Editorial

Topical Issue on many particle spectroscopy of atoms, molecules, clusters and surfaces editorial

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Abstract. Many particle spectroscopy is a subject of continued interest to many experimental and theoretical groups worldwide. It is based on the coincidence spectroscopy of minimum two particles coming from the same elementary process. It is a very powerful tool for studying not just atoms and molecules but also more extended electronic systems such as clusters and surfaces. Due to the large variety of its applications, it is really an interdisciplinary research field. This Topical Issue presents a state-of-the-art description of current research activities in the field of many particle spectroscopy. The contributions to this Issue represent original research results on both experimental and theoretical studies, involving the interaction of various projectiles, like photons, electrons, ions with atoms, molecules, clusters and surfaces.

1 Introduction

In the early decades of atomic physics, one could detect only one out of the particles (no matter how many there were) that were produced in an elementary atomic process, or at least there was no information about multiple detections. The coincidence technique that was introduced a little more than 50 y ago represented a qualitative jump in this area as well. Using this method, one can simultaneously measure the parameters of two particles that were produced in the same elementary atomic process. Later triple or even quadruple, coincidences became measurable.

At the beginning, both the primary particle starting the atomic physics process and the two particles in the final state, detected in coincidence, were mainly electrons. This (e,2e) technique dominated the field of interest even twenty years ago [1], but publications with ion or photon projectiles also appeared. During the last two decades, the fast development of synchrotrons and lasers caused significant changes, primarily in the nature of the projectiles. Publications with photon projectiles gradually became the majority [2,3], and then, they became dominant [4,5].

The objective of this Topical Issue is to assess the state of the art in the current understanding of a variety of basic phenomena in the charged particle dynamics in atoms, molecules, clusters and at surfaces such as:

- collision induced physical, chemical and biological reactions, ultrafast dynamics, charge-exchange processes, collective as well as single-particle excitation and ionization, electron–electron correlation effects in atoms and in solids, excitation and single and multiple ionization of various targets, energy loss, scattering and channelling of primary particles, electron and photon emission processes.

2 Experimental advances in electron and ion impact processes

The experimental study of atoms by means of electron projectiles is a traditional field of interest. Such a work is reported by Borovik et al. [6], where the excitation-autoionization (EA) cross section for the 5p6 subshell in Ba atoms was determined in an incident electron energy range from 15.61 eV up to 600 eV. The data were obtained by measuring the total intensity of ejected-electron spectra arising from the decay of the 5p6n1l1n2l2n3l3 autoionizing states. They found that the energy dependence of the cross section is characterized by the presence of a strong resonance structure in the near-threshold energy region. Genevriez et al. [7] reported on the experimental determination of absolute, total cross sections for electron-impact double ionization of helium in its metastable 1s2s2S state and of the helium negative ion He− (1s22p4P). Cross sections were measured for impact energies ranging from threshold to 1000 eV using the animated crossed beams tech-
phosphate molecules experimentally and theoretically in the energy range from 50 eV to 250 eV [14]. The experimental set-up based on a crossed beam technique comprising of an electron gun, a single capillary gas needle and a detection system with a channeltron was used to measure differential cross sections. The absolute scale for the cross sections was obtained by relative-flow method using argon gas as a reference. For the interpretation of the measured data, the partial expansion method was used. Although the calculation procedure was crude, they found excellent agreement between the shapes of measured and calculated data.

3 Theoretical advances

3.1 Photon-induced processes

The interest towards the interpretation of photon-induced processes is continuously growing. Numerous calculations were performed for the photon projectile–atom target combination. The photo-ionization of rubidium in strong infrared laser fields based on ab initio calculations was investigated [15]. The bound and the continuum states were described with Slater orbitals and Coulomb wave packets, respectively. The bound state spectra were calculated with the variational method. The authors found that it reproduced the experimental data within a few percent accuracy. The effects of the shape and the parameters of the pulse to the photo-ionization probabilities and the energy spectrum of the ionised electrons were shown. We note that these calculations may provide a valuable contribution at the design of laser and plasma-based novel accelerators, the CERN AWAKE experiment.

Lopez and Arbo have elucidated the relevance of the Coulomb potential in the interference structures observed in the momentum distribution of atomic ionization using different theoretical models [16]. They found that by increasing the importance of the Coulomb potential in the phase of the semi-classical approximations, the separation among the interference fringes grows. They also have shown that not only the role of the Coulomb potential is crucial for the formation of the interference structures, but also it needs to be properly accounted for in the theory. Novikovskiy et al. [17] presented a detailed theoretical analysis of the 1s photo-ionization of neon. It was found that the most significant many-electron correlation in computing photo-ionization of inner shells is the rearrangement of the outer shells caused by the inner vacancy. Further noticeable effects are: (1) the polarization of the ion core by the outgoing photoelectron and (2) the coherent effect of double excitation/ionization.

Three articles [18–20] deal with the different photo-ionization processes of argon. Among them, Lagutin and co-workers studied the two-photon ionization of the 3p shell of Ar in the above-threshold ionization (ATI) exciting-photon energy region [18]. The ab initio calculations were performed using perturbation the-
ory and the correlation function technique. The latter enables to perform a summation over the complete set of intermediate states emerging in the transition amplitude. Generalized two-photon ionization cross sections were calculated taking into account many-electron correlations. The calculations demonstrated that the two-photon ionization of Ar at the 3p\(^+\) threshold is almost entirely a collective process. The decisive contribution in the above-threshold two-photon 3p\(^+\) ionization at the exciting-photon energies corresponding to the 3p\(^-\)\(\ldots\)d giant resonance comes from the Auger-like many-electron correlations of \(e'de'd\ldots3pe_f\) type. Gryzlova presented theoretical studies of two-photon sequential double ionization of Ar for photon energies in the region of Rydberg autoionizing states 3p\(^1\) (1\(^D\)) nl of the ion Ar\(^{++}\) overlapping with the particle-hole autoionizing states 3s3p\(^6\)np of neutral Ar [19]. They found that the atomic and ionic autoionizing states lead to sharp variations of the angular correlation function between the two outgoing electrons, as well as in the angular distributions of the first and the second emitted electrons. A strong influence of the second step ionization on the first ionization step was demonstrated. In the third contribution, Orimo et al. presented comparisons between quantum and classical calculations for above threshold ionization of an Argon atom interacting with a strong laser pulse [20]. The time-dependent complete-active-space self-consistent field (TD-CASSCF) method and the classical trajectory Monte Carlo (CTMC) method were used for the cases of quantum and classical calculations, respectively. The authors discussed the differences between the results obtained by the TD-CASSCF and the CTMC simulations.

For the photo-ionization of various molecules, the investigations were carried out to study the effect of the strong laser field [21], the interchannel mixing [22] and the angular distribution parameters [23]. Shvetsov-Shilovsk et al. published a pioneer work regarding the semi-classical approach for molecular target [21]. They extended the semi-classical two-step model for strong-field ionization that describes quantum interference and accounts for the Coulomb potential beyond the semi-classical perturbation theory to the hydrogen molecule. In the simplest case of the molecule oriented along the polarization direction of a linearly polarized laser field, they predicted significant deviations of the two-dimensional photoelectron momentum distributions and the energy spectra from the case of atomic hydrogen. Specifically, for the hydrogen molecule the electron energy spectrum falls off slower with increasing energy, and the holographic interference fringes are more pronounced than for the hydrogen atom at the same parameters of the laser pulse. Rearrangement of the electron shells accompanying inner-shell photo-ionization of the CH\(_4\) molecule was also studied theoretically [22]. Novikovskiy and co-workers calculated the K-shell photo-ionization cross sections and the corresponding photoelectron angular distribution parameters in different approximations using the single centre method. They found a strong mixing of the partial ionization channels in the vicinity of the 1s ionization threshold, caused by the non-spherical part of the molecular potential, which results in a qualitative difference between the electronic rearrangement effects in molecules, as compared to atoms. Novikovskiy et al. also published theoretical results for photo-ionization cross sections and photoelectron angular distribution parameters of the closed-shell CH\(_4\), NH\(_3\), H\(_2\)O and CO molecules [23]. For the neon-like molecules, calculations were performed in two approximations: in the spherical single-orbital and in the non-spherical many-orbital approaches. In the case of 1s\(_1\) (1s) shells of CH\(_4\), NH\(_3\) and H\(_2\)O, the photo-absorption cross sections obtained in the simplified FC SO approximation fortuitously coincide with the results of the more accurate RAC SC calculations.

After exchanging the target, the photoelectron spectra simulations were performed for nanotips as well. The photoelectron trajectories emitted from silver nanoparticles were calculated using the classical trajectory Monte Carlo method, where the image force towards the surface was taken into account [24]. It was shown that the code developed for these special simulations describes the experimental findings reasonably well. Significant effect of the image acceleration to the calculated electron spectra was observed. They found that the calculated energy distributions of photoelectrons are in agreement with the recent experiments.

### 3.2 Electron-induced processes

The laser-assisted (e,2e) collision [25] is a sort transition between the photon and electron projectiles. For the normal (e,2e) processes—which dominated the program in 2000—nowadays they only perform a small amount of calculations. Zaytsev et al. studied the laser-assisted fast (e,2e) collisions on atomic hydrogen both in perturbative and in non-perturbative regimes of laser radiation. The authors calculated the multi-photon triple differential cross sections in asymmetric coplanar kinematics employing the first Born approximation in the projectile–target interaction. They have shown that in both radiation regimes, their method exhibits high efficiency for different net numbers of photons exchanged between the colliding system and the laser field.

For electron projectiles, calculations for double ionization of helium [26] and electron Monte Carlo simulations in solids were also presented [27, 28]. Zaytsev et al. presented fully differential cross sections for the double ionization of Helium by fast electron impact [26]. Ionization amplitudes were obtained by solving in the entire space, to first order, the corresponding three-body-driven Coulomb Schrödinger equation. The comparison with two other ab initio first-order calculations (CCC and GSF) shows that the obtained FDCS shapes were very similar. For certain geometrical situations, however, the authors found a substantial magnitude difference when the two electrons are ejected with 4 eV each. Being slower for this lower energy case, the two electrons interact more (stronger correlation). The authors attributed the magnitude difference to the
3.3 Particles, antiparticles, exotic particles

The influence of the sign of charge of the projectiles for the cross sections for light projectiles [29] as well as for muons and pions [30] was also presented. Positron- and electron-impact ionization of the 1b₁ and 3a₁ orbitals of H₂O was studied by CDW-EIS model at an impact energy of 81 eV [29]. Fully differential cross sections were calculated and contrasted after a proper average procedure over molecular orientations. Double binary peaks were observed for positron-impact and coplanar geometries, while only single binary peaks are exhibited for electron-impact ionization. For the denominated perpendicular planes, similar structures are observed, with an enhancement or decrease in the binary and recoil lobes. Forward electron emission was analysed identifying the electron capture to the continuum structure for positron impact. A high narrow peak and a huge dip for positron and electron impact are, respectively, observed, structures already seen in previous ionization studies involving both light and heavy projectiles. The K-shell ionization cross sections by positively and negatively charged muons and pions have been published at low energies with the CTMC and the ECPSSR [30]. The obtained results are in good agreement with each other and also with the CC calculations for muons on Cu. The ECPSSR cross sections by negative projectiles are larger than the PWBA, and the values for positive projectiles are in the opposite direction. The reasons can be ascribed to the binding-energy effect of the target electron and the Coulomb-deflection effect of the projectile. In the energy region considered here, the latter effect is dominant. At the same projectile velocity, the cross section for pions is almost the same as that for muons, but the deviation from the PWBA is slightly larger for muons. This is explained as the difference in the Coulomb-deflection effect.

Following the work with muon projectiles, the energy shifts and relative radiative rates of electronic Kα x-rays were presented for light muonic atoms with various states of the muon by Mukoyama [31]. The calculations were based on some simplified assumptions, but n dependence of the muonic orbital on the energy shifts and relative rates was obtained. The author found that the l dependence is small. It was assumed that electron vacancies created during muon cascade are quickly refilled. However, for light muonic atoms this assumption may not be valid. The calculations indicated that the number of 2p electrons at the moment of electronic K-x-ray emission plays an important role in energy shifts and relative radiation rates. The knowledge of electron vacancy distribution in cascade processes is essential to obtain more accurate information from analysis of electronic X-rays for light muonic atoms. For this purpose, we may need further experimental and theoretical studies on light muonic atoms.

3.4 Collisions with heavy particles

For the case of heavy projectiles, calculations were presented for targets of helium [32] and lithium atoms [33], as well as for water molecules [34], and neutral atoms and hydrogen molecules [35] collisions. Differential cross sections for charge-exchange and single and double electronic emission in collisions of protons with He-atoms at intermediate impact energies were theoretically evaluated by the classical trajectory Monte Carlo methods [32]. The models incorporate momentum-dependent terms to the Hamiltonian in order to avoid the classical autoionization of He. The theoretical results for single capture and single ionization were compared to available experimental data. The role of the electron–electron correlation effects in double ionization processes was analysed by inspecting the angular and energetic dependence of the electronic emission spectra at different impact energies. Bondarev et al. considered the single ionization of lithium atoms in collisions with p and O⁸⁺ projectiles [33]. Doubly differential cross sections for ionization were reported within a relativistic non-perturbative approach and compared with the recent measurements. Otranto and co-workers studied theoretically, using the classical trajectory Monte Carlo method, the electron production following single and multiple ionization of water by bare ion impact [34]. The obtained results may provide a benchmark against experimental data collected in different laboratories and other theoretical data obtained by means of distorted wave methods. During the simulations, ten electrons in the molecule were explicitly considered, in contrast to previous formulations based on a single active electron description of the target. The authors presented a simple scaling of the cross sections. The
collisional radiative models used in the modelling of beam emission spectroscopy diagnostics neglect atom–atomic collisions because of a lack of sufficiently detailed atomic data. Filling this scantly, Asztalos and coworkers presented 4-body classical trajectory Monte Carlo simulations to calculate the cross sections for various channels in collisions between $H + H_2$ and $Li + H_2$ for a wide range of projectile energies [35]. Based on the calculated cross sections, a simplified version of the collisional radiative model has been derived. The authors have shown that the model is suitable to obtain the beam attenuation in neutral gases outside of the confined plasma region. A strong density dependence has been found for each beam species.

### 3.5 Molecules and attophysics

Finally, in this issue the works with hydrocarbon molecules [36] and the generation of attosecond laser pulses [37] were presented. Zhao et al. [36] studied theoretically the Auger effect after inner-valence ionization of several unsaturated and saturated cyclic and linear hydrocarbon molecules. These prototype molecules were chosen such that the effects of the different characteristics of aromaticity ($\pi$ electrons, conjugation, cyclic geometry) on the Auger decay can be investigated separately. The authors have shown that among these molecules, the ones having $\pi$ electrons can undergo Auger decay after inner-valence ionization. Furthermore, the results reported suggest that conjugation allows for several open Auger decay channels, while aromaticity limits the range of the latter. Last but not least new theoretical and numerical results were presented regarding isolated attosecond XUV soft X-ray pulses that can be generated by Thomson backscattering of a high-intensity single-cycle near infrared laser pulse on a suitable nanobunch of MeV electrons [37]. The theoretical investigations of Hack et al. have shown that the Thomson backscattering of a NIR laser pulse on a suitable relativistic electron nanobunch is a promising source of an isolated attosecond XUV soft X-ray pulse, having advantageous features. Based on the analysis of the coherence factor, the authors derived a simple formula for the cut-off frequency of the collective radiation spectrum, which could also be useful in designing the corresponding experiments.

### 4 Concluding remarks

Many particle spectroscopy has continued its significant progress during the previous years. The objective of this issue was to assess the state of the art in the current understanding of a variety of basic phenomena: in the charged particle dynamics in atoms, molecules, clusters and at surfaces such as collision-induced physical, chemical and biological reactions, ultrafast dynamics, charge-exchange processes, collective as well as single-particle excitation and ionization, electron–electron correlation effects in atoms and in solids, excitation and single and multiple ionization of various targets, energy loss, scattering and channelling of primary particles and electron and photon emission processes. However, a significant number of interesting problems are still unresolved and many interesting fields of physics are waiting for investigations. It is still open to investigate the interaction between many electronic systems either in ion–atom, ion–molecule, ion–cluster or ion–surface collisions. As a new feature, in the last years, attoscience applying lasers came to the fore [38–43]. Attosecond physics is a new and rapidly developing field driven by recent advances in laser technology. Attosecond science holds the promise to observe and to control the optical-field-driven electronics working at clock speeds six orders of magnitude faster than current conventional electronics. Combining this extremely small time-scale with nanodimensional materials gives us fairly new techniques for new discoveries, especially applying the technique of the many particle spectroscopy.

All the old and new questions like physical and chemical phenomena induced by the interaction of particles (singly up to highly charged ions, atoms and clusters, electrons and photons) with atoms, molecules, clusters and surface and the bulk of solids and also liquids remain the key topics of the many particle spectroscopy. The present Topical Issue, based on the works reported at the International Conference on Many Particle Spectroscopy of Atoms, Molecules, Clusters and Surfaces (MPS-2018), summarized and highlighted the current understanding of a variety of basic phenomena in the charged particle dynamics in atoms, molecules, clusters and at surfaces such as collision induced physical, chemical and biological reactions, ultrafast dynamics, charge-exchange processes, collective as well as single-particle excitation and ionization, electron–electron correlation effects in atoms and in solids, excitation and single and multiple ionization of various targets, energy loss, scattering and channelling of primary particles and electron and photon emission processes.

The MPS conference series continues, and the next conference was planned for 2020 in Turku, Finland. However, due to the escalating coronavirus pandemic and the unforeseeable duration of the disruption of activities, it is postponed either to 2021 or 2022. Similarly to the previous MPS conferences, it will focus on the interaction of light and charged particles (ions and electrons) with various forms of matter, ranging from atoms to nanoparticles and surfaces. In particular the latest experiments, techniques and theoretical results involving multiple particles, their interaction (correlation, scattering, dynamics, multi-photon absorption) and detection (such as coincident experiments) are presented.

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Author contributions

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