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Molecular treatment of $H^+ + He^+(1s)$ collisions including pseudostates

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We report close-coupling calculations in a basis of molecular states, modified with a common translation factor, and augmented with a set of pseudostates, for $H^+ + He^+$ collisions for impact energies from 9 to 300 keV/amu.

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In recent work [1] we have shown that use of the molecular approach, modified with a common translation factor [2] (CTF), permits us to obtain accurate values for electron-loss cross sections for a very large range of nuclear velocities [up to $v \approx 3$ a.u. for $He^{2+} + H(1s)$ collisions]. However, in an analysis of the workings of the method [3] we found that, although in the higher-energy range the close-coupling treatment describes the first steps of ionization, this ionizing flux is trapped and accumulated in the charge-transfer channels, thus yielding the well-known failure (overestimation of the charge-transfer cross section) of the method at high v. Moreover, in some cases the ionizing flux is also trapped by the excitation channels [4]. Hence, although these accumulation effects can be predicted *a priori* from the energy correlation diagram together with estimates of the ionization cross sections [4], the situation with regards to the performance of the CTF approach at the higher nuclear velocities is clearly unsatisfactory. A possible connection between these workings of the molecular approach and the so-called "saddle-point" ionization mechanism [5–7] and "hidden crossing" methods [8,9] was indicated in [3]. Furthermore, it was concluded in that reference and in [4] that (i) in order to calculate the ionization cross section in the framework of a molecular expansion, augmentation of the basis with a set of pseudostates is needed, just as it is in plane-wave modified atomic expansion calculations [10–16], and (ii) even though the accumulation of ionizing flux mainly takes place for the highest-lying molecular channels, pseudostates are needed to obtain a proper convergence of the partial charge-exchange cross sections corresponding to the lower-, as well as higher-lying states, at nuclear velocities larger than the electronic ones.

In the present work we report close-coupling calculations for $H^+ + He^+(1s)$ collisions, using a semiclassical, impact-parameter treatment, and a basis of 14 exact eigenstates of the HeH^{2+} quasimolecule (the $n=1$ and $n=2$ capture channels and $n=2,3$ excitation channels) enlarged with a set of functions that are specifically built so as to cover the region between the nuclei, in analogy with the three-center atomic approach [17,18]. The basis set is given in Table I and the same CTF as in [1] was employed.

The program employed to generate the molecular data corresponding to the HeH^{2+} eigenstates was developed in [19–23]. The systems of differential equations for the expansion coefficients were integrated with the program developed in [24]. Additional one-dimensional numerical integration techniques were developed to obtain the data corresponding to the additional basis functions of Table I.

Diagonalization of the electronic Hamiltonian in the basis

TABLE I. Basis set. The molecular basis functions are of the form $\Psi_{nlm}(\lambda,\mu,\phi;Q_a,Q_b,R)=\Lambda(\lambda;Q_a,Q_b,R)f(\mu)\Omega(\phi)$, where λ, μ, and ϕ are the prolate spheroidal coordinates, Q_a, Q_b are the nuclear charges used to define Λ, and n, l, m the united-atom quantum numbers. For $f(\mu)=M(\mu;R)$, Ψ_{nlm} is an exact eigenfunction of the molecular Hamiltonian ($H_{\rm el}=-\frac{1}{2}\nabla_r^2 - Q_a/r_a - Q_b/r_b$).

n	l	m	Q_a	Q_b	$f(\mu)$
1	0	0	1	2	
2	1	0			
2	0	0			
3	2	0			
2	1	1			
3	0	0			
3	1	0			$M(\mu,R)$
4	3	0			
3	1	1			
3	2	1			
3	2	2			
4	2	0			
5	4	0			
4	3	1			
2	1	1			
3	1	1			
3	2	1	3	6	$\exp[-0.5(\mu-1/3)^2]$
1	0	0			
1	0	0			
2	1	0			
3	2	0	1	2	$\exp[-13(\mu-1/3)^2]$
4	3	0			
1	0	0			
2	1	0			
3	2	0	1	2	$\exp[-13(\mu+1/3)^2]$
4	3	0			

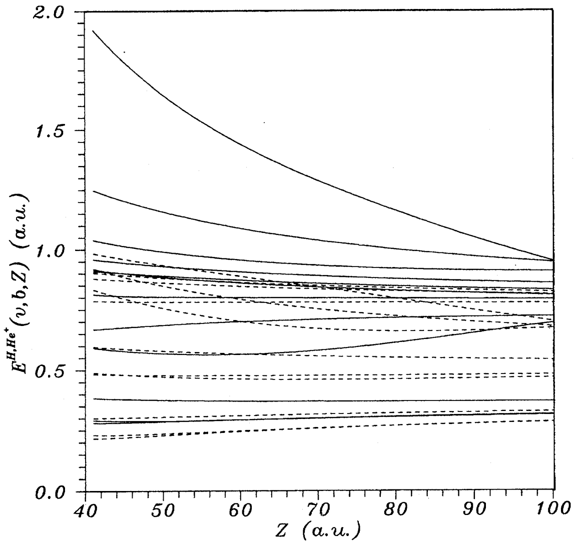

FIG. 1. Expectation values of the H (——), and He$^+$ (– –) atomic Hamiltonians for the (orthogonalized) pseudostates indicated in Table I modified with the CTF of Ref. [1] (with the electron position vector defined with the origin in the respective nuclei), as functions of the nuclear coordinate $Z=vt$, for a representative nuclear trajectory with relative velocity $v=2.0$ a.u. and impact parameter $b=1.0$ a.u.

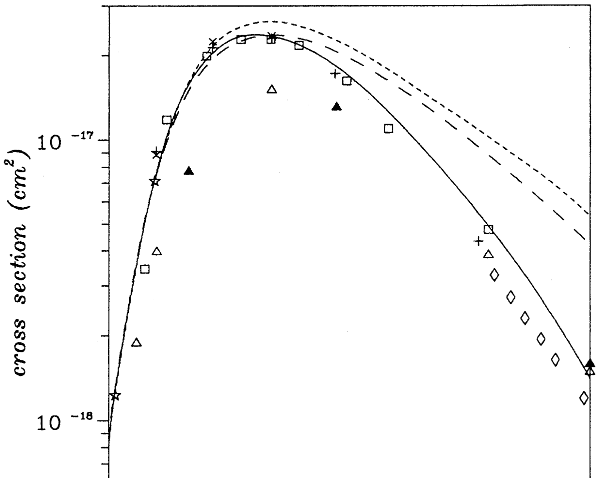

FIG. 2. Total cross section for the reaction $H^+ + He^+(1s) \rightarrow He^{2+} + H(1s)$ as a function of the nuclear velocity. (——) denotes the present results using a basis with the 14 molecular functions and the 12 pseudostates detailed in Table I; (– –) denotes the present results using the 14 molecular functions of Table I; (— —) denotes the present results using the lowest 83 molecular functions (the $n=1$, 2, 3, and 4 capture channels and the $n=2$, 3, 4, 5, 6, and 7 excitation channels). Other theoretical results: (△) Bransden and Noble [26]; (△) Bransden et al. [13]; (+) Winter [14]; (×) Winter [18]; (★) Winter et al. [27]; (◇) Belkić et al. [28]; (□) Fritsch and Lin [11].

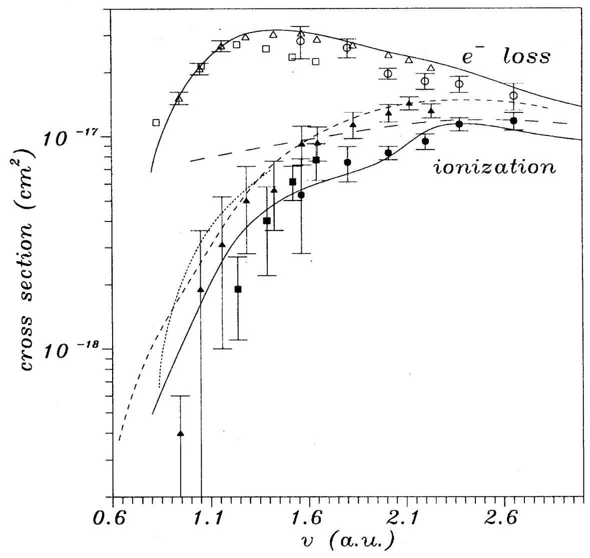

FIG. 3. Total cross sections for electron loss and ionization in $H^+ + He^+(1s)$ collisions as functions of the nuclear velocity. (——) denotes the present results obtained with the basis of Table I. Other theoretical data for ionization: (- - -) Winter [18]; (— —) Reading et al. [32]; (– –) Errea and Sanchez [33]. Experimental data: (△,▲) Rinn et al. [29]; (□,■) Peart et al. [30]; (○,●) Watts et al. [31].

then yields a set of pseudostates in addition to the exact bound states (see, e.g., Fig. 2 of Ref. [3] for the correlation diagram). The (orthonormal) close-coupling basis is then obtained by multiplying these functions by the CTF. We have checked that the pseudostate energies lie in the continuum spectrum of both (moving) atoms at large internuclear dis-

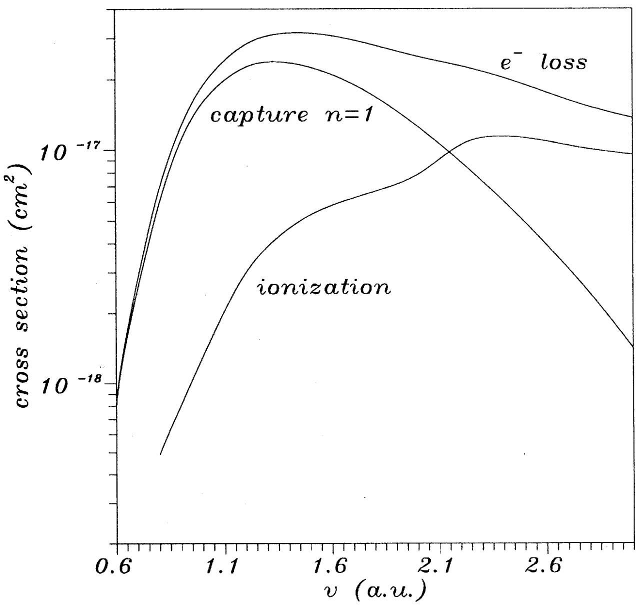

FIG. 4. Total cross sections for charge exchange into H($n=1$), ionization, and electron loss for $H^+ + He^+(1s)$ collisions calculated with the present molecular treatment including pseudostates (see Table I).

tances, so that exit through these channels can be ascribed to ionization [25,7]. An illustration is given in Fig. 1, where we plot for a typical trajectory the expectation value of the atomic Hamiltonians for the pseudostate wave functions, modified with the CTF employed, and with the electronic position vector defined with respect to either nucleus.

Our calculated cross section for the $H^+ + He^+(1s) \rightarrow H(1s) + He^{2+}$ collision is given in Fig. 2, and compared to those of accurate atomic close-coupling treatments and to continuum distorted-wave results [28]. The cross section for exit through all pseudostates is given in Fig. 3 and is seen to closely correspond to the experimental data for ionization; also included in this figure are the results for electron loss. Moreover, in order to show the interplay between capture and ionization in the intermediate velocity regime, cross sections for the mainly populated electron capture channel $[H(n=1)]$, ionization, and electron loss calculated with our molecular treatment including pseudostates are presented in Fig. 4.

In summary, we have performed close-coupling calculations carried out in a basis of molecular states, modified with a common translation factor, and augmented with a set of pseudostates obtained with the same criterion as in the three-center approach [17,18]. The purpose of this paper is to show that, at least for the benchmark reaction $H^+ + He^+$ treated, the inclusion of the pseudostates permits us to offset the difficulties of the molecular approach. Thus, a proper convergence of the charge-exchange cross sections is obtained, and the ionization cross section can be calculated. In addition, the present findings are encouraging with respect to the application of the molecular approach in the whole range of intermediate impact energies. However, to reach a definite appraisal as to its relative performance with respect to other methods is difficult at this time because it depends on the programs available, and especially on experience with regard to the optimal choice of pseudostates, which is mostly lacking—the present work being only a first step in this direction. Finally, we point out that CTF-modified molecular bases have the advantage that the "history" of the collision process can be analyzed; then, pseudostate calculations may permit us to explicitly check whether a connection with the controversial saddle-point classical mechanism exists.

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[1] L. F. Errea, C. Harel, H. Jouin, J. M. Maidagan, L. Méndez, B. Pons, and A. Riera, Phys. Rev. A **46**, 5617 (1992).
[2] S. B. Schneiderman and A. Russek, Phys. Rev. **181**, 311 (1969).
[3] L. F. Errea, C. Harel, H. Jouin, L. Méndez, B. Pons, and A. Riera, J. Phys. B **27**, 3603 (1994).
[4] L. F. Errea, L. Méndez, and A. Riera, J. Phys. B (to be published).
[5] R. E. Olson, Phys. Rev. A **27**, 1871 (1983).
[6] R. E. Olson, Phys. Rev. A **33**, 4397 (1986).
[7] G. Bandarage and R. Parson, Phys. Rev. A **41**, 5878 (1990).
[8] S. Y. Ovchinnikov and E. A. Solov'ev, Sov. Phys. JETP **63**, 538 (1989).
[9] M. Pieksma and S. Yu Ovchinnikov, J. Phys. B **24**, 2699 (1991).
[10] I. M. Cheshire, D. F. Gallaher, and A. J. Taylor, J. Phys. B **3**, 803 (1970).
[11] W. Fritsch and C. D. Lin, J. Phys. B **15**, 1255 (1982).
[12] J. F. Reading and A. L. Ford, Phys. Rev. A **21**, 124 (1980).
[13] B. H. Bransden, C. J. Noble, and J. Chandler, J. Phys. B **16**, 4191 (1983).
[14] T. G. Winter, Phys. Rev. A **25**, 697 (1982).
[15] N. Toshima, J. Phys. B **25**, L635 (1992).
[16] N. Toshima, Phys. Rev. A **50**, 3940 (1994).
[17] T. G. Winter and C. D. Lin, Phys. Rev. A **29**, 3071 (1984).
[18] T. G. Winter, Phys. Rev. A **37**, 4656 (1988).
[19] A. Salin, Comput. Phys. Commun. **14**, 121 (1978).
[20] A. Salin, Comput, Phys. Commun. **15**, 443 (1978).
[21] C. Harel and H. Jouin, J. Phys. B **21**, 859 (1988).
[22] C. Harel and H. Jouin, Europhys. Lett. **11**, 121 (1990).
[23] H. Jouin and C. Harel, J. Phys. B **24**, 3219 (1991).
[24] C. Gaussorgues, R. D. Piacentini, and A. Salin, Comput. Phys. Commun. **10**, 224 (1975).
[25] C. O. Reinhold and C. A. Falcon, J. Phys. B **21**, 1829 (1988).
[26] B. H. Bransden and C. J. Noble, J. Phys. B **14**, 1849 (1981).
[27] T. G. Winter, G. J. Hatton, and N. F. Lane, Phys. Rev. A **22**, 930 (1980).
[28] Dz. Belkic, R. Gayet, and A. Salin, At. Data Nucl. Data Tables **51**, 59 (1992).
[29] K. Rinn, F. Melchert, and E. Salzborn, J. Phys. B **19**, 3717 (1986).
[30] B. Peart, K. Rinn, and K. Dolder, J. Phys. B **16**, 1461 (1983).
[31] M. F. Watts, K. F. Dunn, and H. B. Gilbody, J. Phys. B **19**, L355 (1986).
[32] J. F. Reading, A. L. Ford, and R. L. Becker, J. Phys. B **15**, 625 (1982).
[33] L. F. Errea and P Sánchez, J. Phys. B **27**, 3677 (1994).