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Double-electron-capture processes in B^{4+}+He collisions

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The double-capture processes involved in the $B^{4+}(1s)+\mathrm{He}(1s^2)$ collision have been calculated by means of an *ab initio* configuration-interaction method followed by a semiclassical dynamical treatment. The results are compared to previous theoretical works in order to analyze the adequacy of model potential approaches.

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I. INTRODUCTION

Electron capture of multiply charged ions in collision with neutral atoms has been widely investigated both in astrophysics and plasma fusion research. Formally, single- and double-electron capture at low collision energies are dominated by specific curve crossings where transitions may occur and both processes may be described by the same methods. In practice, the number of channels generally involved in double capture [1], as well as the possible interactions with Rydberg states [2] or with the continuum, especially for highly charged ions, create difficulties in handling such calculations. In some cases, however, double-capture channels may be populated directly, leading to important double-capture cross sections—the process may even be dominant in the resonant He^{2+}+He collision [3–5]—and a complete calculation is possible.

We report here a molecular treatment of the B^{4+}+He system in the 0.3–13 keV/amu energy range using an *ab initio* configuration-interaction method for the determination of the potential-energy curves and couplings, followed by a semiclassical collisional treatment including electron translation effects. This system has been already studied theoretically within the framework of the semiclassical close-coupling formalism with two-electron atomic orbitals by Fritsch and Lin [6] and Hansen and Taulbjerg [7] using different model potentials. Their results are in good agreement for single-electron capture, but differ by about a factor 5 for double capture, perhaps owing to the model potential used, as stated by Hansen and Taulbjerg [7]. In order to go further, we have undertaken an alternative approach of this collisional system by means of a full electron molecular expansion method, focusing our attention on the double-electron-capture mechanism.

II. COMPUTATIONAL METHOD

Since the effect of spin orbit is of negligible importance in the energy range of interest, only the $^2\Sigma$ and $^2\Pi$ states correlated to the entry channel $\{B^{4+}(1s)+\mathrm{He}(1s^2)\}\ ^2\Sigma$ and the $\{B^{3+}(1s2l)+\mathrm{He}^{+}(1s)\}$ and $\{B^{2+}(1s2l2l')+\mathrm{He}^{2+}\}$ configurations have been considered in the calculation. The potential-energy curves have been calculated in the interatomic distance range 2–20 a.u. by means of an *ab initio* methods with configuration-interaction according to the CIPSI (configuration interaction by perturbation of a multiconfiguration wave function selected iteratively) algorithm [8] with a threshold $\eta=0.01$ ensuring a fair description of the perturbation contribution to the wave function.

For boron, we have used the contracted $6s,4p,2d$ basis of Gaussian functions previously optimized on the $B^{3+}(1s2s)$ ion [9], which had been shown to provide a particularly fair description of the $B^{2+}(1s2l2l')$ levels involved in the double-capture process. For helium, we took the $4s,1p$ contracted basis, already optimized for multicharged ion-helium collisions [10].

The radial coupling matrix elements between all pairs of states of the same symmetry have been calculated by means of the finite-difference technique:

$$g_{KL}(R)=\langle\Psi_K|\partial/\partial R|\Psi_L\rangle=\lim_{\Delta=0}1/\Delta\langle\Psi_K(R)|\Psi_L(R+\Delta)\rangle,$$

with the parameter $\Delta=0.0012$ a.u. as previously tested and using the boron nucleus as origin of electronic coordinates. The rotational coupling $\langle\Psi_K|iL_y|\Psi_L\rangle$ has been calculated directly from the quadrupole moment tensor between elec-

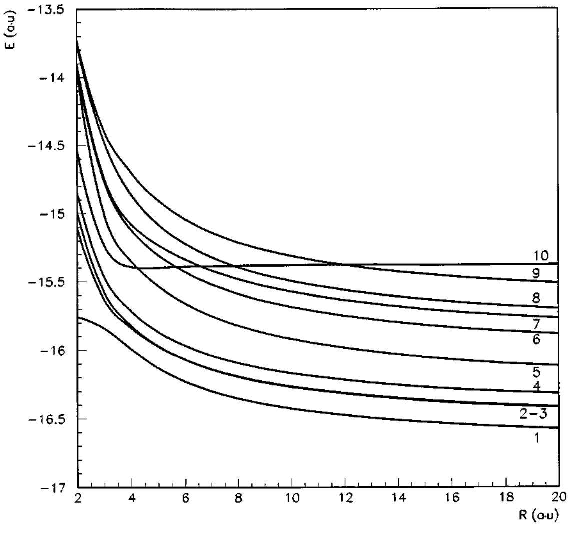

FIG. 1. Adiabatic potential-energy curves for the $^2\Sigma$ states of BHe^{4+}: 1 and 2, Σ states dissociating to $\{B^{3+}(1s2s)\ ^{1,3}S+\mathrm{He}^{+}(1s)\}$; 3 and 4, Σ states dissociating to $\{B^{3+}(1s2p)\ ^{1,3}P+\mathrm{He}^{+}(1s)\}$; 5, Σ state dissociating to $\{B^{2+}(1s2s^2)^2S+\mathrm{He}^{2+}\}$; 6 and 7, Σ states dissociating to $\{B^{2+}(1s2s2p)\ ^2P+\mathrm{He}^{2+}\}$; 8, Σ state dissociating to $\{B^{2+}(1s2p^2)^2D+\mathrm{He}^{2+}\}$; 9, Σ state dissociating to $\{B^{2+}(1s2p^2)^2S+\mathrm{He}^{2+}\}$; 10, Σ state dissociating to $\{B^{4+}(1s)+\mathrm{He}(1s^2)\}$.

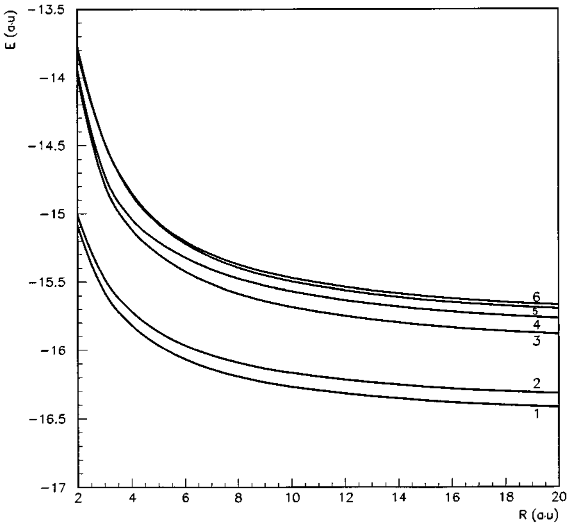

FIG. 2. Adiabatic potential-energy curves for the $^2\Pi$ states of BHe^{4+}: 1 and 2, Π states dissociating to $\{B^{3+}(1s2p)^{1,3}P + He^{+}(1s)\}$; 3 and 4, Π states dissociating to $\{B^{2+}(1s2s2p)\ ^2P + He^{2+}\}$; 5 and 6, Π states dissociating to $\{B^{2+}(1s2p^2)^2D + He^{2+}\}$.

tronic wave functions leading also to the consideration of translation effects in the collision dynamics. In the approximation of the common translation factor developed by Errea, Mendez, and Riera [11], the radial and rotational coupling matrix elements between states Ψ_K and Ψ_L may indeed be transformed respectively into [12]

$$\langle \Psi_K | \partial/\partial R - (\epsilon_K - \epsilon_L) z^2/2R | \Psi_L \rangle,$$

$$\langle \Psi_K | iL_y + (\epsilon_K - \epsilon_L) zx | \Psi_L \rangle,$$

where ϵ_K and ϵ_L are the electronic energies of states Ψ_K and Ψ_L and z^2 and zx are the components of the quadrupole moment tensor. This expression is applicable for any choice of the origin of the electronic coordinates. We have taken the boron nucleus as the origin of electronic coordinates in the molecular structure calculation. The collision dynamics has been treated by semiclassical methods in the 0.1–0.7 a.u. velocity range using the EIKONXS program [13] and including radial and rotational couplings as well as electron translation effects.

III. RESULTS AND DISCUSSION

The adiabatic potential-energy curves of the $^2\Sigma$ and $^2\Pi$ states are presented respectively in Figs. 1 and 2. The asymptotic values obtained from the configuration interaction performed at 20 a.u. corrected by the Coulombic repulsion term (neglecting the $1/R^4$ diffusion term) at this distance are reported in Tables I and II and show good agreement with experimental [14] (single-electron-capture levels) and theoretical data taking into account relativistic correction terms [15] (double-electron-capture levels), especially for exit channels.

TABLE I. Comparison with experiment [14] of asymptotic energy values for single-electron-capture levels (in a.u.).

Level	CIPSI calculation	Experiment [14]
$B^{4+} + He$	1.345	1.331
$B^{3+}(1s2p)^1P + He^+$	0.258	0.257
$B^{3+}(1s2p)^3P + He^+$	0.161	0.161
$B^{3+}(1s2s)^1S + He^+$	0.157	0.155
$B^{3+}(1s2s)^3S + He^+$	0.0	0.0

TABLE II. Comparison with theoretical data [15] of asymptotic energy values for double-electron-capture levels (in a.u.).

Level	CIPSI calculation	Calculation [15]
$B^{4+} + He$	0.938	0.971
$B^{2+}(1s2p^2)^2S + He^{2+}$	0.605	0.600
$B^{2+}(1s2p^2)^2D + He^{2+}$	0.420	0.423
$B^{2+}(1s2s2p)^2P + He^{2+}$	0.349	0.341
	0.234	0.236
$B^{2+}(1s2s^2)^2S + He^{2+}$	0.0	0.0

The double-capture exit channels show strong avoided crossings between successive $^2\Sigma$ states at, respectively, $R = 4.2$, 5.65, 6.6, 7.78, and 12.1 a.u., leading to a quasidiabatic shape for the curves. The corresponding radial coupling matrix elements are very sharp, as shown in Fig. 3. No evidence of any avoided crossing is shown on the $^2\Pi$ adiabatic potential-energy curves. Using these data, we have performed the collisional treatment in the semiclassical framework, owing to the velocity range of interest. In accordance with previous calculations [6,7], the one-electron-capture cross-section levels are in the range from 1.0×10^{-16} cm^2 (for $v = 0.1$ a.u.) to 3.3×10^{-16} cm^2 (for $v = 0.5$ a.u.) for capture on the $2p$ level and the values are lower for capture on the $2s$ level, in the $(0.03–0.95) \times 10^{-16}$ cm^2 range for velocities between 0.1 and 0.7 a.u. The cross sections of double-electron capture are presented in Figs. 4–6 (solid curves) and are compared directly to the previous calculation of Fritsch and Lin (dotted curves) and Hansen and Taulbjerg

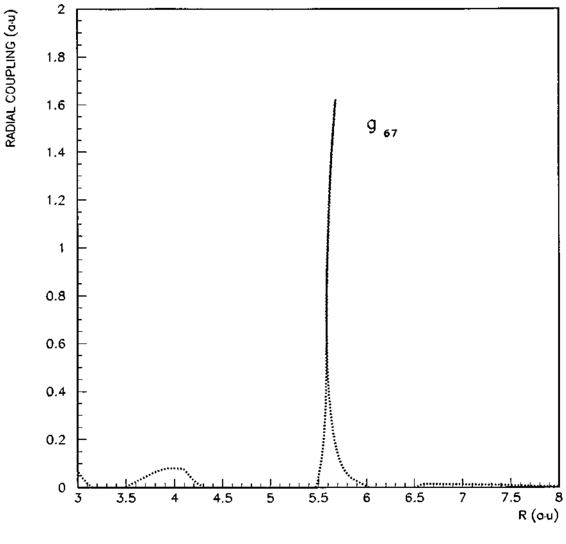

FIG. 3. Nonadiabatic radial coupling matrix elements between $^2\Sigma$ states.

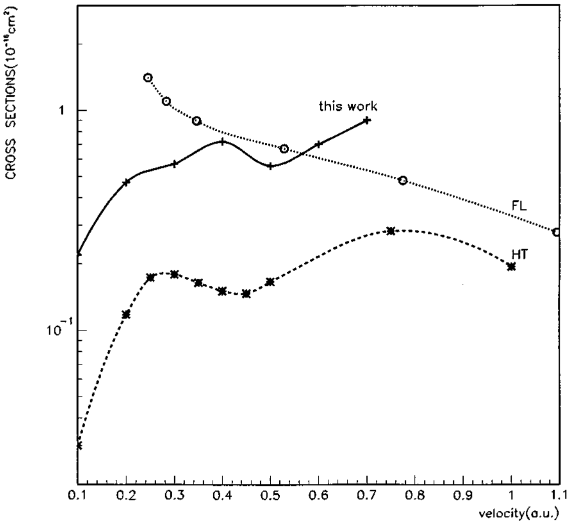

FIG. 4. Partial cross sections on the $\{B^{2+}(1s2s^2)+He^{2+}\}$ level: —, this work; ······, Fritsch and Lin [6]; - - - -, Hansen and Taulbjerg [7].

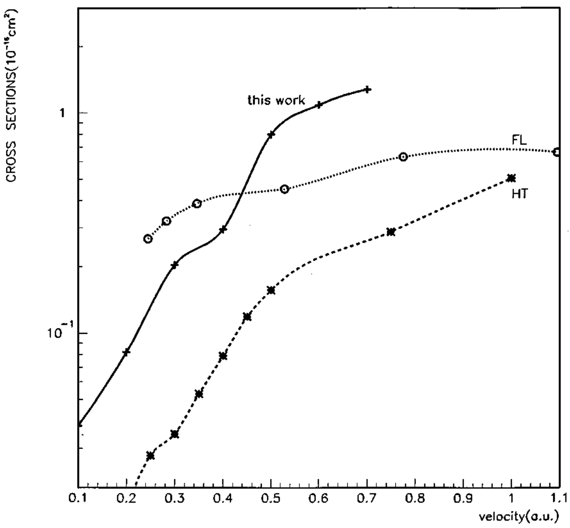

FIG. 6. Partial cross sections on the $\{B^{2+}(1s2p^2)+He^{2+}\}$ levels (same caption as in Fig. 4).

(broken curves) in the same energy range. Our molecular treatment taking into account the three electron interactions seems to be well adapted to describe precisely the $B^{2+}(1s2l2l')$ levels, the correlation effects between $1s$ and $2l$ orbitals being included in the configuration-interaction calculation.

From the present results, our work is shown to be in better agreement with the absolute values of the partial cross sections obtained by Fritsch and Lin [6], especially for the capture on the $B^{2+}(1s2s2p)$ level for which the accordance is quite good, than with the calculation of Hansen and Taulbjerg [7]. Nevertheless, for the variations of the cross sections, our results reproduce quite well the calculations of Hansen and Taulbjerg [7] for the capture on $B^{2+}(1s2s^2)$ and $B^{2+}(1s2p^2)$ levels, which recurs by the total double-capture cross sections (Fig. 7), although their values remain underestimated at all velocities. The complete collapse of the cross sections at lower energies seems yet not very realistic. As we are dealing with an adiabatic representation calculation, these comparisons may be driven mainly at low energies, but the consideration of translation effects could allow us to extend our calculation to higher energies.

IV. CONCLUSION

This work provides an all-electron calculation of the $B^{4+}+He$ double-capture process. Such an approach gets rid of the frozen-core approximation to represent the $1s$ electron and so provides a reliable evaluation of the relaxation of the $1s$ electron in the description of the $B^{2+}(1s2l2l')$ levels, which is certainly enhanced here as we are dealing with open shell systems. In the model potential approach, a careful choice of the potential is thus needed in order to obtain accurate results in such systems with more than two electrons.

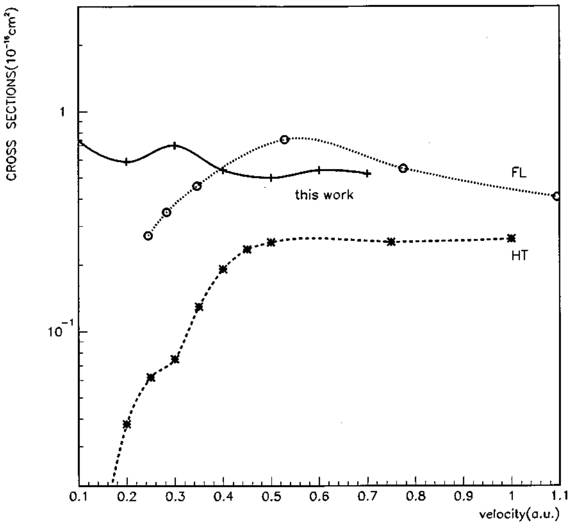

FIG. 5. Partial cross sections on the $\{B^{2+}(1s2s2p)+He^{2+}\}$ levels (same caption as in Fig. 4).

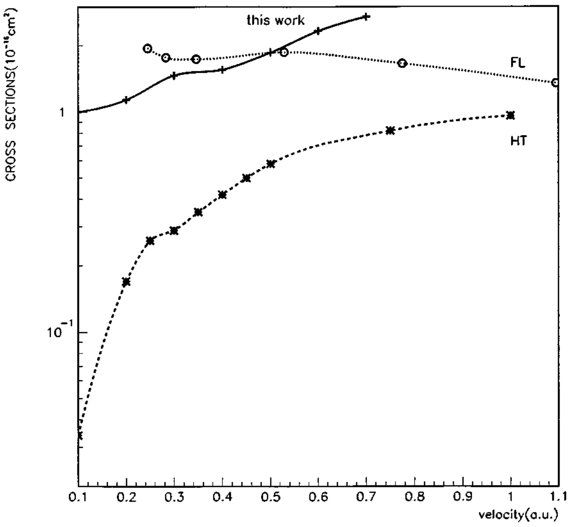

FIG. 7. Total double-electron-capture cross sections (same caption as in Fig. 4).

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