Theoretical charge-exchange Galilean invariant cross sections for the $B^{3+}+He$ collision

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Galilean invariant cross sections were calculated for one-electron capture in collisions of B^{3+} with He at velocities between 0.063 and 0.63 a.u. The collision was described within the framework of the perturbed stationary-state approach with the potential-energy curves and nonadiabatic couplings computed with highly correlated configuration-interaction wave functions. A procedure was also proposed to incorporate Galilean invariance without the explicit calculation of translation factors and a method developed to solve the coupling integrals. Cross-section results are in good agreement with existing experimental and theoretical data.

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I. INTRODUCTION

Collision processes involving multicharged ions and neutral atoms have been a subject of continuous research interest [1,2]. These studies have been motivated not only academically with theoreticians seeking a better understanding of the theories describing the collisions and their approximations [3-5] but also by the scientific and technological applicability associated with such processes [6].

Reactions in interstellar medium [7–10], controlled thermonuclear reactions [11,12], and the development of lasers in the ultraviolet and soft-x-ray regions [13-16] are examples of research areas where ion-atom collisions are very important.

In this study we have focused out attention on the collision of boron ions with helium atoms according to the equation

$$B^{3+}(1s^2)+He(1s^2)\rightarrow B^{2+}(1s^2nl)+He^{+}(1s)\ ,$$

and for velocities in the range of 0.063–0.63 a.u. It is well know, however, that in this range of velocities a correction in the electronic movement due to the nuclear motion become important since the molecular method usually employed to treat this problem does not obey the asymptotic condition of the collision [17], and Schrödinger's equation is not invariant under a Galilean transformation in this context. As a consequence, to incorporate this invariance, a translation factor [4] is generally included in the molecular expansions describing such collisions.

The importance of boron in controlled thermonuclear fusion experiments and the suitability of four-electron systems to high-level electronic description make the $[BHe]^{3+}$ system ideal as a model to test solutions to the problem of the translation noninvariance of the cross section.

In this paper, using highly correlated electronic wave functions of the configuration-interaction type, cross sections for one-electron capture are calculated within the framework of the perturbed stationary-state (PSS) [5] approach. A proposal to eliminate the calculation of translational factors as in the usual approach is also presented. In Sec. II, a brief account of the theory underlying both the electronic structure calculation and the collision cross sections are presented, and the steps leading to the elimination of the translation factors explained. Section III contains the principal results and a discussion of their meaning. Finally, in Sec. IV the main conclusions are presented.

II. METHODOLOGY

A. Electronic structure

The electronic structure was described at the configuration-interaction (CI) level as implemented in the MELD [18] codes, and having the Hartree-Fock configuration as the zero-order function. Single and double excitations relative to the Hartree-Fock configuration were then generated and selected by second-order perturbation theory using an energy threshold of 1.0×10^{-6} a.u. Although singly excited configurations do not contribute to the energy, in this order they were kept, and the final wave function restricted to 1000 terms. Electronic energies and wave functions were finally obtained as the lowest eigenvalues and eigenvectors of the CI Hamiltonian matrix for the states of $^1\Sigma^+$ and $^1\Pi$ symmetries. These calculations have been carried out assuming C_{2v} point-group symmetry.

In the calculation of the molecular orbitals to be used in the CI excitation process, the sets of Cartesian Gaussians $(11s,6p)/[5s,4p]$ for boron [19] and $(6s,1p)/[4s,1p]$ helium [20] were employed. The boron set was still augmented with three d-type polarization functions with coefficients 1.11, 0.402, and 0.145 [19].

B. Scattering equation, radial and rotational couplings

As it is well known, in the perturbative stationary-state (PSS) [21] method the nuclear motion is described classically, whereas the electronic movement is treated in a

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quantum manner. Within this context, the wave function can be written as

$$\Psi(r,t)=\sum_{n\Lambda} a_{n\Lambda}(t)\Psi^{\mathrm{CI}}_{n\Lambda}(r;R(t)) \times\exp\left\{-i\int E_{n\Lambda}(R(t))dt\right\}, \quad (1)$$

where $a_{n\Lambda}(t)$ is the time-dependent perturbation coefficient, $E_{n\Lambda}$ is the Born-Oppenheimer CI energy of the state $n\Lambda$, and Λ is the total orbital angular momentum of the state $n\Lambda$.

For a total wave function given by expression (1), the PSS scattering equation reduces to

$$i\frac{da_{n\Lambda}(t)}{dt}=\sum_{n'\Lambda'} a_{n'\Lambda'}(t)\langle\Psi^{\mathrm{CI}}_{n\Lambda}|H_{\mathrm{el}}-i\frac{v^2t}{R}\frac{\partial}{\partial R} +\frac{vb}{R^2}L_y|\Psi^{\mathrm{CI}}_{n'\Lambda'}\rangle \times\exp\left\{-i\int_0^t(E_{n'\Lambda'}-E_{n\Lambda})dt'\right\}, \quad (2)$$

where v is the classical nuclear relative velocity, b is the impact parameter, H_{el} is the electronic Hamiltonian, and L_y is the y component of the total electronic angular momentum in the molecule reference system.

Equation (2) clearly shows that the terms $\partial/\partial R$ and iL_y couple different Born-Oppenheimer states, and which allow the total wave function to evolve into these states as a function of a classical parametric time. These couplings terms are known as the radial and rotational couplings, respectively, and are given explicitly by the expressions

$$\langle\Psi^{\mathrm{CI}}_n|\frac{\partial}{\partial R}|\Psi^{\mathrm{CI}}_{n'}\rangle=\sum_i C_i^n\frac{\partial C_i^{n'}}{\partial R}+\sum_{\alpha\beta}P^{nn'}_{\alpha\beta}\langle\Phi_\alpha|\frac{\partial}{\partial R}|\Phi_\beta\rangle \quad (3)$$

and

$$\langle\Psi^{\mathrm{CI}}_n|iL_y|\Psi^{\mathrm{CI}}_{n'}\rangle=\sum_{\alpha\beta}P^{nn'}_{\alpha\beta}\langle\Phi_\alpha|z\frac{\partial}{\partial x}-x\frac{\partial}{\partial z}|\Phi_\beta\rangle, \quad (4)$$

where the C_i^n's are the CI expansion coefficients for state n, Φ_α's are the orthonormal and symmetry-adapted configuration state functions, $P^{nn'}_{\alpha\beta}$ is the transition density matrix, R is the internuclear distance, and x and z are electronic coordinates.

In this work, the derivatives of the CI expansion coefficients were computed by finite differentiation, and Eq. (2) was solved using the PAMPA program [22] modified by Errea, Mendez, and Riera [23] to include what is known as the common electronic translation factor if so required.

C. Transition and diffusion amplitudes and cross sections

After the solution of Eq. (2), the transition amplitude (t_{jf}) for each trajectory is computed as the scalar product of the total wave function in the limit of $t\to\infty$ and the wave function of the final state (f)[$t_{jf}=\lim_{t\to\infty}a_f(t)$], subject to the initial conditions $a_j(-\infty)=1$ and $a_f(-\infty)=0$.

The diffusion amplitude can then be expressed by the integral

$$f_{jf}(\theta,k)=ik\int_0^\infty db\, bJ_M(2kb\sin(\theta/2))[t_{jf}(b)-\delta_{jf}], \quad (5)$$

where j and f represent the initial and final states, respectively; k is the linear momentum; and J_M is the cylindrical Bessel function of order $M=|\Lambda_j-\Lambda_f|$. This integral was solved with the aid of the EIKON program [24] modified by Harel.

Cross sections were finally computed by the expressions

$$\frac{d\sigma_{jf}(\theta)}{d\Omega}=|f_{jf}(\theta,k)|^2 \quad (6)$$

and

$$\sigma_{jf}=\int d\Omega\frac{d\sigma_{jf}(\theta)}{d\Omega}=2\pi\int_0^\infty db\, b|t_{jf}(b)-\delta_{jf}|^2. \quad (7)$$

D. Cross sections and their origin dependence

The problem of the origin dependence of the solutions to Eq. (2) and the associated Galilean noninvariant cross sections were discussed by Bates and McCarroll [17] late in the 1950s. Plane waves describing the translation of electrons bound to a nucleus that moves relative to the origin of the coordinate system have been introduced in the literature as an *ad hoc* attempt to incorporate Galilean invariance and have since been known as translation factors (TF) [17,25–27].

As shown by Bates and McCarroll [17], the expansion of Eq. (1) does not obey the asymptotic condition of the collision. For a fixed origin, the dynamic couplings depend on the origin of the integration, and therefore this dependence is also transferred to the cross sections. Explicitly, this dependence can be written as

$$\langle\Psi^{\mathrm{CI}}_n|\frac{\partial}{\partial R}\Big|_{O'}|\Psi^{\mathrm{CI}}_{n'}\rangle =\langle\Psi^{\mathrm{CI}}_n|\frac{\partial}{\partial R}\Big|_{O}|\Psi^{\mathrm{CI}}_{n'}\rangle+\frac{R_{OO'}}{R}\langle\Psi^{\mathrm{CI}}_n|iP_z|\Psi^{\mathrm{CI}}_{n'}\rangle \quad (8)$$

and

$$\langle\Psi^{\mathrm{CI}}_n|iL_y\Big|_{O'}|\Psi^{\mathrm{CI}}_{n'}\rangle =\langle\Psi^{\mathrm{CI}}_n|iL_y\Big|_{O}|\Psi^{\mathrm{CI}}_{n'}\rangle-R_{OO'}\langle\Psi^{\mathrm{CI}}_n|iP_x|\Psi^{\mathrm{CI}}_{n'}\rangle, \quad (9)$$

where O and O' are the origins of two different electronic coordinate systems, $R_{OO'}$ is the separation vector between these origins, and p_x and p_z are the components of the electronic linear momentum operator.

This origin dependence introduces physically unacceptable situations like transitions at infinity when the Stark effect is also present. In the usual formulation without the TF, the radial coupling ($\langle\partial/\partial R\rangle$) is a con-

stant and the rotational coupling ($\langle iL_y \rangle$) behave asymptotically as R, whereas decays varying as R^{-3} and R^{-2} would be expected [28].

E. Galilean invariance without the translation factor

As it is well known, Galilean invariance is initially implicit in Schrödinger's equation, and its solutions are expected to preserve this property. When the adiabatic approach is used to separate the various modes of motion of a molecular system the localization of the origin of the electronic coordinates is critical to maintaining Galilean invariance during the collision.

In this work we are proposing an alternative solution to this problem which we named the central-field approach. The physical basis underlying the procedure used in this work to avoid the explicit calculation of translation factors is very similar to that describing the interaction of two bodies governed by a radial potential of a Coulombic (or gravitational) type; that is, it can be reduced to the description of an effective particle of reduced charge (or mass) subjected to a central field with the origin in the center of charge (or mass) of the system. The choice of an origin other than that of the central field gives rise to the appearance of noninertial forces and the motion will consequently become more complex to describe. Different choices of origins imply different descriptions.

The calculation of the radial coupling using the CI methodology can ultimately be reduced to a sum of integrals of the type $\langle \varphi_B | \partial/\partial R | \varphi_K \rangle$, which is essentially, in its most general case, a two-center, one-electron integral, which depends parametrically on the internuclear distance. This two-center problem can basically be transformed to a central-field-type description by choosing an origin $\mathbf{P}_{ij}$ defined by the relation

$$\mathbf{P}_{ij}=\frac{\alpha_j}{\alpha_i+\alpha_j}\mathbf{B}+\frac{\alpha_i}{\alpha_i+\alpha_j}\mathbf{A}\ , \tag{10}$$

where α_i and α_j are the exponents of the Gaussians centered on atoms A and B, respectively, located by the vectors $\mathbf{A}$ and $\mathbf{B}$. This relation is the usual one of transforming the product of two Gaussians on different centers to a single Gaussian on another intermediate center [29]. The center defined in this way can be seen as having an effective charge which depends both on the electronic atomic distribution and on the nuclei separation.

In this work, every integral contributing to a dynamical coupling is calculated as a central-field problem. It is important to point out, however, that the choice of an origin is made *a posteriori;* that is, first the coupling operator is applied to the Gaussian basis and then the integral is carried out analytically, choosing as origin that of the central field defined by Eq. (10).

This way of approaching the calculation of the dynamic couplings renders easy the interpretation of the problems that usually arise in the limit of separated atoms. For a fixed origin, if both functions are centered on the same atom, the parametric dependence on R still exists, since that origin is now at infinity and is not coincident with the center of force, the only exception being when $R=0$.

Using this approach, the matrix elements between unnormalized Cartesian Gaussians (φ) defining the radial and rotational couplings can then be written as [30]

$$\begin{aligned}\langle \varphi_B | \partial/\partial R | \varphi_K \rangle = &\exp\left\{\frac{-\alpha_B\alpha_K R^2}{\alpha}\right\} G\left[\frac{N+1}{2}\right] G\left[\frac{L+1}{2}\right] \\ &\times\left\{\sum_{b=0}^{m_B}\sum_{k=0}^{m_K+1}(\hat{\mathbf{B}}\cdot\hat{\mathbf{R}})^b\times(\hat{\mathbf{K}}\cdot\hat{\mathbf{R}}^{k+1})\begin{bmatrix}m_B\\ b\end{bmatrix}\begin{bmatrix}m_K+1\\ k\end{bmatrix}\left[\frac{\alpha_K R}{\alpha}\right]^b\left[\frac{\alpha_B R}{\alpha}\right]^k\right. \\ &\left.\times G\left[\frac{M-b-k}{2}\right]\alpha^{-(N+L+M-b-k+2)/2}[f_{\text{rad}}]\left[\frac{(m_K+1-k)(m_K-k)}{(m_K+1)}-\frac{\alpha_K(M-b-k)}{\alpha}\right]\right\}\end{aligned} \tag{11}$$

and

$$\begin{aligned}\langle \varphi_B | i\hat{L}_y | \varphi_K \rangle = &\exp\left\{\frac{-\alpha_B\alpha_K R^2}{\alpha}\right\} G\left[\frac{N}{2}\right] G\left[\frac{L+1}{2}\right] \\ &\times\left\{\sum_{b=0}^{m_B}\sum_{k=0}^{m_K+1}(\hat{\mathbf{B}}\cdot\hat{\mathbf{R}})^b(\hat{\mathbf{K}}\cdot\hat{\mathbf{R}})^k\times\begin{bmatrix}m_B\\ b\end{bmatrix}\begin{bmatrix}m_K+1\\ k\end{bmatrix}\left[\frac{\alpha_K R}{\alpha}\right]^b\left[\frac{\alpha_B R}{\alpha}\right]^k\frac{\alpha^{-(N+L+M-b-k+3)/2}}{2(m_K+1)}\right. \\ &\times\left[G\left[\frac{M-b-k}{2}\right]\left[N(m_K+1-k)(m_K-k)-\frac{(M-b-k)kN\alpha_K}{\alpha}-n_K(M-b-k)(m_K+1-k)\right]\right. \\ &\left.\left.+\frac{2R}{\alpha^{1/2}}G\left[\frac{M-b-k+1}{2}\right][f_{\text{rot}}](m_K+1-k)(\alpha_K N-\alpha n_K)\right]\right\}\ ,\end{aligned} \tag{12}$$

where $\alpha=\alpha_B+\alpha_K$, $N=n_B+n_K$, $L=l_B+l_K$, and $M=m_B+m_K$; the variables n, l, and m can take the value 0 or a positive integer and define the angular part of the Cartesian Gaussian functions ($x^n y^l z^m e^{-\alpha r^2}$) used in the construction of the molecular orbitals; $\hat{\mathbf{B}}$ and $\hat{\mathbf{K}}$ are unit vectors in the direction of the position vectors of the atoms where the bra and ket functions are centered, respectively, with the z axis containing both atoms; $\hat{\mathbf{R}}$ is the unit vector in the direction of the internuclear vector $\mathbf{R}$; and $\binom{m}{n}$ is the binomial coefficient. The function $G(\xi)$ is defined to be equal to zero if ξ is an even integer, and equal to the gamma function $\Gamma(\xi/2)$ if ξ is an odd integer.

The terms f_{rad} and f_{rot} in Eqs. (11) and (12) are equal to α_B/α and zero, respectively, for a central-field origin, and equal to 0.5 and $(\alpha_K-\alpha_B)/2\alpha$ for the geometric center. When both functions are on the same atom, Eq. (11) is null for the central field, since as implicit in the definition of the origin, there is now no dependence on the internuclear distance.

An important result now contained in these equations is that for a central-field origin the radial coupling ($\langle \partial/\partial R \rangle$) decays as R^{-3}, and the rotational coupling ($\langle iL_y \rangle$) decays as R^{-2} for very large internuclear distances, and therefore eliminates the physically unacceptable transitions at infinity when the Stark effect is also present and therefore avoids the use of the *ad hoc* TF.

III. RESULTS AND DISCUSSION

The potential-energy curves of the five lowest adiabatic singlet states of $[BHe]^{3+}$ which correlate with the first four asymptotic atomic channels are shown in Fig. 1. A typical repulsive covalent-ionic behavior is clear in this figure. The entrance channel is covalent and the exit channels are ionic. An avoided crossing at $\sim 4.5a_0$ between the states $1\,^1\Sigma^+$ and $2\,^1\Sigma^+$ is responsible for the metastablity of the ground state and gives rise to a potential well of $\sim 1.38\times10^4$ cm^{-1} deep. Such metastability, however, is not important for medium or high collision energies. The state $2\,^1\Sigma^+$ avoids another crossing at $\sim 7.0a_0$ with the state $3\,^1\Sigma^+$ describing the entrance channel.

Radial couplings ($\partial/\partial R$) calculated with the origin at the central field (CF), expected to give similar results as those with the origin at the geometric center (GC) plus TF, and those computed at the GC without the TF are displayed in Figs. 2 and 3. Rotational couplings are shown in Fig. 4. From these figures one can see that the CF (or GC+TF) and the GC without the TF approaches give very similar results for certain pair of states; however, at large distances, the incorrect asymptotic behavior of the GC approach without the TF is made very clear. Some of the radial couplings ($\partial/\partial R$) with Stark effect are constants at large R for the GC integration, but in the CF (or GC+TF) calculation they decay properly as R^{-3}.

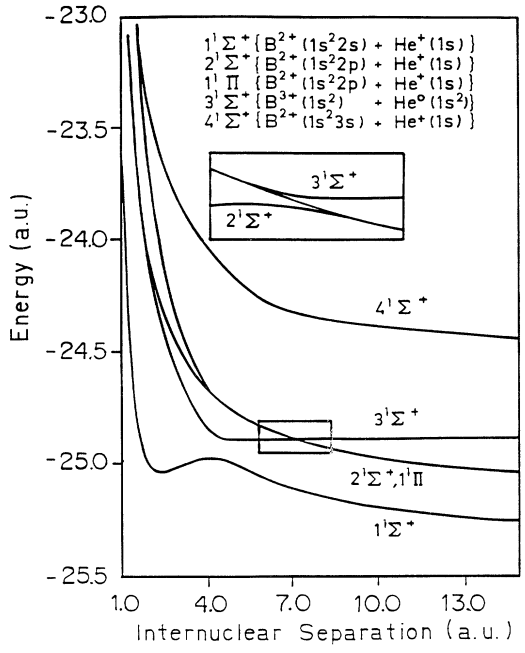

FIG. 1. Potential-energy curves for the lowest-lying electronic states of the quasimolecule $[BHe]^{3+}$.

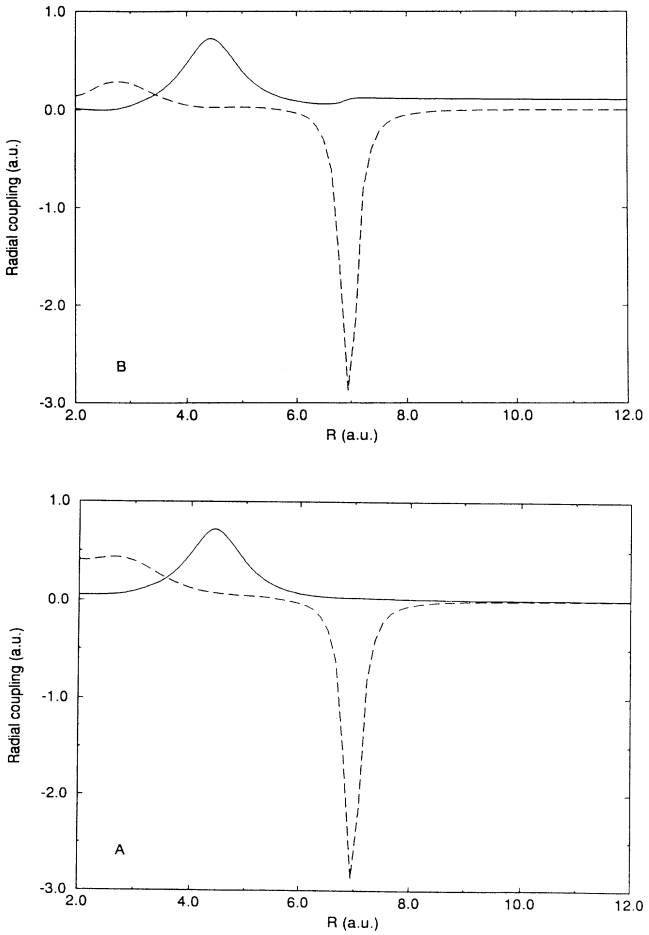

FIG. 2. Radial coupling as a function of the internuclear distance. (a) Origin at the central field. (b) Origin at the geometric center, without translation factors. ——, $1\,^1\Sigma^+-2\,^1\Sigma^+$; — — —, $2\,^1\Sigma^+-3\,^1\Sigma^+$.

In the same manner, the rotational couplings (iL_y) increase as R in GC calculations and decay as R^{-2} in the CF (or GC+TF) approach.

Total, partial, and relative cross section results for one-electron capture using the semiclassical approach are collected in Table I. The letters A and B label the CF calculations with and without the inclusion of the state $1\,^1\Pi$, respectively. The values represented by the letter C are those in the GC without the TF, and those labeled by the letters D and E include the TF until first and second orders in the velocity, respectively. Note that the results obtained with the CF approach (A) proposed in this study are very similar to those calculated with the usual TF method (D and E) but differ significantly from those computed without the TF (C).

The results for the total cross section calculated in this

TABLE I. Total, differential, and relative cross sections (10^{-16} cm^2) for the system $[BHe]^{3+}$ for several relative velocities (in 10^7 cm/s).

Veloc.	$\sigma\Sigma(2s)$	$\sigma\Sigma(2p)$	$\sigma\Pi(2p)$	$\sigma\Sigma(3s)$	σ_t	σ_{2p}	σ_{2s}/σ_{2p}
			A. CF with the inclusion of the $^1\Pi$ state				
1.383	2.827	1.981	4.235	0.016	9.060	6.216	0.455
1.575	3.460	2.298	4.063	0.020	9.842	6.361	0.544
1.947	4.657	1.854	4.048	0.039	10.600	5.902	0.789
3.085	7.741	1.217	3.473	0.038	12.470	4.690	1.651
4.375	8.789	2.070	4.072	0.025	14.960	6.142	1.431
6.191	9.024	1.199	4.569	0.076	14.870	5.768	1.565
9.779	7.394	1.278	3.461	0.224	12.360	4.739	1.560
13.830	5.744	1.728	3.232	0.536	11.240	4.960	1.158
			B. CF without the inclusion of the $^1\Pi$ state				
1.383	3.116	4.786		0.016	7.917		0.651
1.575	3.901	4.504		0.021	8.428		0.866
1.947	5.016	4.195		0.029	9.239		1.196
3.085	8.481	2.806		0.027	11.310		3.023
4.375	10.120	2.691		0.056	12.870		3.761
6.191	9.719	4.123		0.042	13.880		2.357
9.779	7.850	4.727		0.086	12.670		1.661
13.830	6.708	3.626		0.419	10.760		1.850
			C. Geometric center (GC)				
1.383	2.876	1.964	4.001	0.006	8.846	5.965	0.482
1.575	3.513	2.191	3.786	0.012	9.502	5.977	0.598
1.947	4.682	1.699	3.664	0.025	10.070	5.363	0.873
3.085	7.898	0.083	2.947	0.017	11.690	3.773	2.093
4.375	9.133	1.358	2.879	0.078	13.450	4.237	2.156
6.191	10.020	0.943	2.718	0.077	13.760	3.661	2.737
9.779	8.110	2.313	1.522	0.162	12.110	3.835	2.115
13.830	7.816	1.620	2.461	0.431	12.330	4.081	1.915
			D. Geometric center (GC) with TF (first order in velocity)				
1.383	2.776	2.062	4.125	0.008	8.972	6.187	0.449
1.575	3.407	2.334	3.936	0.013	9.690	6.270	0.543
1.947	4.598	1.803	3.893	0.023	10.320	5.696	0.807
3.085	7.683	1.185	3.384	0.018	12.270	4.569	1.682
4.375	8.791	2.100	4.055	0.049	14.990	6.155	1.428
6.191	9.120	1.318	4.681	0.049	15.170	5.999	1.520
9.779	7.418	1.321	3.579	0.156	12.470	4.900	1.514
13.830	5.648	1.989	3.556	0.385	11.580	5.545	1.019
			E. Geometric center (GC) with TF (first and second orders in velocity).				
1.383	2.780	2.052	4.111	0.008	8.951	6.163	0.451
1.575	3.415	2.319	3.917	0.013	9.663	6.236	0.548
1.947	4.611	1.785	3.865	0.023	10.280	5.650	0.816
3.085	7.729	1.148	3.327	0.018	12.220	4.475	1.727
4.375	8.908	1.939	3.988	0.048	14.880	5.927	1.503
6.191	9.241	1.145	4.618	0.049	15.050	5.763	1.604
9.779	7.307	1.413	3.666	0.193	12.580	5.079	1.439
13.830	5.131	2.143	3.986	0.418	11.680	6.129	0.837

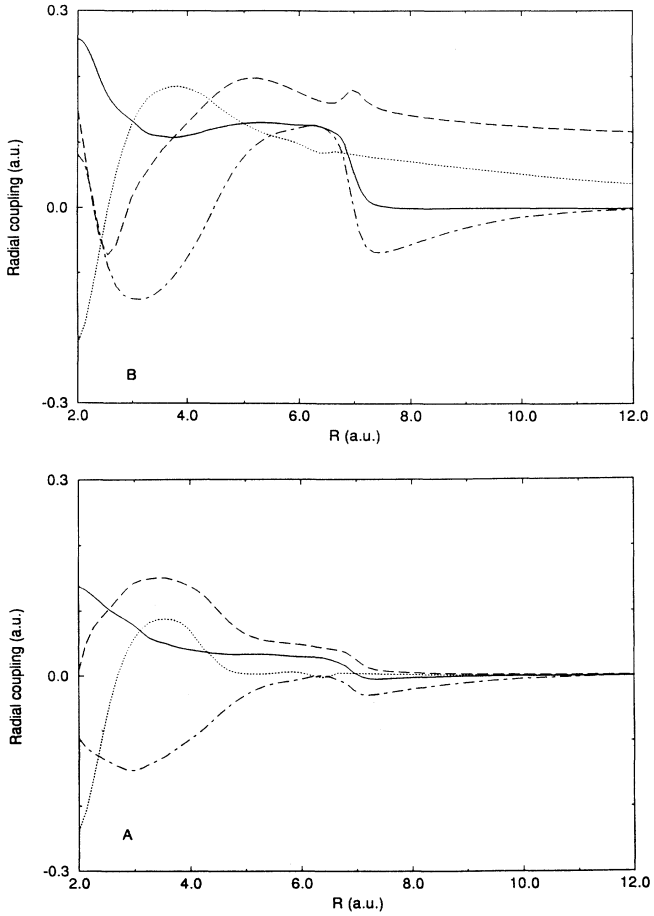

FIG. 3. Radial coupling as a function of the internuclear distance. (a) Origin at the central field. (b) Origin at the geometric center, without translation factors. ——, $1\,^1\Sigma^+-3\,^1\Sigma^+$; . . . ., $1\,^1\Sigma^+-4\,^1\Sigma^+$; — — —, $2\,^1\Sigma^+-4\,^1\Sigma^+$; —·—·—, $3\,^1\Sigma^+-4\,^1\Sigma^+$.

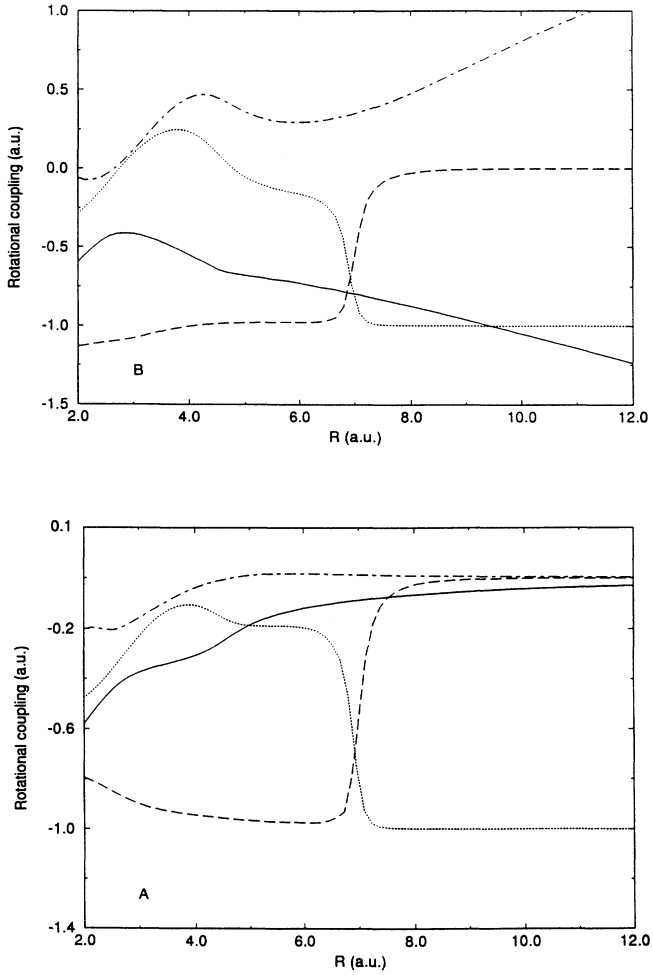

FIG. 4. Rotational coupling as a function of the internuclear distance. (a) Origin at the central field. (b) Origin at the geometric center, without translation factors. ——, $1\,^1\Sigma^+-1\,^1\Pi$; . . . ., $2\,^1\Sigma^+-1\,^1\Pi$; — — —, $3\,^1\Sigma^+-1\,^1\Pi$; —·—·—, $4\,^1\Sigma^+-1\,^1\Pi$.

work are compared in Fig. 5 with the experimental studies of Zwally and Cable [31], Crandall [32], Gardner *et al.* [33], and Iwai *et al.* [34], and with the theoretical results of Shipsey, Browne, and Olson [35], and of Crandall [32] for the remote capture of two electrons. Note in this figure the similar velocity dependence between these sets of data, especially the experimental ones. The total cross section calculated in this work and the theoretical results of Shipsey, Browne, and Olson [35] also have similar velocity dependence in the range of velocities studied, but while our values show a closer agreement with the more recent experimental study of Iwai *et al.* [34], those of Shipsey, Browne, and Olson [35] are concordant with the older experimental results of Zwally and Cable [31]. Recent theoretical results by Hansen, Dubois, and Nielsen [36] (not included in Fig. 5) seem to lie between the data of Iwai *et al.* and of Zwally and Cable. As to the total cross section for the remote capture of two electrons of Crandall [32], one can say that the capture channel is represented by the state $7\,^1\Sigma^+$, associated with the configuration $\{B^{1+}(1s^2 2s^2)\,^1S_0+He^{2+}\}$, and is 29.25 eV higher in energy than the ground state. As discussed by Crandall, the capture of two electrons must occur sequentially with the first electron captured at $\sim 7.0a_0$ and the second at $\sim 2.0a_0$.

In Fig. 6 are displayed the theoretical data of Zwally and Cable [31] for the total and partial cross sections using the Landau-Zener model, the theoretical results of Shipsey, Browne, and Olson [35] using the semiclassical approximation, data based on the central-field approach proposed in this work, and calculations using the geometric center without the translation factor. It is interesting to note that the calculation of the total cross section with the origin at the geometric center and without the inclusion of the translation factor is very similar to that reported by Shipsey, Browne, and Olson, despite the oscillation of the $2p_z$ cross section (σ_{2p}). This fact seems to be an indication that the problem of the non-Galilean invariance is the reason for the lower values of Shipsey, Browne, and Olson compared to those of our study. In fact, the effect of the translation motion of the

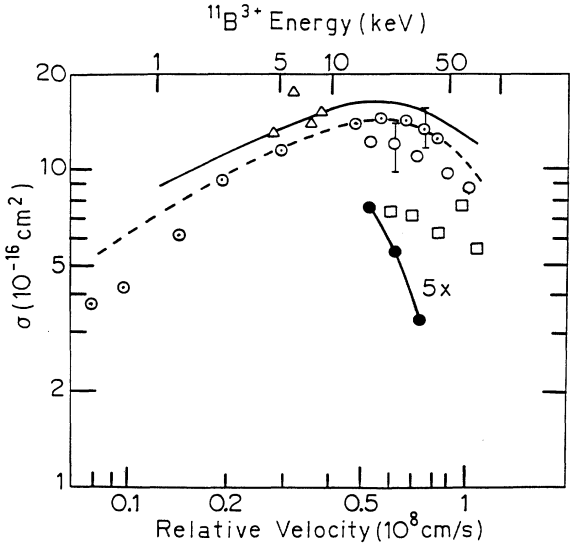

FIG. 5. Total cross section for the collision $B^{3+}+He$. ⊙⊙⊙, expt. Ref. [31]; ○○○, expt. Ref. [32]; □□□, expt. Ref. [33]; △△△, expt. Ref. [34]; — — —, theor. Ref. [35]; ●●● (two-electron capture), expt. Ref. [32]; ——, this work.

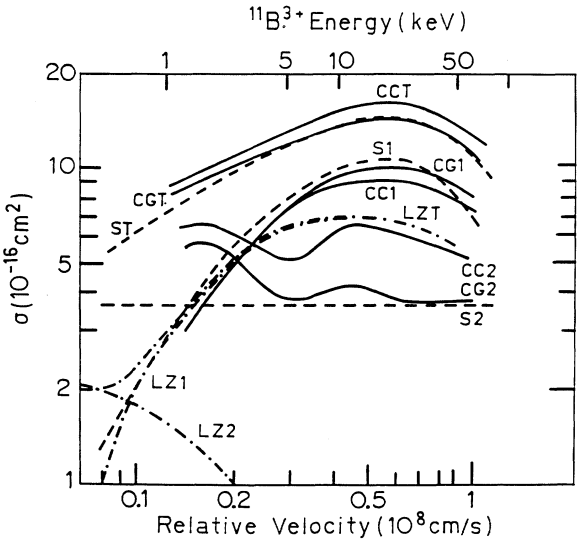

FIG. 6. Partial and total cross sections for the collision $B^{3+}+He$. —·—·—· ($LZ1$, partial cross section σ_{2s}; $LZ2$, partial cross section σ_{2p}; LZT, total cross section σ_t), Ref. [31]; — — — ($S1,\sigma_{2s}$;$S2,\sigma_{2p}$;ST,σ_t), Ref. [35]; —— (CC, central field; CG, geometric center without TF; the extensions 1, 2, and t refer to σ_{2s}, σ_{2p}, and σ_t), this work.

electrons in the computation of the coupling matrix elements was neglected in the study of Shipsey, Browne, and Olson.

Although the importance of electron correlation has recently been stressed by Hansen, Dubois, and Nielsen [36] in a study where a comparison between one- and two-electron models was made, we would like, however, also to call attention to the importance of the core correlation in the description of the entrance channel, since correlating four electrons increases the interaction between the entrance channel with the other channels and therefore increases the cross section. It is also worth pointing out that the results of Hansen, Dubois, and Nielsen for the cross sections included the electronic translational factor and, as pointed out above, they seem to lie between those of Zwally and Cable [31] and the more recent determination of Iwai *et al.* [34], with which our calculation shows a closer agreement. Unfortunately, with the exception of the study by Iwai *et al.*, the unavailability of explicit numerical values of the cross sections in the published works so far does not permit a more direct comparison to be made.

Also, as to a possible justification for the oscillatory behavior of σ_{2p}, one can point out that the first oscillation ($v\sim1.5\times10^7$ cm/s) is due to the first pseudocrossing, for in this energy region there is practically a transfer to a state whose asymptotic limit is described by the configuration $\{B^{2+}(1s^2 2p^1)+He^+(1s)\}$. As σ_{2p} decreases, σ_{2s} increases, for the greater the velocity the more population is transferred to the state $1\,^1\Sigma^+$. Also, the greater the velocity, the more effective the rotational coupling, with σ_{2p} showing another oscillation at $\sim4.4\times10^7$ cm/s.

Experimental and theoretical values for the relative cross section $[I(2s)/I(2p)$ or $\sigma_{2s}/\sigma_{2p}]$ are shown in Fig. 7. As discussed by Matsumoto *et al.* [37], by a direct comparison with the theoretical results of Shipsey, Browne, and Olson [35], the experimental results might be showing a loss of intensity of the products in the $2p$ sate. Since, as shown in Fig. 6, the results of Shipsey, Browne, and Olson seem to underestimate the partial cross section σ_{2p}, it is expected that the relative cross section should still become even lower. In fact, the results of this work displayed in Fig. 7 support an even larger loss in intensity than that originally discussed by Matsumoto *et al.* The same behavior was also displayed more recently in the calculation of Hansen, Dubois, and Neilsen of

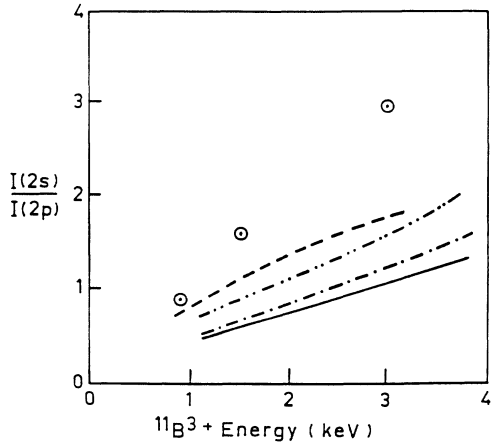

FIG. 7. Relative partial cross sections (σ_{2s}/σ_{2p}) for the collision $B^{3+}+He$. ⊙⊙⊙, Ref. [37]; — — —, Ref. [35]; –··–··–, this work (central field) without the state $^1\Pi$; —·—·—, this work (geometric center) without TF; ——, this work (central field).

the relative cross section, with their best values also underestimating the experimental results.

We also note that the probability of electron capture as a function of the impact parameter presented by Hansen, Dubois, and Neilson is very similar to our results [30], with a disagreement only for $b \leq 2$ a.u. For $v = 0.2$ a.u. and $b_{\max} \simeq 4$ a.u., the total cross section ($\sigma_t = \pi b_{\max}^2$) is estimated to be equal to 50 a.u.^{2} ($\simeq 1.4 \times 10^{-15}$ cm^2).

Finally, in Fig. 8 we have collected the reduced differential cross sections (RDCS, in cm^2) ($\theta \sin\theta d\sigma/d\Omega$) for one-electron capture as a function of the reduced angle τ ($\tau = E\theta$, in keV deg) calculated using the eikonal approximation as implemented in the EIKON program [23]. Clearly, the scattering is more favorable at small angles, and a maximum total cross section should occur for velocities in the range 0.20–0.28 a.u. It can also be seen that the maxima in Fig. 8 remain invariably in the same region of τ, independently of the velocity considered.

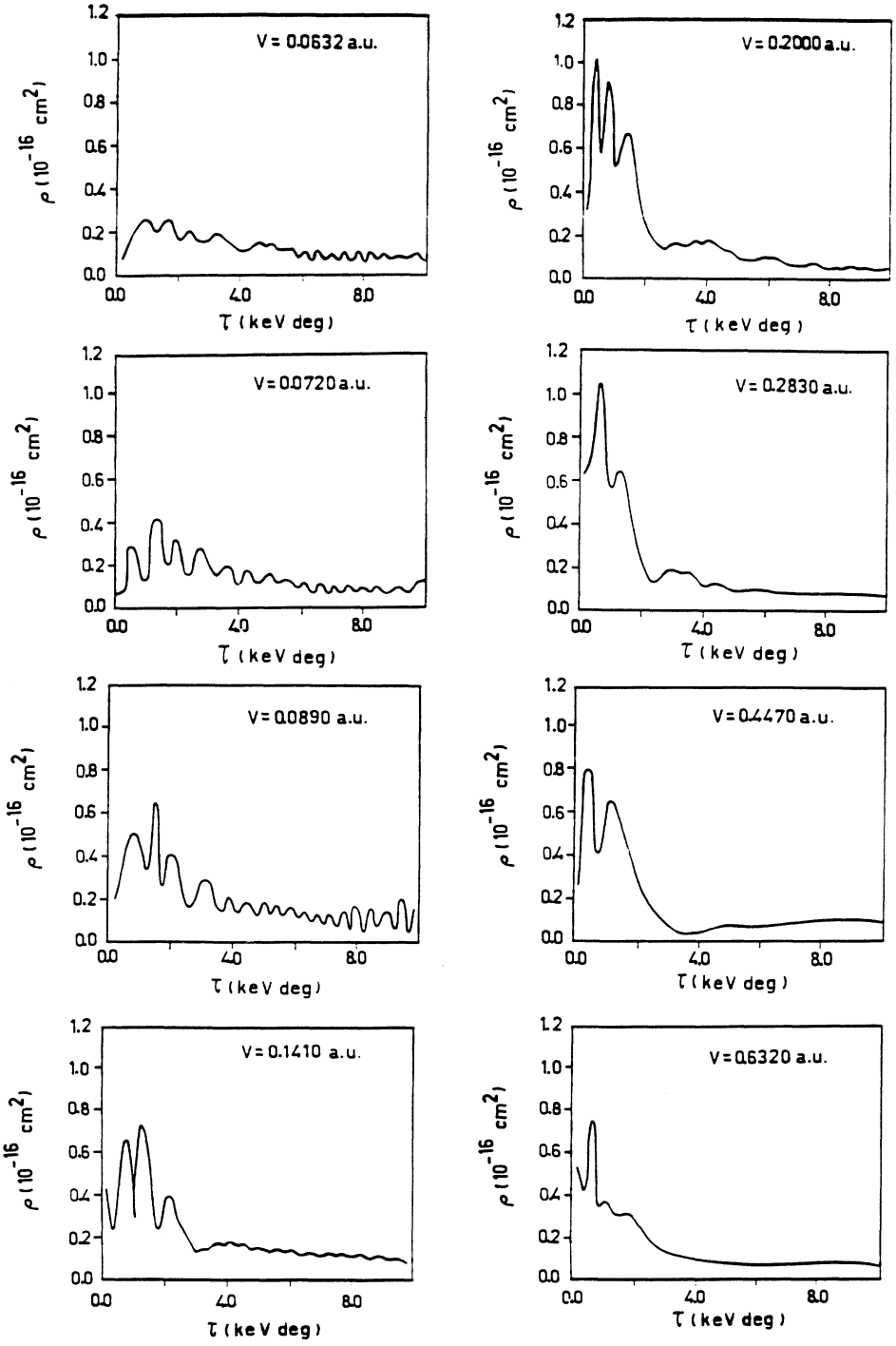

FIG. 8. Reduced differential cross sections for several velocities of the system B^{3+} + He.

This fact shows that the angle θ_{max} corresponding to the maximum is approximately proportional to the reciprocal of the collision energy. These points imply that the system obeys, approximately, the stationary phase approximation, and that the oscillations in the RDCS are certainly Stueckelberg oscillations; they have been measured by Roncin *et al.* [38]. Concerning the structure of the RDCS, further studies are needed for its correct interpretation.

IV. CONCLUSION

A proposal has been made which avoids the introduction of translation factors in an *ad hoc* manner to account for the Galilean noninvariance of the cross section. The method proposed here is aimed at giving results equivalent to that which uses translation factors, but dispenses with their use. In addition, it elucidates the Galilean noninvariance problem, about which confusing interpretations have been found in the literature. A model calculation for the $[BHe]^{3+}$ system shows very good agreement with the traditional approach.

Concerning the collision $B^{3+}+He$, its entrance channel can be represented by the state $3\,^1\Sigma^+$; around $7.5a_0$, the first couplings appear with the radial coupling transferring population from the initial state to the $2\,^1\Sigma^+$ state and the rotational coupling connecting the $3\,^1\Sigma^+$ and $1\,^1\Pi$ states. For $R<7.5a_0$ there is always a rotational coupling with the $3\,^1\Sigma^+$ and $2\,^1\Sigma^+$ states. Part of the population of the $2\,^1\Sigma^+$ state is also transferred to the $1\,^1\Sigma^+$ state by radial coupling for $R\sim4.5a_0$, and delocalized couplings are responsible for exchange population among all states, including the $4\,^1\Sigma^+$ state, for $R<4.5a_0$.

As to the partial cross sections, that of $2p$ reaches its maximum for $v\sim1.6\times10^7$ cm/s, since the radial coupling at $R\sim7.5a_0$ is predominant for this velocity. An increase in the $2s$ partial cross section is also observed for increasing velocities until $\sim6.2\times10^7$ cm/s, since the radial coupling is more effective at $R\sim4.5a_0$. A second maximum ($v\sim4.4\times10^7$ cm/s) is also presented by the $2p$ partial cross section as a result of the importance of the rotational coupling at high velocities. At very high energies, the diabaticity of the system causes a decrease in the total cross section at higher velocities.

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