Charge exchange between H(1s) and fully stripped heavy ions at low-keV impact energies*

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Approximate cross sections for charge transfer between ground-state atomic hydrogen and completely stripped ions of C, N, O, Ne, Si, and Ar have been obtained in the velocity range 6×10^6–7×10^7 cm/sec. In these collisions, electron capture occurs predominantly into high-lying orbitals of the product heavy ion. The calculations are made using the Landau-Zener theory modified for application to a multistate system. The peak cross sections are found to increase by about a factor of 5 in going from C^{+6} (≈ 21 Å^2) to Ar^{+18} (≈ 110 Å^2) and the cross-section curves tend to "flatten out" for the heavier ions where three or four crossings contribute to the charge exchange. At the higher energies, the cross sections become roughly equal to $1.4 \times 10^{-16} Z^{3/2}$ cm^2.

I. INTRODUCTION

Collisional interactions of multicharged heavy ions with atomic and molecular systems at keV energies are of considerable importance in such diverse fields as radiation research, controlled-thermonuclear-fusion plasma studies, and multi-charged heavy-ion source development. In recent years, there has been an explosive growth of research activities directed toward studying collisions of multicharged ions at high-keV and MeV energies which has been stimulated by the availability of ion sources and accelerators in this energy range.[1] However, comparatively little work, either experimental or theoretical, has been done at lower collision energies, where the lack of suitable multiply-charged ion sources has severely limited laboratory investigations.

Recognizing the need for cross-section information, we have begun a program to study theoretically some of these relatively-low-energy collisional processes. In this paper we report the results of calculations of electron-capture cross sections for collisions between hydrogen atoms and several fully stripped heavy ions in the range of velocities below the hydrogenic orbital velocity. In these systems, capture occurs predominantly into high-lying orbitals of the resultant ion and the occurrence of well-defined distant curve crossings which account for most of the charge transfer makes it feasible to utilize hydrogenic wave functions in the Landau-Zener model to obtain reasonable estimates of the relevant cross sections.

II. POTENTIAL CURVES

To demonstrate the approach followed, we will refer specifically in the next few paragraphs to the representative capture reaction

$$C^{+6} + H \rightarrow C^{+5}(n) + H^+ , \qquad (1)$$

where n refers to a given quantum level for the hydrogenic C^{+5} ion.

The long-range interactions between the initial collision pair H-C^{+6} and between three possible H^+-$C^{+5}(n)$ reaction products in which the electron is transferred during the collision to $n = 5$, 4, or 3 orbitals of the C^{+5} ion are depicted schematically in Fig. 1. The asymptotic initial-state interaction can, to first order, be represented by an attractive polarization potential, whereas the long-range H^+-$C^{+5}(n)$ interaction is dominated by the strong Coulomb repulsion. Thus for the exothermic processes shown, the curve crossings are seen to occur at progressively smaller interatomic separations R with a decrease in n.

Actually, because the coupling-matrix elements associated with the various transitions decrease rapidly with increasing internuclear separation, it was found necessary in practice to evaluate the final-state electrostatic interactions more precisely. Thus the crossing distance R_c corresponding to electron transfer from H to $C^{+5}(n)$ is obtained by solving the equation
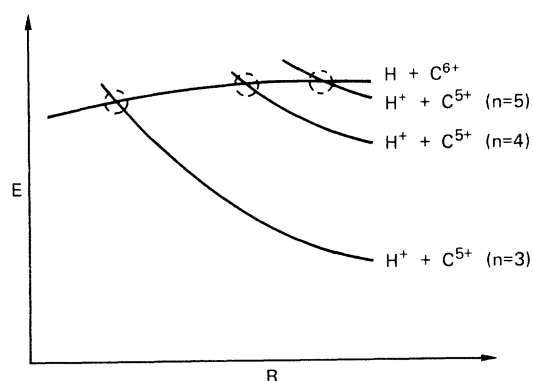

FIG. 1. Schematic representation of the long-range potential interactions between C^{+6} and H(1s) and between three possible H^+-$C^{+5}(n)$ collision partners.

$$\Delta E - \frac{9}{4}\frac{Z^2}{R_c^4} - \frac{Z^2}{R_c}$$

$$+ \frac{1}{16}\left(\frac{n}{ZR_c}\right)^4 [17n^2 - 3(n-1)^2 + 19] + V_n = 0, \qquad (2)$$

where the energy defect for these hydrogenic systems corresponding to level n is given by

$$\Delta E = \tfrac{1}{2}(Z^2/n^2 - 1), \qquad (3)$$

where Z is the initial-state ion charge. The second term in Eq. (2) is the polarizability interaction (second-order Stark interaction) for the initial collision partners. The third term corresponds to the nuclear Coulomb repulsion. The fourth term is the second-order Stark interaction for the resultant collision pair.[2] Finally, the quantity V_n represents the electrostatic interaction in the final state between the proton and the electron. The question of appropriate asymptotic wave functions to be used in these determinations will be discussed later.

It is of interest, in connection with application of the Landau-Zener technique, to consider the adiabatic potential curves for the $(CH)^{+6}$ system. Of all possible $(CH)^{+6}$ potential curves, one can identify a subset of "interacting" or "noncrossing" terms associated with the initial C^{+6}-H(1s) state which has σ symmetry.[3] The usual interpretation of the Wigner-Von Neumann noncrossing rule for diatomic molecules[4,5] does not hold for these one-electron diatomic-molecule systems but must be modified in light of the additional symmetry associated with the separability of the Schrödinger equation in prolate spheroidal coordinates for such systems. The problem has been analyzed in some detail by Power[3] and others.[6,7] A modified noncrossing rule emerging from the separability condition, and rules correlating united-atom states and separated-atom states for one-electron diatomic-molecule systems, have been derived.[3,6] Some of the relevant "interacting" potential curves for the H-C^{+6} system are shown in Fig. 2. The nuclear repulsion energies have not been included in these calculations. The curves were generated using a program developed by Power[8] based on a separation of the Schrödinger equation in prolate spheroidal (elliptical) coordinates. The limiting forms for the elliptical coordinates in the separated-atom limit (as the internuclear separation $R \to \infty$) are parabolic coordinates. It becomes appropriate in this limit to use hydrogenic wave functions expressed in parabolic coordinates with associated parabolic quantization $|n, n_1, n_2, m\rangle$, where n_1 and n_2 are the parabolic quantum numbers and
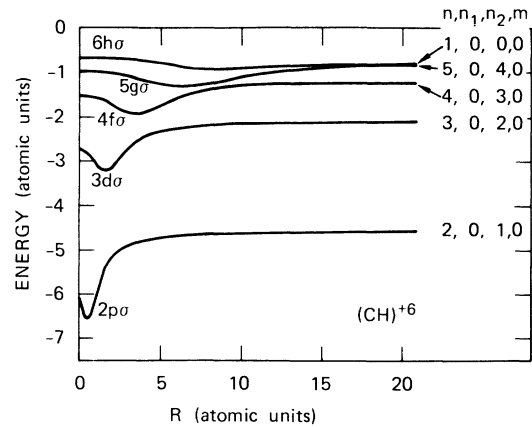
$$n = n_1 + n_2 + |m| + 1. \qquad (4)$$

FIG. 2. Set of "interacting" adiabatic-potential curves associated with the C^{+6}-H(1s) collision systems showing the characteristic pseudo crossings. The curves are labeled on the left-hand side by the relevant united-atom quantum numbers and on the right-hand side by the separated-atom parabolic quantum numbers. The nuclear repulsion energies have not been included in these curves. The separated-atom limit for the upper curve corresponds to H(1s), whereas for each of the other terms it corresponds to a $C^{+5}(n)$ level. For $R > 20$, the two upper curves diverge and, in the asymptotic limit, the level 5, 0, 4, 0, of C^{+5} lies below the level 1, 0, 0, 0 of H.

The set of "interacting" σ terms shown in Fig. 2 are labeled on the left-hand side by their united-atom quantum numbers (n, l, m) which, according to the modified noncrossing rule,[3] satisfy the conditions

$$n - l - 1 = 0 \text{ and } m = 0. \qquad (5)$$

The curves are labeled on the right-hand side by the correlated separated-atom parabolic quantum numbers (n, n_1, n_2, m) with $n_1 = m = 0$. The asymptotic limit for the upper curve corresponds to the atomic hydrogen (1, 0, 0, 0) state (equivalent to the spherical-coordinate hydrogen 1s state). For all other curves, the dissociation limit corresponds to a $C^{+5}(n)$ level. Note that whereas the Wigner-Von Neumann rule provides that all σ terms arising from a given asymptotic n level are "interacting," the one-electron diatomic-molecule crossing rule is much more restrictive, specifying in this case that only one of these, the term associated with the $(n, 0, n-1, 0)$ separated-atom state, is in this category. A set of clearly defined pseudocrossings is evident in Fig. 2. The diabatic curves sketched in Fig. 1 can be obtained to a reasonable approximation from the adiabatic curves of Fig. 2 by adding the nuclear repulsion Z/R to the adiabatic terms and allowing the curves to cross in the pseudocrossing regions. For comparison a similar set of interacting adiabatic potential curves for the Ar^{+18}-H system is shown in Fig. 3.
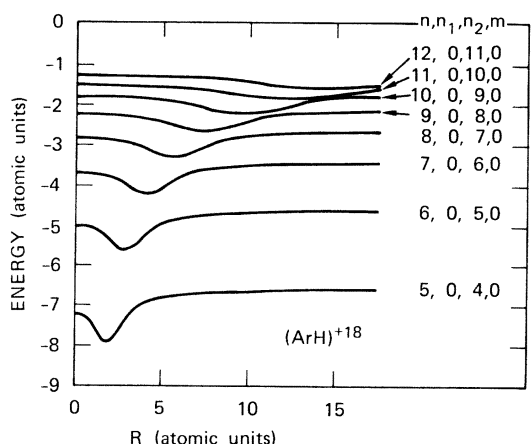
FIG. 3. Set of "interacting" adiabatic-potential curves associated with the Ar^{+18}-H(1s) collision system. The dissociation limit for each of the curves corresponds to an $Ar^{+17}(n)$ level.

III. LANDAU-ZENER METHOD

According to the Landau-Zener model,[9,10] the probability of a transition between two terms at a pseudocrossing corresponding to internuclear separation R_c (or, equivalently, the probability of remaining on the diabatic curve) is given by

$$p = \exp(-2\pi U_{12}^2/v_r \Delta F),\qquad(6)$$

where

$$\Delta F = \frac{d}{dR}(U_{11} - U_{22})\big|_{R=R_c}\qquad(7)$$

The generalization of Eqs. (6)–(8) to the multistate system is obvious.

The coupling-matrix elements corresponding to internuclear separation R are determined as discussed by Bates and Moiseiwitsch[11] from the relation

$$U_{1j} = |S_{1j}(\rho_{1j} - \beta_j) - \sigma_{1j}|/(1-S_{1j})^2,\qquad(11)$$

where, referring to Fig. 5, the two-center integrals S_{1j}, ρ_{1j}, and σ_{1j} are given by

$$S_{1j} = \int_\tau \varphi_1(\vec{r}_1)\,\varphi_j(\vec{r}_j)d\tau,\qquad(12)$$

$$\sigma_{1j} = \int_\tau \frac{\varphi_1(\vec{r}_1)\,\varphi_j(\vec{r}_j)}{r_1}d\tau,\qquad(13)$$

and the radial velocity at the crossing point is

$$v_r = v_0[1 - U_{11}(R_c)/E - b^2/R_c^2]^{1/2}.\qquad(8)$$

Here $U_{12}(R_c)$ is the relevant coupling-matrix element, v_0 and E are the initial relative velocity and kinetic energy, respectively, $U_{11}(R_c)$ and $U_{22}(R_c)$ are the diabatic potentials, and b is the impact parameter.

For the case where there are only two states (1 and 2) and a single crossing the total probability of transition after the two transversals of the crossing region during the collision is approximated by summing over the two possible ways of making the transition. Thus [referring to Fig. 4(a)],

$$P_{12} = 2p(1-p).\qquad(9)$$

This expression can be generalized to the case of N states and $N-1$ crossings by summing over the possible paths necessary to make the transition from state 1 to state j where $2 \le j \le N$. It should be recognized that by employing this technique of adding probabilities rather than amplitudes, interference effects are neglected. The procedure can be thought or as an averaging over probability oscillations which arise as the collision parameters are varied. Denoting the probabilities of remaining on the diabatic curve at each crossing, starting from the outermost crossing, as $p_2, p_3, \ldots, p_j, \ldots, p_N$ [see Fig. 4(b)], we find that the total probability of a transition occurring from state 1 to state j corresponding to a crossing separation R_{cj} during a collision is given by

$$P_{1j} = (p_2 p_3 \cdots p_j)(1-p_j)\{1 + (p_{j+1}p_{j+2}\cdots p_N)^2 + (1-p_{j+1})^2 + [p_{j+1}(1-p_{j+2})]^2 + [p_{j+1}p_{j+2}(1-p_{j+3})]^2$$

$$+ \cdots + [p_{j+1}p_{j+2}\cdots p_{N-1}(1-p_N)]^2\},\quad j < N-1,$$

$$= (p_2 p_3 \cdots p_{N-1})(1-p_{N-1})[1 + P_N^2 + (1-P_N)^2],\quad j = N-1,\qquad(10)$$

$$= 2p_2 p_3 \cdots p_N(1-p_N),\quad j = N.$$

$$\rho_{1j} = \int_\tau \frac{\varphi_j^2(\vec{r}_j)}{r_1}d\tau.\qquad(14)$$

In Eq. (11), β_j is the polarization energy (second-order Stark energy) of the final-state heavy ion in the field of the proton and was determined for the relevant states using the expressions given by Bethe and Salpeter.[2]

The appropriate asymptotic wave functions are the hydrogenic parabolic wave functions corresponding to the various potential curves as shown in Fig. 2 for the C^{+6} on H system with the listed quantization.[12]

It was found convenient for purposes of computation of the two-center integrals involved in the
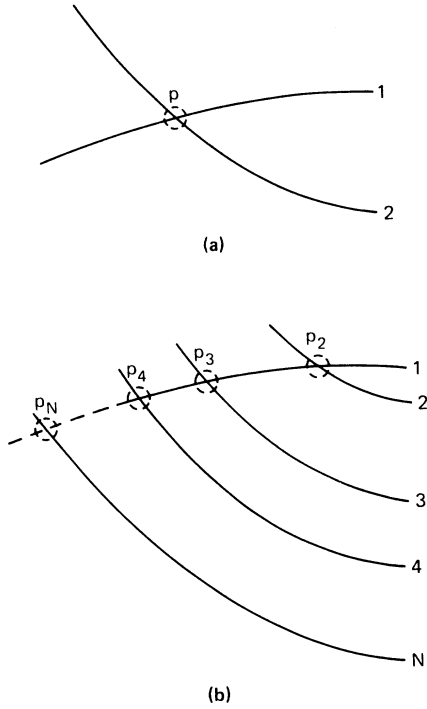
(a)

(b)

FIG. 4. Potential curve crossings. (a) Two states and one crossing, (b) N states and N-1 crossings.

matrix-element determination to transform from parabolic to spherical coordinates. Thus we obtain for the parabolic wave functions of the final-state hydrogenic heavy ions (referring to Fig. 5 for coordinate notation)

$$\varphi_j = |n,0,n-1,0\rangle$$

$$= \frac{1}{\sqrt{(\pi n)}} \frac{1}{(n-1)!} \alpha^{3/2} e^{-\alpha r_j}$$

$$\times \sum_{i=0}^{n-1} (-1)^i \frac{(n-1)!^2}{(n-i-1)!(i!^2)} [\alpha r_j (1 + \cos\theta_j)]^i, \quad (15)$$

and for the ground state hydrogen atom

$$\varphi_1 = |1,0,0,0\rangle = (1/\sqrt{\pi})e^{-r_1}. \quad (16)$$

Here $\alpha = Z/n$ and j is an ordering index, which, appropos to the previous discussion, orders those ion states to which transitions can take place from highest to lowest in energy.

The matrix elements can then be evaluated analytically since each of the two-center integrals involved [Eqs. (12)–(14)] can be reduced to sums of terms involving integrals of the form $\int x^m e^{-\mu x} dx$ (where m is an integer and $\mu > 0$), each of which has a closed-form solution. Thus we find

$$S_{1j} = \frac{2\pi N}{2^{n-1} R_{cj}^n} \sum_{l=0}^{n-1} (-1)^{l+1} \binom{n-1}{l} \sum_{k=0}^{2l+a} \frac{(2l+a)!}{k!}$$

$$\times \left\{ \exp(\alpha R_{cj})[I_1(\alpha+1, g, R_{cj}) - R_{cj}I_1(\alpha+1, g-1, R_{cj})] \right.$$

$$- \exp[(\alpha-2)R_{cj}] \sum_{s=0}^{k} (-1)^s \binom{k}{s} (2R_{cj})^{k-s}[I_2(\alpha-1, d, R_{cj}) - R_{cj}I_2(\alpha-1, d-1, R_{cj})]$$

$$\left. + \exp[(\alpha+2)R_{cj}] \sum_{s=0}^{k} (-1)^{s+k} \binom{k}{s} (2R_{cj})^{k-s}[I_1(\alpha+1, d, 2R_{cj}) - R_{cj}I_1(\alpha+1, d-1, 2R_{cj})] \right\}, \quad (17)$$

where

$$a = 1, \quad (18)$$

$$N = \alpha^{n+1/2}/[\pi n^{1/2}(n-1)!], \quad (19)$$

$$g = 2(n-l) + k - 1, \quad (20)$$

$$d = 2(n-l) + s - 1, \quad (21)$$

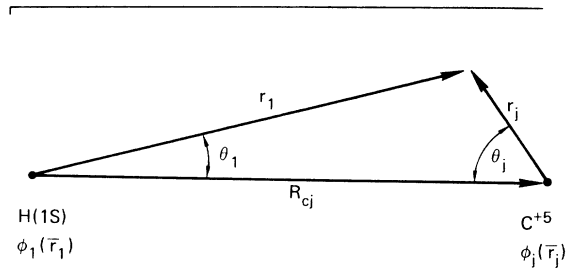and the functions I_1 and I_2 are given by

FIG. 5. Coordinate system for two-center integral computation.

$$I_1(\gamma, m, u) = \exp(-\gamma u) \sum_{k=0}^{m} \frac{m!}{k!} \frac{u^k}{\gamma^{m-k+1}} \qquad (22)$$

and

$$I_2(\gamma, m, u) = I_1(\gamma, m, u) - I_1(\gamma, m, 2u) . \qquad (23)$$

The integral σ_{1j} is determined by exactly the same expression, but with $a = 0$.

Evaluation of the ρ_{1j} integral produces a similar result, but so many terms are involved in the summations that roundoff error becomes a problem in the final computation. To circumvent this difficulty, a multipole expansion of the ρ_{1j} integral was made and the evaluation carried out term by term. The expression converges rapidly enough so that in all cases seven terms are sufficient for a final determination accurate to within 1%.

Once the matrix elements are computed, the cross sections may be determined in the conventional impact-parameter formulation. Thus the partial cross section for capture into a given level of the resultant hydrogenic ion may be expressed as

$$Q_j = 2\pi \int_0^{b_j} b\, P(b, E)\, db . \qquad (24)$$

Here b_j is the limiting impact parameter for which the distance of closest approach is equal to the crossing separation R_{cj},

$$b_j = R_{cj}[1 - U_{11}(R_{cj})/E]^{1/2} . \qquad (25)$$

The total cross section for capture is finally given by

$$Q_c = \sum_j Q_j , \qquad (26)$$

where the summation is over all levels for which there is appreciable transfer. In practice, for the systems considered, it was found that in general only a few crossings contributed significantly to the overall charge transfer. For the most distant crossings, the coupling is weak enough so that the system can be considered to move along the initial diabatic potential curve with small probability of capture taking place. On the other hand, for close crossings in the region of considerable overlap, the coupling is so strong that again negligible net electron transfer occurs.

IV. COMPUTATIONAL RESULTS AND DISCUSSION

A. Landau-Zener cross sections

Using these procedures, coupling-matrix elements and crossing separations for electron capture into various levels of final-state ions C^{+5},

N^{+6}, O^{+7}, Ne^{+9}, Si^{+13}, and Ar^{+17} were computed and are listed in the third and fourth columns of Table I. These represent, for each of the ions, the group of levels into which capture predominantly occurs. For C^{+5}, the transfer takes place primarily into the $n = 4$ level, whereas for the other ions considered two to four levels share in the capture process.

Another important consideration to emphasize here is that in accordance with the one-electron diatomic-molecule noncrossing rule, for each of these n levels, the transitions are primarily into the parabolic states with $n_2 = n - 1$. This implies that the product ions are distributed over all of the various l levels corresponding to a given n. Because the wave functions of the hydrogenic ion form a complete set in either parabolic or spherical coordinates, the wave function in parabolic coordinates $\varphi_{n n_1 n_2 m}$ can be expressed as a linear combination of the wave functions in spherical coordinates Ψ_{nlm}. Thus, for example, the distribution in spherical coordinate states for the resulting $C^{+5}(n)$ ion can be written[13]

$$\varphi_{4030} = \tfrac{1}{2}[\Psi_{400} - (3/\sqrt{5})\Psi_{410} + \Psi_{420} - (1/\sqrt{5})\Psi_{430}] . \qquad (27)$$

Estimates of the coupling-matrix elements at the crossings can also be obtained from the adiabatic potential curves. These independent determinations are of interest in that they provide a reasonable check on the magnitudes of the matrix elements obtained with atomic wave functions. In a two-state system, if one assumes linearity of the diabatic terms in the region of the avoided crossing, it is a reasonable approximation to take the matrix element as equal to one half the minimum separation between the adiabatic terms.[14] Estimates of a number of matrix elements and crossing distances for several of the systems studied were obtained by noting the internuclear separations and curve separations corresponding to the points of closest approach of the curves. The assumption is made in this procedure that only the two close-lying curves interact and that the influence of other states can be neglected. The values obtained are also listed in Table I where they are compared with the same quantities computed using formulas (2) and (11). In general, the two sets of the matrix elements are in reasonable agreement considering the differences in the two approaches. It should be noted that the total capture cross sections are dominated by the contributions from the more distant crossings where the use of atomic wave functions is expected to be valid. The values of the computed crossing separations R_{cj} are, in general, smaller than those ob-

TABLE I. Coupling-matrix elements and crossing separations for electron capture from H(1s) into various final-state levels. The unprimed quantities were obtained by direct computation. The primed quantities were derived from an analysis of the pseudocrossings observed in the adiabatic-potential curves for each system (Ref. 8). The number in parentheses associated with each U_{1j} and U'_{1j} value is the power of 10 which multiplies it.

Final-state ion	n level	U_{1j} (a.u.)	R_{cj} (a.u.)	U'_{1j} (a.u.)	R'_{cj} (a.u.)
C^{+5}	4	5.09 (−2)	7.3	5.0 (−2)	8.1
N^{+6}	5	9.19 (−3)	11.4	1.2 (−2)	11.6
	4	9.57 (−2)	5.7	1.2 (−1)	6.4
O^{+7}	6	6.60 (−4)	16.8	9.8 (−4)[a]	16.8[a]
	5	4.78 (−2)	8.3	5.0 (−2)	8.9
	4	1.07 (−1)	5.0	1.9 (−1)	5.4
Ne^{+9}	7	1.96 (−3)	16.2	3.0 (−3)[a]	16.1[a]
	6	4.13 (−2)	9.4	4.6 (−2)	10.0
	5	9.93 (−2)	6.1	1.5 (−1)	6.5
Si^{+13}	9	3.35 (−3)	17.3	5.3 (−3)[a]	17.2[a]
	8	2.89 (−2)	11.9	3.5 (−2)[a]	12.2[a]
	7	7.59 (−2)	8.4	9.8 (−2)	8.9
Ar^{+17}	11	3.06 (−3)	19.3	5.0 (−3)[a]	19.2[a]
	10	1.92 (−2)	14.4	2.6 (−2)	14.6
	9	5.35 (−2)	10.9	6.6 (−2)	11.3
	8	8.59 (−2)	8.4	1.3 (−1)	8.6

[a] Values added in proof.

tained from the potential curves. This, however, is not surprising in view of the fact that the actual diabatic crossing does not necessarily coincide with the point corresponding to the minimum approach of the adiabatic-potential curves, which was the convenient rule we used to estimate these quantities.

Plots of the total cross sections for electron capture from ground-state H atoms to C^{+6}, N^{+7}, O^{+8}, Ne^{+10}, Si^{+14}, and Ar^{+18} in the range of relative velocities from 6×10^6 to 7×10^7 cm/sec are presented in Fig. 6. A scale in terms of the laboratory kinetic energy of the C^{+6} ion is also included. The highest velocity displayed is considerably smaller than the hydrogenic orbital velocity. This ensures that the velocity range is indeed in the near-adiabatic region and reduces considerably the effect of neglecting momentum transfer of the electron. The lower limit on velocity is always such that the relative energy is much greater than any of the relevant coupling-matrix elements for these systems, which is a condition for applicability of the Landau-Zener formula.

The cross-section curves in the energy range considered, with the exception of the lower-energy N^{+7} data, show a definite systematic pattern. The maximum cross sections obtained increase monotonically with Z, the increase from C^{+6} to Ar^{+18} being about a factor of 5, reflecting the occurrence of contributing crossings at larger internuclear

separations for the higher-Z systems. The curves also tend to become flatter for these heavier ions because of the "smearing-out" effect of a number of important crossings (three or four) contributing significantly over a range of energies.

The Z dependence of the cross sections deserves further consideration. Dividing each cross section by $Z^{3/2}$ and replotting these reduced quantities, we obtain the curves shown in Fig. 7. The curves converge in the velocity range above about 3 or 4
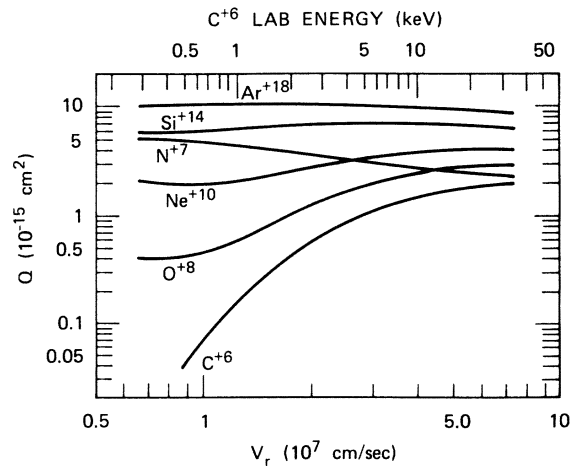

FIG. 6. Total Landau-Zener cross sections for electron transfer between H(1s) and various stripped ions.
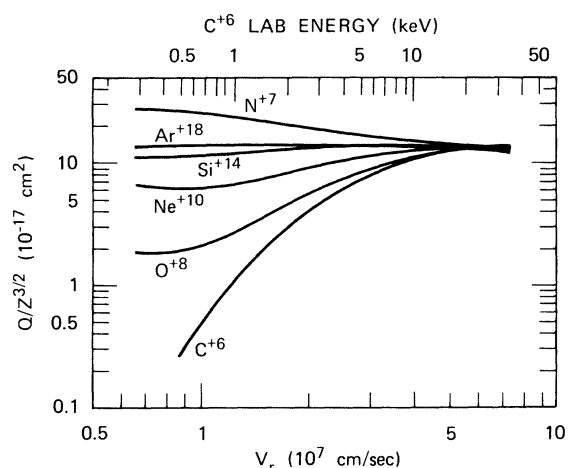
FIG. 7. Reduced capture cross sections corresponding to curves of Fig. 5. Each of the cross sections of Fig. 6 is divided by its associated value of $Z^{3/2}$.

$\times 10^{7}$ cm/sec. Thus for the higher energies the transfer cross sections can be represented to a reasonable approximation by the relation

$$Q_t \approx 1.4 \times 10^{-16} Z^{3/2} \text{ cm}^2 . \tag{28}$$

The N^{+7} curve should not be considered anomalous. In this case, there are only two important crossings and the interaction is such that the more distant crossing has a large enough matrix element to provide a strong maximum in the region of velocities around 6×10^{6} cm/sec. The C^{+6}-H system has only one significant crossing and the cross-section curve exhibits the typical Landau-Zener two-state threshold behavior.

B. Improved calculations

The deficiencies and limitations of the two-state Landau-Zener model have been well documented during the last 15 years.[15-19] Both experimental results and more refined theoretical efforts indicate that the application of the Landau-Zener formula leads, in general, to underestimates of the peak cross sections and to shifts in the position of the peak value with respect to relative collision velocity. A major part of the problem lies in the fact that, contrary to what is assumed in the Landau-Zener model, the transition region, in effect, extends over a considerable range in R over which the coupling can vary appreciably. Moreover, interference effects are neglected completely. Ovchinnikova[19] has recently made a systematic investigation of the effect of certain characteristic interaction parameters on the magnitudes and energy dependences of the inelastic cross sections obtained for a two-state, single-crossing model. Her analysis was made using an improved (relative

to the Landau-Zener case) linear model to obtain the more accurate transition probabilities. In terms of this theory, two of the important parameters are

$$A = (2/\pi)(R_c/\delta R)^{1/2} \tag{29}$$

and

$$\nu = 2\gamma_e \delta R , \tag{30}$$

where

$$\delta R = U_{12}/\Delta F \tag{31}$$

and γ_e is an effective exponential decay constant for the coupling term. Here, $1/A$ is a measure of the width of the transition region relative to R_c and ν characterizes the extent to which the coupling changes in the effective-interaction region ($A = \infty$ and $\nu = 0$ for the Landau-Zener case). Changes in A affect the cross-section maximum significantly but have very little influence on the position of the peak. The increase in the cross section with decrease in A can be attributed mainly to the increased contribution of peripheral (tunneling) collisions with $b \gtrsim R_c$. On the other hand, the effect of an increase in ν is primarily to shift the cross-section peak to lower energies.

The Ovchinnikova theory would seem to be particularly appropriate for application to the C^{+6}-H system where a single crossing predominates. The calculated values of A and ν for this case are 2.33 and 0.829, respectively. The quantity ν was obtained directly from the R dependence of computed matrix elements. These values suggest significant
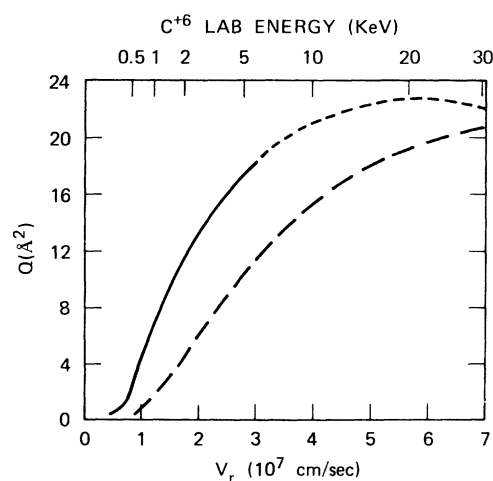

FIG. 8. Charge-transfer cross sections for the C^{+6}-H(1s) collision system. (a)--, Landau-Zener computations; (b)—, quantum close-coupling calculations; (c)---, extrapolation of quantum close-coupling calculations based on Ovchinnikova's analysis (Ref. 19).

corrections to the Landau-Zener results are re-
quired. Unfortunately, only a few correction
curves covering a very limited range of param-
eters were given by Ovchinnikova, making a quan-
titative determination of the cross sections diffi-
cult, particularly in the threshold region.

To obtain more accurate cross sections for the
C^{+6}-H system, therefore, we proceeded in the fol-
lowing way: In the threshold and lower-velocity
range, we employed a quantum close-coupling
method to calculate the cross sections. The quan-
tal equations for a two-state system incorporating
the previously discussed potentials were solved
for the S matrix at each energy over the appropri-
ate range of partial waves using the logarithm de-
rivative algorithm given by Johnson.[20] In the equa-
tions, the coupling term was set equal to the arith-
metic mean[21] of U_{12} and U_{21}. The results are shown
by the solid curve in Fig. 8 up to a velocity of
3×10^7 cm/sec. At the higher velocities where the
close-coupling method becomes very expensive,
we then employed the Ovchinnikova corrections to
extrapolate the cross-section curve to 7×10^7
cm/sec (shown as the small-dash line in Fig. 8).
At $v = 3 \times 10^7$ sec^{-1} and below, the cross sections
derived from the Ovchinnikova analysis were in
reasonable agreement with the close-coupling cal-
culations, taking into consideration the interpola-
tion errors involved in the former determinations.
Hence we believe the extrapolation to higher vel-
ocities is valid. These results may then be com-
pared with the Landau-Zener calculations which
have been replotted in Fig. 8 as the large-dash
curve. The shapes of the cross-section curves
are qualitatively similar. However, the close-
coupling curve is clearly shifted towards lower
velocities and the peak cross sections are about
15% higher.

No additional calculations or corrections have
been made for the other systems studied, each of
which included two or more strongly contributing
crossings. The Ovchinnikova analysis was not ap-

plicable in its present form to these multicrossing
systems. However, the correctional parameters
A and ν could be evaluated for each of the cross-
ings, and on the basis of these evaluations some
qualitative inferences could be made. In general,
both the "shift" and "magnitude" corrections are
expected to be smaller than in the case of C^{+6}-H,
particularly for the heavier systems such as
Ar^{+18}-H and Si^{+14}-H. The "shift" corrections are
further reduced in importance for these systems
by the smearing-out effect of the several contribu-
ting crossings.

V. CONCLUDING REMARKS

Clearly, the set of calculations presented here
can be considered only as an initial exploratory
step toward the solution of a very complicated
class of collision problems.[22] In general, for a
two-state, single-crossing system, application of
the Landau-Zener theory with its neglect of tunnel-
ing leads to underestimates of the peak cross-sec-
tion values and shifts of the peaks to lower colli-
sion velocities. Extension of the model to a multi-
state, multicrossing system brings up additional
complications which have yet to be checked out by
experiment and more refined theory. Finally,
possible contributions due to rotational coupling
have been neglected in this presentation. Never-
theless, despite their limitations, we believe the
calculations serve a valuable purpose by delineat-
ing the dominant capture processes and giving
reasonable cross sections over a considerable en-
ergy range. Because of the nature of the approxi-
mations made, the calculated cross sections are
probably underestimates of the "true" cross sec-
tions with uncertainties of about a factor of 2.

[1]See, for example, *Proceedings of the International Con-
ference on Inner Shell Ionization Phenomena and Future
Applications, Atlanta, 1972,* edited by R. W. Fink
et al., CONF-720404 (Natl. Tech. Information Service,
U. S. Dept. of Commerce, Springfield, Va., 1972).
[2]H. A. Bethe and E. E. Salpeter, *Quantum Mechanics of
One and Two-Electron Atoms* (Springer, Berlin, 1957),
p. 232.
[3]J. D. Power, Philos. Trans. R. Soc. 274, 663 (1973).
[4]J. Von Neumann and E. Wigner, Z. Phys. 30, 1467

(1929).
[5]K. Razi-Nagvi and W. Byers Brown, Int. J. Quant. Chem.
6, 271 (1972).
[6]S. S. Gershtein and V. D. Krivchenkov, Zh. Eksp. Teor.
Fiz. 40, 1491 (1961) [Sov. Phys.-JETP 13, 1044 (1961)].
See also I. V. Komarov and S. Yu. Slavyonov, J. Phys.
B 1, 1066 (1968).
[7]C. A. Coulson and A. Joseph, Int. J. Quant. Chem. 1,
337 (1967).
[8]This program developed by J. D. Power, is now avail-
able as Program No. 233 from the Quantum Chemistry
Program Exchange, Chemistry Dept., Indiana Uni-
versity, Bloomington, Ind. 47401.

[9]L. Landau, Phys. Z. Sowjetunion 2, 46 (1932).

[10]C. Zener, Proc. R. Soc. London A 137, 696 (1932).

[11]D. R. Bates and B. L. Moiseiwitsch, Proc. Phys. Soc. A 67, 805 (1954).

[12]Reference 2, p. 29.

[13]K. Omidvar, Phys. Rev. 153, 121 (1967).

[14]R. E. Olson, F. T. Smith, and E. Bauer, Appl. Opt. 10, 1848 (1971).

[15]D. R. Bates, Proc. R. Soc. A 257, 22 (1960).

[16]Yu. P. Mordvinov and O. B. Firsov, Zh. Eksp. Teor. Fiz. 39, 427 (1960) [Sov. Phys.-JETP 12, 301 (1961)].

[17]C. A. Coulson and K. Zalewski, Proc. R. Soc. A 268,
437 (1962).

[18]E. E. Nikitin, Adv. Quant. Chem. 5, 135 (1970).

[19]M. Ya. Ovchinnikova, Zh. Eksp. Teor. Phys. 64, 129 (1973) [Sov. Phys.-JETP 37, 68 (1973)].

[20]B. R. Johnson, J. Comp. Phys. 13, 445 (1973).

[21]D. R. Bates, H. C. Johnston, and I. Stewart, Proc. Phys. Soc. Lond. 84, 517 (1964).

[22]See also L. P. Presnyakov and A. D. Ulantsev, Kvant. Electron. 1, 2377 (1974) [Sov. J. Quant. Electron. 4, 1320 (1975)] for a general analysis of charge-transfer processes involving highly charged ions and atoms.