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Nils Andersen · Klaus Bartschat

Polarization, Alignment, and Orientation in Atomic Collisions

Second Edition

Springer

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Foreword to the Second Edition

The study of polarization effects in atomic collisions physics is almost as old as the field itself. Indeed, the problem of the polarization of light emitted from atoms excited by electrons with kinetic energy just above threshold presented the new quantum mechanics with one of its earliest challenges. The knowledge of absolute total and differential cross sections is crucial for applied problems in which collisional processes play a major role, such as atmospheric and plasma systems, but it is polarization studies that probe collision dynamics in detail. In the case of electron polarization, this is due to the fact that both Pauli and magnetic (spin-orbit) interactions are connected directly with electron spin. Fluorescent photon polarization gives us a snapshot of the final target state—its alignment and orientation—created by the collision.

The topic of polarization effects and multipole descriptions of atomic excitation has had an illustrious history in physics. A series of seminal reviews and monographs are available, but perhaps no one has worked harder to codify the field and generalize and unify the overarching concepts and notational structure than Professors Andersen and Bartschat. This book represents the summary of their extensive efforts. It defines, standardizes, and exposits beautifully the topic of polarization and multipole phenomena in atomic collisions.

The appearance of this second edition is well-timed. While topics such as post-interaction electron vortices and collisions with heavy, open-shell atoms in the "outback" of the periodic table represent exciting new challenges, the field of atomic collisions is essentially mature (due, in large part, to the efforts of the authors!). A broad summary of the field, with a detailed list of up-to-date case studies, is needed now to spur on the next generation of researchers.

At the end of this second edition, the authors point the way to new horizons. For example, while electron impact excitation of light atoms is now essentially a solved problem, the study of electron impact excitation of molecular hydrogen is in its infancy. There will be much new physics arising from studies of polarization effects with molecular targets in the coming century, and this book provides a solid basis for that new effort.

Lincoln, Nebraska, USA

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Foreword to the First Edition

The field covered by this book has been the focus of broad activities over the past decades. Individual researchers, small groups, and centers of excellence (thus or similarly named) contributed to the enormous progress of our knowledge of polarization, alignment, and orientation in atomic collisions.

A comprehensive overview of these developments has been given in a series of reviews published in Physics Reports by groups of researchers headed by the authors of the present monograph. Since these articles give a detailed and (at the time of their publication) complete survey of the field, I was somewhat surprised when I learned that Andersen and Bartschat were preparing a book on almost the same subjects covered by their earlier reviews. I must admit that I was first a little bit skeptical, wondering what the new message of such an enterprise should be. However, when I went through the manuscript of the book it did not take long to convince me that here a new and extremely useful approach has been developed.

In contrast to the aforementioned reviews, it is the purpose of the present publication to give an *introduction* to this area of modern atomic physics. The time of such a project is well chosen since, from the wealth of separate experimental and theoretical results, a coherent picture has been put together in the past decade. It is therefore quite appropriate to speak of a "relatively mature field" as the authors do. This does not mean, however, that its development will soon level off. I rather believe that the field will continuously grow, thereby shifting from simple atomic systems to molecular and even more complex systems.

A requirement for this growth is, of course, that a number of bright researchers can be enthused for such topics, a task which the present monograph is perfectly suitable to fulfill. Its concept differs from the technical reviews written so far that strive for completeness while giving a well-structured compilation and careful analysis of the existing data, thus aiming at the researcher already familiar with the field. But for the curious scientist trying to get an idea of the matter, the material accumulated there may be overwhelming, if not discouraging. The much more compact form of the present introduction is, however, appropriate for becoming, in a reasonable time, familiar with the basic concepts as well as with the latest developments. A feature of the book adding much to its appeal is the links between a variety of processes that seem to be unconnected, since a general framework was established that allows for a superior treatment of different phenomena.

Owing to the wide scope of the field, the authors are frequently compelled to present and comment on the facts without being able to give detailed derivations such as those found in textbooks. The reader who wants to get deeper insight into one topic or the other has to resort to other sources. This turns out not to be a problem since the authors assist by providing plenty of references not only to the primary literature, but also to introductory books.

Working through the book, the reader soon will notice a few features that give the subject its particular flavor. First of all, it is a fine blend of experimental and theoretical work without rigid borderlines between these two sections of physics. The principal reason for this is that most of the research has been done in coordination between experimentalists and theorists, where the partners of the two sections defined and solved tasks for each other. Personally, I found this to be the most rewarding aspect when working in this field. As a result of this close cooperation, intuitive models were developed so that the reader does not have to put up with results in the form of abstract parameters that cannot be easily visualized. In fact, the "charge cloud movies" provided on the accompanying CD present a delightful example of such a visualization, having become possible through recent advances in data and image processing.

A special feature of the book is that it really goes back to the roots. Part III gives a selection of fundamental papers published between 1925 and 1976 that were crucial for the development of the field. I welcome this idea very much and not only because it is often necessary for gaining a proper perspective to go back to the primary sources. One also gets an impression on how the style of publications has changed over the years. Finding that in this respect the early papers compare favorably with most modern ones, one might be encouraged to return to the old standards. Besides, as a consequence of the information explosion, easy access to early literature is no longer granted in most libraries.

Needless to say, the monograph benefits considerably from the fact that the authors have participated actively in the field over the years with a great amount of fundamental and instrumental contributions. This, together with the effort they had to go through in writing their comprehensive reviews, enabled them to give a complete picture of polarization, alignment, and orientation in atomic collisions. Graduate students and researchers will derive abundant profit from it when studying this subject of central importance.

Münster, Germany Joachim Kessler

Preface to the Second Edition

Since the first edition of this book, a number of significant developments took place regarding both the experimental studies of polarization, alignment, and orientation phenomena and the theoretical treatment, especially concerning numerical calculations. Even though we are not aiming for a comprehensive review, it seemed appropriate to prepare a second edition of this book in order to highlight some of these developments.

Rather than changing much of the original text (except for fixing a few minor printing mistakes), we decided to provide updates via additional (sub)sections throughout the book. The most significant change is the splitting of what used to be Chap. 11, *Related Topics and Applications*. Photo-driven processes now have their own chapter, since this field almost exploded with the rapid development of new-generation light sources such as free-electron lasers. Furthermore, we added experimental developments such as the magnetic angle changer and the reaction microscope, as well as new experimental benchmark data that were obtained with these improved detection techniques. Regarding the numerical treatment, much progress has been made in developing convergent close-coupling techniques, either formulated in momentum space (CCC) or in coordinate space using the R-matrix with pseudo-states (RMPS) approach. Furthermore, rapid advances in computational resources (hardware and software) have made explicitly time-dependent formulations a competitive technique even in some steady-state arrangements. They are, of course, necessary to describe short-pulse intense laser-matter interactions.

Note that there are three other books in this Springer Series that deal with topics also covered in the present book, namely:

1. *Plasma Polarization Spectroscopy* by T. Fujimoto and A. Iwamae (2008);
2. *Angle and Spin Resolved Auger Emission* by B. Lohmann (2009);
3. *Perfect/Complete Scattering Experiments* by H. Kleinpoppen, A.N. Grum-Grzhimailo, and B. Lohmann (2009).

We have tried to minimize the overlap with the above books and essentially referred to the first two in our short subsections on Auger electrons and plasma polarization spectroscopy. Regarding perfect/complete experiments, especially for electron collisions, our treatment is more extensive, especially regarding the “natural” coordinate system, detailed cases studies, and the numerous examples presented in Part II of the book.

Finally, instead of providing a CD with supplemental material as in the first edition, the charge cloud movies and historical papers are now made available through electronic depositories at 10.1007/978-3-319-55216-3_7, 10.1007/978-3-319-55216-3_8, 10.1007/978-3-319-55216-3_10, and 10.1007/978-3-319-55216-3_13.

Copenhagen, Denmark Nils Andersen
Des Moines, USA Klaus Bartschat

Preface to the First Edition

Since the early work of Étienne Malus, polarization studies have played an increasingly important role in science as a tool for understanding natural phenomena. In the field of atomic collision physics, the polarization of photons and electrons emerging from the collision zone is in many cases intimately related to the dynamical evolution of the collision complex. Therefore, a quantitative understanding of the origin of the observed polarization and the development of appropriate concepts for describing the emission process have been a central goal of theoretical and experimental studies since the early days of collision studies in the 1920s. The idea of a "perfect" or "complete scattering experiment" introduced in the late 1960s, as well as the concept of "alignment" and "orientation," was of crucial importance for the further advancement of the field. The latter allowed for a proper disentanglement of dynamical and geometrical features and aimed at describing the shape of the collisionally excited atomic electron cloud and its intrinsic currents.

Since then, systematic and coordinated theoretical and experimental investigations have gradually led to a very satisfactory situation concerning the understanding and accurate description of many fundamental electronic and atomic collision processes in Nature. Thus, at the end of the 1990s, atomic collision theory has developed into a mature state in which collision-induced polarization phenomena for a few benchmark systems have been measured and predicted with an unprecedented accuracy and degree of detail over a wide range of impact energies. At the same time, these studies often reveal a very detailed and direct picture of the collision dynamics. Hence, the experimental methods, the general framework, and the numerical approaches have now been developed to a level that provides an excellent starting point for the study of even more complex collision problems. Apart from being of high intrinsic interest for the community of atomic physicists, this gain in understanding is also expected to be useful for applications in neighboring fields of science, such as surface, solid state, and nuclear physics, astronomy, and the physics of lasers, plasmas, and planetary atmospheres.

Based upon current knowledge, the present book aims at introducing the non-expert reader into this field without having to go through the individual papers or the comprehensive, technical reviews in the literature. With this in mind, Part I of the book describes polarized light (Chap. 2) and polarized electrons (Chap. 3), experimental and theoretical methods for scattering studies (Chap. 4), the density matrix formalism as a convenient tool for the theory of measurement (Chap. 5), and basic numerical methods (Chap. 6) that are widely used in calculations supporting ongoing experiments. This part of the book is aimed primarily toward graduate students in physics and has been used as a basis for graduate courses in atomic physics. Therefore, some chapters are supplemented with suggested problems.

Part II presents in a systematic way a series of case studies selected with the aim of illustrating applications of the framework developed in Part I to fundamental atomic collision processes for electronic (Chap. 7) and heavy-particle (Chap. 8) impact. No attempt is being made toward a complete coverage, but rather to "tell a story" concentrating on a few benchmark systems. Chapters 9 and 10 on propensity rules and particle-impact ionization, respectively, address further topics of intense current research. These sections, together with Chap. 11 on selected applications of polarization studies in other areas of physics, indicate the potential of the formalism and its expected impact on future research. Hence, in addition to the graduate student reader mentioned above, this part is intended for active researchers in atomic collision physics who would like to place their own work in a broader perspective and to researchers in neighboring fields who want to evaluate the potential of applying polarization studies in their own field.

With the form of presentation chosen for this book, an uninitiated reader may be carried to the frontier of the field in a short time and with a relatively modest effort. On the other hand, the approach hides the long, fascinating, and sometimes tortuous development which, with numerous detours, has led to the present situation. Furthermore, it does not always give sufficient credit to the early pioneers on whose joint efforts this presentation rests. In particular, it hides the interesting and often very educational paths along which the critical concepts were developed. In an attempt to remedy this situation, we have selected for Part III some of the early, pathbreaking publications in this field from the period 1925–1975. Due to space limitations, a few sections from the longer papers have been omitted, and sometimes, short initial notes of the research results have been chosen instead of the longer follow-up publications that give more results and sometimes important details. Consequently, the book is accompanied by a CD-ROM that contains all the papers of Part III, as well as a few related publications. We have used these papers successfully as reading material in graduate student courses to give a flavor of what really happened when the principal ideas were born. Furthermore, the CD-ROM contains movies of theoretically predicted electron charge clouds and currents for some of the cases discussed in Part II.

Many people have helped us during the preparation of this book. We are particularly indebted to Gordon Drake for suggesting the book project as a follow-up to our contributions to the "Handbook on Atomic, Molecular, and Optical Physcis" and to Maria Taylor and Jenny Wolkowicki for administering the project with Springer-Verlag, to, Bill Baylis, Albert Crowe, Friedrich Hanne, Joachim Kessler, Mette Machholm, Bill McConkey, Andy Mikosza, Jim Williams, Dehong Yu, and

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Copenhagen, Denmark — Nils Andersen
Des Moines, USA — Klaus Bartschat

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We thank Gordon Drake, Karin Louzada, Tom Spicer, and Sam Harrison from Springer for their encouragement to prepare this second edition and all our colleagues for their willingness to provide the material that we requested and the permission to use it.

Finally, we thank our families, in particular Jette, Teresa, Camilla, Nick, and Erika, for their patience with us while we worked on this book.

Contents

Notation

Vectors Vectors will be indicated by boldface italic symbols $\boldsymbol{r}$.

Matrices Matrices and operators will be indicated by boldface roman symbols $\mathbf{T}$.

Quantum numbers such as the orbital, spin, and total electronic angular momenta; the nuclear spin; and the total angular momentum will be indicated by italic and script symbols, e.g., ℓ, L, s, S, j, J, I, F.

To label standard abbreviations for angular momenta of atomic states, we use roman characters, i.e., S for $L = 0$, P for $L = 1$, D for $L = 2$, and F for $L = 3$.

There are many occasions in this book, where the term “velocity” is used instead of “speed,” i.e., the scalar magnitude of the vector velocity. Since this is the common nomenclature in the field, we decided to conform with it.