Solid state and orbital theories

Solid State and Molecular Theory: A Scientific Biography. By John C. Slater. Pp. 357. (Wiley-Interscience: New York and London, March 1975.) £10.25.

JOHN SLATER started research in 1923 and was from the first concerned with atomic, molecular and solid state theory. Nobody could be better qualified to tell the story of the development of these subjects, and this Slater has done in a very personal way.

Of the days before quantum mechanics there are some curious sidelights. On a visit to the Cavendish and Copenhagen he became convinced of the existence of photons, but found that Bohr refused to consider the idea and dissuaded him from publishing—and that still rankles. Then came 1925 and 1926 and the startlingly sudden formulation of quantum and wave mechanics, which Slater describes. Of this period Slater says there seemed to be among theoretical physicists two types: one prosaic, matter of fact and willing to indicate the argument behind what he did; the other like a magician, waving his hands as if he were drawing a rabbit out of a hat. Though admiring—who could not?—the achievements of some of the latter, Slater puts himself in the former category. I would agree, and it is in thorough and detailed work on solids and molecules, a description of which forms the main part of the book, that he has made his greatest contributions. Particularly charming is his account of the early days of many-electron wave functions, when Wigner, Hund and others entered the field with their *"Gruppenpest"*, the pest of group theory, as disgruntled people who had never studied the subject in school described it. By his introduction of the "Slater determinant" he provoked the remark that "Slater has slain the *Gruppenpest*"—and, as he says, his paper was universally popular.

The account of the application of advanced computers to problems of molecular wave functions occupies the last part of the book. Slater has been involved with this for the last 10 years since he retired from MIT. As he points out, this kind of work had to await the development of the computer, and could not have been done earlier. In this Slater is clearly in his element. His likes and dislikes come out strongly, both as regards persons and methods. He likes a clearly defined problem, complicated enough to be difficult but simple enough for the computer of the day. Approximate methods, valid for even more complicated problems, are less to his taste. Thus the pseudopotential is not mentioned and the work of the English school using such methods is rather summarily dismissed. Curiously, for a physicist who has done so much for metal theory, there is no mention of Landau's work on the nature of the Fermi surface. Slater, one feels, draws a line round himself and the computer, and those outside it are the handwaving magicians. But within this circle Slater's achievements are second to none and all his friends and colleagues will hope that his present very successful work will continue for many years. **Nevill Mott**

Orbital Theories of Molecules and Solids. Edited by N. H. March. Pp. xiv+385. (Clarendon: Oxford; Oxford University Press: London; November 1974.) £10.75.

IN 1973 Charles Coulson celebrated his 60th birthday and part of the tribute paid to him by his students and close collaborators is this book. It is essentially a review of the current state of those research fields to which the greater part of his scientific life was dedicated.

The book divides into two distinct areas in spite of all the efforts of the authors to maintain continuity. The solid state part begins with a general survey by Pincherle of the present state of band theory calculations. Then Altmann presents a detailed review of the often misunderstood cellular methods and shows in a convincing way that their neglect is not justified. If those papers stress the orbital concept in its delocalised form the next two redress the balance by considering the atoms. The editor, March, contributes a masterly review of the theory of the potential around atoms and around defects in crystals and shows how many-body effects can be assimilated into what may be considered a typical orbital concept. The different kinds of defect that can occur in crystals of different types is the subject of Lidiard's chapter. He demonstrates, more convincingly than in any other chapter, the fruitful interplay between molecular and solid state ideas. The extent to which this field has been organised and analysed theoretically is impressive.

The molecular half of the book begins with a most useful account by McWeeny of the electronic properties of molecules. He stresses the role of density matrices in unifying and simplifying these properties and although he refers to a large number of spin and magnetic properties the reader is given simple interpretations of their origin. Although Coulson is best known for his molecular orbital work he was prepared to use other theories when they suited his purpose. It is fitting, therefore, that the next chapter, by Balint-Kurti and Karplus on atoms in molecules, should use valence bond ideas to obtain calculated molecular energies in better accord with experiments than simple molecular orbital results could ever give.

The book concludes with two articles which carry the subject into different regions. Murrell presents a careful look at the theory of intermolecular forces and shows that, though caution is needed in some instances, the traditional division into additive components can still be justified despite all the complications of a more sophisticated theory. Craig brings the book back to the theme of molecules and solids with an up-to-the-moment account of the theory of excitons in molecular solids. Here, the nature of the free molecule and of its association in the solid, a major interest of Coulson's, are seen to contribute equally to an understanding of the complicated structure of the excited states of molecules in crystals.

The death of Charles Coulson came as a bitter blow to those who looked to him for new research ideas and new insights into old truths. This book which demonstrates both the enduring quality of his own basic ideas and the sound training he gave his students will be a worthy memorial to him. **G. G. Hall**