

John C. Slater and the quantum theory of matter

QUANTUM THEORY OF ATOMS, MOLECULES AND THE SOLID STATE: A Tribute to John C. Slater. Per-Olov Löwdin, ed. 641 pp. Academic Press, New York, 1966. \$25.00

by Joseph G. Hoffman

"There are many areas . . . in which the name of Slater is synonymous with progress in physical understanding." Thus writes Robert S. Mulliken in "John Clarke Slater: His Work and a Bibliography." The 41 technical papers by 69 contributors provide a measure of the stimulus and leadership that Slater gave to quantum mechanics in its beginnings in the late twenties.

His scientific career began in 1924 with the paper on compressibility of alkali halides, his PhD research under Bridgman at Harvard. The period 1928 to 1933 is marked by his unique work in atomic, molecular and metallic structures. A classic paper from this period, "Cohesion in Monovalent Metals" (1930), is reproduced here and commented upon by Per-Olov Löwdin.

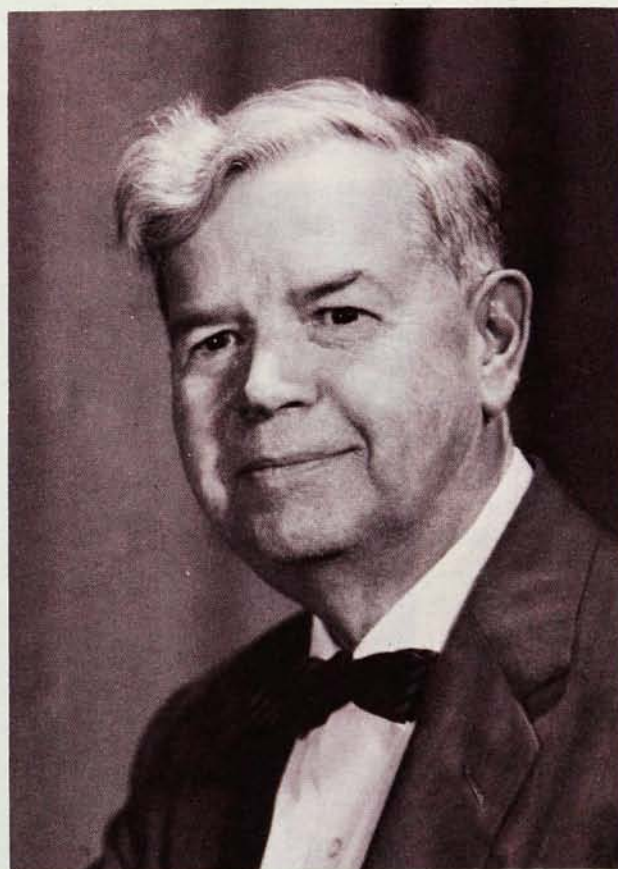
Slater's scientific contributions are all the more remarkable in view of the fact that he was made head of the department of physics at MIT in 1930, and held that position until 1951. He was a successful scientist-administrator. Insight into this aspect of his work is given in the "Biographical Note of Appreciation" by Phillip M. Morse. He writes: "John knew, in detail, what all of us were doing and gave encouragement when needed. Daily teas in the Moore Room served to bring the graduate students and faculty together, and the Slater's small house overlooking the Charles River beyond Lars Anderson Bridge, served as a social center for department members." Much effort was given to planning and teaching undergraduate courses while at the same time his own research, and that of graduate students, developed the new quantum theory. By the end

of 1933 he had set forth lasting concepts in quantum theory among which were the Slater determinant, the Slater-type orbitals, and the directed valence in polyatomic molecules. In the following 6 years he was active in the development of the modern theory of the solid state. World War II interrupted this work. In 1939 he took up war work on microwaves. His principles of design of the magnetron won him the Presidential Certificate of Merit.

Slater's persistent search for theoretical explanations of our empirical knowledge of the properties of matter led to a remarkable series of pioneering ideas. Well over 100 papers and 11 books are the record of his creative explorations such as: the quantum-

mechanical virial and the Slater augmented-plane-wave method (APW) for calculating energy bands in solids; the concept of damped electron waves in solids; the extension of Bloch's band theory of ferromagnetism and its relation to the band theory of solids; the explanation of abnormal diamagnetic effects in superconducting solids by means of spin-wave theory. As the editor's preface points out: Slater's "achievements" are so fundamental and numerous that there is hardly any area of the quantum theory of matter that is not basically influenced by his work."

An impressive series of papers on a wide variety of topics in this volume are contributed by the leaders in quantum-mechanical theory of mole-



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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."

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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

