Chapter 1
Introductory Remarks

Structural analysis of atoms and molecules in their ground and excited states belong to topics of *atomic and molecular spectroscopy* including actions of static or dynamical fields on free atoms and molecules. Atoms, molecules, ions, electrons, photons can also collide with each other which causes a large series of phenomena that we call *atomic and molecular collision processes*.

Physically important properties of such collision processes are their development as a function of time, the various types of interactions between the colliding partners, the intensities of all these processes as a function of initial conditions, such as the relative energies of the colliding atomic particles, their mutual potential energies and their quantum numbers before and after the collision. The total entity of all these physical processes of atomic collisions is determined both by atomic structure as well as by parameters of the collision processes. While atomic and molecular structure is an important parameter in collision processes, atomic collision dynamics is the central problem of the physics of atomic collision processes.

A huge number of possible atomic and molecular collision processes exists; any arbitrary atom or ion can collide with another atom or ion or with an electron or photon. The energies of the colliding atomic particles can be chosen arbitrarily; after the collision, the particles involved propagate in all possible directions. The manifold character of collisions requires a classification and ordering system based upon physical processes; these will be described and developed up to a certain point. A more introductory description of atomic and molecular collision processes can be found in the specialized literature, e.g. Johnson (1982).

Since about the 1960s, the field of research on atomic and molecular collisions has advanced through a variety of new development of experimental and theoretical methods; these have led to a more detailed understanding of quantum-mechanical collision dynamics. In analogy with nuclear and elementary-particle physics, especially the *technology of coincidence and spin experiments* have contributed to the advancement of new knowledge of atomic and molecular collision physics. Applications of atomic and molecular collision processes are found in astrophysics, atmospheric physics, plasma physics, nuclear fusion physics and chemical reactions. We want to

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emphasize that the present book also refers to the article in honor of Ben Bederson (Kleinpoppen et al. 2005) but does not claim to represent an approach to review on *Perfect and-or complete Scattering Experiments*; it only encloses a selection of topics of our personal choices. More detailed reviews are available and are partly listed in the references, e.g. Andersen and Bartschat (2000), Becker and Crowe (2001), Hanne et al. (2003).

The existing data of complete/perfect scattering experiments provide a deep insight into physical mechanisms of atomic and molecular scattering processes. They reveal what types of processes and interactions occur or compete with each other in the collisional process.

Scattering amplitudes and their phase differences and also atomic target parameters extracted from these type experiments have successfully been applied *as most sensitive tests of modern collision theories*. Coincidence and spin experiments do not, in selected cases, average or sum over atomic cross sections for various sub-processes or interactions of the collisional processes. Such coincidence and spin experiments resulting in collision amplitudes, phases and target parameters have been classified as *third generation* type of experiments going well beyond the more limited kind of information obtained from differential (*second generation* type of experiments) or total (*first generation* type of experiments) cross section measurements.

In a detailed analysis of complete/perfect atomic and molecular collisions we are dividing the task into the various sub-parts, namely on electron-photon coincidence experiments, on atomic and electron spin experiments and comparisons between electron and positron scattering.

Only recently a start has been made to combine spin and coincidence experiments; we will briefly refer to this newest development.

While Chap. 2 is devoted to the general analysis methods and the detection of the scattering residuals, i.e., electrons, ions, atoms, or molecules which might, if still excited, decay further by photon emission or another scattering process, we will focus on the discussion of nowadays angle and spin resolved Auger emission experiments and related research in Chap. 3. As has been pointed out in Chap. 2 such kind of experiments yield more refined information about the electron emission process, particularly the scattering phase. This can be seen as a step towards a complete experiment, i.e., to determine all elements of the describing density matrix, as has been first requested by Bederson (1969a, b). The basics of the Auger effect and the early experiments will be shortly reviewed. Ongoing, open shell atoms will be discussed, focusing on the angular distribution of the excited sodium KLL Auger transitions. The investigation of open shell atoms yields surprising results concerning the cross section, as well as the angular distribution, due to the open shell character. Eventually, the angle and spin resolved Auger emission analysis will be investigated, experimentally and numerically, stressing the example of the angle and spin resolved resonantly excited $\mathrm{Ar}^*(2\mathrm{p}_{1/2}^{-1}4\mathrm{s}_{1/2})_{J=1}$ and $\mathrm{Ar}^*(2\mathrm{p}_{1/2}^{-1}3\mathrm{d}_{3/2})_{J=1}$ states and their subsequent $\mathrm{L}_2\mathrm{M}_{2,3}\mathrm{M}_{2,3}$ Auger emission in detail. For the generation of the intermediate excited Rydberg state two different mechanisms will be considered.

As a prerequisite to angle and spin polarized Auger emission a deep inner shell hole must be generated which should either be aligned and/or oriented with respect to its magnetic sublevels. Particularly, the process of photoexcitation reveals several advantages with respect to its theoretical description and, due to the availability of 3rd generation synchrotron beam sources, allows for a large variety of experimental approaches. Complementary, we will investigate the generation of these oriented and/or aligned hole states via photoionization, where particularly emphasis will be given to closed (sub-)shell atoms, e.g. the rare gases or the earth alkalis. The available numerical results will be compared to the experimental data. In addition, alignment and orientation of open-shell atoms are investigated, and, as a new field, orientation and alignment of radioactive elements are explored.

As an alternative process electron impact excitation of Auger states will be considered. Only a sparse number of experiments have been carried out applying this method. Though, it yields information about the Auger process which cannot be accessed in photoionization/excitation experiments.

A challenging task of performing quantum mechanically complete experiments is molecular photoionization. This is because the anisotropic molecular potential seen by the photoelectron causes an admixture of an unlimited number of outgoing partial waves. This process may be visualized for localized core electrons as partial wave mixing due to the intramolecular scattering of the photoelectron on its way out. This will be demonstrated by investigating the angle resolved molecular Auger emission from CO molecules.

The angle and spin resolved studies of the Auger decay in a combination with detection of the polarization state of the residual ion leads to complete experiments for the Auger decay; i.e. all the complex decay amplitudes can be determined. We will discuss such experiments and present their first results for both resonant and normal Auger processes. Having the validity of a two-step model of the reaction as a necessary prerequisite, the experiments for the Auger decay provide a showcase for complete experiments for so-called *half collision* processes.

Increasing brightness and wavelength tunability of synchrotron radiation sources, including those with variable polarization of the photon beam, allowed to extend considerably the photoionization studies. In combination with angle and spin resolved electron spectroscopy and laser techniques these studies developed to the level of complete photoionization experiment. Chapter 4 is concerned with phenomena related to complete experiments in photoionization. Atomic Auger decay and atomic photoionization have in common the fact that in both cases the process can be completely characterized by a small number of angle-independent partial wave amplitudes. The latter can be extracted from different kind of measurements: observation of angular distributions of photoelectrons from isotropic and polarized targets, spin polarization of photoelectrons, polarization of residual photoions, coincidence between photoelectron and secondary products of the photoionization. The discussion of the above phenomena is preceded by general theoretical introduction on complete experiment for photoionization. Special sections deal with nonresonant two-photon ionization, features of photoionization in the region of resonances and non-dipole effects in atomic photoionization.

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