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Unified treatment of slow atom-atom and ion-atom collisions. II. Applications to $H^+ + H$ and $C^{6+} + H$ collisions

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A unified treatment of ion-atom collisions proposed earlier [Phys. Rev. A **31**, 590 (1985)] is applied to study excitation and charge transfer in $H^+ + H$ and $C^{6+} + H$ collisions. This method expands the time-dependent electronic wave function in terms of traveling atomic orbitals of the two collision centers at large internuclear separations which is matched to the solution in the inner region where it is expanded in terms of molecular orbitals without translational factors. The results for $H^+ + H$ are shown to agree with recent elaborate close-coupling calculations and with experiments. For $C^{6+} + H$ collisions, the partial cross sections for capture to $n = 5$ of C^{5+} are in better agreement with the atomic expansion calculation of Fritsch and Lin than with the molecular orbital expansion of Green *et al.*

I. INTRODUCTION

Inelastic processes in ion-atom collisions in the low- to intermediate-energy region have been the subject of extensive theoretical study in recent years. Almost all of the theoretical models use the semiclassical impact-parameter formulation and expand the time-dependent electronic wave functions in terms of the stationary molecular orbitals (MO's) or in terms of the traveling atomic orbitals (AO's) of the collision system. However, it has been recognized that either approach has its intrinsic limitations. The AO expansion method cannot appropriately account for the relaxation of the electronic orbitals during slow collisions and the MO expansion in the perturbed stationary-state (PSS) approximation has difficulties in incorporating the translational motion of the electrons in the asymptotic regions. Various methods have been introduced aiming at solving these difficulties. Within the AO expansion scheme the AO + model[1] and the triple-center AO expansion[2] method were proposed. Both approaches introduced united-atom atomic orbitals in the expansion to account for the relaxation of the electronic orbitals at close collisions. Within the MO expansion scheme, various translational factors have been introduced[3,4] into the formalism and several applications to simple collision systems have emerged in the last few years.

In a recent article[5] (hereafter referred to as I), the authors proposed a new model by adopting the better features of the AO and MO expansions in each region of the configuration space into a unified treatment of ion-atom collisions. In this model the time-dependent electronic wave functions are expanded in terms of traveling atomic orbitals of the two moving centers at large internuclear separations. In the interaction region, the wave functions are to be solved variationally. For slow collisions, however, they are expanded in terms of molecular orbitals. The solutions in the two regions are matched at two internuclear separations. This model is similar to the R-matrix method[6] for the solution of time-independent Schrödinger equation. The model was applied to $H^+ + He^+$ collisions in I and a similar method was applied by Winter and Lane[7] to $He^{++} + H$. The results from both calculations agreed quite well with other elaborate close-coupling calculations based either on AO or on MO expansion and with experiments.

In this article, we apply the model to two different collision systems: the symmetric $H^+ + H$ collisions and the asymmetric $C^{6+} + H$ collisions. In the first case we want to test the reliability of the present method for obtaining accurate partial cross sections, in particular, the excitation and charge transfer to $2s$ and $2p$ states. Theoretical calculations for these processes have a long standing history, but only in the last few years the theoretical results from various models[2,3,8,9] and experiments are beginning to converge qualitatively in the energy region from 1 to 10 keV. On the other hand, quantitative agreement for the small $2s$ channel is still not entirely satisfactory. There is a 32% difference between the largest and smallest values obtained at 2 keV among the various elaborate close-coupling methods. Since experimental data are not accurate enough to resolve the discrepancy, it is desirable to see if the difference originates from the lack of including higher channels or from the defects of some other models. The present calculation also serves to test this new approach and to assess the sensitivity of the method with respect to the matching parameters chosen.

For the second collision system, the dominant processes are the electron capture to $n = 4$ states of the C^{5+} ions. New experimental results[10] on the total capture cross sections are in agreement with the results from the large-scale calculation based on the 35-state AO expansion[11] and those based on the 33-state MO expansion.[12] However, the two calculations predict different cross sections for capture to the $n=5$ states. According to the MO expansion method, there is a significant amount of capture to the $n=5$ states for energies below 0.4 keV/amu while according to the AO expansion there is little contribution from the $n=5$ states. Our present calculations agree with the results from the AO expansion.

The main features of the model description as used in the present investigation and the calculational procedures are outlined in Sec. II. Results of the calculations are presented and discussed in Sec. III. Finally, Sec. IV contains some concluding remarks. Atomic units are used throughout.

II. THEORETICAL METHOD

We adopt a semiclassical impact parameter formulation. In this model, the basic equation for describing the time development of the electronic motion is the time-dependent Schrödinger equation. For the one-electron collision systems investigated here, the equation for the time-dependent wave function $\Psi(\mathbf{r},t)$ is

$$\left[-\tfrac{1}{2}\nabla^2-\frac{Z_T}{r_T}-\frac{Z_P}{r_P}\right]\Psi(\mathbf{r},t)=i\frac{\partial}{\partial t}\Psi(\mathbf{r},t)\ , \qquad (1)$$

where the first term is the kinetic energy of the electron; Z_P is the charge of the projectile; Z_T is the charge of the target atom; and r_T, r_P, and r are the distances of the electron measured from the target, the projectile, and the chosen origin, respectively. If the wave function $\Psi(\mathbf{r},t)$ is expanded in terms of some basis functions $\{U_i(\mathbf{r},t)\}$,

$$\Psi(\mathbf{r},t)=\sum_i a_i(t)U_i(\mathbf{r},t)\ , \qquad (2)$$

then following the standard procedure, Eq. (1) can be reduced to a set of linear coupled equations,

$$\underline{I}\,\underline{S}\,\underline{A}=\underline{M}\,\underline{A}\ , \qquad (3)$$

where $\underline{S}$ and $\underline{M}$ represent the overlap matrix and coupling matrix, respectively, and the column matrix $\underline{A}$ represents the time-dependent expansion coefficients. In the inner MO region, the electronic Hamiltonian is diagonal and the coupling matrix $\underline{M}$ is due to the nuclear motion. In the outer AO region, the potential due to the two collision centers is the source of the coupling matrix $\underline{M}$.

In Fig. 1, we show the configuration space divided into two regions: the outer region where the charge cloud around the two moving centers overlaps only slightly and the inner region where the electron cloud spreads over the two centers equally. In the outer region, the electron around each center is traveling with the moving collision center, thus an expansion of the wave function in terms of two-center traveling atomic orbitals is suitable. In the inner region, the translational energy of the electron is relatively small and it is therefore appropriate to expand the wave function in the inner region in terms of molecular orbitals neglecting the translational motion. At the two boundaries $-t_0$ and t_0, it is assumed that both expansions are adequate and the solutions can be matched.

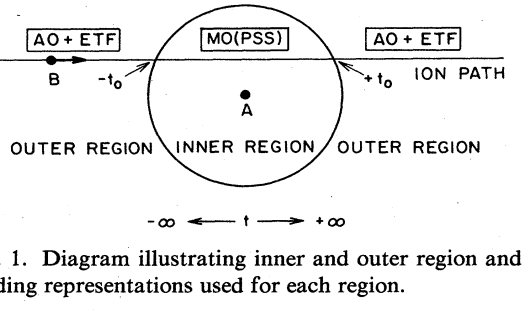

FIG. 1. Diagram illustrating inner and outer region and corresponding representations used for each region.

In practical applications, the time-dependent wave function is first expanded in terms of atomic orbitals,

$$\Psi(\mathbf{r},t)=\sum_i a_i(t)\tilde{\phi}_i^{\mathrm{AO}}(\mathbf{r}_T)+\sum_j b_j(t)\tilde{\phi}_j^{\mathrm{AO}}(\mathbf{r}_P)\ , \qquad (4)$$

where $\tilde{\phi}_i^{\mathrm{AO}}(\mathbf{r}_c)$ is a traveling atomic orbital (including a proper plane-wave translational factor) centered at c. With the expansion (4), a set of linear coupled equations [see (3)] is obtained which is integrated from $t=-\infty$ to $t=-t_0$. From $t=-t_0$ to $t=t_0$, $\Psi(\mathbf{r},t)$ is expanded in terms of molecular orbitals,

$$\Psi(\mathbf{r},t)=\sum_k C_k(t)\phi_k^{\mathrm{MO}}(\mathbf{r};\mathbf{R})\ . \qquad (5)$$

Since the molecular orbitals are orthogonal, the overlap matrix S in the resulting linear coupled equations [see (3)] is a unit matrix. To integrate the coupled equations (3) in the inner region, the initial values of the coefficients at $t=-t_0$ have to be determined. They are obtained by projecting $\Psi(\mathbf{r},-t_0)$ onto each MO, i.e.,

$$C_k(-t_0)=\langle\phi_k^{\mathrm{MO}}(\mathbf{r};R_0)\,|\,\Psi(\mathbf{r},-t_0)\rangle\ , \qquad (6)$$

where $R_0=R(-t_0)$. The calculation and the relevant matrix elements in the inner region are similar to those in the conventional PSS model. Instead of applying the MO expansion to large R, we reexpand $\Psi(\mathbf{r},t_0)$ in terms of a two-center AO expansion (4) for $t=t_0$ and integrate the resulting equations in the AO basis from t_0 to $+\infty$ to extract scattering amplitudes. The initial coefficients $\{a_i(t_0),b_j(t_0)\}$ at t_0 are obtained by projecting $\Psi(\mathbf{r},t_0)$ onto each atomic orbital. Since the atomic orbitals on different centers are not orthogonal, we have to solve the following algebraic equations:

$$a_i+\sum_{j=1}^{N_P} b_j\langle\tilde{\phi}_i^{\mathrm{AO}}\,|\,\tilde{\phi}_j^{\mathrm{AO}}\rangle=\langle\tilde{\phi}_i^{\mathrm{AO}}\,|\,\Psi(\mathbf{r},t_0)\rangle\ , \qquad i=1,2,\ldots,N_T$$

$$(7)$$

$$b_j+\sum_{i=1}^{N_T} a_i\langle\tilde{\phi}_j^{\mathrm{AO}}\,|\,\tilde{\phi}_i^{\mathrm{AO}}\rangle=\langle\tilde{\phi}_j^{\mathrm{AO}}\,|\,\Psi(\mathbf{r},t_0)\rangle\ , \qquad j=1,2,\ldots,N_P$$

where N_T and N_P are the number of atomic orbitals included in the expansion (4) for the target and the projectile center, respectively.

The probability $P_j(b)$ for charge transfer to a particular jth state is given by

$$P_j(b)=|\,b_j(+\infty)\,|^2 \qquad (8)$$

for each impact parameter b and each given energy E. The cross section to the ith state is obtained by integrating over impact parameters.

This unified treatment takes advantage of the most suitable basis sets in each portion of the configuration space during the collision. However, it introduces some small uncertainties depending on the choice of matching parameters and the basis functions used. As a rule, if the matching is made at a larger internuclear separation, then a larger molecular basis in the inner region is required to represent the traveling character of the electron cloud in this region. If the matching is made at a smaller internuclear separation, then a larger traveling AO basis set is needed in the outer region to account for the relaxation of the electronic cloud. If this outer region is extended throughout the whole configuration space, as in the AO + model,[1] then a larger basis set, including united-atom orbitals, is required. The conventional perturbed stationary state (PSS) approximation extends the "inner" MO region to all allowed values of R. Since the basis functions in the PSS model do not satisfy the asymptotic boundary conditions, spurious couplings in the outer region are introduced.

The internuclear separations R_0 where matching is made can be determined at where the charge cloud begins to break apart. In this region, the dominant molecular orbitals can be expressed as linear combination of atomic orbitals (LCAO). This criterion was used in I. A similar conclusion was obtained from the work of Winter and Lane[7] through the examination of electron density during the collision. In these two studies, it was shown that the results are not sensitive to the choice of matching parameter R_0. In principle, the basis set has to be changed if R_0 is changed. Our experience is that the results are not very sensitive to the parameter R_0 used even if the basis set is fixed.

Since the basis set used in each region is not complete, the total probabilities are not conserved at the matching. This loss of unitarity is important only at the second matching point. As the two nuclei separate, the charge cloud grows bigger and some part will emerge traveling with the target and some part with the projectile. These parts are easily represented in terms of expansions using atomic orbitals moving with the two centers. However, there is also a component propagating outward as time increases which is not well represented by the two-center AO functions. This behavior of the charge cloud evolution was demonstrated by Shakeshaft[13] for $H^+ + H$ at 40 keV. We can attribute the loss of unitarity at matching to ionization probabilities. Our calculations clearly show that the loss of unitarity becomes more significant at higher collision energies. This is consistent with the general behavior of ion-atom collisions where ionization becomes dominant at higher collision energies. However, this assessment has to be checked in later calculations to see if the results are stable against the choices of basis sets. The loss of unitarity in the present calculations is generally less than 10% except at the highest energy point for $H^+ + H$ collision where the loss of probability is 16%. In our present calculation, we have renormalized the probability at the matching point so that it can be easily compared with the close-coupling results. (This may not be really desirable if the unitarity loss at matching can be attributed to ionizations.) All the calculations reported here have been carried out using a straight-line trajectory for heavy particle motion for collision energy above 1 keV/amu, and a Coulomb trajectory for $E < 1$ keV/amu.

III. RESULTS AND DISCUSSION

A. Symmetric $H^+ + H$ collisions

In the last few years many elaborate calculations based on the general close-coupling scheme have been applied to study the excitation and charge transfer to $2s$ and $2p$ states. Among them are the 10-state MO expansion,[3] the 40-state AO + expansion,[14] the 36-state triple-center AO expansion,[2] and the 150-state Hylleraas basis function expansion. The results from these calculations for the first time explain the qualitative behavior of the experimental total cross sections[15–20] for charge transfer and excitation to $2s$ and $2p$ states. In the 1–15 keV region, the $2p$ states are populated mostly via the $2p\sigma$ and $2p\pi$ rotational coupling, the cross sections for $2p$ are larger than for $2s$, and the results are explained well by those models where the rotational coupling is appropriately included. The situation for the $2s$ is different. It is populated via the weak radial coupling. The cross section is small. Although the energy dependence of the calculated $2s$ total cross sections agree with experiments, the discrepancies between theories are about 30% at lower energies. The large discrepancies among experimental data also make definite assessment of theoretical calculations difficult.

We have employed 10 MO's (the five lowest *gerade* and five lowest *ungerade* states) to expand the time-dependent wave function in the inner region and 20 AO's ($1s$, $2s$, $2p$, $3s$, $3p$, and $3d$) on each center in the outer region. To test the sensitivity of the calculated probabilities to the matching radius R_0, we listed in Table I the probability for charge transfer to $2s$ state at $b=2$ a.u. and $E=5$ keV. Recall that this is a weak channel, and results in the table indicate that the probability does not depend sensitively on the matching radius in the 3 to 6 a.u. region. The results reported below are from calculations using $R_0=4.5$ a.u.

In Fig. 2 the $bP(b)$ vs b for electron capture to $2s$ and $2p$ states obtained from the present calculation are shown at $E=1.56$ and 11.1 keV. In comparison with the results (not shown) from the 22-state AO + model,[8] and from the 36-state triple-center AO expansion model,[2] there is a good agreement in the overall shape of $bP(b)$ for each case. On the other hand, the values at the peak from the

TABLE I. $2s$ capture probability $P(b)$ times the impact parameter b as a function of the matching radius R_0 (a.u.). $E=5$ keV, $b=2$ a.u.

R_0 (a.u.)	$bP(b)$
3.0	0.0208
4.0	0.0219
5.0	0.0227
6.0	0.0224

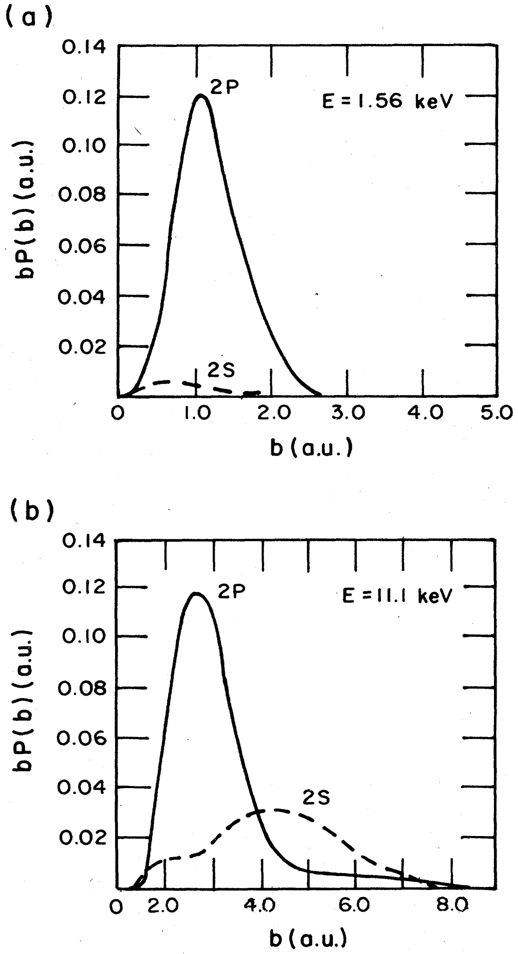

FIG. 2. Probability times impact parameter versus impact parameter for $H^+ + H$ collision at (a) $E = 1.56$ keV and (b) $E = 11.1$ keV.

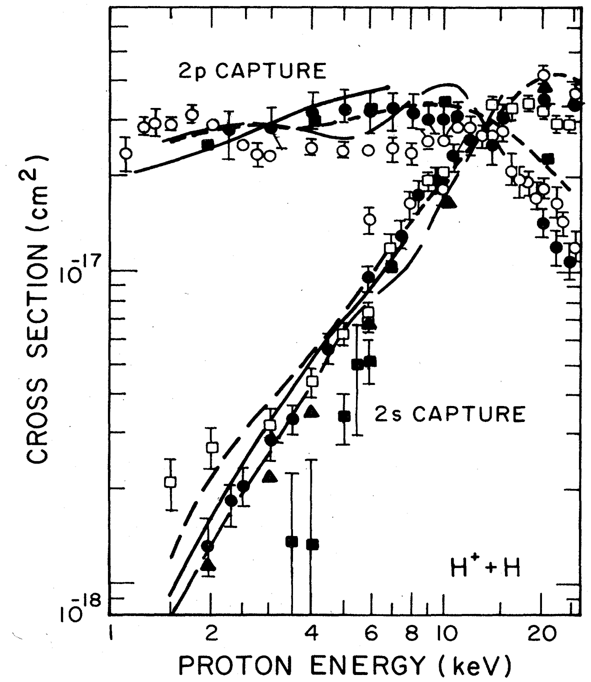

FIG. 3. Electron capture to $2p$ and $2s$ states. Theory: $2p$ (■), $2s$ (▲), present; solid line, MO, Ref. 3; dashed line, AO +, Ref. 8; long dash, triple center, Ref. 2. Experiment: ●, Refs. 15 and 20; ○, Refs. 16 and 17; ■, Ref. 18; □, Ref. 19.

present calculation at both energies are lower by about 6—10 % for the $2s$ and 12—14 % for the $2p$ as compared with the triple-center results, while the latter results are 9—25 % and 14—18 % lower than the AO + results. These discrepancies are probably due to the different size of basis sets used in each calculation.

The electron capture cross sections to $2s$ and $2p$ states obtained from experiments and from the results of several elaborate calculations are shown in Fig. 3. Among the theoretical calculations are the 10-state MO expansion,[3] the triple-center AO expansion,[2] and the AO + model.[8] For the $2p$ capture, the present result lies between the MO and the AO + results below 3 keV, and it stays close to the AO + result at $E > 5$ keV. In comparison with experiments, the present results agree better with those from Refs. 15 and 20. The present calculation does not predict the pronounced dip structure of $2p$ capture near 5 keV as shown in the triple-center AO calculation. The position of the cross-section maximum is consistent with other calculations.

The capture cross sections to $2s$ are also shown in Fig. 3. The present results are in good accord with other elaborate close-coupling calculations shown in the figure as well as with experiments. However, there are still significant discrepancies among the theoretical calculations. For example, the 36-state triple-center values differ from the 22-state AO + values by 31%, 22%, and 17% at energies of 1.56, 5.16, and 11.1 keV, respectively. The present results, on the other hand, differ from the triple-center results by 8%, 5%, and 5% at the above energies, respectively. The discrepancies at lower energies probably can be attributed mostly to the AO + model where the basis set is less "complete" in comparison with other calculations.

B. Asymmetric $C^{6+} + H$ collisions

We have also applied the present unified treatment to $C^{6+} + H$ collisions using 25 MO's (all MO's which correlated to the $n = 4$ and 5 manifolds of C^{5+} and the $1s$ of H) and 27 AO's (26 states of $n = 4$ and 5 of C^{5+} and $1s$ of H). According to the previous work of Green *et al.*[12] and of Fritsch and Lin,[11] transitions to other channels are small and states correlated to those channels are not included in the present calculation. The sensitivity of the results with respect to the matching radius R_0 was also tested. It was chosen at the optimum value of 6 a.u. in the present study. By changing R_0 within ±20% of the optimum value, the largest fractional change of probability is about 15%. Loss of unitarity at the matching lies typically between 0.05 to 0.13 for the basis set chosen, the

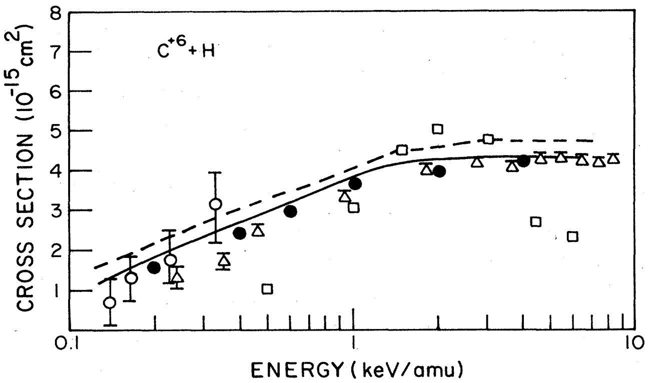

FIG. 4. Total electron capture cross section for C^{6+} + H collision. Theory: ●, present; solid line, AO+, Ref. 11; dashed line, MO, Ref. 12. Experiment: ○, Ref. 21; □, Ref. 22; △, Ref. 10.

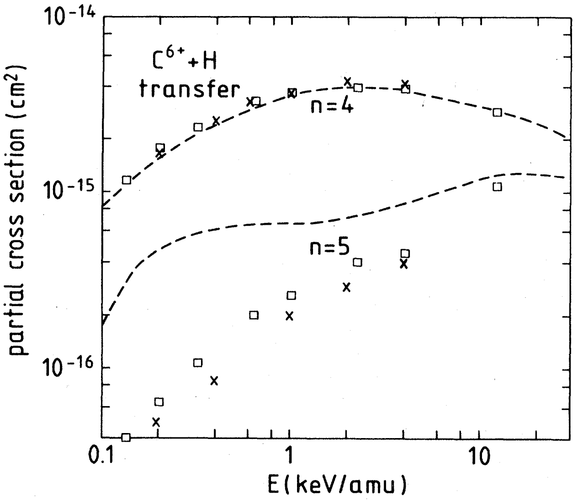

FIG. 5. Partial cross sections for transfer into C^{5+} $n=4$ and $n=5$ orbitals in C^{6+} + H collisions. Results of the 33-state MO investigation (Ref. 12) are shown in dashed lines, results of the 35-state AO study (Ref. 11) are indicated by open squares, and the present results are given in crosses.

larger value corresponding to higher energy collisions.

We first compare the total capture cross sections with experiments. In Fig. 4 the result from the measurement of Panov *et al.*,[21] the earlier data of Phaneuf *et al.*,[22] and the recent result from Meyer *et al.*[10] are shown together with the results from the 33-state MO expansion of Green *et al.*,[12] the 35-state AO expansion of Fritsch and Lin[11] and from the present calculation. The result from the present work agrees in general, quite well with the AO result and with the most recent data of Meyer *et al.*

The general agreement among the theoretical calculations for total capture cross sections is somewhat misleading. In fact, a critical test is to compare the predicted (n,l) distributions. In Table II, the partial cross sections from the present work are tabulated. They are to be compared with Table I of Ref. 11. In Fig. 5 we show the n distribution calculated from the three models. We notice that the results for $n=4$ agree with each other among the three calculations. For the $n=5$ cross sections, the present work agrees with the AO results while the MO model predicts much higher values.

We also compare the l distribution for the $n=4$ manifold. Recall that the total capture cross sections to $n=4$ calculated among the three models are basically identical. By comparing Table II with Table I and Fig. 4 of Ref. 11, we notice that the agreement among the three models for l distribution is quite good, although the present results tend to be closer to the AO results.

IV. CONCLUSION

We have applied a unified theory of ion-atom collisions to study the partial cross sections in H^+ + H collisions

TABLE II. Cross section (10^{-15} cm^2) for electron capture into C^{5+} l sublevels. n, principal quantum number; P_l, normalized l-sublevel cross section.

E (keV/amu)	n	σ_n	P_0	P_1	P_2	P_3	P_4
0.20	4	1.66	0.04	0.12	0.33	0.51	
	5	0.03					
0.40	4	2.31	0.07	0.14	0.36	0.43	
	5	0.08					
0.60	4	3.11	0.08	0.16	0.39	0.37	
	5	0.14	0.08	0.18	0.33	0.22	0.19
1.0	4	3.54	0.09	0.20	0.41	0.30	
	5	0.20	0.05	0.11	0.26	0.35	0.25
2.0	4	3.83	0.11	0.23	0.42	0.24	
	5	0.27	0.03	0.09	0.16	0.33	0.35
4.0	4	3.79	0.08	0.22	0.41	0.29	
	5	0.38	0.02	0.08	0.13	0.32	0.42

and in $C^{6+} + H$ collisions. The results are compared with other elaborate close-coupling calculations. We conclude from the comparison that the present method is capable of giving accurate partial cross sections for capture and excitation to $2s$ and $2p$ states in $H^+ + H$ collisions. We have also shown that the total capture cross section for $C^{6+} + H$ from the present study agrees very well with the most recent experimental data, and the partial cross sections to the $n=5$ states agree with the AO calculations rather than with the MO calculations.

In conclusion, we have shown that the present method, with a small basis set in each region of the configuration space, can produce not only reliable total cross sections but also accurate partial cross sections. Together with the positive results from I and from Ref. 7, we can conclude that this unified theory can provide reliable results for one-electron collision systems. However, the challenge is to apply this method to many-electron collision systems. Applications of the model to two-electron collision systems are underway.

We have also studied the dependence of the calculations on matching parameters. In this connection it is appropriate to remark on the work of Dickinson and McCarroll[23] and of Salin.[24] In the work of Ref. 23, as in the present work, the authors also considered the inner and the outer regions. The PSS model was applied in the inner region where the MO's were matched to the outer region smoothly by introducing a damped electron translational factor. In their model calculations, the matching was carried out at a very large radius using a two-state approximation. It was discussed in Ref. 24 that such a procedure is inappropriate. Our approach differs from these authors in that we adopt the matching radius at where the charge cloud begins to break apart and a larger basis set was used in both regions. In a test calculation for $H^+ + H$ system, we purposely chose a matching radius around 10 a.u. with a fixed basis set. The results were shown to depend sensitively on where the matching was made. To obtain results independent of matching parameters at such a large matching radius, a much larger MO basis set is needed, although it is not clear how large the basis set must be for it to be adequate.

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