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Transfer ionization process $p+\mathrm{He}\rightarrow\mathrm{H}^0+\mathrm{He}^{2+}+e^-$ with the ejected electron detected in the plane perpendicular to the incident beam direction

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A joint experimental and theoretical study of the transfer ionization process $p+\mathrm{He}\rightarrow\mathrm{H}^0+\mathrm{He}^{2+}+e^-$ is presented for 630-keV proton impact energy, where the electron is detected in a plane perpendicular to the proton beam direction. With this choice of kinematics we find the triple-differential cross section to be particularly sensitive to angular correlation in the helium target. There is a good agreement between the experimental data and theoretical calculations.

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Multiple-differential cross sections of fragmentation processes in atomic collisions provide valuable information on the nature of electron correlation in atomic systems [1,2]. However, the double-electron transitions induced by collisions with photons and particles are extremely sensitive to both static and dynamic electron correlation [3]. Therefore, coincidence studies of double-electron transitions with fragmentation are among the most advanced methods for understanding how correlation works. Over the last decade there has been increasing interest to study the double ionization and ionization excitation by photon and particle impacts [4–7]. These processes, though sensitive to electron correlation, are, however, strongly affected by post-collision interactions between the charged particles in the final state [8]. Transfer ionization is another double-electron process with fragmentation. For proton impact the projectile captures one electron, which becomes atomic hydrogen, and one could therefore expect that post-collision Coulomb interactions with the scattered projectile would be neutralized and the full sensitivity to target correlation effects would be apparent.

First, multiple-differential cross sections for the transfer ionization process,

$$p^+ + \mathrm{He} \rightarrow \mathrm{H}^0 + \mathrm{He}^{2+} + e^-, \tag{1}$$

have been measured using the COLTRIMS technique [9–11]. The experiments reveal that (i) the ejected electron is predominantly emitted into the backward direction, (ii) the direction of maximum ejection is insensitive to the impact energy but shows some dependence on the momentum transfer, and (iii) the captured electron, recoil He^{2+} ion, and ejected electron always have comparable momenta. Godunov, Whelan, and Walters [12] produced a simple theoretical model that explained the observed qualitative features in terms of target correlation and gave quantitative predictions for triple-differential cross sections (TDCSs), which explicitly demonstrated the sensitivity to terms beyond the $(ns)^2$ in a multiconfiguration Hartree-Fock description of the target, confirming a suggestion first made by Schmidt-Böcking *et al.* [10,11]. Results of their calculations within the first-order collision model with wave functions allowing for angular electron correlation for the initial state reproduced the effects observed experimentally in multiply differential cross sections. Particularly, (a) there is a propensity for the ejected electron to be detected in the backward direction to the incident protons and (b) the direction of maximum ejection is insensitive to the impact energy but shows dependence on the momentum transfer.

In a recent paper [13] we presented a joint theoretical and experimental study of the transfer ionization process (1) in a coplanar geometry where the incident proton, the collision fragments, and the momentum transfer vector all lay in the same plane. All particles in the final state were detected in triple coincidence. The fully differential measurements were in a good agreement with the theoretical model, where the target was described by a wave function containing both radial and angular correlation terms. Our theoretical calculations demonstrated a clear target dependency, and we thus concluded that the two-electron processes in fast transfer ionization reactions occurred mainly due to initial-state correlations, and post-collision electron correlations had only a minor influence on the final-state momentum pattern.

In this paper we explore a novel kinematical arrangement that we have chosen especially in the belief that the resulting cross sections would be even more sensitive to the angular correlation than the previous ones. Atomic units are used through the paper unless otherwise stated.

In the model of [12] the transition amplitude consisted of the sum of two terms: a "transfer-first" term,

$$f_{tr} = -\frac{\sqrt{\mu_i\mu_f}}{(2\pi)^4}\int \frac{-4\pi Z_p}{|\vec{s}_0-\vec{s}|^2}\varphi^F_{1s}(\vec{s})d\vec{s}\int \psi^{(-)^*}_{\vec{k}_2}(\vec{r}_2)\exp[i\vec{r}_1\cdot\vec{Q} - i\vec{r}_2\cdot\vec{Q}/(M_t+1)]\Phi_i(\vec{r}_1,\vec{r}_2)d\vec{r}_1d\vec{r}_2, \tag{2}$$

where $\mu_i=M_p(M_t+2)/(M_p+M_t+2)$ is the reduced mass of the projectile and the helium atom; $\mu_f=(M_p+1)(M_t+1)/(M_p+M_t+2)$ is the reduced mass of the hydrogen atom

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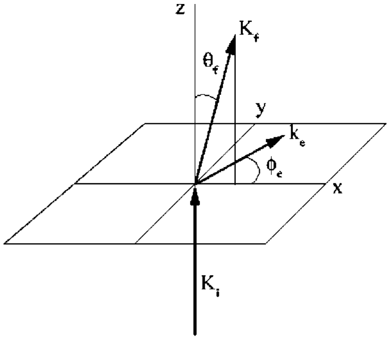

FIG. 1. Collision geometry for the transfer ionization process.

and the helium ion He$^+$; M_p is the mass of the proton and M_t is the mass of the helium nucleus; $\psi_{\vec{k}_2}(\vec{r}_2)$ is the Coulomb wave function for the ionized electron in the field of the He^{2+} ion [normalized as $\langle\psi_{\vec{k}}|\psi_{\vec{k}'}\rangle=(2\pi)^3\delta(\vec{k}-\vec{k}')$]; $\varphi_{1s}^F(\vec{s})$ is the Fourier transform of the hydrogen ground state; the momentum transfer is $\vec{Q}=(M_t+1/M_t+2)\vec{K}_i-\vec{K}_f$ and $\vec{s}_0=\vec{K}_i-\vec{K}_f(M_p/M_p+1)$; $\vec{K}_i$ and $\vec{K}_f$ are the momenta of the incoming projectile and the scattered particle, respectively; and $\Phi_i(\vec{r}_1,\vec{r}_2)$ is the ground state of the helium atom. The "ionization-first" amplitude is given by

$$f_{ion}=-\frac{\sqrt{\mu_i\mu_f}}{(2\pi)^4}\int\frac{-4\pi Z_p}{|\vec{s}_0-\vec{s}|^2}\varphi_{1s}^F(\vec{s})d\vec{s}\int\psi_{\vec{k}_2}^{(-)^*}(\vec{r}_2)\exp\{i\vec{r}_1\cdot(\vec{s}-\vec{s}_0+\vec{Q})+i\vec{r}_2\cdot[\vec{s}_0-\vec{s}-\vec{Q}/(M_t+m)]\}\Phi_i(\vec{r}_1,\vec{r}_2)d\vec{r}_1d\vec{r}_2. \quad (3)$$

We note that in the transfer-first amplitude f$_{tr}$, the transfer and ionization processes are separable; this is not the case for the ionization-first amplitude f_{ion}. Consequently the dependence on the initial state $\Phi_i(\vec{r}_1,\vec{r}_2)$ is much more transparent in the transfer-first case. The triple-differential cross section as a function of the scattered angle, Ω_f, and the energy E_e and the angle Ω_e of the ionized electron is the coherent sum of both amplitudes, i.e.,

$$\frac{d^3\sigma}{dE_e d\Omega_e d\Omega_f}=2\frac{K_f k_e}{K_i}|f_{tr}+f_{ion}|^2. \quad (4)$$

Here k_e is the momentum of the ejected electron. The cross section thus depends on both mechanisms and their interference.

The wave function $\Phi_i(\vec{r}_1,\vec{r}_2)$ for the helium ground state was calculated in the multiconfigurational Hartree-Fock approximation (MCHF) [14]. The full set calculations with both radial and angular correlation included $(ns)^2$, $(ps)^2$, and $(nd)^2$ terms with $n\leqslant 4$. These configurations yield about 97% of the correlation energy. Allowing for radial correlation only [$(ns)^2$ configurations] yields 41% of the correlation energy for the ground state.

Let us now define our kinematical conventions. We assume that we have a regular right-handed set of axes x,y,z and corresponding spherical polar coordinates r,θ,ϕ. The incident proton comes in along the z axis and the H^0 is detected at an angle θ_f with respect to the axis z in the xz plane ($\phi_f=0$) (Fig. 1). In this paper we will consider the situation where the electron, with coordinates (θ_e,ϕ_e), is detected in the xy plane, i.e., $\theta_e=\pi/2$, the TDCS will be given as a function of ϕ_e.

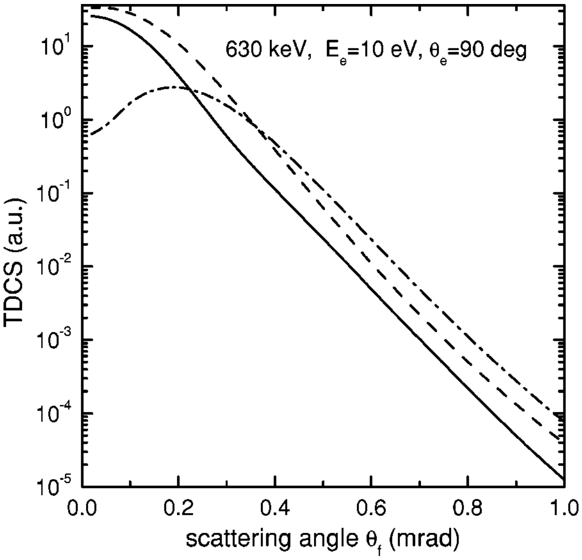

FIG. 2. Triple-differential cross section for transfer ionization in a proton-helium collision at $E_i=630$ keV in the coplanar arrangements ($\phi_e=180°$). Electron emission energy E_e is 10 eV, and the electron emission angle is 90°. Theory: solid line, calculations include both (2) and (3) amplitudes with radial and angular correlations in the initial-state wave function; dashed line, calculations with the transfer-first mechanism (2) only; chain line, calculations with the ionization-first mechanism (3) only.

In our earlier work [13] we compared theory and experiment in a coplanar arrangement; in this case we found the amplitudes (2) and (3) to be of equivalent size. However, angular correlation affects the transfer- and ionization-first amplitudes differently. We have therefore sought out kinematical arrangements where theory predicts that the either ionization-first amplitude is much smaller than the capture-first amplitude or vice versa. Figure 2 shows the transfer ionization cross section for proton-helium collision as a function of the scattering angle with the electron ejected in the plane perpendicular to the incident beam direction, and the azimuthal angle $\phi_e=180°$. The transfer-first mechanism dominates at small scattering angles. As the scattering angle increases, the ionization-first mechanism is stronger than the transfer-first one. The small scattering angle is therefore an ideal one for the dynamical study of the target correlation.

The present experiment was performed at the van de Graaff accelerator of the Institut für Kernphysik at the University Frankfurt. The H$^+$ beam of 630 keV was collimated by two sets of adjustable slits to a beam size of about 0.5×0.5 mm^2 at the target. The beam was cleared from charge-state impurities by a set of electrostatic deflector plates 15 cm upstream from the target. At 15 cm downstream a second set of electrostatic deflector plates separated the primary (charged) beam from the now neutral H^0 ejectiles. This H^0 beam intersected a supersonic He gas jet with a density of 5×10^{11} atoms/cm^2 and 1 mm diam at the intersection. The H^0 particles were detected with a position- and time-sensitive

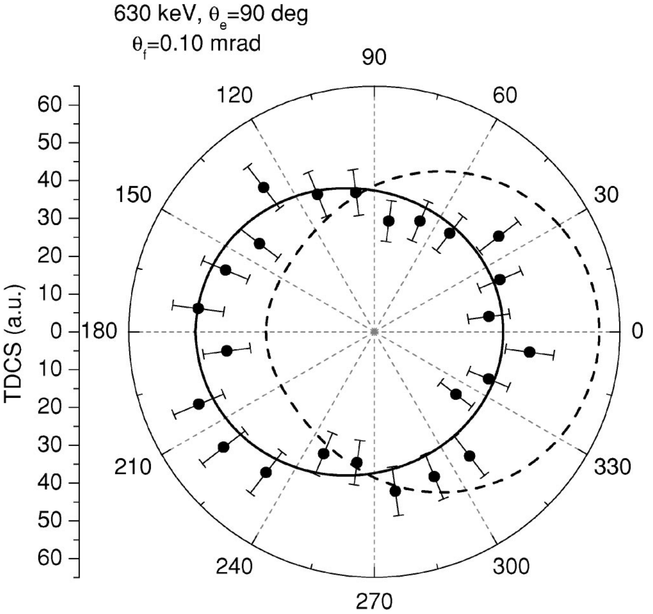

FIG. 3. Triple-differential cross section for transfer-first ionization in the perpendicular plane for proton-helium collision at $E_i = 630$ keV; the scattering angle is 0.1 mrad and is integrated over electron emission energy. Theory: solid line, calculations include both (2) and (3) amplitudes with radial and angular correlations in the initial-state wave function; dashed line, the initial state includes radial correlations only. Experiment: COLTRIMS measurements normalized to the full theoretical calculations.

40-mm multichannel plate (MCP) detector. The recoil ions were accelerated by an electrostatic field of 4.8 V/cm at the target. A three-dimensional time and space focusing field geometry [15,16] was used to minimize the degrading influence of the extended reaction volume on the momentum resolution. A resolution $\leqslant 0.1$ a.u. was achieved. The electrons were guided by a magnetic field of $\leqslant 13.5$ G and accelerated 20 cm by the same electrical field onto a 120-mm MCP detector with delay line anode; a time focusing geometry was used here, too. Events were recorded in a three-particle coincidence (e^--H^0-He^{2+}). By measuring the time of flight and the position of impact on the detectors, we obtained the initial momentum vectors of the recoil ion and the electron. Six of a total of nine momentum components were thus measured directly. The momentum of the H atom, and hence the angle θ_f, was calculated from the measured He^{2+} and the electron distribution by using momentum conservation. Energy conservation was used for offline background suppression. The hydrogen atom is detected at angle θ_f with respect to the beam direction; the triple-differential cross section is presented as a function of the detected electron angle ϕ_e.

Unfortunately, because of the nature of the experimental technique and the uncertainties inherent in the measurement, it was not possible to give meaningful results for fixed energies of the ejected electrons; instead, experimental results are presented over all electrons detected in the perpendicular plane. Therefore, our theoretical cross sections are integrated over ejected energies from 0 to 500 eV.

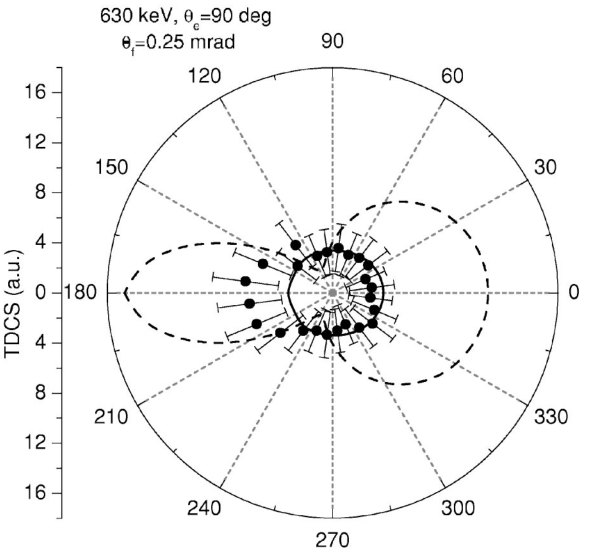

FIG. 4. Triple-differential cross section for transfer-first ionization in the perpendicular plane for proton-helium collision at $E_i = 630$ keV; the scattering angle is 0.25 mrad and is integrated over electron emission energy. Notation as in Fig. 2.

In Figs. 3–5 we present measured and calculated differential cross sections of transfer ionization as a function of the azimuthal electron emission angle ϕ_e in the perpendicular plane geometry for three scattering angles, i.e., 0.1, 0.25, and 0.55 mrad.

At small scattering angles (Fig. 3) the cross section calculated using the ionization-first amplitude (3) is dramatically smaller than that corresponding to the transfer-first amplitude (2). This arrangement is thus ideal for focusing on the transfer-first term. Allowing for angular correlation in the initial-state wave function changes the qualitative behavior of the cross section, resulting in a shift of the cross section toward the direction of 180°, whereas calculations with ra-

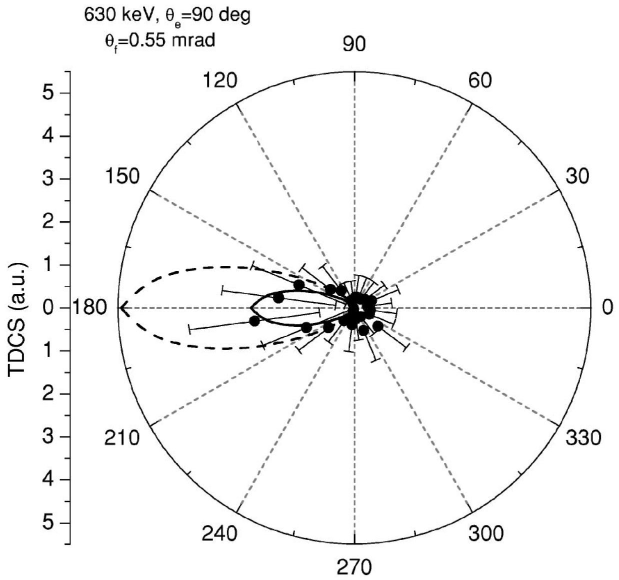

FIG. 5. Triple-differential cross section for transfer-first ionization in the perpendicular plane for proton-helium collision at $E_i = 630$ keV; the scattering angle is 0.55 mrad and is integrated over electron emission energy. Notation as in Fig. 2.

dial correlation only demonstrate quite the opposite effect, i.e., shift toward small angles. Calculations with both radial and angular correlations agree well with experiment.

As the scattering angle increases (Fig. 4), the contribution from the second mechanism (ionization first) becomes comparable with the transfer first. The cross sections are a result of strong destructive interference between amplitudes. Experimental distribution appears more peaked toward 180° than the full calculation predicts.

For larger scattering angles (Fig. 5) the ionization first dominates, however, destructive interference with the transfer-first amplitude is still strong and affects the resulting cross sections on an absolute scale. The cross section is peaked toward 180°. This feature is determined by collision kinematics, such as the binary encounter peak in single ionization. Angular correlation in the initial state has a very minor effect in this case. Since the ionization-first mechanism is less sensitive to correlation, large scattering angles are less favorable for studying correlation effects.

In summary, we have performed calculations and measurements for multiple-differential cross sections of transfer ionization of helium by a 630-keV proton impact with the ejected electron detected in the plane perpendicular to the incident beam direction. The theoretical model includes two principal mechanisms of transfer ionization for this kinematic arrangement. The wave function of the helium atom includes both radial and angular electron correlation. The results presented here demonstrate that the perpendicular plane geometry for transfer ionization, together with the small scattering angles, is a very good case for studying effects of target electron correlation.

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[1] E. Weigold and I. E. McCarthy, *Electron Momentum Spectroscopy* (Plenum/Kluwer, New York, 1999).

[2] R. Moshammer, J. Ullrich, M. Unverzagt, W. Schmitt, P. Jardin, R. E. Olson, R. Mann, R. Dörner, V. Mergel, U. Buck, and H. Schmidt-Böcking, Phys. Rev. Lett. **73**, 3371 (1994).

[3] J. H. McGuire, *Electron Correlation Dynamics in Atomic Collisions* (Cambridge University Press, Cambridge, 1997).

[4] O. Schwarzkopf, B. Krässig, J. Elmiger, and V. Schmidt, Phys. Rev. Lett. **70**, 3008 (1993).

[5] A. Lahman-Bennani, J. Phys. B **24**, 2401 (1991).

[6] C. Dupre, A. Lahmam-Bennani, A. Duguet, F. Mota-Furtado, P. F. O'Mahony, and C. Dal Cappello, J. Phys. B **25**, 259 (1992).

[7] R. Moshammer, J. Ullrich, H. Kollmus, W. Schmitt, M. Unverzagt, O. Jagutzki, V. Mergel, H. Schmidt-Böcking, R. Mann, C. J. Woods, and R. E. Olson, Phys. Rev. Lett. **77**, 1242 (1996).

[8] J. Rasch, P. J. Marchalant, Colm T. Whelan, and H. R. J. Walters, in *Many-Particle Spectroscopy of Atoms, Molecules and Surfaces*, edited by J. Berakdar (Kluwer/Plenum, New York, 2001).

[9] V. Mergel, R. Dörner, K. Khayyat, M. Achler, T. Weber, O. Jagutzki, H. Lüdde, C. L. Cocke, and H. Schmidt-Böcking, Phys. Rev. Lett. **86**, 2257 (2001).

[10] H. Schmidt-Böcking, V. Mergel, R. Dörner, T. Weber, O. Jagutzki, H. Lüdde, L. Schmidt, and J. Berakdar, in *Correlation, Polarization and Ionization in Atomic Systems*, AIP Conf. Proc. No. 604 (AIP, New York, 2001), p. 120.

[11] H. Schmidt-Böcking, V. Mergel, R. Dörner, C. L. Cocke, O. Jagutzki, L. Schmidt, T. Weber, H. J. Lüdde, E. Weigold, J. Berakdar, H. Ceredquist, H. T. Schmidt, R. Schuch, and A. Kheifets, Europhys. Lett. **62**, 477 (2003).

[12] A. Godunov, Colm T. Whelan, and H. R. J. Walters, J. Phys. B **37**, L201 (2004).

[13] M. Schöffler, A. L. Godunov, Colm T. Whelan, H. R. J. Walters, V. S. Schipakov, V. Mergel, R. Dörner, O. Jagutzki, L. Ph. H. Schmidt, J. Titze, E. Weigold, and H. Schmidt-Böcking, J. Phys. B **38**, L123 (2005).

[14] C. Froese Fischer, in *Atomic, Molecular and Optical Physics Reference Book*, edited by G. W. F. Drake (AIP, New York, 1996), Chap. 21.

[15] R. Dörner, V. Mergel, O. Jagutzki, L. Spielberger, J. Ullrich, R. Moshammer, and H. Schmidt-Böcking, Phys. Rep. **330**, 95 (2000).

[16] R. Dörner, V. Mergel, L. Spielberger, M. Achler, Kh. Khayyat, T. Vogt, H. Bräuning, O. Jagutzki, T. Weber, J. Ullrich, R. Moshammer, M. Unverzagt, W. Schmitt, H. Khemliche, M. H. Prior, C. L. Cocke, J. Feagin, R. E. Olson, and H. Schmidt-Böcking, Nucl. Instrum. Methods Phys. Res. B **124**, 2 (1997).