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Book review

Hyperspherical harmonics and generalized Sturmians (Progress in theoretical chemistry and physics), John S. Avery, Kluwer, Dordrecht, 1999, ISBN 0–792–36087–7

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This is a new book by John Avery on a topic to which he has made pioneering contributions. In 1989, he published the book "Hyperspherical harmonics: applications in quantum theory" (Reidel texts in mathematical science), which in the last decade has been a key reference for an increasing number of quantum chemists, attracted by the prospect of applying hyperspherical techniques to solve quantum mechanical problems. Using these techniques, solutions to the N-particle Schrödinger equation are searched for in a $3N$-dimensional space, parameterized as a radius and the $3N$–1 angles of a hypersphere. The ten years since the publication saw considerable progress in the applications, notably in atomic, molecular and nuclear physics, and in chemical reaction dynamics. This new book is a timely update, particularly for those interested in developments in electronic structure theory.

In the book, the mathematical apparatus is described carefully. A detailed account is given of the connections among the theory of hyperspherical harmonics, momentum-space quantum theory, and generalized Sturmian basis functions; these methods should permit the solution of many-particle problems directly, beyond the self-consistent-field approximation. Particular attention is given to many-electron Sturmians based on the choice of the attractive potential of the nuclei in the system as a reference potential. This choice offers as advantages the diagonal matrix representation of the nuclear attraction potential and the vanishing of the kinetic energy term from the secular equation; this enforces the automatic optimization of the Slater exponents of the atomic orbitals. The worked out examples suggest good convergence properties and prospects that excited states can also be obtained with reasonable accuracy.

There is one important further connection that in the opinion of the present reviewer will prove fruitful in the near future: it is with modern advances in angular (and hyperangular) momentum theory, since these basis sets arise naturally as Lie-group representations and, therefore, belong to the theory of special functions and orthogonal polynomials. Their dissemination may even provide a breakthrough in computational quantum theory, allowing all integrals to be obtained in closed form.

The exposition of the material is complete and the coverage of the literature exhaustive. The new theoretical tools made available here to scholars and students may help to remove some bottlenecks in the progress of theoretical and computational chemistry, such as those associated with singularities at cusps.

This book should find its place on the shelves of theoretical chemists as a good companion to other well-known books by this author: "Creation and annihilation operators" and "Quantum theory of atoms, molecules and photons". He also has coedited books collecting contributions from various authors on selected topics of interest to quantum chemistry, "Dimensional scaling in chemical physics" (edited by D.R. Herschbach, John Avery and O. Goscinski, Kluwer, Dordrecht, 1993) being particularly related to the scope of the present book.

We should be grateful to John Avery not only for his continuing efforts to disseminate with his pedagogically inspired books the innovative aspects of quantum chemistry, but also for his attention to social and economic problems (see his book "Progress, poverty and population: Re-reading Condorcet, Godwin and Malthus!", Cass, London, 1997), whose solutions will also depend on the awareness of the scientific community.