

not so long ago that almost all children at school over (and often under) the age of 12 had to learn Latin and Greek. Surely classical languages are even less natural and comfortable than science — for the British that is. There is no reason to suppose that they presented much difficulty to the ancient Greeks or Romans.

Fashion is always hard to understand: you may just as well ask why over the past two years women have abandoned pale stockings for black ones as seek reasons for the abysmal ignorance of science in Britain. In deploring this state of affairs,

Wolpert is strongly supported by Walter Bodmer who points to the lack of scientists in government or administration: after all, they have “an approach to thinking about problems in a rational way”. Unfortunately neither of them proposes a solution, but if this book raises the image of the scientist in the eyes of the British public — as it certainly will if they believe what they read — it will have served a useful purpose. □

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Configuring it out

Rodney J. Bartlett

Methods in Computational Chemistry. Vol. 1, Electron Correlation in Atoms and Molecules. Edited by Stephen Wilson. Plenum: 1987. Pp.363. \$78, £43.35.

ANY COLLECTION of review papers on an active research area depends on two factors to distinguish it from an excess of similar volumes: the novelty of the topics addressed, and the presentation, scholarship and depth of the contributions. This book, the first in a new series, deserves high marks on both counts.

A defining characteristic of the articles is the emphasis on approaches to electron correlation which are usually called ‘many-body’ (that is, many-electron) methods. These methods include many-body perturbation theory (MBPT), coupled-cluster (CC) theory and propagator approaches, all of which are addressed at length in various chapters. Although no single review deals primarily with the oldest class of correlated methods, configuration interaction (CI) and its very modern unitary group implementations,

many of the contributions, and particularly that of Jankowski *et al.*, discuss the considerable contribution of modern CI.

Electron correlation in atoms, as opposed to molecules, frequently receives too little attention today from the quantum chemistry community. Jankowski restricts himself to atomic theory as studied by methods which (except for symmetry considerations) are also applicable to molecules. This review largely deals with contemporary thinking on the subject, but it also reminds the reader of the origins of a body of essential developments, now often forgotten.

Today, few research topics in electron correlation are expanding as rapidly as the coupled-cluster and their finite-order MBPT approximations, reviewed by Urban *et al.* New developments occur almost daily in this field, and this thorough review highlighting recent events and key references, and pointing the way towards future advances, is unusually timely. Particularly useful is the authors’ discussion of properties other than the energy in CC theory, including analytical derivatives. The thoroughness of the treatment, which includes many numerical results, strongly recommends this contribution.

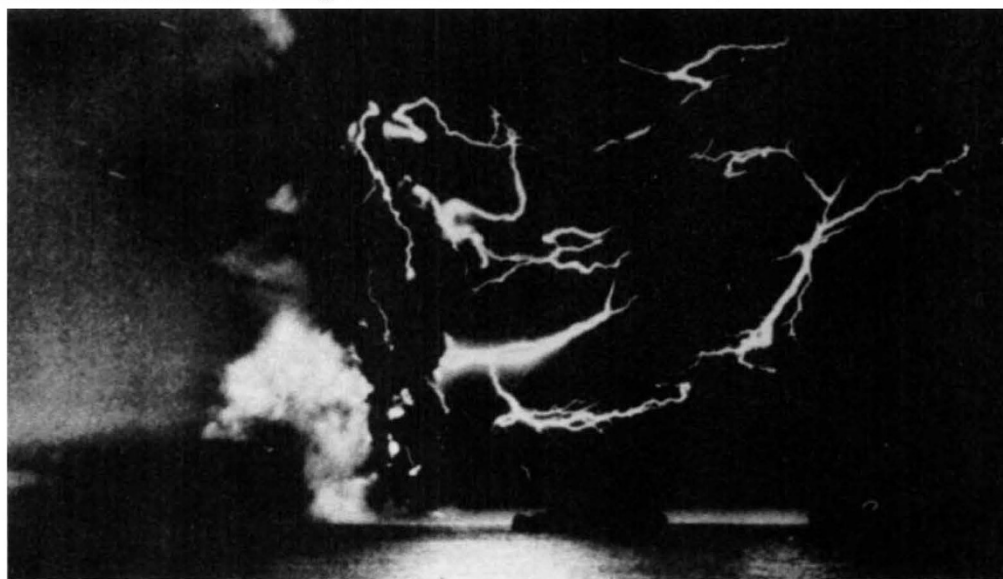
At the core of any correlated method

lies an integral transformation. The methods for doing such transformations have been known for some time, yet few authors have critically assessed the different approaches. One particularly important question addressed in the book is whether an integral transformation is the best strategy for many problems. Ways to avoid most of a transformation, such as the so-called coefficient matrix approaches, would be recommended for large-molecule calculations, for example.

Different approximations for electron correlation have their strengths and weaknesses, yet underlying any such method is another approximation, of perhaps greater importance, which might be termed the (primitive) basis set problem — or the limitation in describing the wavefunction for a molecule in terms of a limited number of atomic orbitals for each atom. Green’s function Monte Carlo (GFMC) methods potentially offer a way to avoid such basis set problems. For electrons, however, other kinds of approximation pertaining to the location of wavefunction nodes and the existence of vastly different ‘time’ scales for inner and valence electrons introduce problems that have proved difficult to resolve. Also, the extreme computational demands of GFMC are a limiting factor in applications to molecules. The article by Wells takes the reader through the developing GFMC area, delineating the ‘fixed-node’ and ‘short-time’ approximations, and how they may be removed.

Each of the reviews in this collection is well written and up to date. The book as a whole is well worth the attention of quantum chemists, and the high quality of the contents augurs well for future volumes in the series. □

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Flashes of brilliance — lightning in the volcano cloud over Surtsey, near Iceland, in December 1963. The November eruption resulted in the formation of an island nearly 1 kilometre long and 100 metres above sea level. The picture is taken from The Lightning Discharge by Martin A. Uman, just published by Academic Press as part of their International Geophysics Series. Price is \$49, £31.50.