

cules and solids. Among the names, taken at random, are Coulson, Longuet-Higgins, Condon, Massey, Hirschfelder, Mulliken, Pauling, the Pullmans, Fröhlich, Van Vleck, Bardeen, Schockley and Löwdin. Subjects range from "Collisions of Slow Positrons with Atoms," through "Charge Transfer Complexes in Biochemistry," and "The Size of an Exciton in a Molecular Crystal," to "Superconductors and Superfluids." The paper by A. C. Wahl on "Pictures of Molecular Orbitals" recalls Slater's paper of 1931 on "Directed Valence in Polyatomic Molecules," which had

many photographs of molecular models. Earl Callen has a short and witty paper on "Quantum A Go Go." H. C. Longuet-Higgins concludes his paper on "Second Quantization in the Electronic Theory of Molecules" with the sentence: "Creation and annihilation operators in molecular quantum mechanics are here to stay," and in his bibliography, the 1929 paper by J. C. Slater has the notation: "The birth certificate of the Slater determinant."

All the contributed papers are at a high level of excellence: They constitute a volume that is not only a tribute to a great man but is also a

substantial landmark in quantum theory. A perusal of these papers reveals the correctness of Leland C. Allen's remark in his paper on "A New Approach to Many-Electron Theory at Intermediate Densities": "There is no question that Slater's influence on the course of science will be even greater during the next 35 years than it has been in the past 35."

* * *

Joseph G. Hoffman is professor of physics and a member of the Center for Theoretical Biology at the State University of New York at Buffalo.

APW calculations for the beginner

AUGMENTED PLANE WAVE METHOD: A GUIDE TO PERFORMING ELECTRONIC STRUCTURE CALCULATIONS. By Terry Loucks. 256 pp. W.A. Benjamin, New York, 1967. Cloth \$10.00, paper \$4.95

by John C. Slater

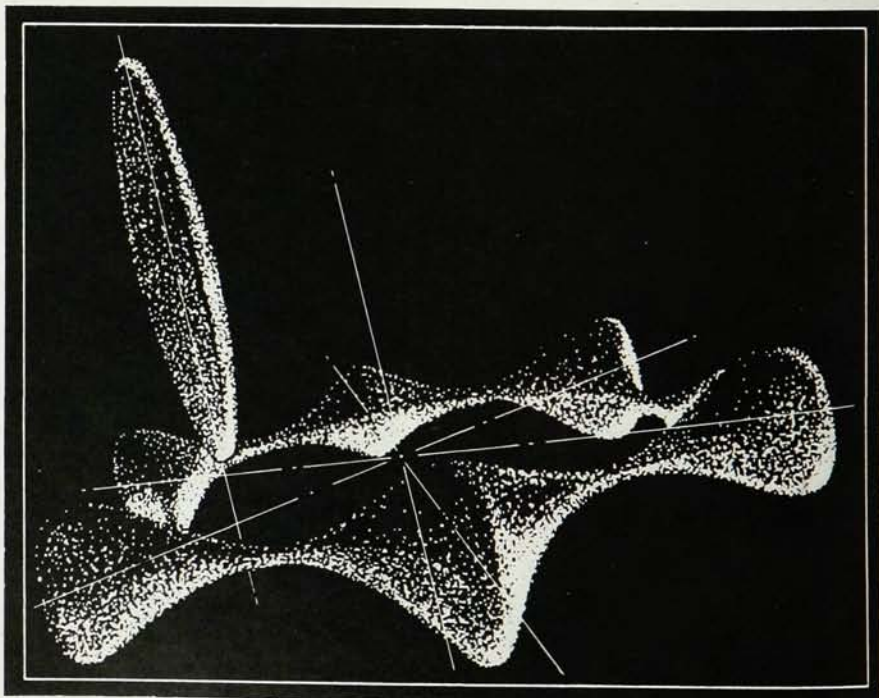
During the last few years, we have seen a great many books on physics in a new format: photo-offset reproductions of lecture notes or other types of rather informal presentations, often supplemented by reproductions of papers fundamental to the field under discussion. This is one of them. There are really three parts to it: the general descriptive text that grew out of a set of lectures given in the summer of 1965 at Iowa State University; a detailed description of computer programs for carrying out the calculations, together with reproduction of the programs; and copies of 17 leading papers dealing with the augmented-plane-wave method. The result is an invaluable compendium of material on the augmented plane-wave method that should be of great use in introducing graduate students and more mature workers to this addition to our repertoire of mathematical approaches to the theory of solids. It forms one of the "Frontiers in Physics" series (David Pines, editor) that has already included a considerable number of very useful books of the same general type. The reviewer agrees with the opinion expressed in the editor's foreword to the series, to the effect that rather informal publication like the present volume forms a

very valuable way of communicating information in a rapidly expanding field.

The augmented-plane-wave method is a device for solving the problem of motion of a single electron in a periodic potential, such as it encounters in a crystal, if an approximation by a self-consistent-field method reduces the many-body problem to a one-electron problem. The reviewer takes a very personal interest in the method, since he introduced it in a paper in the *Physical Review* in 1937, and most of

the development has been by his students and in his research group at MIT. Terry Loucks, the author of this excellent work, is one of the few physicists who did not obtain their training in the MIT group that has taken up the method. This puts him in a particularly strategic position to evaluate the method and its potentialities as a partly outside observer.

In the 100-odd pages of text that form the first part of this work, Loucks first critically compares the various methods now in use for energy-band



calculations: the OPW or orthogonalized-plane-wave method; the closely related pseudopotential method, applied particularly to the NFR or nearly free-electron case; the KKR or Korringa-Kohn-Rostocker method; and the APW or augmented-plane-wave method, most closely related to the KKR method. The OPW and pseudopotential methods have been most useful for the so-called "simple crystals," metals such as sodium, magnesium and aluminum, and semiconductors such as silicon and germanium.

The APW method, on the contrary, is the best one for crystals containing transition elements, and containing heavy atoms. The applications described in this book are to metallic crystals with only one atom in the unit cell, but the method has been applied as well to more complicated elements, and to many compounds. The book contains a good bibliography, and information about all the crystals that have been treated by the method. Too recent for inclusion are some papers, some not yet published, on the application of the method to ferromagnetic and antiferromagnetic crystals. For problems of this latter type, the method and the closely related KKR method are practically required, since they are the only ones capable of handling the transition elements in an *a priori* fashion.

The part of the theory to which Loucks has made the most significant contribution is the adaption of the method to atoms heavy enough to require relativistic treatment. This means at least the latter half of the periodic table. There is a good discussion of all the points connected with setting up the relativistic calculation, a method that remarkably enough is not much more difficult than the nonrelativistic version.

After the textual material, there are nearly 50 pages devoted to details of computer programs for making calculations. This is particularly useful, for the method so far has been used, as was indicated in an earlier paragraph, almost entirely by the students of the reviewer, who got their training at MIT. Loucks worked up his programs by himself, and this volume should help others to do the same. Many workers in other institutions who have been using the pseudopo-

tential and other methods, feeling that they were simpler, might well be inspired by this book to learn the more powerful methods of the APW technique.

Finally, as was mentioned earlier, there are facsimile reproductions of 17 of the leading papers that have so far appeared, dealing either with the techniques of the method or with energy-band calculations made by use of it. These are well chosen and furnish a very valuable supplement to the material presented in the earlier part of the text.

It is only fair to say that this text does not cover all aspects of the APW method. For one thing, the matter of symmetry and of the application of group theory to the study of energy bands in crystals is almost completely omitted. For the very simple crystals under discussion by Loucks, this is not unreasonable; the simplification of the problem that can be brought about by use of group-theoretical methods is not necessary in order to get useful results. But as one goes to more complicated crystals, with many atoms in the unit cell (not treated in this volume), group theory becomes increasingly necessary to bring the problem within the range that can be handled with present computers. It may be appropriate to point out that an extensive review article on the method, now under preparation by L. F. Mattheiss,

J. H. Wood, and A. C. Switendick, will provide a great deal of additional material, and when it is published, it should provide a useful supplement to the present book.

There are advantages, however, in simplicity, and the opinion of the reviewer is that the book of Loucks contains just about the amount of detail that should be found in a text intended to give the reader a first acquaintance with the method.

* * *

John C. Slater is Institute Professor Emeritus at MIT and graduate research professor of physics and chemistry at the University of Florida.

Subtle and eclectic history

THE ROLE OF MATHEMATICS IN THE RISE OF SCIENCE. By Salomon Bochner. 386 pp. Princeton U. Press, Princeton, N. J., 1966. \$9.00

by Eugene P. Wigner

This is not an easy book to read or review. Its purpose is, if we believe its title, to describe the role that mathematics plays in the sciences, and it describes much of this. However, it does much more—it gives a history of mathematics as seen by the author, and this is a delightful history. Almost every page has some subtle observa-

Reviewed in This Issue

- 91 LÖWDIN, ed: Quantum Theory of Atoms, Molecules and the Solid State:
A Tribute to John C. Slater
 - 92 LOUCKS: Augmented Plane Wave Method:
A Guide to Performing Electronic Structure Calculations
 - 93 BOCHNER: The Role of Mathematics in the Rise of Science
 - 95 KARGON: Atomism In England From Hariot to Newton
 - 97 LEDERER, HOLLANDER, PERLMAN: Table of Isotopes
 - 99 DUGDALE: Entropy and Low Temperature Physics
 - 101 MENDELSSOHN: The Quest for Absolute Zero:
The Meaning of Low Temperature Physics
 - 103 GOURDIN: Unitary Symmetries and Their Application to High Energy Physics
 - 103 OREAR: Fundamental Physics
 - 105 CLEGG: High Energy Nuclear Reactions
 - 105 BASS: Elements of Probability Theory
 - 107 WU: Kinetic Equations of Gases and Plasmas
 - 107 FUHS: Instrumentation for High Speed Plasma Flow
-