Many-body Theory of Atomic Structure and Photoionization

This page is intentionally left blank

Many-body Theory of Atomic Structure and Photoionization

Editor

T.-N. Chang

Univ. of Southern California

World Scientific

Singapore • New Jersey • London • Hong Kong

Published by

World Scientific Publishing Co. Pte. Ltd.

P O Box 128, Farrer Road, Singapore 9128

USA office: Suite 1B, 1060 Main Street, River Edge, NJ 07661

UK office: 73 Lynton Mead, Totteridge, London N20 8DH

MANY-BODY THEORY OF ATOMIC STRUCTURE AND PHOTOIONIZATION

Copyright © 1993 by World Scientific Publishing Co. Pte. Ltd.

All rights reserved. This book, or parts thereof, may not be reproduced in any form or by any means, electronic or mechanical, including photocopying, recording or any information storage and retrieval system now known or to be invented, without written permission from the Publisher.

For photocopying of articles in this volume, please pay a copying fee through the Copyright Clearance Centre, Inc., 27 Congress Street, Salem, MA 01970, USA.

ISBN 981-02-0876-6

981-02-0877-4 (pbk)

Printed in Singapore.

Dedicated to the memory of
Hugh P. Kelly and Robert T. Poe

This page is intentionally left blank

PREFACE

Recent rapid advancement of experimental techniques, such as the laser cooling and ion trap, together with the increasing availability of high-resolution intense light sources, including high power laser and dedicated synchrotron radiation with extended wavelength, have opened up the possibility for a more detailed quantitative study of the many-body interactions in complex atoms. At the same time, the calculational difficulties experienced earlier by many theoretical approaches, due to the computational limitation, have been reduced substantially by the application of a fast growing new-generation of high power computers. Physical interpretations of atomic processes dominated by complex many-body effects, which were intractable in the past, can now be identified and demonstrated systematically.

This book is targeted at advanced graduate students and scientists who would like to become familiar with the recent theoretical and experimental progress in this fast developing research subject. I have put together a collection of detailed review chapters on many of the recent advances in the many-body theory of atomic structure by leading theorists on their respective specialized approaches. Emphasis is given to the photoionization dominated by the resonance structures, which reveals the effect of the multi-electron interactions in atomic transitions involving highly correlated atomic systems. Recent experimental advancements, including applications of intense lasers and synchrotron radiation, both separately and jointly, are also reviewed by leading experimentalists.

The first two chapters of this volume summarize the recent development and applications of the nonrelativistic and relativistic Many-Body Perturbation Theory in atomic systems. Chapter three presents a comprehensive review of the R-matrix theory of atomic and molecular processes. Chapter four details a high-precision configuration-interaction method for smaller atoms. Chapter five reviews the recent applications of hyperspherical coordinate method to single- and multiphoton processes in two-electron atoms. The next three chapters represent a collection of reviews on the recent advances using L^2 basis functions methods. Chapter nine illustrates the role of many-electron effects on Auger transitions in terms of a few specific examples. The last three chapters summarize the recent experimental progress. Specifically, Chapter ten discusses the multiple excitation in photoionization of outer valence shell at energy below the ionization threshold of the inner shell electron. Chapter eleven presents a comprehensive review of atomic structure effects in multi-

photon processes induced by laser excitation. Finally, in Chapter twelve, the many-body interactions in photoionization of excited atoms and ions are examined by a combined application of synchrotron radiation and intense laser.

Not included in the present volume are a few important theoretical approaches, which have been examined extensively elsewhere. The successful earlier applications of the **Random-Phase Approximation** approach by **M. Ya. Amusia** and his co-workers in the 70's, have been reviewed in a recent book *Atomic Photoeffect*. Other earlier successful efforts include works based on the **Relativistic Random-Phase Approximation** approach by **W. R. Johnson** and his co-workers in the late 70's and early 80's. Substantial progress in many-body theory has been made more recently by **I. Lindgren** and his co-workers on the **Coupled-Cluster** approach. Highly successful applications to complex atoms have also been carried out with the combined **Quantum Defect and Eigenchannel R-matrix Method** by **C. H. Greene**, **M. Aymar** and their co-workers.

I would like to dedicate this volume to **Hugh P. Kelly** and **Robert T. Poe**, who started in the same research laboratory at Berkeley and pioneered the applications of the Brueckner-Goldstone theory to atomic systems in the late 60's and early 70's. Their efforts have led to numerous successful applications of the Many-Body Perturbation Theory to physical processes in atomic systems. Hugh Kelly, with his genuine enthusiasm to basic research, has inspired a generation of atomic physicists, including myself. His insistence to complete the first chapter of this volume a few days before passing away is a moving testimony of his love and dedication to atomic physics. Bob Poe, in addition to his early contributions to atomic theory and high-energy experiment, is also remembered by many of us of his warmth and personal dedication to the development of sciences and technology in Taiwan. His vision and effort, before his untimely death in 1984, have led to the establishment of the Institute of Atomic and Molecular Sciences at the Academia Sinica in Taiwan and the recent completion of the synchrotron radiation facility, also in Taiwan. Both Hugh and Bob are greatly missed by all of us.

I am grateful for the cooperation and patience of friends and colleagues who have contributed to this volume. I would like to thank Dr. Z. W. Liu for his help in completing the final typing of Chapter one. I would also like to acknowledge the support of the editors and staff of World Scientific.

Tu-nan Chang
Los Angeles
Summer 1993

CONTENTS

Dedication		v
Preface		vii
Chapter 1	Recent Many-Body Perturbation Calculations of Photoionization Cross Sections <i>Hugh P. Kelly</i>	1
Chapter 2	Relativistic Many-Body Theory Applied to Highly-Charged Ions <i>Walter R. Johnson</i>	19
Chapter 3	R-Matrix Theory of Atomic and Molecular Processes <i>Philip G. Burke</i>	47
Chapter 4	Precision Configuration-Interaction Calculation for Atomic Systems with a $1s^2$ -Core <i>Kwong T. Chung</i>	83
Chapter 5	Hyperspherical Coordinate Description of Single- and Multiphoton Processes in Two-Electron Systems <i>Anthony F. Starace</i>	107
Chapter 6	Non-variational Multiconfiguration Hartree-Fock Calculations for Continuum Wave Functions <i>Charlotte Froese Fischer</i>	143
Chapter 7	L^2 Basis Function Methods for the Electronic Continuum. Photoionization and Some Related Processes <i>V. Carravetta, P. Spizzo and Roberto Moccia</i>	175
Chapter 8	B-Spline Based Configuration-Interaction Approach for Photoionization of Two-Electron and Divalent Atoms <i>Tu-nan Chang</i>	213
Chapter 9	Many-Electron Effects on Auger Transitions <i>Mau Hsiung Chen</i>	249
Chapter 10	Multiple Excitation Processes in Photoionization <i>James A. R. Samson</i>	271
Chapter 11	Atomic Structure Effects in Multiphoton Processes: An Experimental Perspective <i>Louis F. DiMauro</i>	297
Chapter 12	Many-Body Interactions in Photoionization of Excited Atoms and Ions <i>François J. Wuilleumier</i>	349