

Excitation and charge transfer in $\text{He}^+ + \text{H}$ collisions. A study of the origin dependence of calculated cross sections

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A treatment of the $\text{He}^+ - \text{H}$ collision is presented in an impact-parameter formalism for collision energies 0.5–30 keV. The origin dependence of the calculated total cross sections is studied in detail. It is shown that the branching ratio between reactions $\text{He}^+(1s) + \text{H}(1s) \rightarrow \text{He}^+(1s) + \text{H}(2p)$ and $\text{He}^+(1s) + \text{H}(1s) \rightarrow \text{He}(1s2p) + \text{H}^+$ oscillates as a function of the origin of electronic coordinates chosen in the calculation. This oscillation is strong enough so that at nuclear velocity 0.5 a.u., either both reactions are competitive or one of them can have a cross section twice as large as that of the other. Likewise the cross section for the reaction $\text{He}(1s^2) + \text{H}^+ \rightarrow \text{He}^+(1s) + \text{H}(1s)$ can either be negligible or comparable to those of the other reactions. We study the oscillatory behavior of the charge-exchange-transition probability as a function of $1/v$. We show the similarity, for high velocity, between non-resonant and resonant charge-exchange processes, the origin of the damping factor, and the influence of the rotational coupling on the transition probabilities as functions of $1/v$. A connection between Lichten's and Demkov's models is established.

I. INTRODUCTION

This paper presents a treatment of $^4\text{He}^+(1s) + \text{H}(1s)$ collisions with the use of a molecular approach with some of the energies and couplings calculated in the preceding article.¹ Its aim is to provide a molecular treatment that includes as many relevant states as possible within the framework of the standard perturbed stationary states approach. We also study an important consequence of the well-known difficulty of the standard molecular method, which is the origin dependence of the calculated cross sections. Although this problem is, in principle, solved by using a modified molecular approach which includes translation factors, in our opinion there are not sufficient examples in the literature to enable workers to realize to what extent calculated cross sections depend on the origin chosen to calculate them, when translation factors are not used. Moreover, as discussed in the previous article¹ (see also Errea *et al.*,²), this origin dependence may appear in disguise when using a treatment that incorporates translation factors. It is, therefore, of utmost importance to ascertain the extent of the problem using the standard treatment. Finally, we shall also discuss the behavior of the charge-exchange transition probability versus the inverse nuclear velocity, for fixed ΘE . Our analysis of this behavior is still valid when translation factors are included.

II. TOTAL CROSS SECTIONS

Total cross sections for the reactions

$$^4\text{He}^+(1s) + \text{H}(1s) \rightarrow ^4\text{He}^+(1s) + \text{H}(2p), \quad (1)$$

$$^4\text{He}^+(1s) + \text{H}(1s) \rightarrow ^4\text{He}(1s2p \ ^{1,3}P) + \text{H}^+, \quad (2)$$

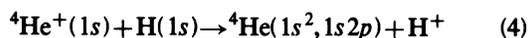
$$^4\text{He}(1s^2) + \text{H}^+ \rightarrow \text{He}^+(1s) + \text{H}(1s), \quad (3)$$

have been calculated in an impact-parameter formalism, using the energies and couplings for the states $0^1\Sigma$ and $1^{1,3}\Sigma$ described in Ref. 1, and $1^{1,3}\Pi$ and $2^{1,2}\Pi$ described in Ref. 3. The other Σ states presented in the previous paper cannot be included because of the residual radial couplings as $R \rightarrow \infty$, unless translation factors are included in the molecular expansion.

The basic mechanism which is responsible for the processes (1), (2), and (3) is as follows. The system is initially represented by a statistical mixture of $1^1\Sigma + 1^3\Sigma$ molecular states [see Figs. 1 (a) and 1(b) of the previous article¹]. These states are coupled rotationally to the states $1^{1,3}\Pi$ and $2^{1,3}\Pi$ (primary mechanism).⁴ The radial couplings $\langle 1^{1,3}\Pi | (d/dR) | 2^{1,3}\Pi \rangle$ provide the secondary mechanism that further governs the branching ratio between reactions (1) and (2); the radial coupling $\langle 0^1\Sigma | (d/dR) | 1^1\Sigma \rangle$ determines the cross section of the inverse of reaction (3).

The program PAMPA of Gaussorgues *et al.*⁵ was

modified to integrate the anomalous rotational couplings, as explained in the appendix of Ref. 3. Our results for reactions (1) and (2) are plotted in Figs. 1 and 2, respectively, with the origin of electronic coordinates placed on either the hydrogen atom or the nuclear center of mass. These results are very similar to those found in Ref. 1. We have also included the experimental data without the (very wide) error bars, for the sake of clarity. For the whole energy range considered (0.5–30 keV), the cross sections calculated with the origin placed on the center of mass agree better with experiment^{6–9} than those obtained with the origin on the proton. Clearly, one would also obtain similar results using the center of nuclear charge, which lies close to the center of mass for ${}^4\text{HeH}^+$. These facts were explained in Ref. 1 with the help of a mechanism involving a two-state ($1^{1,3}\Pi$ and $2^{1,3}\Pi$) model. We have also included in Fig. 2 the results for the inverse of reaction (3), and the total cross section for the reaction



because the experimental data in that figure correspond to all possible final states of He. Our calculated contribution of the inverse of reaction (3) to reaction (4) falls within the experimental errors.

In Fig. 3 we present our calculated total cross section for reaction (3) with the origin placed on the center of mass, together with the experimental data^{10,11} and the low-velocity theory of Hughes and Crothers¹²; their agreement with experiment is remarkable taking into account the approximations involved in their calculation.

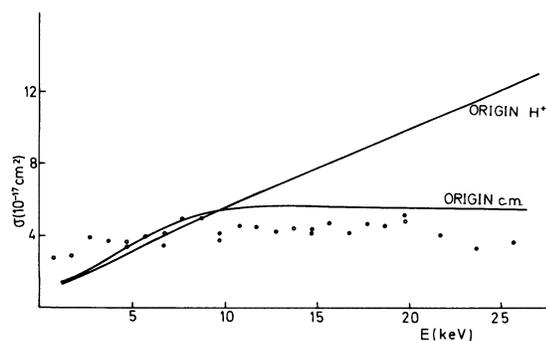


FIG. 1. Total cross section for reaction ${}^4\text{He}^+(1s) + \text{H}(1s) \rightarrow {}^4\text{He}^+(1s) + \text{H}(2p)$. Experimental data: \circ see Ref. 6; \bullet see Ref. 7.

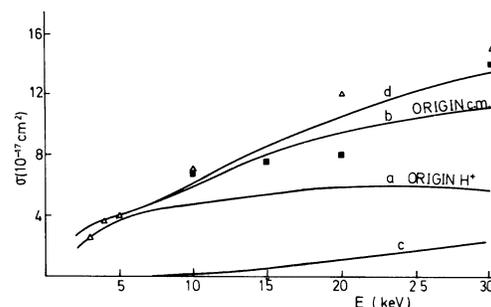


FIG. 2. Total cross section for reaction ${}^4\text{He}^+(1s) + \text{H}(1s) \rightarrow {}^4\text{He}(1s2p, {}^1,3P) + \text{H}^+$ (a and b). Total cross section for reaction ${}^4\text{He}^+(1s) + \text{H}(1s) \rightarrow {}^4\text{He}(1s^2) + \text{H}^+$ (c), with origin at the center of mass. This cross section is $\frac{1}{4}$ of that for reaction (3) of text since triplet states cannot contribute to reaction (c). Total cross section for reaction ${}^4\text{He}^+(1s) + \text{H}(1s) \rightarrow {}^4\text{He}(1s^2, {}^1S; 1s2p, {}^1,3p) + \text{H}^+$ with origin at the center of mass (d). Experimental data: \blacksquare , see Ref. 8; \triangle , see Ref. 9.

III. ORIGIN DEPENDENCE OF THE CROSS SECTIONS

It is interesting to explicitly study the dependence of the cross sections on the origin of electronic coordinates chosen to perform the collision calculations, for the three reactions (1)–(3), and for a fixed nuclear velocity. As an example, in Fig. 4 we present our results for $v = 0.49$ a.u. (impact energy 24 keV). The results for reactions (1) and (2) oscillate with the position of the origin while those for reaction (3) vary monotonically, in that range. Depending on the origin chosen, reaction (3) may be negligible (origin on He^{2+}), or it may compete with

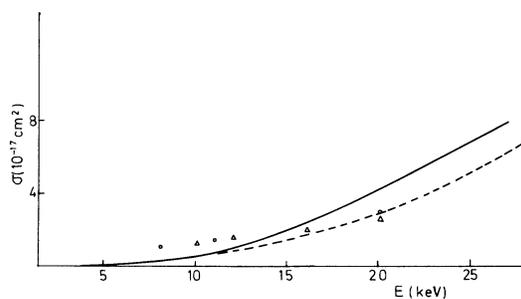


FIG. 3. Total cross section for reaction ${}^4\text{He}(1s^2) + \text{H}^+ \rightarrow {}^4\text{He}^+(1s) + \text{H}(1s)$. —, Our results; - - -, low velocity theory. See Ref. 12. Experimental data: \triangle , see Ref. 10; \circ , see Ref. 11.

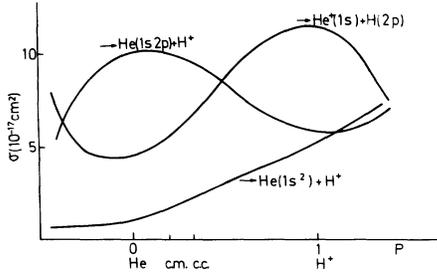


FIG. 4. Origin dependence of reactions (1), (2), and (3) of text. We plot the total cross section for impact $E=24$ keV as function of $p=0A/R$, where $0A$ is the distance from He^{2+} to the origin of electronic coordinates. The positions of the center of mass (c.m.) and center of charge (c.c.) are also indicated.

the processes (1) and (2) (origin H^+). This is a striking example of the limitations of the standard molecular approach, and it shows quite clearly that there is no privileged origin for the study of these reactions.

On the other hand, given the form of the couplings, the shape of the curves in Fig. 4 can be easily predicted. As explained in Ref. 1, a two-state model can be used to explain qualitatively the behavior of the radial couplings $\langle 1^{1,3}\Pi | (d/dR) | 2^{1,3}\Pi \rangle$ and cross sections:

$$\begin{aligned} \chi_1 &\simeq \cos\theta\phi_1 - \sin\theta\phi_2, \\ \chi'_1 &\simeq \sin\theta'\phi'_1 + \cos\theta'\phi'_2, \\ \chi_2 &\simeq \sin\theta\phi_1 + \cos\theta\phi_2, \\ \chi'_2 &\simeq -\cos\theta'\phi'_1 + \sin\theta'\phi'_2. \end{aligned} \quad (5)$$

for the singlet (χ_1, χ_2) and triplet (χ'_1, χ'_2) Π states. The functions ϕ and ϕ' represent diabatic states, which at large R are quasiatomic in character:

$$\begin{aligned} \phi_1 &\underset{R \rightarrow \infty}{\sim} \phi_{\text{H}}, \quad \phi'_1 \underset{R \rightarrow \infty}{\sim} \phi'_{\text{H}}, \\ \phi_2 &\underset{R \rightarrow \infty}{\sim} \phi_{\text{He}}, \quad \phi'_2 \underset{R \rightarrow \infty}{\sim} \phi'_{\text{He}}. \end{aligned} \quad (6)$$

At high-impact energies, the transition probability for reactions (1) and (2) will be

$$p_{\text{H}} \propto \cos^2\theta(0) + 3 \sin^2\theta'(0) \quad (7)$$

for reaction (1), and

$$p_{\text{He}} \propto \sin^2\theta(0) + 3 \cos^2\theta'(0)$$

for reaction (2). The dependence of both θ and θ' on the origin of electronic coordinates is easily seen to be linear in the parameter p , which is the distance of the origin from the He^{2+} nucleus divided by R :

$$\begin{aligned} \theta(R) &= \int_R^\infty \left\langle \chi_1 \left| \frac{d}{dR} \right|_{\text{He}} \chi_2 \right\rangle dR \\ &+ p \int_R^\infty \langle \chi_1 | \Gamma | \chi_2 \rangle dR \end{aligned} \quad (8)$$

with a corresponding expression for θ' , where $-i\Gamma$ is the matrix of the electronic linear momentum along the z axis. Accordingly, for $R=0$ we have

$$\begin{aligned} \theta(0) &= \int_0^\infty \left\langle \chi_1 \left| \frac{d}{dR} \right|_{\text{He}} \chi_2 \right\rangle dR \\ &+ p \int_0^\infty \langle \chi_1 | \Gamma | \chi_2 \rangle dR \\ &= \theta \Big|_{\text{He}(0)} + p\beta \end{aligned} \quad (9)$$

with a similar expression for $\theta'(0)$. From Fig. 2 of Ref. 3, we calculate

$$\begin{aligned} \theta \Big|_{\text{He}(0)} &= 1.65, \quad \beta = -1.79 \\ \theta' \Big|_{\text{He}(0)} &= -0.22, \quad \beta' = 1.75. \end{aligned} \quad (10)$$

Substitution of Eq. (9) in Eq. (7) yields the oscillating structure seen in Fig. 4. A similar reasoning using an exponential model can explain the shape of the curve corresponding to reaction (3).

IV. OSCILLATION OF THE NONRESONANT ELECTRON CAPTURE PROBABILITY

In Fig. 5(a), 5(b), and 5(c) we present our results, with origin on the center of nuclear mass, together with those of Keever and Everhart,¹³ corresponding to the transition probability of reaction (3) for fixed ΘE and as a function of the inverse nuclear velocity. To do this we have made a correspondence between the scattering angle Θ and the input parameter of the trajectory, according to Rutherford's formula. We also include the results of Burns and Crothers¹⁴ obtained using the same low-energy theory as Hughes and Crothers.¹² The same remark can be made as the goodness of their agreement with experiment, while our results reproduce the structure and position of the extrema. Our calculations permit us to study an important point which is the purpose of the work Burns and Crothers¹⁴: What is the origin of the oscillations in the transition probabilities?

Fite *et al.*,¹⁵ and Lichten¹⁶ mention that there is no experimental evidence in favor of the distinction

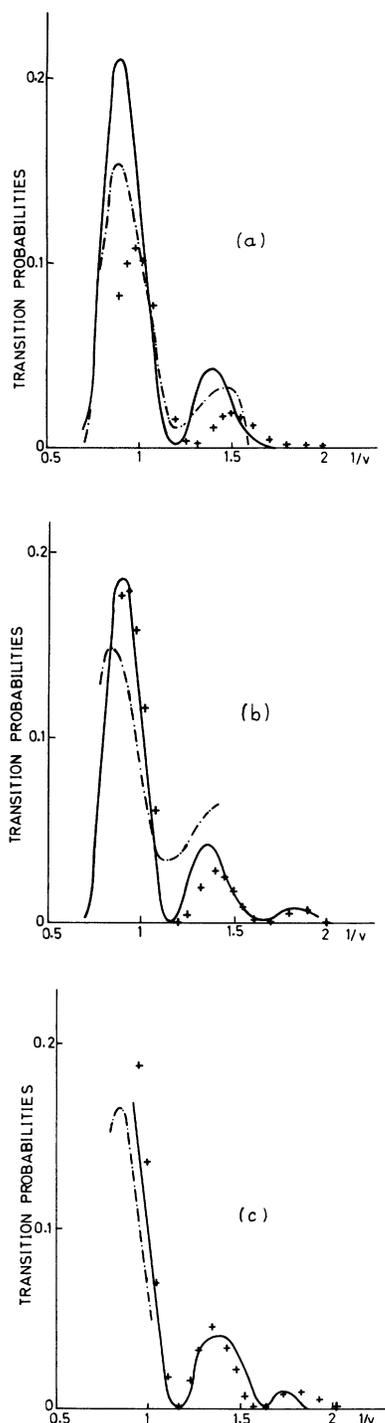


FIG. 5. Transition probability for reaction (3) of text at fixed ΘE . +, Our results; —, low velocity theory (see Ref. 14); - - - -, experimental data (see Ref. 23). $\Theta E = 20$ deg keV (a); $\Theta E = 40$ deg keV (b); $\Theta E = 400$ deg keV (c). E is the impact He^{2+} energy. Notice the change of scale with respect to Refs. 14 and 23 where H^+ impact energy was used.

made by Bates and Lynn¹⁷ between resonant and nonresonant charge exchange. In his discussion, Lichten uses for the probability of charge exchange an empirical modification of the formula employed for the symmetric case, introducing a damping term. To calculate the phase of the oscillations, he stops the integration of the energy difference at a given point λ , which corresponds to a sudden transition from the separated atoms to a molecular ion. It is not clear, however, which is the justification of this cutoff, and how to determine it *a priori*. In view of our results, and more specifically, of the fact that when the center of nuclear mass is used as the origin of electronic coordinates, the area under the radial coupling $\langle 0'\Sigma | d/dR | 1'\Sigma \rangle$ is approximately $\pi/4$, we can establish a connection between the symmetric resonant, symmetric nonresonant, and nonsymmetric nonresonant cases.

In a resonant case, when adiabatic wave functions are used for large internuclear distances, the system is initially represented by a mixture of two molecular states, gerade and ungerade, which evolve independently, and the interference between the corresponding wave functions for $t \rightarrow \infty$ produces the oscillations in the transition probability; the area between the g and u energy curves determines the phase of the oscillation [Fig. 6(a)]. In an analogous way to the $\text{H}^+ + \text{H}$ case, Lichten¹⁸ explained the oscillations in the transition probability corresponding to double charge exchange in $\text{He}^{2+} + \text{He}$ collisions, using a nonadiabatic [molecular orbital (MO)] representation for all internuclear distances. Then, the two energies have different limits as $R \rightarrow \infty$, and as the integral of the energy difference diverges, Lichten also introduced a cutoff parameter λ . We have shown¹⁹ that this parameter should be taken to characterize the boundary zone between the regions where MO and valence band (VB) descriptions are adequate. Lichten's model must then be interpreted as a sudden approximation method, in which the interference that produces the oscillations arises solely from the energy difference between the MO curves, and a change of representation to the atomic states place for $R = \lambda$.

Lichten used again the same approach¹⁶ for the nonsymmetric nonresonant case (HeH^+) where the energy difference between the exact adiabatic states is nonzero as $R \rightarrow \infty$. Although this case is physically different from the previous one, it is formally similar, and it can be treated in the same way. The difference is that in the nonsymmetric nonresonant case the adiabatic energies are not degenerate for $R \rightarrow \infty$, while they are exactly so in the resonant

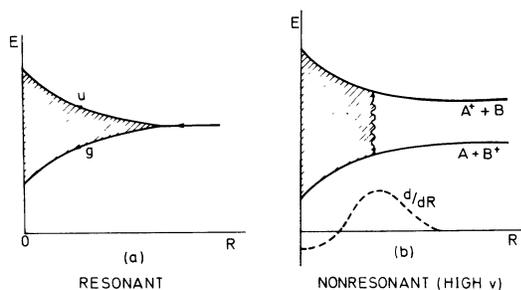


FIG. 6. Equivalence between resonant and (high-velocity) nonresonant charge exchange. Phase of the transition probability vs $1/v$ is determined by (a) the area between the g and u energy curves, and (b) the area between the energy curves up to approximately the value of R for which the radial coupling has a maximum.

case: the situation Lichten found in this case is due to his using a nonadiabatic representation at large R . The similarity between the two cases is that a cutoff is also needed in the integration of the energy difference. In the nonsymmetric nonresonant case, this cutoff represents a transition from the VB (localized) to the MO (delocalized) regions; in an adiabatic representation, the transition zone is characterized by a maximum in the radial coupling [Fig. 6(b)]. At high velocities and large- R values the system is well represented by VB structures, and it suffers a (sudden) transition to MO structures at a distance which corresponds to the maximum of the radial coupling $R_{\max} = \lambda$. Using the standard molecular model, the phase of the oscillations is then determined by the shaded area in Fig. 6(b). On the other hand, at very low velocities there will be no oscillations in the transition probability, because the system will follow adiabatically the molecular curve which corresponds to the entrance channel. The damping of the oscillations follows from the change between the two velocity regimes.

Since the process we are discussing is due to delocalization effects, the Demkov²⁰ exponential model is applicable, because the area under the coupling $\langle 0' \Sigma | d/dR | 1' \Sigma \rangle$ equals approximately $\pi/4$ when the origin of electronic coordinates is placed near the nuclear center of mass. This model assumes that the two states involved have a constant energy difference, and are coupled by an exponential electrostatic interaction H_{12} . At high velocities, this model also implies a sudden transition from a VB to a MO structure at the point where $H_{12} = \Delta E/2$. The phase of the oscillations of the transition probability is then determined²⁰ by the integral over the interaction term H_{12} . We shall now establish the connection between Lichten's and Demkov's ap-

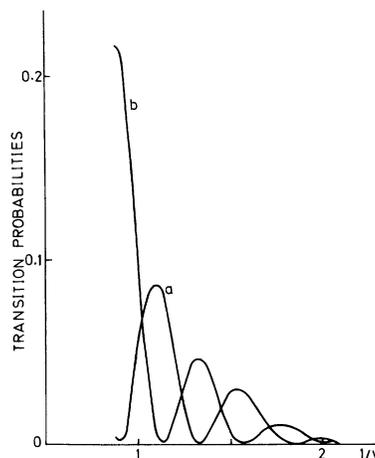


FIG. 7. Transition probabilities for reaction (3) of text at $\Theta E = 400$ deg keV. (a) Results for a two- Σ -state model. (b) Same as (a) including the rotational coupling to a Π state. Just as in the resonant case, including the rotational coupling causes a phase shift of $\pi/4$ in the transition probability.

proaches.

The wave functions used in Demkov's model to represent the states of interest can be added and subtracted to obtain a new representation for $R < R_{\max}$ (where $H_{12} = \Delta E/2$). This change of representation takes us from a model with constant energy difference and exponential interaction to another with constant interaction and exponential energy difference. For $R < R_{\max}$, Demkov's treatment²⁰ is equivalent to assuming that the collision is elastic for each state of the new model and, therefore, the phase of the oscillations is determined by the integral of the energy difference up to the transition point R_{\max} , just as in Lichten's approach.

An important characteristic of the resonant charge-exchange process is that when one of the two Σ states involved in the transition is rotationally coupled to a Π state, there is a phase shift of $\pi/2$ on the oscillations of the charge-exchange-transition probability versus v^{-1} . In our work we have tested whether the same phenomenon appears for the nonresonant case. We have calculated (see Fig. 7) the transition probability for $\Theta E = 400$ deg keV using a two- Σ -state model and a two- Σ , one- Π -state model. The $\pi/2$ phase shift is clearly shown in this figure and is due to the fact²¹ that at high velocities the effect of the rotational coupling is simply to change the sign of the coefficient of the wave function that represents the Σ state.

In short, our findings support the claim^{15,16} that, at high velocities, there is no real difference between

resonant and nonresonant charge-exchange-transition probabilities versus v^{-1} , and this applies both to the phase of the oscillations and to the $\pi/2$ phase shift (see Refs. 19 and 21).

It should be noticed, however, that the previous discussion has been made for one specific choice of origin (in the region of the center of nuclear mass, or of nuclear charge, of ${}^4\text{HeH}^+$) of electronic coordinates. For other choices, the shape of the oscillations is very different, and does not conform to the experimental values.

V. CONCLUSIONS

We have presented a collisional treatment of excitation and charge-transfer processes in ${}^4\text{He}^+(1s) + \text{H}(1s)$ collisions. Reasonable agreement with experimental data is obtained, for the energy range 2–30 keV, when a seven-term molecular expansion is used, and the origin of electronic coordinates is chosen to be in the neighborhood of the center of nuclear mass.

We have explicitly calculated the origin dependence of the total cross sections of reactions (1)–(3) for fixed nuclear velocities. Dramatic effects of this dependence are as follows.

(a) The oscillations in the branching ratio of reaction (1) and (2) begin to be important at $v = 0.3$ a.u. For example, at $v = 0.49$ a.u. (see Fig. 4) reactions (1) and (2) can be competitive, or either one can have a cross section twice as large as that of the other one.

(b) The calculated cross section for reaction (3) can either be negligible or comparable to those for reactions (1) and (2).

These results illustrate the extent of the momentum-transfer problem in the standard molecular approach to atomic collisions.

Furthermore, we have shown the following: (i) the similarity, for high nuclear velocities, between nonresonant and resonant charge-exchange transition probabilities versus v^{-1} ; for high nuclear velocities, Demkov's model yields oscillations for this probability, just as the simple elastic scattering in the resonant case. (ii) The lower the nuclear veloci-

ty, the less diabatic is the behavior of the system, and therefore, the similarity between the resonant and nonresonant cases, resulting in a damping of the oscillations. (iii) For velocities which are not too low, the rotational coupling $1\Sigma - 1\Pi$ has exactly the same effect as for the symmetric resonant case, that is, it adds a constant $\pi/2$ phase shift to the transition probability.

Burns and Crothers¹⁴ have presented two treatments for reaction (3) in a range of energies going up to high values of E . Since for the energy range considered in our work their high-velocity approach—which includes the effect of translation factors—yields results which are in worse agreement with experiment than those from their low-velocity theory, we only have compared our calculated transition probabilities with their results with the latter theory.

Finally, a point of interest is to see whether the origin of electronic coordinates that yields results in good agreement between calculated and experimental cross sections also yields good results for the phase and position of the extrema of the charge-exchange transition probability versus v^{-1} . This is not necessarily so, in principle, because the trajectories which dominate the charge-exchange cross sections are not, in general, those which determine the transition probabilities for fixed ΘE . While it is significant that the same origin (center of mass, or center of charge) reproduces well both experimental quantities, from our study it is clear that one should not conclude that these centers are, in any sense, privileged origins.²²

At high velocities, the dependence of total cross sections and transition probabilities on the origin of electronic coordinates chosen to perform the calculations should be taken into account, since either agreement or disagreement with experimental data may be a consequence of the origin chosen. In our opinion, this is a point which, at present, is not sufficiently emphasized in the literature.

ACKNOWLEDGMENTS

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- ¹A. Macías, A. Riera, and M. Yáñez, *Phys. Rev. A* **27**, 206 (1982), preceding paper.
- ²L. F. Errea, L. Méndez, and A. Riera, *J. Phys. B* **15**, 101 (1982).
- ³A. Macías, A. Riera, and M. Yáñez, *Phys. Rev. A* **23**, 2941 (1981).
- ⁴J. Fayeton, J. C. Houbert, M. Barat, and F. Masnou-Seews, *J. Phys. B* **9**, 461 (1976).
- ⁵C. Gaussorgues, R. D. Piacentini, and A. Salin, *Comput. Phys. Commun.* **10**, 223 (1975).
- ⁶R. A. Young, R. F. Stebbings, and J. W. McGowan, *Phys. Rev.* **171**, 85 (1968).
- ⁷D. A. McKee, J. R. Sheridan, J. Geddes, and H. D. Gilbody, *J. Phys. B* **10**, 1679 (1977).
- ⁸R. E. Olson, A. Salop, R. A. Phaneuf, and F. W. Meyer, *Phys. Rev. A* **16**, 1867 (1977).
- ⁹G. J. Lockwood, G. H. Miller, and J. M. Hoffman, *Bull. Am. Phys. Soc.* **21**, 1266 (1976).
- ¹⁰S. K. Allison, *Rev. Mod. Phys.* **30**, 1137 (1958).
- ¹¹J. B. Hasted (private communication) in Ref. 12.
- ¹²J. G. Hughes and D. S. F. Crothers, *J. Phys. B* **10**, L605 (1977).
- ¹³W. C. Keever and E. Everhart, *Phys. Rev.* **150**, 43 (1966).
- ¹⁴W. D. Burns and D. S. F. Crothers, *J. Phys. B* **9**, 2479 (1976).
- ¹⁵W. L. Fite, A. C. H. Smith, and R. F. Stebbings, *Proc. R. Soc. London, Ser. A* **268**, 527 (1962).
- ¹⁶W. Lichten, *Phys. Rev.* **139**, 27 (1965).
- ¹⁷D. R. Bates and N. Lynn, *Proc. R. Soc. London, Ser. A* **253**, 141 (1959).
- ¹⁸W. Lichten, *Phys. Rev.* **131**, 229 (1963).
- ¹⁹V. López, A. Macías, R. D. Piacentini, A. Riera, and M. Yáñez, *J. Phys. B* **11**, 2889 (1978).
- ²⁰Y. N. Demkov, *Zh. Eksp. Teor. Fiz.* **45**, 195 (1963) [*Sov. Phys.—JETP* **18**, 138 (1964)].
- ²¹R. McCarroll and R. D. Piacentini, *J. Phys. B* **3**, 1336 (1970).
- ²²In the limit $R \rightarrow 0$ the center of nuclear charge was used as a privileged origin by K. Taulbjerg, J. Vaaben, and B. Fastrup, *Phys. Rev. A* **12**, 2325 (1975). See also D. S. F. Crothers and N. R. Todd, *J. Phys. B* **14**, 2233 (1981) and V. H. Ponce, *ibid.* **14**, 2823 (1981). See, however, in Ref. 2, a discussion on how the calculated results are affected by the extent of the region where the switching factor is made to tend to zero. Moreover, even in cases where a privileged origin could be justified in a formalism which includes translation factors, we see no reason to prefer this origin in the standard treatment (without translation factors).
- ²³H. F. Helbig and E. Everhart, *Phys. Rev.* **136**, A674 (1964).