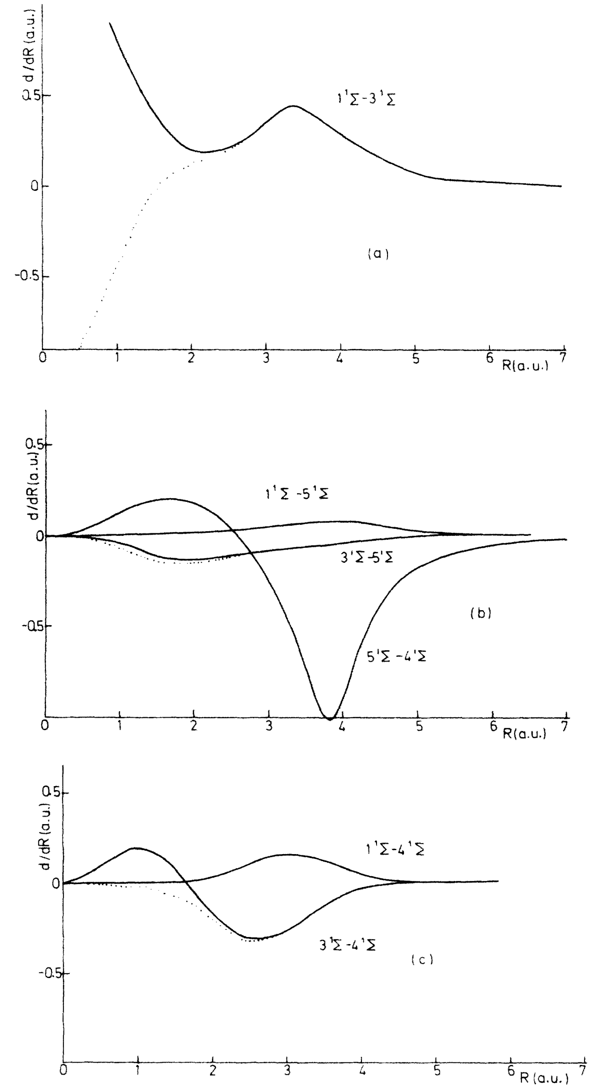

FIG. 2. Modified radial couplings between (a) $1\,^1\Sigma$-$3\,^1\Sigma$; (b) $1\,^1\Sigma$-$5\,^1\Sigma$, $3\,^1\Sigma$-$5\,^1\Sigma$, and $5\,^1\Sigma$-$4\,^1\Sigma$; (c) $1\,^1\Sigma$-$4\,^1\Sigma$ and $3\,^1\Sigma$-$4\,^1\Sigma$. · · · ·, with CTF of Eqs. (2) and (3) with $\beta=1.5$ and $p_0=0$. ——, with CTF of Eqs. (2) and (3) with $\beta=1.5$ and $p_0=1$.

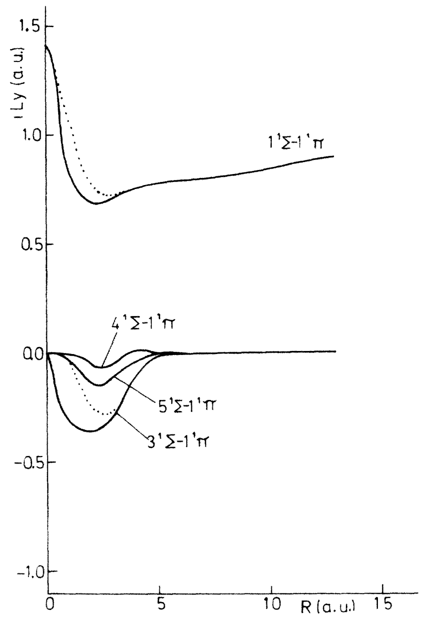

FIG. 3. Modified rotational couplings between $1\,^1\Sigma$, $3\,^1\Sigma$, $4\,^1\Sigma$, and $5\,^1\Sigma$ states and the $1\,^1\Pi$ state. Conventions as in Fig. 2.

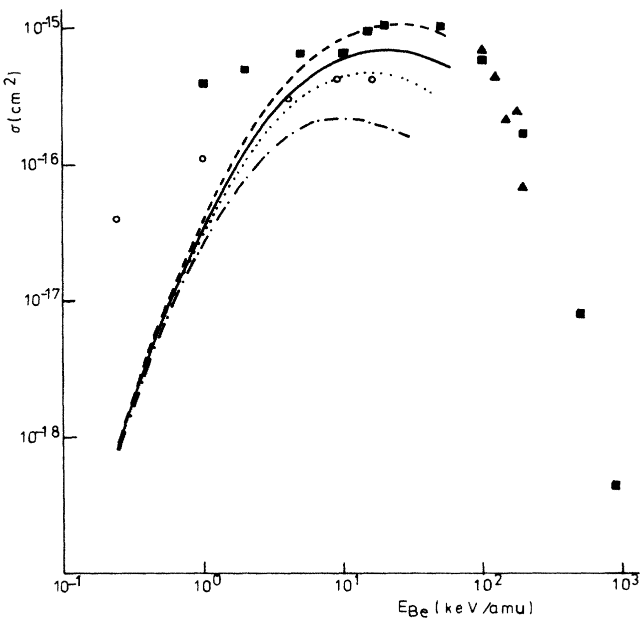

FIG. 4. Cross sections for reaction (9) (single charge exchange). ——, same results as in Table I using CTF of Eqs. (2) and (3), — — —, results calculated without CTF and origin on the He nucleus; · · · ·, results calculated without CTF and origin on nuclear center of charge; —·—·—·, results calculated without CTF and origin on the Be nucleus. ■, theoretical results (UDWA) of Suzuki *et al.* (Ref. 26). △, theoretical results (CTMC) of Olson (Ref. 27). ○, experimental results of Iwai *et al.* (Ref. 28) for one-electron capture in C^{4+} + He collisions.

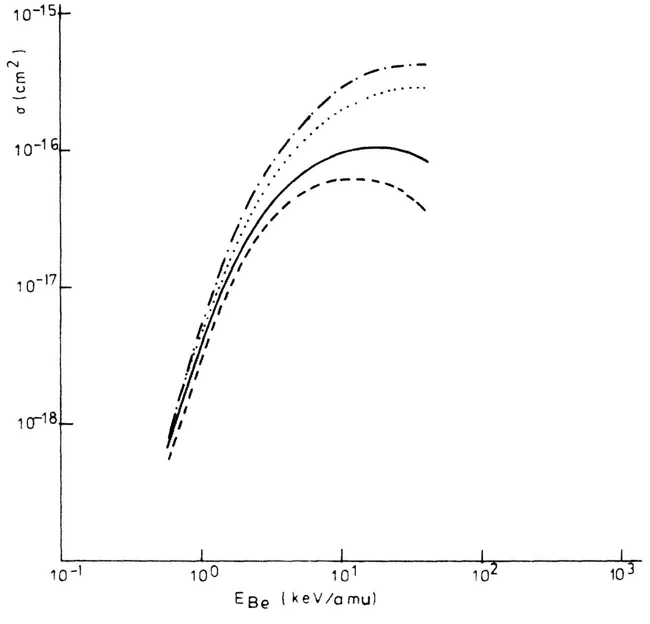

FIG. 5. Cross sections for reaction (10) (double charge exchange); conventions as in Fig. 4.

change yielding $Be^{2+}(2s^2,2s\,2p,2p^2)+He^{2+}$.

The $2\,^1\Sigma$ and $6\,^1\Sigma$ states are not included in the treatment because of their lack of appreciable interaction with the other channels, as explained in Ref. 6.

For comparison, we have also performed calculations with the perturbed stationary states (PSS) expansion [i.e., without translation factors, $U=0$ in Eq. (1)] and three "intuitive" choices for the origin of electronic coordinates: the position of either nucleus and of the center of nuclear charge. These results are presented in Fig. 4 (single charge exchange) and Fig. 5 (double charge exchange). The former ones are compared to the theoretical data of Suzuki *et al.*[26] using the unitarized distorted-wave approximation (UDWA), and Olson[27] using the classical trajectory Monte Carlo method. Given the fact that the UDWA approach usually performs poorly[26] at energies which are lower than that of the cross-section maximum,

TABLE I. Calculated cross sections for reactions (9) (σ_s) and (10) (σ_d) with the molecular wave functions of Ref. 6 and the CTF of Errea *et al.* [Eqs. (2) and (3)] with $\beta=1.5$.

v (a.u.)	E (keV/amu)	σ_s (10^{-16} cm^2)	σ_d (10^{-16} cm^2)
0.1	0.25	0.0077	0.000 35
0.15	0.56	0.0895	0.0060
0.2	1.00	0.3302	0.0345
0.3	2.25	1.518	0.2414
0.4	4.00	3.094	0.5064
0.5	6.25	4.483	0.7855
0.6	9.00	5.564	0.8728
0.7	12.25	6.201	1.007
0.8	16.00	6.516	1.097
0.9	20.25	6.711	1.054
1.0	25.00	6.825	0.9562

and that the same holds for our molecular approach with a CTF (Refs. 23 and 24) for energies beyond that maximum, the agreement between the theoretical results can be taken as very good.

As mentioned before, no experimental data is available for either single or double electron exchange in $Be^{4+}+He$ collisions. Nevertheless, it is of some interest to compare our results to the measurements of Iwai *et al.*[28] for one-electron capture in $C^{4+}+He$ collisions; the partial agreement between these data and ours (see Fig. 4) will be discussed below. A list of some of our results obtained with the CTF is presented in Table I. We have explicitly checked that our calculated cross sections were practically invariant to the choice of the parameter p_0 in the CTF [Eq. (3)].

Comparison between Figs. 4 and 5 shows that in $Be^{4+}+He$ collisions, single charge exchange dominates double electron transfer for the whole range of impact energies treated. A second conclusion, of interest to the theorist, is the importance of the introduction of translation factors in the study of these processes (9) and (10). For example, if one performs calculations without translation factors (PSS approach) and with the origin of electronic coordinates situated at the Be nucleus, we see from Figs. 4 and 5 that one obtains the incorrect result that two-electron transfer dominates one-electron transfer for impact $E>7$ keV/amu—although the error could be guessed by performing the same calculation with the center of nuclear charge or the He nucleus as alternative origins. A parallel situation with respect to charge exchange versus excitation cross sections in the PSS approach was reported by Macías *et al.*[29] We also see from Figs. 4 and 5 that with none of our choices for the origin of electronic coordinates can the PSS approach reproduce the cross sections calculated using translation factors—a normal situation in the intermediate energy range.

To analyze the mechanism of processes (9) and (10), we present in Figs. 6 and 7 the corresponding transition probabilities $P(b)$ times impact parameter b, as functions of b, for incident energies $E=4$ and 9 keV/amu. We have defined

$$P_s(\Sigma)=\lim_{t\to\infty}|a_{1\Sigma}(t)|^2\,, \tag{11}$$

$$P_s(\Pi)=\lim_{t\to\infty}|a_{1\Pi}(t)|^2 \tag{12}$$

for single charge exchange, and

$$P_d=\lim_{t\to\infty}[\,|a_{4\Sigma}(t)|^2+|a_{5\Sigma}(t)|^2] \tag{13}$$

for double charge exchange. As reasoned in Ref. 6, while the autoionizing character of the molecular channels involved in the processes can be ignored in the collision treatment, autoionization *after* the collision is very important[8-14] in the present case, since the doubly excited Be^{2+} ions eventually emit an electron. Then, the probability P_d of Fig. 7 can be used to predict electron emission spectra, because, as we shall see later on, only the $Be^{2+}(2s2p\,^1P)$ exit channel is appreciably populated.

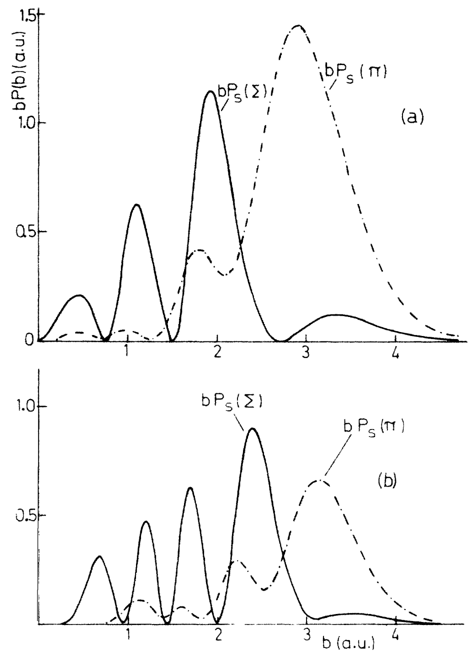

FIG. 6. Plot of $bP_s(\Sigma)$ (——) and $bP_s(\Pi)$ (— — —) vs the impact parameter b where $P_s(\Sigma)$ and $P_s(\Pi)$ are defined in Eqs. (11) and (12) for an impact energy of (a) 9 keV/amu, (b) 4 keV/amu.

It can be seen from Figs. 6 and 7 that transitions only occur for trajectories with impact parameters $b<4$ a.u., and are clearly caused by the $1\,^1\Sigma$-$3\,^1\Sigma$ and $3\,^1\Sigma$-$4\,^1\Sigma$ radial couplings. The Π state has little influence on the dynamics of these primary mechanisms; its elimination from the molecular basis of Eq. (1) yields results that are practically identical to those of Figs. 4 and 5. In fact (see Fig. 6) its effect is to share the population between the exit channels $Be^{3+}(2p_z)+He^{+}(1s)$ and $Be^{3+}(2p_x)+He^{+}(1s)$, by a (relatively) long-range mechanism, involving the slowly (R^{-2}) decreasing rotational coupling between the corresponding quasidegenerate

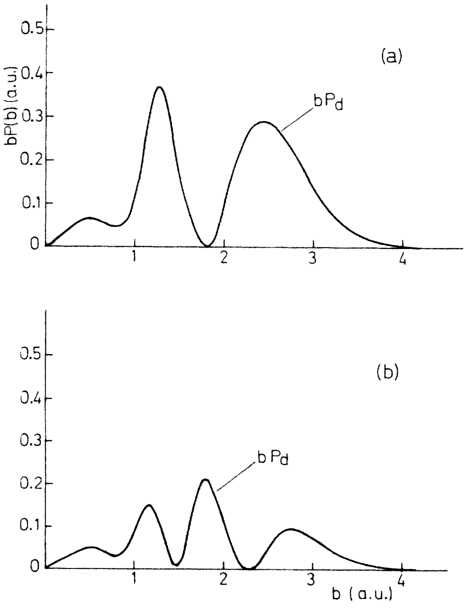

FIG. 7. Plot of $bP_d(b)$ (——) vs b where P_d is defined in Eq. (13), for an impact energy of (a) 9 keV/amu, (b) 4 keV/amu.

molecular states[6] (see Fig. 3). The "history" of the collision process is simply visualized if one plots, as in Figs. 8(a) and 8(b), the individual state populations $|a_n(t)|^2$ as functions of time for collisions with trajectories $b=2.0$ a.u. (dominant exit through Σ channel) and $b=3.0$ a.u. (dominant exit through Π channel) for an impact energy $E=9$ keV/amu. We also see in these figures how exit to autoionizing Be^{2+} species exclusively proceeds through $3\,^1\Sigma$-$4\,^1\Sigma$ and $4\,^1\Sigma$-$5\,^1\Sigma$ transitions so that only the $Be^{2+}(2s\,2p\,^1P)$ state is obtained, as mentioned in the previous paragraph.

Finally, comparison between our calculated single electron-transfer cross section in Table I and Fig. 4, and the corresponding one for $C^{4+}+He$ collisions, shows some agreement in the region of the cross-section maximum, and a clear departure from this agreement at lower energies. In fact, this comparison is of great interest from the practical point of view, since if one could treat $C^{4+}+He$ instead of $Be^{4+}+He$ collisions—and analogously fill the corresponding $1s^2$ inner shells for heavier $X^{n+}+He$ systems—one would avoid the whole issue raised by our recent work[1,3,4,6] in what concerns the formal autoionizing character of the molecular channels, and the uselessness of standard quantum chemical programs and techniques to evaluate their energies and couplings. This is obviously because the relevant CHe^{4+} molecular states are *not* autoionizing. It is worth looking into this point in some detail.

Firstly, the differences in Fig. 4 between $C^{4+}+He$ and $Be^{4+}+He$ cross sections are unlikely to be due to omission of higher excited states in our treatment. Moreover, it is known[30,15] that double electron capture dominates over single electron capture in the former case at low energies, while we obtain higher single charge-transfer cross

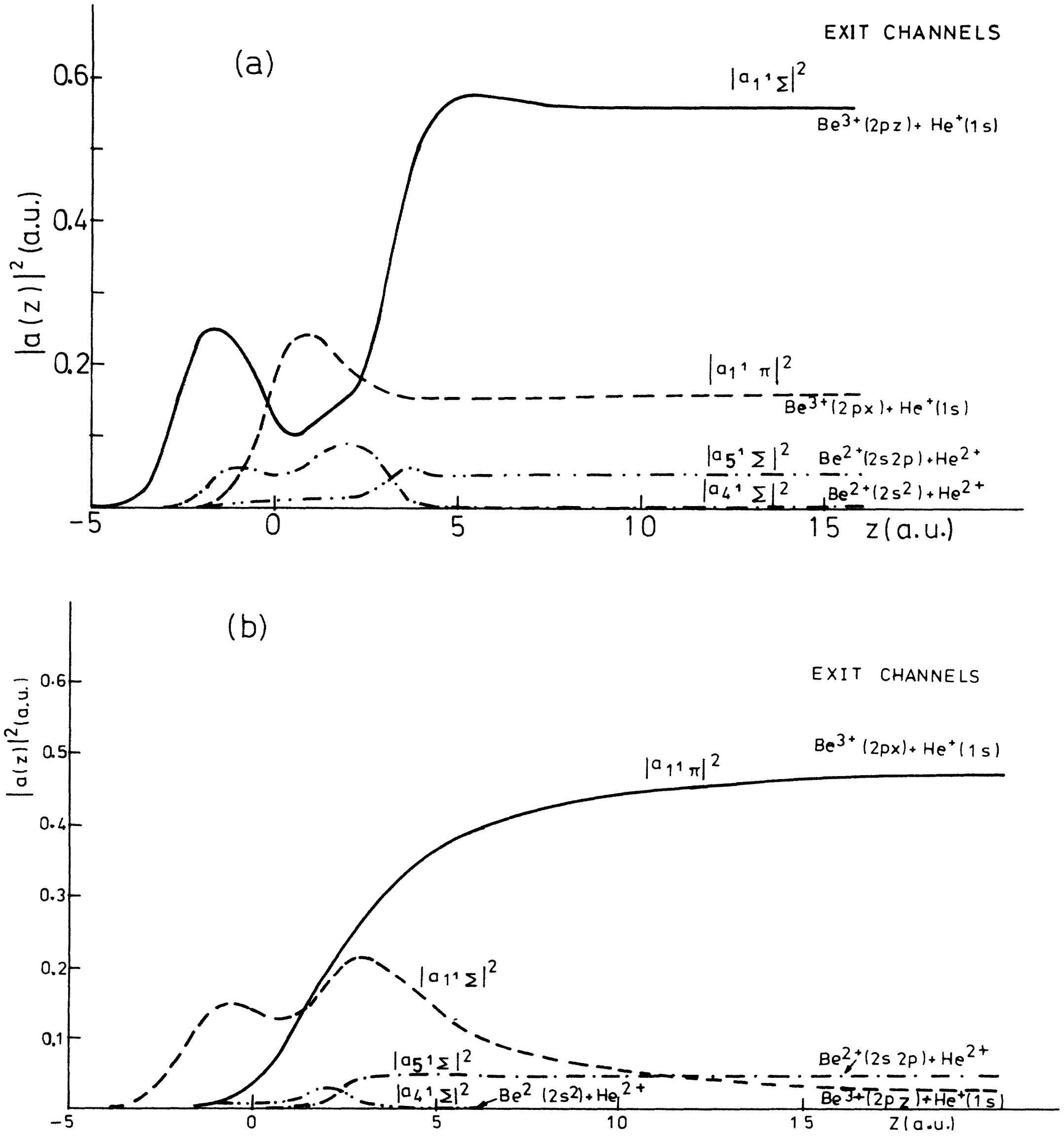

FIG. 8. Plot of the values of the occupation number $|a_1\,^1\Sigma|^2$, $|a_1\,^1\Pi|^2$, $|a_4\,^1\Sigma|^2$, and $|a_5\,^1\Sigma|^2$ as functions of $Z=vt$. (a) $E=9$ keV/amu and $b=2.0$ a.u., and (b) $E=9$ keV/amu and $b=3.0$ a.u.

sections. Secondly, the shape and magnitude of the cross sections are very sensitive to the position, and concomitant width, of the $1\,^1\Sigma$-$3\,^1\Sigma$ and $3\,^1\Sigma$-$4\,^1\Sigma$ pseudocrossings (shown in Fig. 1) where transitions occur. Then, the explanation for the differences is simply that the interaction between the outer, and the inner $1s^2$, shells of C^{4+} cause a shift in both positions and a corresponding change in the energy separations in the CHe^{4+} case, with respect to $BeHe^{4+}$, which are sufficient to significantly alter the transition probabilities from one to the other system. Agreement between both single charge-exchange cross sections at $E \simeq 10$ keV/amu is then probably accidental.

Hence, CHe^{4+} is not "the same" as $BeHe^{4+}$, and a solution of the practical problem caused by the infinitely excited nature of the molecular channels in the latter system is not achieved by introducing an artificial inner shell. Rather one should introduce in the quantum chemistry calculations a pseudopotential to prevent collapsing of the outer shells—and thus avoid the appearance of the $1s\sigma nl\sigma$ Rydberg series and $1s\sigma\epsilon\sigma$ discretized continuum. A rigorous and elegant way to achieve this is provided by the Feshbach method. This justifies the considerable programming effort invested in our implementation of this method.[1,4,6]

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