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# Electron Momentum Spectroscopy

Erich Weigold
*The Australian National University*
*Canberra, Australia*

and

Ian E. McCarthy
*Flinders University of South Australia*
*Adelaide, Australia*

Springer Science+Business Media, LLC

Library of Congress Cataloging-in-Publication Data

Weigold, Erich.
Electron momentum spectroscopy / Erich Weigold and Ian E. McCarthy.
p. cm. -- (Physics of atoms and molecules)
Includes bibliographical references and index.

1. Electron spectroscopy. I. McCarthy, I. E. (Ian Ellery), 1930- II. Title. III. Series.

QC454.E4 W45 1999
539'.1'0287--dc21

99-047695

ISBN 978-1-4613-7164-9 ISBN 978-1-4615-4779-2 (eBook)
DOI 10.1007/978-1-4615-4779-2


Originally published by Kluwer Academic / Plenum Publishers in 1999
Softcover reprint of the hardcover 1st edition 1999

10 9 8 7 6 5 4 3 2 1

A C.I.P. record for this book is available from the Library of Congress.

# Preface

Electron momentum spectroscopy (EMS), or (e,2e) spectroscopy, is a powerful tool for investigating the electronic structure of matter. It can be considered as a microscope that reveals how the electrons move rather than where they are. Of course, we know from quantum mechanics that the two pictures, the one for momentum and the one for position in space, are completely equivalent. The advantage of the momentum space microscope is that the macroscopic energies and momenta of the probes involved (electrons) are quite close to the atomic counterparts, ensuring good resolution in the measurements. Another advantage of the momentum space microscope is that it automatically involves the measurement of energies or energy differences in the samples being studied, a feat that is very difficult to achieve in ordinary microscopes. Thus, it is also a spectroscopy.

Given the continuing expansion in the range of applications of the technique to the study of the electronic structure of atoms, molecules, and solids, as well as recent major advances in experimental techniques, it seemed to us an appropriate time to write a book that would serve as a comprehensive introduction to the technique, covering both theory and experiment. With the development of multiparameter detection techniques, polarized and monochromated electron sources, aligned and oriented targets, experimental techniques have made enormous advances in recent years. This is particularly so in its application to the study of the structure of condensed matter samples, including single-crystal, polycrystalline, and amorphous samples. The experimental problems peculiar to condensed matter targets, resulting from their high electron density, are discussed in some detail. Even though enormous technical strides have been made, further significant developments are under way. We have attempted to give experimentalists sufficient detail to enable the motivated reader to design and set up a suitable EMS spectrometer and to carry out significant experiments.

The theory of EMS is developed fully. Although it is a difficult problem to calculate the differential cross section for an arbitrary electron impact ionization process, a kinematic region can be identified in which cross sections in agreement with accurate measurements can be calculated with quite simple reaction theory. This is the EMS region of the (e,2e) reaction, and the cross section, as a function of ion recoil momentum and electron separation energy, depends very sensitively on the orbitals and on electron correlations in the target and residual-ion systems. The reaction theory is developed fully for the cases of atomic, molecular, and solid targets. The differential cross section depends directly on the electronic structure amplitude, which is simply the quasiparticle or Dyson orbital or the one-electron momentum-space overlap between the initial target state and the energy selected final ion state. The role of electron correlations in the target and/or ion states on the EMS cross section is fully explored.

Because EMS measures properties of the electronic structure of matter we give an outline of structure theory and recent developments in quantum chemistry treatments of the many-electron problem. This encompasses a discussion of molecular-orbital symmetry, independent-particle models, self-consistent-field orbitals, density-functional theory, other many-body techniques, and electron band theory of a crystal. We also describe how normalized Dyson orbitals can be directly derived from EMS measurements.

We then give in separate chapters results for atoms, molecules, and solids. In each case we attempt to draw out the full extent of the structure information that can be derived from EMS measurements, without attempting a complete coverage of the systems that have been studied. We also point out directions for future developments.

Finally, we give a brief comparison with other reactions that also yield information about electronic structure. These also depend on the removal of an electron and include Compton profile and ($\gamma$,e$\gamma$) measurements, electron annihilation of thermalized positrons, photoelectron spectroscopy, and angle-resolved photoelectron spectroscopy. All of these spectroscopies omit at least one of the three quantities (energy, momentum, and the corresponding density) that can be measured by EMS, but they sometimes have advantages such as better energy resolution. Our purpose is to describe what can be measured by each of these spectroscopies, rather than to give a detailed account of any of them.

We would like to acknowledge the help of Michael Brunger, Anatoli Kheifets, and Maarten Vos in providing some of the data and graphics. We are particularly indebted to Marilyn Holloway, for her patience, good humor, and above all for her expertise in typesetting and preparing the graphics.

*Canberra, Australia* Erich Weigold

*Adelaide, Australia* Ian McCarthy

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