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Ilya G. Kaplan "The Pauli Exclusion Principle: Origin, Verifications, and Applications" 1st Edition, (Wiley, Chichester, West Sussex, 2017)

Book Review

A.V. Luzanov

This book has come from the pen of prof. I.G.Kaplan, one of the bright representatives of the former Soviet science in the field of the molecular quantum mechanics (quantum chemistry) and beyond (radiation processes theory etc). During more than the last quarter of a century, I.G.Kaplan is working in Mexico, now in the Materials Research Institute (Mexico). He has published numerous articles and reviews as well as authoritative monographs (in Russian and English [1,2]) on principal aspects of the general and applied quantum theory. Among his chief achievements are the development of the so-called quantum chemistry without spin, the statistics of quasiparticles in crystal lattices, the prediction of interference phenomena for the molecular photoionization in X-ray region and others. In 2012 the special issue of International Journal of Quantum Chemistry (v. 112, No 18) was published in honor of prof. Ilya Kaplan. His one more book is dedicated to the Pauli exclusion principle, and below a very short review of the book is given.

On my opinion, this is a remarkable book which touches not only the history – very dramatic one, but first of all, the physical nature and a mathematical heart of one of the fundamental quantum principles. Firstly, I would like to lay more stress on deep-seated aspects of the Pauli principle theory. In Kaplan's book one finds the intriguing chapter "Can the Pauli exclusion principle be proved ?". Indeed, even in Landau and Lifshitz's famous quantum mechanics textbook (as in most others) the Pauli principle is actually presented as a rigorously proven mathematical fact. But it is not the case, and the cited chapter clarifies the situation in many respects by cogently nvoking permutation group theory and other considerations. It turns out that, strictly speaking, the Pauli exclusion principle has not accurate theoretical foundation. However, the given by the author a fine group-theoretic argumentation, including a requirement of nondegeneracy for permutational states, and all existing experimental data are agreed with the Pauli principle. This important analysis (published by Kaplan many years ago) seems to be missed by the physical community. The understandable exposition of the Pauli principle theory in this book can improve the situation.

From the above passage one can easily estimate the scientific level of the book. Further, it is worth mentioning several more of the interesting issues of the book. In Chapter 4 very effective methods (also due to the author) for finding the Pauli allowed states in atomic, molecular and nuclear spectroscopy are described. They are evidently more elaborated than in the popular Herzberg's spectroscopy books; for instance, the explicit formulas for characters of reducible representations are presented for all types of polyatomic molecules. Or in chapter 5, the exotic statistics such as modified parafermi statistics (for magnons and excitons), statistics of Cooper's pairs, and fractional statistics, are discussed in some details.

As for me, a small but highly significant, is the book's critical analysis of the

density-functional theory (DFT) The latter has become a working horse of modern computational solid state physics and material science. Practically used DFT techniques have known limitations and inaccuracies (recall Burke's ironic and witty remark about DFT: "The good, the bad and the ugly" [3]). But the state of affairs in this field is not altogether satisfactory. The first important remark was given by McWeeny (one of the founders of many-electron density matrix theory), stating that electron spin is in fact extraneous to the DFT! But Kaplan had moved further and rigorously proved that the one-electron density of a many-electron system does not depend on its total spin. Then, it means that the DFT basic concept of energy functionals depending on electron density only, has no foundation in principle. Therefore, one can state that in their nature DFT practical techniques which are often working well are rather semiempirical ones. This inference is very important for the DFT practitioners, particularly those in the material science who would like to understand the basics behind the usual DFT models and to see how much credence can be given to these models (see also the last paper on this subject [4]).

To summarize, one finds in this book many important statements and results which are concerned with the methodology principles and their consequences for the practical side of using current theories as well. Notice that for presumably less experienced readers the author has supplied a multitude of appendices which in a sense comprise a useful compendium on group theory.

I think it is now clear why I wanted to share my impressions of this book. Of course, it is doubtful whether it is possible, or even desirable, to state that it is a completely ideal book. For instance, I would like to see in the text more results about the unitary group approach and its applications to many-body problems. It would be also interesting to know the authors viewpoint on the original spin-free formulation of many-electron problem due to Fock (I mean the elegant Fock's cyclic symmetry condition). But these are not-so-substantive comments.

The resulting conclusion is clear: we have now the new book which is widened our understanding of many-body quantum theory, and it would be naturally to see the book in most libraries of traditional universities, and material science institutions as well.

References

1. I.G.Kaplan, Symmetry of Many-Electron Systems, Academic Press, New York (1973).
2. I.G.Kaplan, Intermolecula Interactions: Physical Picture, Computational Methods and Model. Potentials; John Wiley & Sons, New York (2006).
3. J.Leszczynski (ed.) Handbook of computational chemistry, Springer, Berlinm (2011), p. 95.
4. I.G.Kaplan. *Mol. Phys.*, **116**, 658 (2018).