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Single- and double-ionization cross sections for angular scattering of fast protons by helium

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The angular scattering of H^+ by He has been investigated for single ionization at energies of 0.5, 1.0, and 3.0 MeV; and for double ionization at 1.0 MeV. The classical-trajectory Monte Carlo method has been used within one- and two-electron models to illustrate the collision dynamics. The angular differential single-ionization cross sections are in good agreement with experiment, and display the combined effects of proton scattering from the He nucleus and its electrons. The relative fraction of double ionization, as a function of scattering angle, shows a maximum at ~0.9 mrad that is in agreement with the experiments of Giese and Horsdal [Phys. Rev. Lett. **60**, 2018 (1988)]. This maximum is found to be due to two uncorrelated scattering events between the H^+ and the He atom's two electrons in the double-ionization reaction from impact parameters different than that for the single-ionization reaction.

Recent experimental data by Giese and Horsdal[1] have displayed a distinct peak at a H^+ scattering angle of ~0.9 mrad for the ratio of double ionization

$$H^+ + He \rightarrow H^+ + He^{2+} + 2e^- , \quad (1)$$

to single ionization

$$H^+ + He \rightarrow H^+ + He^+ + e^- , \quad (2)$$

plus double ionization. The peak position was found to be independent of projectile velocity and was unexpected, since it is outside the maximum deflection of 0.545 mrad for a H^+ by a stationary electron.

Several reasons have been given to explain such a peak. In one paper,[2] it is postulated that on either side of the maximum the H^+ is deflected by the He nucleus with small momentum transfer with an electron, while at the peak the cross section is dominated by large momentum transfer to an electron; calculations by Reading, Ford, and Fang realized a peak at ~0.5 mrad. Another model[3] uses a triple-collision hypothesis, H^+-electron, electron-electron, followed by H^+-electron scattering to predict a sharp peak at 0.96 mrad. However, cross-section calculations were not performed by the author. In contrast to the above, we give a simple explanation which is that near the peak and at smaller angles, the double ionization is dominated by two uncorrelated ionizing collisions with the electrons at large impact parameters where the H^+ deflection by the He nucleus is small compared to that by the electrons.

To verify our explanation, we have employed a series of classical-trajectory Monte Carlo (CTMC) calculations to illustrate the competition in the angular deflection at the H^+ by the He nucleus and its two electrons. The classical Hamiltonian for reactions (1) and (2) can be written as

$$H = p_a^2/2M_a + p_b/2M_b + \sum_i (p_i^2/2m_i + z_a z_i/r_{ai} + z_b z_i/r_{bi}) + z_a z_b/R_{ab} + 1/r_{12} . \quad (3)$$

In Eq. (3), the index a represents the H^+, b the He nucleus, and $i = 1,2$ the two electrons.

Three successive CTMC calculations have been used to investigate the dynamics of the double-ionization reaction at 1 MeV. They are as follows: 1CTMC—a one-electron calculation with the transition probabilities evaluated within the independent electron model to reflect the He target, 2CTMC—a two-electron calculation where both electrons are explicitly included, but the electrons are independent of one another as in a Hartree calculation with the $1/r_{12}$ absent from Eq. (3), and bCTMC—a two-electron calculation within the Bohr model where the full Hamiltonian with the $1/r_{12}$ electron-electron repulsion is incorporated. The 1CTMC and 2CTMC calculations are similar to one another in that the impact parameter dependence of the single- and double-ionization transition probabilities are the same. However, proton deflection by the second electron will be explicitly included in the 2CTMC model, while not in the 1CTMC model. Calculations with the Bohr He atom, bCTMC, further include the electron-electron dynamical correlation. This latter interaction is required by the model of Vegh[3] in order to obtain a peak in the ratio of double to total ionization. Thus, if the Vegh model is correct, the peak will only be present in the bCTMC results.

The nCTMC method used for the 1CTMC and 2CTMC calculations has been described previously.[4] In it, each electron is distributed within a microcanonical model, with a screening constant of $\frac{5}{16}$ to the helium nucleus. Each electron's binding energy was set equal to the experimental first ionization value of 0.903 a.u. All interactions between the H^+, the electrons, and the helium nucleus are included within this three-dimensional model. Previously, the ejected electron spectra have been shown to be correctly predicted[5] by the nCTMC method, lending credence that collisional momentum transfer in ionization is well reproduced. Because the Hamiltonian has not been

separated into nuclear and electronic parts, the momentum-transfer coupling between electrons and heavy nuclei is directly incorporated. Thus, the method is able to describe the dominance of H^+ scattering from the He nucleus at small impact parameters, and by the electrons at large impact parameters with small distances of closest approach between the H^+ and the electrons. No assumption is needed as to a central potential in order to give a relationship between impact parameter and deflection angle. From other work, it is known that such a relationship is invalid for the transverse momentum balance in this system at these energies.[6] The Bohr helium atom, bCTMC, has been described previously[7] and corresponds to both electrons being in a circular orbit and out of phase with one another by 180°.

In Fig. 1 are presented the 2CTMC results for H^+ angular scattering after single ionization, reaction (1). Of the three methods, the 2CTMC single-ionization values should be the most accurate because of the inclusion of both electrons with microcanonical momentum distributions. These calculations are compared to experimental data at 0.5 and 1.0 MeV from Giese and Horsdal[1] and at 3.0 MeV from Kamber *et al.*[8,9] (note: we used the renormalized data from Ref. 9). The differential cross sections are presented in terms of $d\sigma/d\theta$, since then the values are directly proportional to their contribution to the total cross section. This presentation also removes some of the precipitous decrease in $d\sigma/d\Omega$ plots which are simply due to the $\sin\theta$ contribution.

The calculations lie above the Giese and Horsdal data at small angles, but are within the experimental angular resolution except for the smallest angle at 0.5 MeV. However, the direction of the difference is puzzling since the calculated values for the total (integral) cross sections are lower than independently measured values, Table I, due to the lack of including quantal tunneling. Hence, if the data are correct, there must be a very different behavior at $\theta < 0.2$ mrad then given by the calculations in order to obtain the correct total cross sections. The 3-MeV calculations are in good agreement with the experimental values from Kamber *et al.*[8,9] At $\theta < 0.1$ mrad a beam-dump precluded signal acquisition in the experiments.

Of importance is that at 3.0 MeV the 2CTMC calculations clearly display the dominance of H^+ scattering from the ionized electron at $\theta < 0.545$ mrad, along with the large decrease in cross-section magnitude at larger angles where scattering from the He-nucleus dominates. The reason for the large change in magnitude about ~ 0.545 mrad is that at larger angles, only impact parameters $b < 0.1a_0$ contribute to the cross sections. At smaller angles, all other impact parameters contribute ($\sim 99\%$ of the total cross section), with the H^+ deflection primarily determined by the distance of closest approach to the ionized electron, not to the He nucleus.

At the lower energies, 0.5 and 1.0 MeV, no sharp shoulder is observed near 0.545 mrad due to the relatively stronger influence of the Compton profile of the electrons. However, an observable change in slope of the cross sections is found to persist in this region. Numerical studies indicate that at an impact parameter of $0.1a_0$ corresponds to a scattering angle of ~ 1.0 mrad at 0.5 MeV, and that any correspondence between impact parameter and H^+ scattering angle disappears for $b > 0.2a_0$. Hence, even at 0.5 MeV, projectile scattering to angles of ~ 0.9 mrad in single-ionization collisions is primarily due to very small impact parameters where the H^+-helium nucleus interaction dominates.

A similar behavior is found to occur for the double-ionization reaction (2), except that H^+-helium nucleus scattering does not dominate until $\theta > 1.3$ mrad, which again corresponds to very small impact parameter collisions. Scattering at smaller angles is primarily determined by close collisions between the H^+ and the two electrons, not with the He nucleus. It is these very collisions that also contribute $\sim 95\%$ to the total double-ionization cross section.

If a H^+ incoherently scatters off two electrons, each with a maximum deflection angle of 0.545 mrad, the resulting transverse momentum distribution is highly peaked at near two times this angle. Other combinations of H^+ transverse momenta also yield distributions which peak close to the sum of the magnitudes of the two vec-

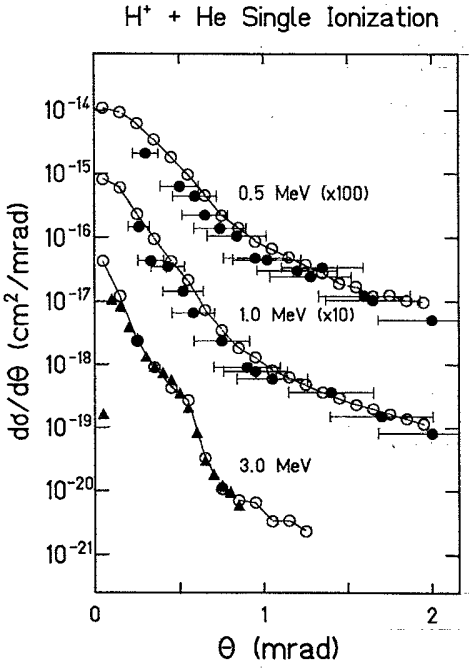

FIG. 1. Angular differential cross sections for H^+ scattering in single-ionizing collisions with He. The 2CTMC results are given by the open symbols with a line drawn to guide the eye. The solid circles at 0.5 and 1.0 MeV are data from Giese and Horsdal (Ref. 1), while the data at 3.0 MeV are from Kamber *et al.* (Ref. 9).

TABLE I. Total cross sections for single ionization. Units are 10^{-18} cm^2, error limits on the 2CTMC calculations are at the one standard deviation level.

E (MeV)	2CTMC	Ref. 10	Ref. 11
0.5	33.3 ± 0.6	37.0 ± 1.5	36.7 ± 3.7
1.0	18.2 ± 0.2	22.6 ± 0.8	21.4 ± 2.1
3.0	5.92 ± 0.08	...	8.68 ± 0.09

tors. Hence, one should expect a maximum in the fraction of double ionization to the sum of single and double ionization in the range between 0.5 and 1.5 mrad (the Compton profile of the electrons must also be considered). The reason being that different impact parameter regions are probed for the single- versus the double-ionization reactions. For $\theta \sim 1.0$ mrad, we find small impact parameter H^+-helium nucleus scattering for single ionization, while H^+-electron scattering at all impact parameters for the double ionization. The fraction of double to total ionization can be expected to decrease to a small finite value at zero angle due to the longer range of the single-ionization reaction and the uncertainty in the scattering angle. A plateau to a constant value in the fraction should occur for $\theta > 1.5$ mrad since the H^+ scattering angle probes the same $b \rightarrow 0.0a_0$ impact parameter range for both reactions (1) and (2).

The calculated double-ionization fraction for 1.0-MeV collisions from the various calculations are compared to the experimental results of Giese and Horsdal[1] in Fig. 2. In Fig. 2(a) are shown the coupled-channel results for Reading, Lord, and Fang.[2] The overall magnitude of this calculation is in good agreement with the data, but the peak is incorrectly predicted at ~ 0.5 mrad. The reason for this discrepancy most likely lies in the assumption of a central potential to relate impact parameter to scattering angle. Experimental data and 2CTMC calculations[6] indicate that the nuclear and electronic degrees of freedom cannot be decoupled in describing the projectile scattering.

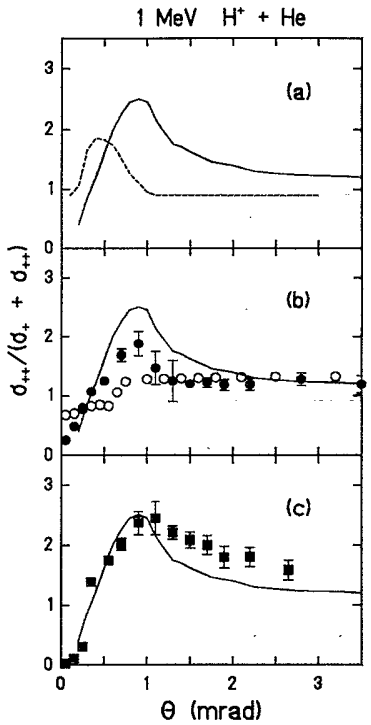

FIG. 2. Fraction of double ionization to total ionization as a function of H^+ scattering angle. The solid line in each of the figures is the fit by Giese and Horsdal to their experimental data (Ref. 1). The dashed line in (a) is the result of the quantal close-coupling (forced impulse method) calculation of Reading *et al.* (Ref. 2). In (b) are shown the 1CTMC results (open circles) and the 2CTMC results (solid circles) with one standard deviation statistical error bars. In (c) are given the bCTMC results (solid squares). In all cases, the CTMC calculated ratios have been divided by 3.

Figure 2(b) presents two sets of independent electron calculations. In the first, the 1CTMC method, the conventional one-electron independent particle model[4] is used to calculate double-ionization transition probabilities from the single-ionization values. The calculated single-ionization angular scattering is weighted by these probabilities to obtain the θ-dependent ratio. One must be careful in this analysis since scattering angle and impact parameter are not uniquely related. Hence, it is not obvious that a peak in the ratio will not arise by using this method. In fact, we see a very slight peak around 0.5 mrad, before the ratio rises to a constant value for $\theta > 1.0$ mrad.

Also shown in Fig. 2(b) are the two-electron 2CTMC results. Although the large-angle values are similar since there is a direct relationship between impact parameter and scattering angle, there are major differences with the 1CTMC calculations at $\theta < 1.5$ mrad. It should be reemphasized that the single- and double-ionization transition probabilities are identical as a function of impact parameter for both the 1CTMC and 2CTMC calculations. Thus, differences in the angular scattering directly reflect the additional electron-scattering center. We find the second electron leads to an enhancement in the ratio around ~ 1.0 mrad giving rise to a peak, and a decrease at $\theta < 0.2$ mrad. An electron-electron $1/r_{12}$ interaction is not required in order to realize the maximum. Thus, the model of Vegh[3] is not supported by these calculations.

To complete our study, the Bohr He model was also used to calculate the ratio, Fig. 2(c), and the maximum is again realized. In Fig. 2, all the classical results have been divided by three in order to normalize the $\theta > 2.0$ mrad data ($b \rightarrow 0.0a_0$). We note that $\sim 99\%$ of the single-ionization total cross section is determined by angles $\theta < 0.3$ mrad, thus the peak shown in Fig. 2 is a very minor component of the total scattering and an inaccurate calculation of the peak magnitude is an insensitive test of a model's ability to predict total cross sections.

In conclusion, the classical calculations presented here indicate that a peak at ~ 0.9 mrad in the angular fraction of double ionization to total ionization is realized within a simple model of an uncorrelated collision of the H^+ with the He atom's two electrons. The results strongly suggest that complicated scattering processes or quantal interference mechanisms are not necessary to understand the collision dynamics; the single- and double-ionization reactions simply probe different ranges of impact parameters for H^+ deflections around 1.0 mrad. Moreover, our conclusions are supported by the fact that the peak position is independent of H^+ energy, indicating that the structure is determined by the distance of closest approach to the electrons and not a direct function of impact parameter. The results demonstrate the invalidity of a central potential approach to ionization reactions at intermediate collision energies, and the necessity of including both the heavy particles and the electrons in determining their transverse momentum balance.

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