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Quantum-theory based event generator for the analysis of kinematically complete experiments

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Abstract. The ‘reaction microscope’, an electron-ion coincidence momentum imaging spectrometer, represents a unique technique to measure multiply differential ionization cross sections for ionic projectiles. Observed discrepancies with theory for singly ionizing collision of 3.6 MeV/u Au⁵³⁺ and 100 MeV/u C⁶⁺ ions severely challenge theoretical models. We present a method based on event-generators, which allows to consistently incorporate instrumental effects into theory. The result of the convolution procedure suggests, that the observed discrepancies are not a result of the experimental resolution, but are of true physical nature.

1. Introduction

Atomic and molecular fragmentation experiments serve as an ideal tool to study few-body dynamics in atomic systems. In this field, the invention of fragment momentum imaging, so-called ‘reaction microscopes’, provides a unique and revolutionary experimental method [1]. Here, for each charged fragment the full momentum vector information can be reconstructed which allows for detailed insights into the collision process. A further outstanding feature is, that a large part of the final-state momentum phase space is covered, such that in principle a comprehensive data set of the studied collision process is acquired. The reconstructed momentum vectors of each fragment are stored in a list – the ‘event-file’ – for each detected collision event. After a sufficiently large sample of events has been gathered, sorting the events accordingly can generate spectra, which reflect the differential cross section for the studied process.

For ion-impact ionization of atoms, the reaction microscope takes a prominent place as it overcomes problems, which in the past basically made kinematically complete experiments for fast ion impact impossible. As a result, the first fully differential cross sections (FDCS) for ionization by ion impact were measured using this method [2]. In this contribution we will focus on two experiments studying ion-impact single ionization of helium by (i) medium velocity (12 au) 3.6 MeV/u Au⁵³⁺ ions, resulting in a huge perturbation of $Z_p/v_p = 4.4$ au (Z_p : projectile charge, v_p : projectile velocity), and realizing the other extreme of a very small perturbation of $Z_p/v_p = 0.1$ au by 100 MeV/u C⁶⁺ ions with a high velocity $v_p = 60$ au as projectiles. In both cases pronounced structures are observed in the absolute FDCS represented as the emission probability of the ejected electron as a function of the emission angle at fixed momentum transfer and ejected electron energy [3,4]. These data proved to

present a severe challenge to theoretical modeling, where for (i) a peak in the electron emission pattern in direction of the incoming projectile is observed and not reproduced by any calculation so far. Even more surprising, an enhancement of electron emission in directions perpendicular to the projectile scattering plane is observed in (ii), which is again in strong contradiction with all theoretical models, where actually already a simplest first order approach using the First Born approximation was expected to hold.

Recently, Olson and Fiol *et al.* claimed in several publications [5,6] that the observed discrepancies can be entirely resolved by considering instrumental effects hereby questioning the reaction microscope technique itself in its ability to provide reliable fully differential data. However, for the 3.6 MeV/u Au⁵³⁺ projectiles [5], they had to assume a very poor resolution, which was by a factor of four worse than the one stated in the experimental papers, to at least reproduce the absolute magnitude of the cross section. For 100 MeV/u C⁶⁺ projectiles [6], these authors claimed that the out-of-plane enhancement could be fully resolved by convoluting a CDW-EIS and even an FBA calculation with the resolution as given in the experimental papers, which however conflicts with the assumption of [5], namely that the resolution is far worse than actually stated by the experimentalists. Furthermore, the assertion of Fiol and Olson is inconsistent with their own previous work, where they found out-of-plane peak structures without accounting for the experimental resolution [7].

In this paper we present a method, which allows to convert the predictions of theoretical modeling into an event-file, similar to the one obtained in the experiment. One major advantage is, that the experimental resolution can be easily implemented into the generated event-file, which effectively results in the convolution of the theory with the instrumental function of the reaction microscope. With our method we can firstly verify that the resolution stated in the experimental papers is correct and that the reaction microscope is indeed capable of providing reliable fully differential benchmark data. Secondly, we show for the 100 MeV/u C⁶⁺ single ionizing collisions, that a convolution of the FBA with the thus confirmed resolution of the reaction microscope does not lead to the effect reported in the work of Fiol *et al.* [6]. While the resolution does have a significant effect on measured cross sections, the above mentioned discrepancies are mostly due to true physics effects. Furthermore, we outline the potential of event-generators of providing deeper insights into theoretical modeling of atomic few-body processes.

2. Event-Generator and Convolution of Theory with Experimental Resolution

Our convolution procedure is based on a so-called event-generator, a method routinely used in high-energy physics, where one is confronted with the problem of complicated instrumental response functions of the complex detection systems. There, such a method using an event-generator is called 'Monte-Carlo simulation', since random number generators play a major role in this technique. Event-generators serve as an alternative way of representing the predictions of a theoretical model. Concerning the convolution of calculated cross sections with the instrumental function, one frequent obstacle is the mismatch of the preferred reference frame, or in other words the different coordinate systems used in theory and by experimentalists. Theoretical calculations naturally use the collision frame determined by the momenta of the incoming and scattered projectile. Every experiment, however, at first instance uses the laboratory-frame, which in the reaction microscope experiment is given by the directions of the projectile beam and the atomic target beam. The transformation into the collision frame has to be performed for each single recorded event, since the projectile can be scattered into different directions in the laboratory-frame. This event-by-event transformation hampers a consistent and complete consideration of the different instrumental effects into calculated cross sections. One example is the consideration of the initial momentum distribution of the target atoms resulting from the finite temperature T of the atomic beam. Here the situation is complicated by the fact, that the initial momentum distributions differ for the directions along and perpendicular the target beam. The reason is, that perpendicular to the atomic beam hot atoms are filtered out by collimation, which is not possible along the target beam directions. Therefore only estimates of the resolution in

the collision frame could be given, however, so far no consistent consideration of the instrumental effects on multiply-differential cross sections was performed.

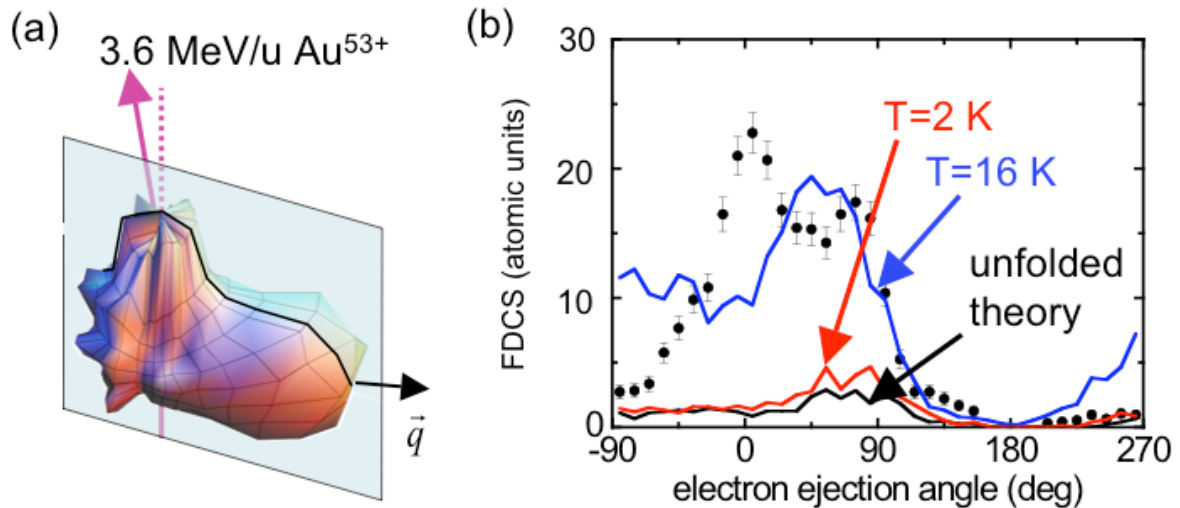


Figure 1. (a) An example result of the experimental fully differential cross section represented as a 3D-image after single ionization of helium by 3.6 MeV/u Au⁵³⁺. The arrow denotes the direction of the scattered projectile. (b) Absolute fully differential cross section results in the scattering plane (depicted in (a)) for fixed momentum transfer ($|\mathbf{q}|=1$ au) and fixed energy of the ejected electron ($E_e=10$ eV). Solid lines: results from the event-generator at different folded experimental resolutions. Points: experimental data.

These problems with folding the calculated cross section with the instrumental function are avoided by employing an event generator technique. The simulated event file has precisely the same structure as the event file generated by the experiment. Like the former, it either contains Cartesian momentum coordinates of the final-state particles or the original coordinates can easily be converted into Cartesian coordinates. The frequency of occurrences of certain momentum combinations in the event file reflects the cross section as predicted by the theoretical model. Differential cross sections can be extracted by analyzing the event-file sorting the events into corresponding histograms and using appropriate kinematic conditions. This way, theoretical modeling can be brought to a form, which is compatible to the data recorded using the fragment imaging technique. Instead of convoluting a calculated cross section, the instrumental effects are implemented into the event-file generated from theory event-by-event and then the cross section is evaluated by analysis of the modified event file.

There are further advantages which arise in the representation of theory by an event-file: Once the event-file has been generated (which is the time-consuming part), coordinate transformations can be performed quickly event-by-event, such that in principle any representation of the cross section can be readily chosen which opens the way to highlight specific aspects in connection with few-body processes (e.g. Dalitz representations [8]). In the field of atomic collisions, such event-files are so far only known from CTMC calculations (classical trajectory Monte-Carlo), which mimics atomic scattering within a classical framework. However, the decisive difference of our event-generator is that in principle any calculation can be used as an input, including models based on quantum theory. Since instrumental effects can never be avoided in differential cross section measurements, event generators therefore provide an ultimate method to benchmark calculations against experimental data.

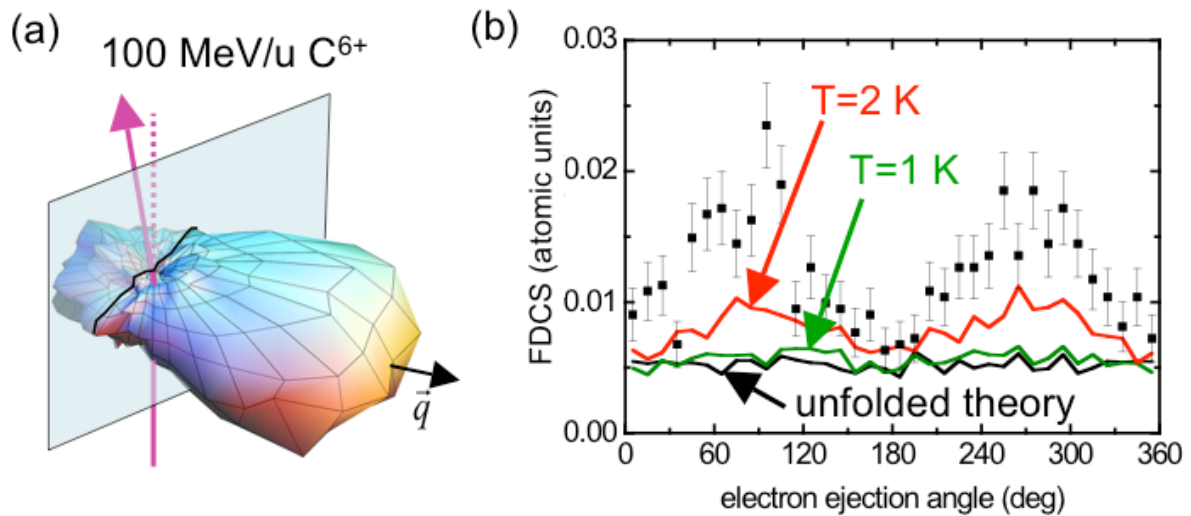


Figure 2. (a) Three dimensional image of the experimental fully differential cross section for 100 MeV/u C⁶⁺ single ionization of helium. The arrow denotes the direction of the scattered projectile. (b) Absolute fully differential cross section results in the scattering plane (depicted in (a)) for fixed momentum transfer ($|q|=0.75$ au) and fixed energy of the ejected electron ($E_e=6.5$ eV). Solid lines: results from the event-generator at different folded experimental resolutions. Points: experimental data.

2.1. Event-Generator: Converting Theory into an Event-File

The general principle of the event-generator has been outlined in [9] and is only briefly discussed here. The method is based on pseudo-random number generators, where a huge number (several billions) of final state momenta is generated, each component uniformly distributed within a specified range. The result is composed into a raw 'event-file', where each event represents a (virtual) collision event consisting of the different final-state momentum components. Until now, each event has equal weight, irrespective of the momentum components. From this raw sample, events are selectively rejected where the selection criterion applied to each single event is the cross section calculated for the point specified by momentum components of the event. The application of this rejection method results in a probability weight for each event, which corresponds to the probability predicted by the underlying model. The generation of the event-file is very time-consuming since firstly a large number of random numbers needs to be generated and secondly because for each event from the raw event-file the cross section has to be evaluated for the rejection procedure which results in the calculation of a large number of cross section points.

Two event-files were generated for the two experiments mentioned in the introduction, one based on a simple first Born model for a comparison with the data obtained in the 100 MeV/u C⁶⁺ single ionization experiment. The second event-file was generated using a theoretical model based on the symmetric eikonal approximation including the nuclear-nuclear interaction (dubbed SEA-NN) presented in [10] in order to compare the result of a model based on perturbation theory at the unusual high perturbation in 3.6 MeV/u Au⁵³⁺ singly ionizing collisions.

2.2. Implementing the Resolution into the Event-File

Once theory has been converted into an event-file, the instrumental function can be implemented in the following way: To each momentum component an appropriate momentum, determined from a model instrumental function, which simulates the experimental resolution, is added event-by-event. We used a Gaussian profile for the model instrumental function, which is discussed in detail in [9]. The modified event-file, now fully afflicted with the resolution, can then be reanalyzed and the extracted spectra represent the convoluted cross section. The described method is far less time

consuming than an analytic convolution, since only random numbers need to be generated and no further calculation of the cross section is necessary.

3. Comparison of Convolved Theory with Experimental Results

With the experimental resolution implemented into the event-file the next step is the comparison of cross sections from theory and experiment extracted from the generated and experimentally recorded event-files. In [9] we analyzed cross sections differential in the Cartesian momentum transfer components transverse to the incoming projectile beam. Here, the observed distributions turn out to be very sensitive to the experimental resolution, and for the 100 MeV/u C^{6+} and the 3.6 MeV/u Au^{53+} collision we were able to infer upper limits of the actual experimental resolution, which resulted to be $T=2$ K for the Jet-temperature, and a beam diameter of 1 mm. From the extracted single differential cross section a temperature of 16 K could be clearly ruled out, which implies that the instrumental effects on fully differential cross sections presented in [6] are drastically overestimated. Further analysis yielded a most realistic estimate of $T = 1.5$ K and a beam size of 0.5 mm. We present the unconvoluted and convoluted FDCS extracted from our generated event file in Figure 1 and Figure 2, showing the cross sections extracted from the generated event-files together with the cross section extracted from the measurement. For 3.6 MeV/u Au^{53+} case, the convolution with the upper limits of our resolution shows almost no effect. Even a strongly exaggerated poor resolution from a $T=16$ K jet-temperature cannot reproduce the dominant peak in the cross section in the 0° direction.

Considering the collision with 100 MeV/u C^{6+} ions, shown in Figure 2, the convolution of the FBA-model with the experimental resolution shows a stronger effect in the plane perpendicular to the scattering plane. Using our upper limits of the experimental resolution leads to a peak structure in the convoluted cross section, qualitatively seen in the experimental data. However, the convoluted theory fails to match the absolute magnitude of the cross section by a factor of two. Furthermore, our result contradicts those published by Fiol *et al.* [6], where the authors claim that by folding in a resolution corresponding to 1 K target temperature results in pronounced structures with the same intensity as seen in the data. However, our study suggests, that a temperature of 1 K alone has essentially no effect. The out-of-plane enhancement for electron emission is not uniquely a result of the experimental resolution but rather is mainly due to the failure of theory to correctly describe the collision. That structures which are of physical nature are present in the plane perpendicular to the momentum transfer has been unambiguously demonstrated in singly ionizing collision with 1 keV electrons corresponding to a similar perturbation as for ion-impact and for identical kinematical parameters [11]. In this respect it is important to note, that the experiment using electrons has a resolution which is a factor of three better than in the ion-impact experiment such that here no effects of the experimental resolution in the out-of-plane cross section are present. We also note that convoluting the FBA with classical elastic scattering between the projectile and the target core using the same event generator technique, the data for C^{6+} impact can be very well reproduced [12].

4. Summary and Conclusions

Event-generators show great potential in the field of atomic and molecular few-body collision processes. This method allows to convert the result from any form of theoretical modeling into an event-file, which documents the collision-by-collision history of a ‘virtual’ experiment. Following advantages arise through the generation of event-files:

- Theoretical modelling is brought into a form, which is more appropriate for the consideration of instrumental effects. Since such effects can never be avoided and any theoretical model can be implemented into the event-generator, this method provides an ultimate method to benchmark calculations against experimental data.
- Coordinate transformations of alternative representations can be easily chosen in the analysis of the event-files. Re-representations of the cross section allow to highlight different aspects and to provide deeper insights into the dynamics of few-body reactions.

In particular the fragment-imaging technique benefits from these advantages, mainly because the recorded data on few-body collision processes is provided as an event-file, too. This allows for the first time to consistently incorporate all known effects, which influence the experimental resolution, into a theoretical cross section. Using upper limits of the experimental resolution, which were verified by studying single differential cross section spectra [6], the discrepancies between theory and experimental data seen in fully differential cross sections for single ionization by 3.6 MeV/u Au⁵³⁺ and by 100 MeV/u C⁶⁺ ions were confirmed. Concluding, with the help of the event-generator method it was demonstrated, that the reaction microscope provides reliable multi-dimensional benchmark data, which still challenge theoretical modeling of charged particle induced break-up processes.

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