Simultaneous capture and ionization in helium

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Data for simultaneous capture and ionization in helium by H^+, He^{2+}, and Li^{3+} are compiled and analyzed in terms of direct and rearrangement mechanisms at high projectile velocity. Some new data for H^+ and He^{2+} are presented and a similarity in the ratio of cross section for capture and ionization to single capture plus capture and ionization for projectiles of charges $Z=2$ and 8 is noted.

The many-electron and many-body problem is central to understanding various areas of physics, chemistry, and biology. In atomic physics the two-body problem and parts of the few-body problem are fairly well understood. For example, single-electron capture and atomic ionization are well in hand at high collision velocities. This three-body knowledge can provide a basis for studies of simultaneous capture and ionization or double ionization[1-19] at high velocities. In this paper we study the ratio of the cross section, σ^{2+}, for simultaneous capture and ionization divided by the cross section, σ^{+}, for single capture in helium. By taking the ratio of a two-electron to a one-electron transition cross section, the effects of the one-electron transition mechanism tend to cancel so that the two-electron mechanism becomes more apparent.

Mechanisms for double ionization have been previously studied[5-7,15] by considering the ratio of double- to single-ionization cross sections in helium. Analysis was done using a combination of the final-state rearrangement mechanism and a direct mechanism where double transitions occur via direct Coulomb interaction of both electrons with the projectile. In the direct mechanism at high velocities in the Born approximation the ratio of cross sections increases with the projectile charge Z and decreases with collision velocity v as $Z^2/(v^2 \ln v)$. These two mechanisms, rearrangement and direct, have been used to analyze cross sections for double ionization in helium in high-energy collisions with protons, heavy ions, electrons, photons, and most recently, antiprotons.[6] Here we extend this analysis to simultaneous capture and ionization and give a unified formulation for the rearrangement and direct mechanisms.

In the pioneering work of Horsdal-Pedersen and Larsen[1] only the rearrangement mechanism was used in analysis of the data. We have compiled additional data and demonstrate here that the direct mechanism can also play an important role in these collisions. We also present some new data for capture and ionization by protons and α particles. At lower velocities we find a peak in the ratio of capture plus ionization to single-capture cross sections for α projectiles. This peak is qualitatively similar to structure seen earlier[2,3] in collisions with projectiles of charge $8+$.

In order to understand a little about the nature of simultaneous capture and ionization we begin with an exact expression for the probability amplitude for multiple capture ionization and capture in an atom collision where the projectile's path is characterized by an impact parameter b. Here the exact probability amplitude may be expressed as

$$a(b)=\left\langle \phi_f \left| T\exp\left[i\int V\,dt \right] \right| \phi_i \right\rangle . \tag{1}$$

Here ϕ_i represents the initial state of the many-electron target and an incident projectile, ϕ_f represents the final state of the system containing both captured and continuum electrons, and $T\exp(i\int V\,dt)$ is the operator containing the interactions V, occurring during the collision. For the purposes of this paper it is sufficient to consider a two-electron system.

A useful starting point for approximation is the independent-electron approximation where electron-electron interactions are neglected. In this approximation whatever happens to one electron does not affect the other electron. Hence capture plus ionization occurs only when both electrons interact directly with the projectile. In this independent-electron approximation or direct (D) picture $\phi_i=\phi_i^1(r_1)\phi_i^2(r_2)$ and $\phi_f=\phi_f^1(r_1)\phi_f^2(r_2)$ and $V=V_1+V_2$ we have

$$\begin{aligned} a_D &= \left\langle \phi_i^1 \left| T\exp\left[i\int V_1 dt \right] \right| \phi_f^1 \right\rangle \\ &\quad \times \langle \phi_i^2 \mid T\exp(iV_2 dt) \mid \phi_f^2 \rangle \\ &= a_{\rm cap} a_{\rm ion} . \end{aligned} \tag{2}$$

Since electron-electron correlation is ignored this amplitude is zero unless V_1 and V_2 both act because $\langle \phi_f^k \mid \phi_i^k \rangle = 0$ for $k=1,2$. Using the Born approximation for the ionization amplitude at large impact parameters one has[11] that

$$a_D \sim a_{\rm cap} Z/v . \tag{3}$$

The difference between the exact amplitude of Eq. (1)

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and the independent-electron approximation (or D) amplitude of Eq. (3) is due to correlation. Two types of correlation are possible. The first is static correlation, i.e, correlation contained in the asymptotic wave functions ϕ_i and ϕ_f. The remaining correlation is contained in the scattering operator in Eq. (1), and we refer to it as scattering correlation.

Static correlation can cause ionization to occur well after the first electron is captured. This corresponds to final-state rearrangement (R). In this picture one may expect that the ratio of capture plus ionization to single capture to be independent of the properties of the projectile, i.e., independent of Z or v. A simple approximate expression for the amplitude for this mechanism may be obtained by regarding the electrons as identical so that with $V_2=0$ in Eq. (1),

$$a_R = a_{\rm cap}\langle \phi_f^2 \mid \phi_i^2 \rangle \ . \tag{4}$$

Here $\langle \phi_i^2 \mid \phi_f^2 \rangle$ is nonzero since the asymptotic Hamiltonians are different initially and finally because the correlation interaction is changed. Thus in the rearrangement mechanism the ionization occurs due to electron-electron correlation.

An expression for the scattering correlation may also be obtained[16] at large impact parameters for weak correlation, namely,

$$a_{\rm sc} = a_{\rm cap}/v^2 \ . \tag{5}$$

This scattering correlation is important at low velocity where there is sufficient time for electrons to interact with one another during the collision. And unlike static correlation where extensive work has been done on correlated static wave functions, techniques have yet to be developed to evaluate this amplitude in detail. At high velocity this scattering correlation amplitude is not as important as the direct or rearrangement amplitude and we shall not discuss it further here.

At high velocities we expect that the direct and rearrangement amplitudes will dominate. Here the cross-section ratio will be independent of Z and v in the rearrangement mechanism and vary as $(Z/v)^2$ in the direct mechanism. This reflects a higher Born contribution as a higher power in (Z/v) in the direct mechanism. Because single capture is not as long ranged as ionization, there is no $\ln(v)$ dependence in our present case.

Experimentally we have performed coincidence measurements of charge-transferred projectiles with the He recoil ions produced in collisions of H^+ and He^{2+} ions on helium atoms. The He^{2+} ions were produced by an electron beam ion source[20] and accelerated by voltages between 6 and 16 keV. After magnetic momentum analysis, the He^{2+} projectile beam was crossed by a beam of He atoms from an injection needle inside a parallel-plate condenser field. The slow He target ions produced were extracted by the electric field, passed a drift tube and were detected by a channel electron multiplier. The projectiles were charge analyzed by a magnet downstream from the collision region and detected by a chevron arrangement of multichannel plates. By using a well-documented time-of-flight coincidence technique,[21] fractions F_i of He^{i+} target ions were determined correlated to single-electron capture by the projectiles. The data for protons were taken by using a similar technique. Protons were extracted from a Penning ion source and accelerated by voltages between 50 and 140 kV. After magnetic momentum analysis the ions passed an arrangement[22] similar to the one described above but designed for high-resolution time-of-flight measurements with fast projectile ions. After the collision, the charged particles in the projectile beam were deflected by an electric field while the fast H atoms produced by single-electron capture continued straight on and were detected by a single-particle detector.[23] Again, by a time-of-flight coincidence technique we determined fractions F_i of He^{i+} target ions correlated to single-electron capture by protons from helium atoms.

In Fig. 1 we present a compilation of data for ionization plus simultaneous capture in helium for bare projectiles of $Z=1$, 2, and 3. In this figure we have plotted the ratio of capture plus ionization to single capture plus capture with ionization cross sections. In addition to our data we show data from several other groups.[1,7,10–13]

At very high velocities we expect this ratio to go to a constant value, independent of projectile charge Z or velocity v. In this region the rearrangement mechanism is expected to dominate, as is evident from Eqs. (3)—(5). As first recognized by Horsdal-Pedersen and Larsen, it is sensible to expect that this high-velocity limit is the same as for photoionization followed by shakeoff since in both cases the initial electron leaves the target quickly. It has been previously noted[18] that the corresponding high-velocity limit for the ratio of double to single ionization is an order of magnitude lower probably due to the fact that the initial electron does not leave quickly and final-state correlation is likely. For our case the high-energy limit of the cross-section ratio does appear to go over to a constant consistent with photon values, and our data confirms the original observations of Horsdal-Pederson and Larsen. We do note that the photon value rests heavily on a single experiment by Carlson[17] in 1967 as well as various theoretical calculations. For projectiles with $Z>1$, however, this high-energy rearrangement limit has apparently not yet been reached experimentally.

Earlier one of us suggested[19] that the direct mechanism might also be important at projectile velocities near a few hundred MeV/amu. Since the cross-section ratio, $\sigma^{2+}/(\sigma^+ + \sigma^{2+})$ varies with Z and v in the direct mechanism but not in the rearrangement mechanism, it was suggested that data for He^{2+} and Li^{3+} projectiles be considered. Data for He^{2+} and Li^{+3} shown in the figure clearly vary with Z and v. A simple calculation for $v>Z$ is also shown in the figure. The D curves shown were obtained by evaluating the ionization probability from the tables of Hansteen, Johnsen, and Kocbach[24] using a screened charge of 1.7 and a binding energy of 14.6 eV for helium. We assume that $\sigma^{2+} \ll \sigma^+$. Uncertainties in this calculation are about 50%, mostly due to the use of hydrogenic, i.e., uncorrelated, wave functions. We have no comparably reliable calculations for capture probabilities for this system, so we choose the value of D to be that of an average $P(b)$, namely $P(b)$ at $b=r_k$, where r_k is the k-shell radius. The velocity dependence of this result is invariant over a range of b, changing by only a few per-

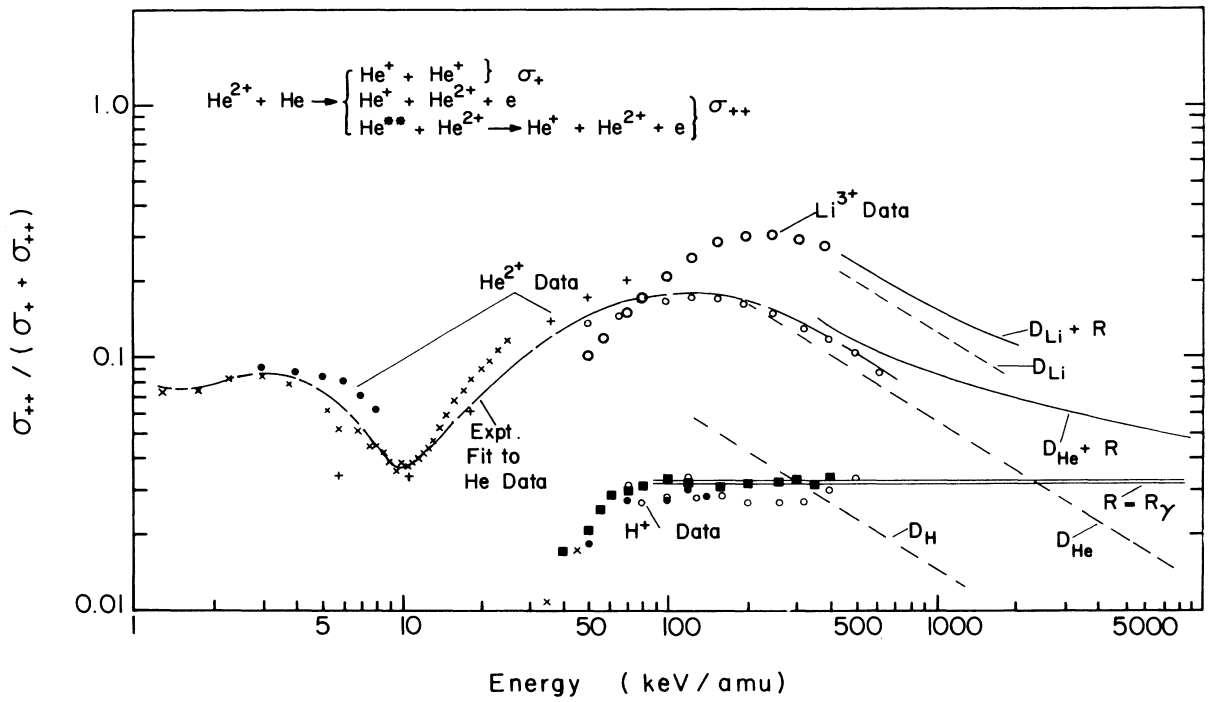

FIG. 1. Ratio of cross sections $\sigma^{2+}/(\sigma^+ + \sigma^{2+})$ for capture plus ionization, σ^{2+}, to single capture, σ^+, plus capture plus ionization vs projectile velocity for impact by H^+, He^{2+}, and H^{3+}. $R = R_\gamma$ is the ratio of single to double ionization by photons. R represents the rearrangement mechanism and D represents the direct mechanism. Symbols for data: ●, present data; □, Horsdal-Pedersen and Larsen (Ref. 1); ○, Shah and Gilbody (Ref. 7); ×, Afrosimov *et al.* (Refs. 11–13); +, DuBois (Ref. 10). Transfer ionization, i.e., double capture to excited states followed by autoionizing action, important at the lower velocities, is included.

cent when b is changed by a factor of 2. The value of R, independent of Z and v, was chosen from experiment, i.e., R is empirical. The sum of the empirical R and our simple D calculations, which are well fit by a $(Z/v)^2$ scaling consistent with the Born amplitude given by Eq. (3), is in good agreement with the He^{2+} and Li^{3+} data. However, our simple calculation, which excludes the possibility of interference between R and D, does not agree with the H^+ data. A more complete calculation properly incorporating both rearrangement and direct mechanisms is apparently required to obtain agreement with all the data shown in our figure. Such a calculation could be useful in understanding the two-electron transition of capture plus ionization.

At high velocities ($v > Z$) and when the direct mechanism is dominant, the observations shown in the figure are consistent with a simple $(Z/v)^2$ scaling. Below the peak at about 100 keV/amu the cross-section ratio drops to an apparent minimum at about 10 keV/amu where there is some spread in observed results. In this region, at about 10 keV our data are in reasonable agreement with the observations of Afrosimov *et al.*[11–13] but not with the lowest energy point observed[10] by DuBois. In the vicinity of a few keV/amu a second low-energy peak is evident. Our own data presented in Fig. 1 tends to confirm the existence of this low-energy peak. We further note that earlier data taken for projectiles of $Z = 8$ on helium[2,3] give qualitatively similar ratios to that shown in Fig. 1. This suggests that the structure in the energy dependence of these ratios may be similar for a range of projectile charges. We present here, however, no simple physical explanation for this structure.

Finally we note that a peak in the angular distribution of the ratio for capture plus ionization to capture has recently been reported by Horsdal *et al.*[25] Horsdal *et al.* interpret this peak as a two-step mechanism where one target electron scattered from the projectile rescatters from the second electron to give capture plus ionization. Such a two-step (or Thomas-type) mechanism is consistent with our picture presented here. If the second step is in fact due to the electron-electron interaction, then we regard this as a correlation mechanism. It could be either rearrangement or scattering correlation depending on whether the correlation is incorporated into the asymptotic wave functions or the scattering operator. However, we note that Briggs has recently suggested[26] that this mechanism could be due in part to multiple interactions between the electron and the projectile, corresponding to our direct mechanism. Measuring this peak for projectiles of different charge could help sort out the nature of this two-step mechanism, since the charge dependence of the direct mechanism differs from the rearrangement mechanism and scattering correlation as illustrated by Eqs. (2)–(5).

In summary we have presented a compilation of data for the two electron transition process of simultaneous capture plus ionization and included some new data. We have found some structure in the ratio of cross sections for capture plus ionization to single ionization that has

some similarity for more than one projectile. At high projectile velocities (above 100 keV/amu) we have presented an explanation of this data in terms of direct and rearrangement mechanisms for two-electron transitions and presented some simple analytic forms for the projectile charge and velocity dependence of these mechanisms. This demonstrates that such a simple analysis, earlier applied to multiple ionization, may also be used in analysis of capture plus ionization.

Note added in proof. H. Knudsen *et al.* (unpublished) have very recently noted that a two-step mechanism could alter the high-energy limit of the cross-section ratio, i.e., $R \neq R_\gamma$, and new data are inconclusive.

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