This is an introduction to the field of many-body atomic physics suitable for researchers and graduate students. Drawing from three major subject areas, atomic structure, atomic photoionization, and electron-atom collisions, this book begins with an introduction to many-body diagrams, and continues with several chapters devoted to each subject area written by leading theorists in that field. Topics in atomic structure include the relativistic theory for highly charged atomic ions and calculations of parity nonconservation. Topics in atomic photoionization include single and double photoionization processes, and photoelectron angular distributions. Topics in electron-atom collisions include the theory of electron impact ionization, perturbation series methods, target dependence of the triply differential cross section, Thomas processes, *R*-matrix theory, close coupling and distorted-wave theory. This volume has been prepared by leading atomic physicists as a tribute to Hugh Kelly, one of the pioneers of many-body theory.

Many-body atomic physics

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Lectures on the application of many-body theory to atomic physics

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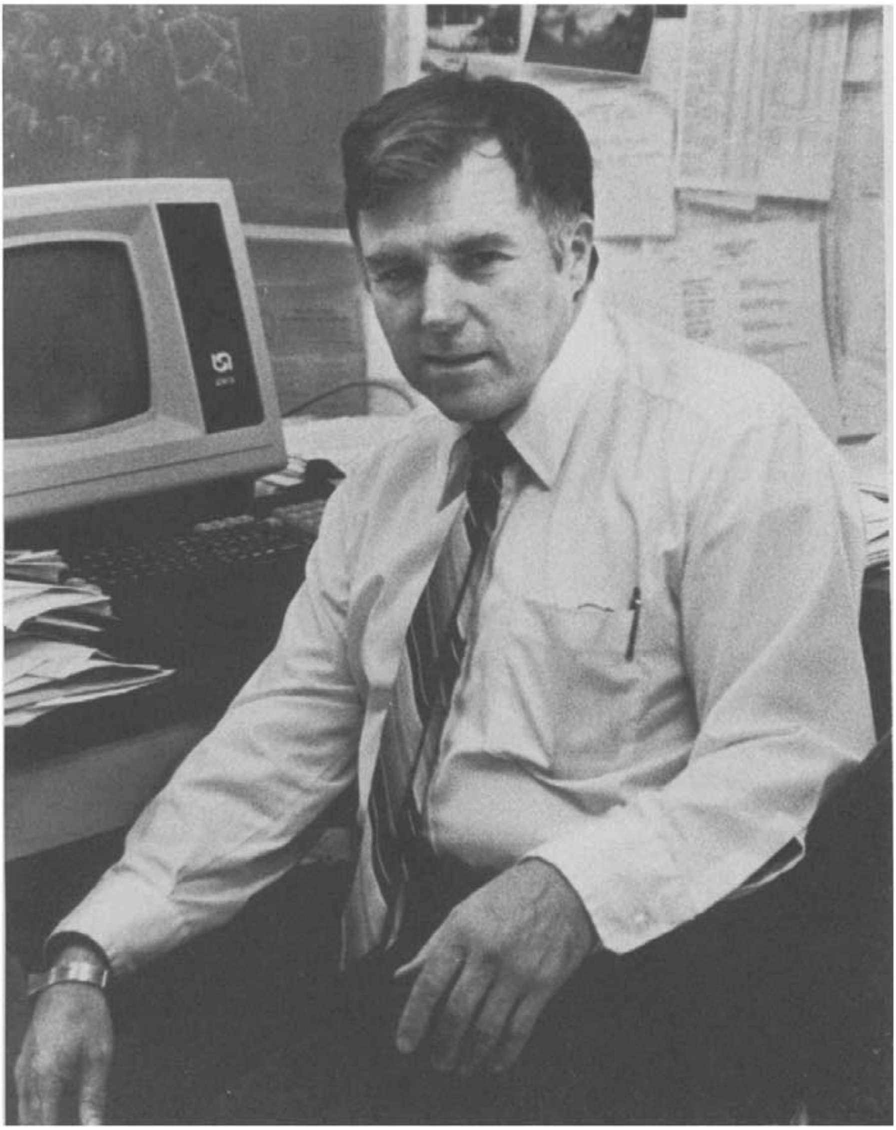

Hugh Kelly in his office at the University of Virginia Physics Department. Photograph courtesy of *Inside UVA*.

Foreword

Hugh Padraic Kelly died on June 29, 1992 after a brave and lengthy struggle against cancer.

Hugh was a graduate of Harvard University, receiving an AB degree in 1953. He continued on to UCLA where he was awarded an M.Sc. degree in 1954. He served in the Marine Corps for three years before returning to graduate school at Berkeley. He worked there with Kenneth Watson, receiving his Ph.D. degree in 1963 and proceeding on to a postdoctoral fellowship with Keith Brueckner at the University of California, San Diego, where he began his seminal work on many-body theory. He was appointed to the faculty of the University of Virginia in 1965. He was a distinguished administrator, serving the University as Chairman of the Department of Physics, as Dean of the Faculty and as Provost.

Hugh was a very special person. He was from his first research paper the leader in the application of many-body perturbation theory in atomic and molecular physics using diagrammatic techniques. He was renowned internationally not only for his brilliant researches but also for his extraordinary personal qualities. He was modest, unassuming, always supportive of others. He had an abundance of creative ideas, which he freely shared. Hugh was the least competitive of people. He saw science as a joint enterprise in which he participated with his friends and students. For all that he was a major figure in scientific research and high level university administration, it is for his warmth and friendship and enthusiasm he will be remembered most.

Hugh was deeply involved in the education of graduate students. This book would have pleased him. Written by his friends and collaborators, it is intended to introduce the application of many-body theory to the new generation that comes after him.

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Preface

Hugh Padraic Kelly is generally recognized by the scientific community as a pioneer in the application of diagrammatic many-body perturbation theory to problems in atomic physics. His work began in the late 1950's and early 1960's with the study of correlation energies in light atoms. From that time, with numerous colleagues and students, he led the development of many-body methods for the treatment of a wide variety of problems in atomic structure, photoionization of atoms, and electron-scattering from atoms. On April 15-17, 1993, some of the leading atomic theorists in the world attended a workshop at the Institute for Theoretical Atomic and Molecular physics at the Harvard-Smithsonian Center for Astrophysics in order to review the application of many-body theory to atomic physics in memory of Hugh Kelly. The organizers of the workshop took advantage of this setting in order to ask the participants to contribute chapters for a textbook on theoretical many-body atomic physics – one that would promote the field to prospective students, as well as would pay tribute to the memory of the field's pioneer. This book is the result of that effort.

This book can be used as a supplement to seminar courses in atomic physics, many-body physics, or quantum chemistry. Each chapter is self-contained and there are cross references between the chapters. Where possible, consistent notation is used in the the various chapters and a key to this notation is included in the Appendix.

There are three main topics with a total of fifteen chapters. The first topic is Atomic Structure and includes chapters 1 through 3. In chapter 1, Ingvar Lindgren surveys the development of atomic many-body perturbation theory from its origin in nuclear physics showing the early role played by Hugh Kelly. Later developments, such as relativistic many-body perturbation theory, calculations performed within the framework of quantum electrodynamics, and coupled-cluster techniques are considered as well. Chapter 1 also includes a review of the mathematical fundamentals of many-body perturbation theory and the construction of many-body diagrams. In chapter 2, Walter Johnson provides a more detailed account of relativistic many-body perturbation theory, and of the use of finite element methods. He applies diagrammatic perturbation theory to the calculation of the energy levels of copper-like atomic ions in order to test our understanding of strong-field quantum electrodynamics. In chapter 3, Steven Blundell, Walter Johnson, and Jonathan Sapirstein review the application of relativistic many-body perturbation theory to the calculation of electroweak neutral current interactions in atoms. With further theoretical and experimental advances, parity non-conservation effects in atoms are likely to provide one of the most precise tests of the standard model of particle physics.

The second topic in the book is atomic photoionization and includes chapters 4 through 7. In chapter 4, James Boyle and Mickey Kutzner review the application of many-body perturbation theory to single photoionization processes in atoms. The emphasis in this chapter is on the evaluation of low-order many-body diagrams, as well as a short review of all-order techniques. Examples drawn from calculations performed on platinum, barium, xenon, and tungsten are provided. In chapter 5, Tu-Nan Chang presents a B-spline based configuration interaction method for the calculation of photoionization processes in two-electron and divalent atoms. This method has proven successful for the calculation of doubly-excited resonance profiles. In chapter 6, Zuwei Liu reviews the application of many-body perturbation theory to the calculation of direct double photoionization processes in atoms. In contrast to single photoionization, the process of double photoionization cannot occur without electron correlation. The focus of this chapter is on those cases where many-body perturbation theory has been applied successfully. In chapter 7, Steven Manson presents an overview of the theory of atomic photoelectron angular distributions. The separation of the angular momentum geometry and the dynamics is highlighted. Examples that illustrate the phenomenology and the physics to be learned from angular distributions are presented.

The third topic in the book is atomic scattering and includes chapters 8 through 15. This topic begins with a subheading of general considerations and includes chapters 8 and 9. In chapter 8, Myron Amusia reviews the application of many-body perturbation theory to electron–atom collisions. A variety of atomic processes are considered, including elastic and resonance scattering, the formation of negative ions, collisions with open-shell and excited atoms, and inelastic electron–atom scattering. In chapter 9, Philip Altick reviews the theoretical aspects of electron impact ionization at high and intermediate energies. The emphasis in this chapter is on the theoretical attempts to model the measured triply differential cross sections, which, minus the spin polarization, provide a complete description of the ionization process.

The next subheading in the topic of atomic scattering is low-order applications and includes chapters 10 through 12. In chapter 10, Don Madison applies Born series methods to the theory of electron impact excitation of atoms. Typical results of first and second order perturbation theory calculations for electron–alkali atom differential scattering are presented. In chapter 11, Cheng Pan and Anthony Starace review the application of many-body perturbation theory to the calculation of electron–atom triply differential cross sections at low energies. The near-threshold energy and angular dependence of two electrons escaping from a positive ion remains a difficult problem in atomic collision physics. In chapter 12, James McGuire, Jack Straton, and Takeshi Ishihara apply Born series methods to the theory of ion–atom charge and mass transfer collisions. The second Born term is found to be the largest Born term at high velocity and corresponds to the simplest allowed classical process — the Thomas process.

The final subheading in the topic of atomic scattering is all-order applications and includes chapters 13 through 15. In chapter 13, Philip Burke presents a summary of the basic *R*-matrix theory of atomic and molecular processes. Applications of the theory are made to low-energy electron scattering by iron ions, electron scattering by atoms and ions at intermediate energies, and multiphoton processes. In chapter 14, Wasantha Wijesundera, Ian Grant and Patrick Norrington provide a brief overview of the Dirac equation *R*-matrix theory for electron–atom collisions. Examples of calculations performed for the resonance structure and cross sections of electron-impact excitations of mercury, lead, and cesium are presented. In chapter 15, Donald Griffin and Michael Pindzola review the close-coupling and distorted-wave theories for the electron-impact excitation and ionization of atomic ions. It is demonstrated that independent-processes calculations have certain advantages for highly ionized species.

The contributors to this book gratefully acknowledge the support of the National Science Foundation of the USA and the Smithsonian Institution for their sponsorship of the workshop held on April 15-17, 1993 in Cambridge Massachusetts. As the organizers of the workshop, we would also like to extend our thanks to the contributors, who, in many cases, made considerable sacrifice in order to participate in the workshop and in this book. We would also like to thank Tom Gorczyca for editorial assistance in the atomic scattering section of the book. Finally, we would like to thank the Directors of the Institute for Theoretical Atomic and Molecular Physics at the Harvard-Smithsonian Center for Astrophysics for their support of this project. These include Alex Dalgarno, Eric Heller, Kate Kirby, and George Victor. Without their support, as well

as the atmosphere provided by the Institute, this project would not have been possible.

As a group, we donate all royalties from the sale of this book to the Hugh P. Kelly Fellowship Fund at the University of Virginia, established in order to support education in theoretical physics.

James J. Boyle
Michael S. Pindzola

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Wasantha Wijesundera, Ian Grant, and Patrick Norrington, the authors of Chapter 14, Electron scattering from atomic targets: application of Dirac *R*-matrix theory, thank Farid Parpia for helpful discussions. All computation for the results presented in Chapter 14 was carried out on the Oxford University Computing Services VAX 8700/8800 cluster, the Rutherford Appleton Laboratory Computer Centre Cray X-MP/416 facility and the University of London Computer Centre Cray X-MP/28 facility. Wasantha Wijesundera was supported by an SERC research grant.

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