## **BOOK REVIEWS**

Selection of books for review is based on the editor's opinions regarding possible reader interest and on the availability of the book to the editor. Occasional selections may include books on topics somewhat peripheral to the subject matter ordinarily considered acceptable.





## The Hartree-Fock Method for Atoms

Author Charlotte Froese Fischer

Publisher John Wiley and Sons, Inc., New York (1977)

Pages 308

*Price* \$22.95

Reviewer Jack Simons

This research-level reference book by Charlotte Froese Fischer represents a major contribution to the numerical calculation of Hartree-Fock (HF) wave functions for atomic systems. Froese Fischer's own research efforts have established her as a leading expert in this area of quantum theory. In fact, many of the computational and numerical analysis tools discussed in this book have resulted from her own scientific investigations. It is my opinion that Froese Fischer's experience and knowledge make her an eminently qualified scientist to undertake the task of presenting an up-to-date overview of numerical HF theory.

The first two chapters of this book are devoted to a review of the HF method as well as various further approximations that are currently very widely used (e.g., UHF, RHF, EHF). The derivation of the HF equations, including a clear treatment of the Lagrange multipliers, is combined with good illustrative numerical results and a discussion of the shapes of the radial wave functions.

Chapters 3 and 4 contain a discussion of several techniques for treating electron correlation in atomic systems. Little attempt is made to cover a wide variety of modern approaches to the correlation problem. Instead, the author emphasizes the perturbation theory approach and the multiconfigurational HF (MCHF) method. The MCHF variational equations are derived, and the results of applying this method to several states of small atoms are clearly discussed. In Chap. 5, Froese Fischer analyzes how one computes atomic expectation values and transition properties at both the HF and correlated levels. As in her earlier treatment of correlation contributions to atomic state energies, the author does not attempt to cover more recent approaches to these problems (e.g., many-body techniques, equations-of-motion theory, or Green's function theory).

In Chaps. 6 and 7, Froese Fischer presents what, in her opinion, represents the optimal numerical methods for use

in HF and MCHF calculations. As in the earlier chapters, the author employs results that have been taken from the literature to illustrate the accuracy and/or limitations of these numerical techniques. Largely through the research efforts of Froese Fischer, the solution procedures for the HF equations outlined in Chap. 6 have become well accepted and widely used within the theoretical chemistry community. Because the MCHF approach to electronic structure investigation is more modern, its numerical methods are not yet as widely known. Hence, it is likely that most researchers in atomic structure theory will derive much benefit from Chap. 7.

In summary, I feel that this book contains an excellent research-level discussion of the numerical approach to HF and MCHF calculations. I believe that scientists whose research is in atomic and molecular physics, theoretical chemistry, or nuclear structure theory should read this book.

Jack Simons (BS, chemistry, Case Institute of Technology, 1967; PhD, chemistry, University of Wisconsin, 1970) has been on the chemistry faculty at the University of Utah since 1971. He is a recognized leader in the application and development of quantum chemical methods to the electronic structure of atoms and molecules. He is especially well known for his pioneering research into the electronic structure of negative molecular ions.

## Traité de Neutronique—Physique et Calcul des Réacteurs Nucléaires

Authors J. Bussac and P. Reuss

Publisher Hermann, Éditeurs des Sciences et des Arts

Pages 662

Price 190 francs

Reviewer H. J. M. Bowen

This volume is, I believe, the first detailed monograph in French describing theories of neutron behavior and their application to nuclear reactors. It is aimed at post-graduate physicists and engineers who wish to understand the methods used to calculate neutron energies, fluxes, and distributions in real and imaginary arrays of fuel elements. It will, therefore, be valuable to all those who are involved in teaching courses on reactor physics, as well as to their students, particularly those from developing countries where French is a second language. The large number of mathematical exercises (without answers) that it provides will help the serious student.

Much of the matter in the first five sections (480 pages) has already been treated in English in the classic monographs by Glasstone and Edlund or Weinberg and Wigner. The mathematical treatment of neutron absorption, diffusion, and thermalization given here is clear and straightforward. The sections concerning applications to homogeneous and heterogeneous reactors incorporate a substantial contribution by such French scientists as A. Amouyal, P. Benoist, and M. Cadilhac that cannot be found in standard texts in English. The last two chapters (130 pages) give an up-to-date summary of French experience with uranium/light water and plutonium/liquid-sodium reactors that I found both original and stimulating.

There are nine mathematical appendixes and a short index; bibliographies are given after each chapter. The book specifically does not cover problems of heat transfer, shielding, and health physics or experimental detection of neutrons. Minor criticisms concern the figures (which are only numbered consecutively by chapter, and whose axes are not always clearly labeled) and the failure to relate all the units quoted to SI (e.g., "pcm" used as units of reactivity). However, jargon terms, such as "pile" for reactor, are not overemphasized, and the style is lucid. All in all, this is a scholarly work that can be recommended.

H. J. M. Bowen is a reader in analytical and radiochemistry at Reading University in England. He is co-author of a book on radioactivation analysis and has written several other books, including one on the chemical applications of radioisotopes.

## **Elements of Nuclear Reactor Design**

Editor Joel Weisman

Publisher Elsevier Scientific Publishing Company (1977)

Pages 466

*Price* \$51.65

Reviewer Roger A. Rydin

To paraphrase the Preface to Elements of Nuclear Reactor Design, "The primary objective of this work is to provide a basic description of the quantitative aspects of nuclear reactor design. An effort has been made to consolidate material scattered throughout the literature and to treat in considerable detail the topics of reactor computations, piping and vessel design practice, fuel element design and reactor safety, which in the past have generally received superficial treatment. The book should be suitable both as a reference and as the sole text for reactor engineering courses."

The announced goals are certainly ambitious. In my opinion they serve as an adequate basis for judging the book. The questions to be answered are:

- 1. Is it a good textbook?
- 2. Is it a good reference book?

Before going into detail, a few statistics are in order. The book consists of 14 fairly distinct chapters averaging 27 pages of text material plus 3 pages of references and problems each. The appendixes contain some mathematical data plus useful physical and thermodynamic data on coolants, fuels, moderators, and cladding materials. Nine different authors contributed to the book.

First, I would like to make a general observation. A reference book and a textbook have somewhat different requirements put upon them. A textbook is supposed to provide a fundamental understanding of a subject starting from basic principles, while a reference work is supposed to summarize the latest high-level design practice. While these two requirements are not inherently incompatible, at a minimum they require extra explanation and coordination of subject matter, i.e., a longer book. I find that the authors of Elements of Nuclear Reactor Design, in a conscious effort to keep chapter lengths in bounds, have opted in the direction of a reference work rather than a textbook. A detailed critique of each chapter follows.

Chapter 1. "Elements of Reactor System Design" by J. Weisman. This is a well-written and informative description of current reactor system designs. The author has wisely refrained from trying to cover every design that has ever been used or conceived of.

Chapter 2. "Reactor Materials" by J. Weisman. The author presents a generally good description of reactor materials and their problems.

Chapter 3. "Thermodynamics of Nuclear Power Systems" by J. Anno. This is a moderately good, logical presentation of thermodynamics as applied to nuclear systems. The author assumes that the reader has had an undergraduate-level course in thermodynamics and is familiar with its basic definitions and vocabulary. He takes an interesting approach to the topic of irreversibility. Unfortunately, some of the problems at the end of the chapter are unrelated to the text.

Chapter 4. "Reactor Physics Computations" by A. Shapiro. This chapter is a quantum jump above the previous chapter in level of difficulty. Here, the author assumes that the reader has had a year of graduate work in reactor theory. While the presentation is reasonable given space limitations, there are a few flaws. Specifically, he does not emphasize that the industry uses two- or three-parameter fits for ultimate generation of most few-group cross sections, and he fails to mention the importance of self-shielding in depletion calculations. His discussion of control rod calculations is archaic. Finally, the problem set is the most difficult set in the book.

Chapter 5. "Nuclear Reactor Shielding" by J. Moteff. This is the longest, and one of the best-written, chapters in the book. It is easy to read, informative, and contains good shielding design suggestions.