01 Dec 2005

Extreme Sensitivity of Differential Momentum Transfer Cross Sections to Target Atom Initial Conditions

Ronald E. Olson
Missouri University of Science and Technology, olson@mst.edu

J. Fiol

Recommended Citation

R. E. Olson and J. Fiol, "Extreme Sensitivity of Differential Momentum Transfer Cross Sections to Target Atom Initial Conditions," *Physical Review Letters*, American Physical Society (APS), Dec 2005.
The definitive version is available at https://doi.org/10.1103/PhysRevLett.95.263203

Extreme Sensitivity of Differential Momentum Transfer Cross Sections to Target Atom Initial Conditions

R. E. Olson*

Physics Department, University of Missouri-Rolla, Rolla, Missouri 65401, USA

J. Fiol†

Instituto Balseiro and Centro Atómico Bariloche, 8400 S. C. de Bariloche, Río Negro, Argentina

(Received 24 June 2005; published 23 December 2005)

Heavy-particle cross sections differential in the momentum transferred to the target are investigated using the classical trajectory Monte Carlo method. With the 3.6 MeV/u Au^{53+} + He system as a test case, it is shown that these cross sections are extremely sensitive to the initial target temperature. In particular, when thermal motion is varied for one of the target's initial momentum components between 0 and 25 K the absolute cross sections vary by orders of magnitude and, in addition, their relative shapes undergo major changes. We find that by setting one of the target's transverse momenta to a temperature of 16 K, previously reported major discrepancies between theory and experiment are removed.

DOI: 10.1103/PhysRevLett.95.263203 PACS numbers: 34.50.Fa, 34.10.+x

In heavy-particle collisions, the study of single ionization cross sections differential in the momentum transferred to the target **Q** is a new and expanding field. In particular, such studies provide the ultimate test of three-body collision theories. However, to date, comparisons between theory and experiment have often been poor, at best. These comparisons have lead to questions of the capability of present theories to provide a three-body description of heavy-particle single ionization processes [1].

In this Letter, we present calculations for the much studied 3.6 MeV/u

$$\mathrm{Au}^{53+} + \mathrm{He} \rightarrow \mathrm{Au}^{53+} + \mathrm{He}^{+} + e$$

system. Data for this reaction have been sorted in various manners, and the results have been particularly puzzling. In the first publications, cross sections differential in the longitudinal momentum transferred to the ionized electron were well reproduced by state-of-the-art continuum distorted wave (CDW) and classical trajectory Monte Carlo (CTMC) calculations [2,3]. However, when these same data were later analyzed to yield doubly differential cross sections dependent on the momentum **Q** transferred to the target, agreement with theory was severely lacking [4]. Still further analyses of the data provided triply differential cross sections as a function of **Q** that again showed poor agreement in both shape and absolute magnitude with calculated values [5–7].

In attempts to provide reasons for the serious discrepancies, theoretical work analyzed the sensitivity of the cross sections to different forms for the interaction potential between the projectile and He nucleus [8,9], included 4-body effects that incorporate the possibility of He^{+} excitation [10–12], investigated the loss of flux due to the presence of double ionization [8,10], and tested the sensitivity of the cross sections to various forms for the wave functions [13]. However, none of these extensive studies has been able to identify a solution or any problems with the theoretical models. In all cases the agreement with experiment remained poor, thus questioning the applicability of well established and tested theories to provide an accurate picture of what has been assumed to be a well-understood atomic process, namely, single ionization resulting from fast, heavy ion impact. Are there new, unknown physical processes involved, or are there fundamental problems with the theoretical models?

The goal of this Letter is twofold; first, we show that agreement between experiment and theory may be resolved without invoking either of the above conclusions, but rather that the discrepancy results from the convolution of the "exact" cross sections with uncertainties invoked for the initial target atom momenta.

Second, and more important, we show that data for cross sections differential in magnitudes related to the projectile deflection are extremely sensitive to the experimental resolutions. As a consequence, even nearly perfect state-of-the-art experiments must accurately determine the attained resolutions in order to make sound comparisons to theoretical results.

In particular, recently measured **Q**-dependent cross sections are extremely sensitive to the experimental resolution in the momentum of the target residual ion. Such measurements are made using the cold target recoil-ion momentum spectroscopy (COLTRIMS) method where two of the three initial state momenta of the target are controlled to first order by the experimental setup of the supersonic jet target, namely, the geometry of the nozzle and skimmers [14]. These determine the momentum uncertainty of the longitudinal and one of the transverse momenta of the target atom. Typical geometries yield uncertainties for these two initial state momenta on the order of $T = 0.5$ K [14]. The third momentum, which is along the jet direction, corresponds to a transverse momentum component of the atom and is determined by the supersonic jet expansion characteristics. In a recent publication, the Au^{53+} experimental conditions for Refs. [2–7] were given and the component along the jet direction was stated to be about 1 K, which corresponds to a momentum spread of 0.15 a.u. [7]. However, it is well known that the transverse momentum of the jet is quite broad due to a small non-Gaussian tail extending to large momenta: see the review by Miller [15] and recent data by Tejeda *et al.* [16]. This large momentum tail can critically affect one component of the recoil ion transverse momentum.

Furthermore, the overall momentum resolution of a COLTRIMS type measurement is rather complex, being a combination of the transverse momentum resolution of both the electron and residual ion along and perpendicular to the jet axis. In addition to the target temperature effect discussed above, which is different in each direction, other factors such as position resolution of the detectors and time resolution due to the electronics, the spatial extent of the target and the beam, lensing in the spectrometer, add to the final experimental uncertainties. For the sake of simplicity we consider in this work a test where only one of the recoil ion's transverse uncertainty was varied to assess and quantify the changes in the differential cross sections.

The availability of the experimental uncertainties now allows us to convolute our theoretical results in order to more precisely simulate experimental results. Here we use the CTMC method, which we have shown yields fully differential cross sections that are in good accord with quantal CDW results [8,11,17]. An advantage of the CTMC approach is that it is essentially a computer experiment that provides a collision-by-collision history of all final state momenta for each ionization event. Thus, it is possible to directly utilize the event files and include the experimental uncertainties in order to study their effect on cross sections differential in $\mathbf{Q}$. Note that this procedure does not modify the magnitude of the total cross section.

When the experimental conditions were applied, the cross section magnitudes were found to increase by approximately a factor of 2 when the quoted value of 1 K was used for the momentum component along the jet direction rather than the ''ideal'' value of zero Kelvin. A further increase in temperature for this momentum component to $T = 16$ K, which corresponds to a factor of 4 increase in the quoted momentum uncertainty from 0.15 to 0.60 a.u., showed that the apparent cross sections differential in momentum transfer $\mathbf{Q}$ changed by orders of magnitude, and, surprisingly, major changes in their shapes also were observed. In particular, the previously unexplained forward focusing of the ionized electrons was realized. This forward focusing was discussed in several publications, which emphasized the failure of three-body theories to reproduce the data [1,5,6]. When we increased the temperature to 16 K, the major differences in the absolute magnitudes of the experimental and theoretical cross sections also decreased from orders of magnitude to less than a factor of 2.

In this work we held fixed the uncertainties in the longitudinal and one of the transverse components of the target nucleus momenta. In order to compare with the experimental data, we include the uncertainties in the momentum of the target atoms in their initial state. For every ionizing trajectory in the CTMC calculations, each component of the residual target momentum was randomly perturbed following a normal distribution. The standard deviation used for each momentum component depends on the temperature T in that direction $\sigma = (2M_R k_T T)^{1/2}$, where M_R is the mass of the target atom and k_T is the Boltzmann's constant. Note that a temperature of 1 K corresponds to a σ value of 0.15 a.u.

The inclusion of the initial state temperature changes drastically the calculated spectra. This is illustrated in Fig. 1 where the three-body CTMC triple differential cross sections (TDCS) $d\sigma/d\Omega_e dE_e d\mathbf{Q}$ as a function of the electron polar angle are shown with temperatures of 0, 1, 4, and 9 K for one of the transverse components of the target's momentum. As in the experiment, the cross sections are averaged over all events in which the electrons are emitted with energy $E_e = 10 \pm 3$ eV, azimuthal projectile-electron angle $\varphi = \pm 10°$, and the projectile transfers $Q = 1.0 \pm 0.2$ a.u. of momentum to the target-electron system.

The absolute magnitude of the cross section in Fig. 1 for very cold targets ($T = 1$ K, momentum uncertainty of 0.15 a.u.) is 100% larger than for ideal zero Kelvin conditions. Additionally, the TDCS are increased approxi-

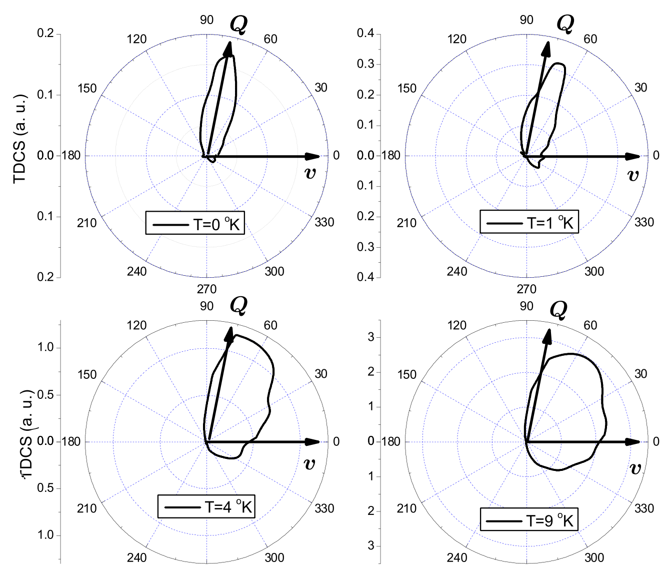

FIG. 1 (color online). Classical trajectory Monte Carlo triple differential cross section for ionization of He by impact of 3.6 MeV/u Au^{53+} for electrons emitted in the scattering plane at 10 eV. The projectile transfers $Q = 1.0$ a.u. of momenta to the target-electron system.

mately by a factor of 7 when raising the temperature to 4 K (momentum uncertainty of 0.30 a.u.). Observe that by increasing the temperature further, not only do the absolute values change by an order of magnitude but also the shapes are strongly modified. The distribution directed along the vector momentum transfer **Q** ($\theta \approx 75°$) for $T = 0$ and 1 K changes to a broader distribution centered at $\theta \approx 50°$ but with important contributions in the forward direction when convoluted with uncertainties corresponding to $T = 9$ K.

The reason for the dramatic modifications obtained when including the initial target's temperature is that the exact ($T = 0$ K) TDCS are rapidly decreasing functions of the momentum transfer **Q** [17,18]. The convolution over the recoil momentum uncertainties includes the contributions from small Q values, whose absolute magnitudes are orders of magnitude larger than those corresponding to the momentum transfer under study. Thus, by increasing the initial state momentum uncertainties, the region of small momentum transfer plays an ever increasing role in the observed TDCS. As a result, the contributions from small Q values, which have a maximum in the forward direction, contribute strongly to the observed spectra. Moreover, the contribution from large Q values is also included in the convolution; for higher temperatures they become increasingly important and eventually lead to a decrease in the absolute magnitude of the resultant cross sections.

We have investigated the sensitivity of the atom's initial temperature for different electron emission energies. In Fig. 2, the TDCS are presented for electron energies of 4, 10, 17.5, and 55 eV with Q constant at 1.0 a.u. Theoretical triple differential cross sections show features already discussed in previous works. The distributions are mainly directed along the position of the binary peak or in a mirror position to it. These two mechanisms, namely, electrons produced in "binary" and "swing-by" collisions correspond to close projectile-electron or projectile-nucleus collisions, respectively, and have been extensively discussed [8,17]. Briefly, swing-by electrons dominate the spectra for larger momentum transfer while at small values of Q the electrons are mainly emitted in the direction of the binary peak. As demonstrated in a previous work, the transition between these two regimes occurs in a small range of Q values [17].

The calculated TDCS for $T = 0$ K disagree notably with the experimental data. The absolute magnitudes are below the data by factors as large as 70 for $E = 4$ eV. Note also that even for ideal $T = 0$ K the convolution over the experimental bin size increases the absolute magnitude by a factor of 2 at $Q = 0.65$ a.u. [11]. The magnitude of TDCS for ideal conditions are closer to the experiment for higher electron energies, but their shapes remain very different and lack the observed forward focusing. However, for a temperature of $T = 0$ K, the convoluted theoretical values change drastically for all electron energies and the shape closely resembles the experimental TDCS. Also, the absolute magnitudes fall within 50% of the data.

In Fig. 3 we present the TDCS for an electron energy of 55 eV and momentum transfers of 0.65 and 1.5 a.u. As expected, for small values of momentum transfer the electrons are mainly emitted in the direction of the binary peak. On the other hand, for large Q values only swing-by electrons are produced, indicating a strong interaction between the two nuclei [17]. Note, however, that the convolution with the initial temperature in the one transverse direction completely nullifies these structures. At $Q = 0.65$ a forward peak is produced that is characteristic of very small Q values. At $Q = 1.5$ a.u., the inclusion of the initial state uncertainty obliterates the structure due to the swing-by electrons and produces the mirror image binary-peak structure. This is because the contribution from smaller Q values produces a binary peak as shown on this and the previous figures. Both of the convoluted calculational trends are displayed in the measurements.

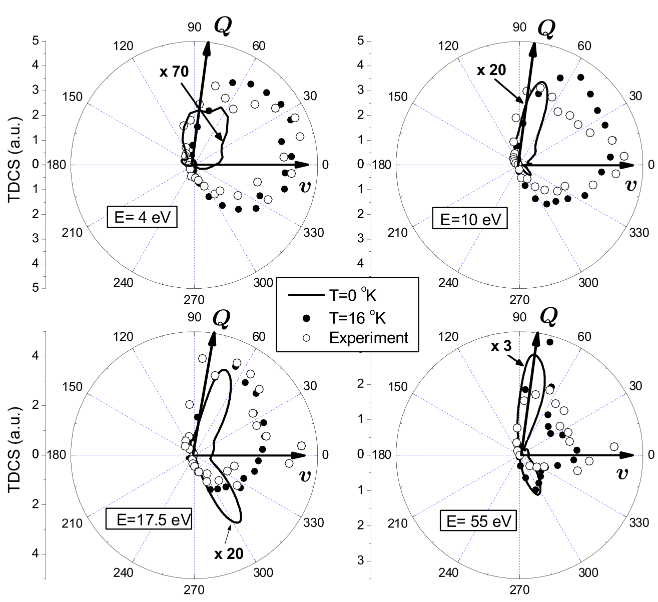

FIG. 2 (color online). TDCS similar to Fig. 1 for temperatures $T = 0$ and 16 K and $Q = 1$ a.u. The electron energies are 4, 10, 17.5, and 55 eV. Experimental data are obtained from [5,7].

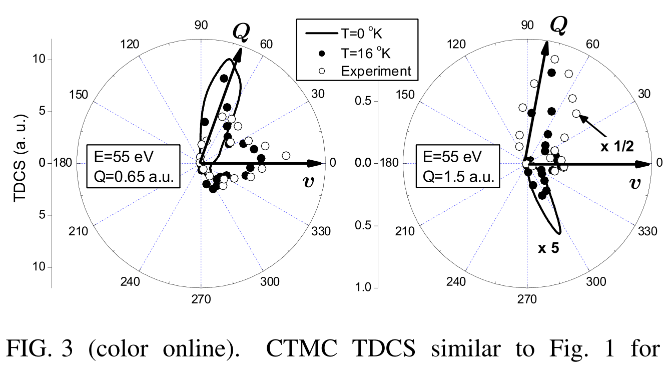

FIG. 3 (color online). CTMC TDCS similar to Fig. 1 for electron energy $E = 55$ eV and momentum transfer $Q = 0.65$ and 1.5 a.u. is compared with the experimental data from Refs. [5].

Thus, in conclusion, we have presented new insight that resolves long-standing questions related to the ability of several theoretical models to describe simple one-electron processes. We have demonstrated the extreme sensitivity of the cross section measurements to initial target atom temperature or momenta when looking at magnitudes related to the momentum **Q** transferred to the target atom. In particular, variation of only one of the target's transverse momenta yielded major changes in both the magnitude and shapes of the cross sections. Our calculations show that if the uncertainty of one of the transverse momentum components of the atom is increased from $T = 1$ to 16 K, the previous serious discrepancies between experiment and well established theories are removed. Unfortunately, our work also implies that even future state-of-the-art experiments where all initial state momenta of the target can be held to less than $T = 0.5$ K, corresponding to He atom momenta values less than 0.10 a.u., the experimental cross section magnitudes will still be approximately 50% larger than "perfect" $T = 0$ K results. Thus, any comparisons between theory and experiment for cross sections differential in momentum transfer **Q** must provide accurately measured uncertainties for the experimental resolutions and a detail of the angular bin sizes of the TDCS in order to be meaningful. Furthermore, our study suggests that the high temperature wings transverse to the jet direction, which have long been thought to be insignificant, may play a major role in both the magnitudes and shapes of cross sections differential in momentum transfer. Future experiments will need to clearly investigate their importance.

Support from the U.S. Department of Energy–Fusion Energy Sciences is gratefully acknowledged.

*Electronic address: olson@umr.edu
†Electronic address: fiol@cab.cnea.gov.ar

[1] M. Schulz, R. Moshammer, D. Fischer, H. Kollmus, D. H. Madison, S. Jones, and J. Ullrich, Nature (London) **422**, 48 (2003).
[2] W. Schmitt, R. Moshammer, F. S. C. O'Rourke, H. Kollmus, L. Sarkadi, R. Mann, S. Hagmann, R. E. Olson, and J. Ullrich, Phys. Rev. Lett. **81**, 4337 (1998).
[3] R. Moshammer, P. D. Fainstein, M. Schulz, W. Schmitt, H. Kollmus, R. Mann, S. Hagmann, and J. Ullrich, Phys. Rev. Lett. **83**, 4721 (1999).
[4] R. Moshammer, A. Perumal, M. Schulz, V. D. Rodríguez, H. Kollmus, R. Mann, S. Hagmann, and J. Ullrich, Phys. Rev. Lett. **87**, 223201 (2001).
[5] M. Schulz, R. Moshammer, A. N. Perumal, and J. Ullrich, J. Phys. B **35**, L161 (2002).
[6] M. Schulz, R. Moshammer, D. Fischer, and J. Ullrich, J. Phys. B **36**, L311 (2003).
[7] D. Fischer, R. Moshammer, M. Schulz, A. Voitkiv, and J. Ullrich, J. Phys. B **36**, 3555 (2003).
[8] J. Fiol and R. E. Olson, Nucl. Instrum. Methods Phys. Res., Sect. B **205**, 474 (2003).
[9] V. D. Rodríguez, Nucl. Instrum. Methods Phys. Res., Sect. B **205**, 498 (2003).
[10] R. E. Olson and J. Fiol, J. Phys. B **34**, L625 (2001).
[11] J. Fiol and R. E. Olson, J. Phys. B **37**, 3947 (2004).
[12] P. D. Fainstein and L. Gulyás, J. Phys. B **38**, 317 (2005).
[13] M. Foster, D. H. Madison, J. L. Peacher, and J. Ullrich, J. Phys. B **37**, 3797 (2004).
[14] J. Ullrich, R. Moshammer, R. Dörner, O. Jagutzki, V. Mergel, H. Schmidt-Böcking, and L. Spielberger, J. Phys. B **30**, 2917 (1997).
[15] D. R. Miller, in *Atomic and Molecular Beam Methods*, edited by G. Sçoles, D. Bassi, U. Buck, and D. Laine (Oxford University Press, New York, 1988), Vol. 1, p. 14.
[16] G. Tejeda, B. Maté, J. M. Fernández-Sánchez, and S. Montero, Phys. Rev. Lett. **76**, 34 (1996).
[17] J. Fiol and R. E. Olson, J. Phys. B **35**, 1759 (2002).
[18] J. Fiol, R. O. Barrachina, and V. D. Rodríguez, J. Phys. B **35**, 149 (2002).