Book Review

Kostas Gavroglu and Ana Simões: *Neither Physics nor Chemistry: A History of Quantum Chemistry*, Cambridge, MA & London: MIT Press, 2012, 351 pp. [ISBN 0262016184]

by Brian T. Sutcliffe

The book has four chapters which are mainly historical, preceded by a chapter in which the issues that the authors propose to raise in their exposition are outlined and followed by a chapter in which they consider the emergence of quantum chemistry as a sub-discipline. The development of the subject up to 1970 is the range of interest. The preface, in which the authors place themselves in the field and thank those who helped and acknowledge those who influenced them, begins with two poems one by Cavafy and the other by Pessoa that, it seems to me, set the tone for the whole work.

The issues that the authors wish to raise are: the historical becoming of the epistemic aspects of quantum chemistry, the emergence of quantum chemistry as a discipline, the contingencies of its development, the effect upon the discipline of the coming of electronic computers, the effects that the emergence of the discipline had on the philosophy of chemistry, and the development of a definite intellectual style in the discipline. They raise these issues in interlinked ways in the four chapters: 'Quantum Chemistry qua Physics', 'Quantum Chemistry qua Chemistry', 'Quantum Chemistry qua applied Mathematics', and 'Quantum Chemistry qua Programming'.

The first chapter deals mainly with the contributions made by Germans, beginning with the work of Walter Heitler and Fritz London and describing Friedrich Hund's contributions together with those of Erich Hückel and Hans Hellmann. The second chapter deals mainly with work performed by US workers but often begun or continued in Europe. The account begins with the work of Gilbert. N. Lewis and its development by Linus Pauling and later George W. Wheland, and the contributions of John. C. Slater and Robert S. Mulliken. They discuss the tensions that developed between the valence bond and the molecular orbital points of view and the attempt by Albert Sherman and John H. Van Vleck to deal even-handedly with the two approaches in their 1935 review 'The quantum theory of valence'. Nevil Sidgwick and Ralph Fowler also get a look in here though as British they

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feature in the next chapter too. The third chapter seems to involve chiefly work done in the UK. It begins with the work of William and Douglas Hartree, goes through the work of John Lennard-Jones, picking up the early works of George Hall, John Pople, and Frank Boys, but concentrating upon the works of Charles Coulson of his pupils, particularly Christopher Longuet-Higgins but also Roy McWeeny and Michael Barnett. The fourth chapter begins in France with the work of Raymond Daudel and later that of Bernard and Alberte Pullman; it goes via Japan and the work of Maseo Kotani to Sweden and the development of Per-Olov Löwdin's group. Then over to the USA to consider the work of Robert Parr, Klaus Ruedenberg, Clemens Roothaan, and Enrico Clementi, these last three in Mulliken's group. But Coulson, Boys, and McWeeny come in here again.

The book is written in an engaging manner and it is thus easy to read. It does not grind any particular axe and so seems objective enough. But the reader will undoubtedly come away with the feeling that Pauling was not such a nice man and that Coulson was an admirable man. Although the authors treat Mulliken as a good communicator, he was very bad at formal lecturing, but he could talk informally in a very clear manner. J. C. Slater as seen here, is a man of patience and forbearance. But he had a formidable temper and if he thought that he was listening to nonsense he could show his contempt in an explosive and very disconcerting manner. The reader might be as surprised as was the reviewer to learn that Douglas Hartree was the great-grandson of Samuel Smiles, the author of 'Self-Help' and one of Mrs. Thatcher's favorite Victorians.

Is the account provided accurate and illuminating? The authors give a nicely nuanced account of the introduction of Gaussian orbitals into quantum chemical calculations. This event is often presented rather crudely and it would seem to exemplify the sort of care that they have taken in such historical matters. On the other hand they say that analytic solutions to the Schrödinger equation are possible for the Helium atom. If only they were right, how happy we should all be. But it is, in my view, a nice kind of slip. I should take these two observations as typifying the presentation as a whole. The history seems accurately and carefully observed but from time to time there are small slips of no real importance. I was a bit disappointed that there was no mention of the work by Henry Eyring and Michael Polanyi on the quantum mechanical theory of reaction rates. This was certainly a quantum mechanical influence on me as a chemistry student in the 1950s and, I should think, on many others too. As for illumination, much of what is recounted in the book actually falls within the range of the reviewer's experience. However I think that the presentation is pretty fair and it certainly illuminated for me some aspects of the development of the subject with which I was unfamiliar

and I am sure that it will do so for others of my age. For younger readers I imagine that it will illuminate the whole of the development.

The authors begin the last chapter by saying

> The story of quantum chemistry has been a story with a happy ending: the happy ending of a tortuous journey [...] beginning [...] with the realization that there could be no analytical solutions to almost all the problems of chemistry using quantum mechanics. [p. 245].

They say that it was the electronic computer that was largely responsible for the happy ending, but they are certainly alive to the ways in which this has generated problems. They quote Alberte Pullman who wondered whether modern (1971) quantum chemistry was principally "the reproduction of known results by means of uncertain methods" or "using known methods to search for unknown results" (*ibid*.).

The last chapter considers the position of quantum chemistry in chemistry as a whole by means of historiographical discussion of the recorded attitudes of participants in the field and of philosophers of science generally and of chemistry in particular. What seems to emerge is that the field developed as a mélange of national styles and the subject-origins of the innovators, mediated by the desire to be 'chemical'. This leads the authors to consider the very puzzling question of how, once quantum mechanics had been allowed into chemistry, chemistry managed to stay 'chemistry' and not get incorporated as part of physics. How has it been possible for chemists to import just enough quantum mechanics to be useful? They draw an interesting parallel with the introduction of thermodynamics into chemistry as Chemical Thermodynamics and argue that here, and in the introduction of quantum mechanics

> chemical theories were formulated by chemists with fundamentally different cultural outlooks compared with those of physicists. Compared with physicists, these chemists expressed a different culture when it came to formulate a theory and to impose their demands on such a theory – such as the constitutive and regulatory role of empirical data in theory building. [p. 258]

In this context they stress the contingency of all this. Things could have come out very differently.

I find their arguments for contingency convincing but I feel that the authors rather under-played the role that molecular structure played in the way that things actually did turn out. They do say that one of the reasons for "proposing new concepts or engaging in discussions about the validity of various approaches" (p. 255) was to make compatible the language of classical structure theory and quantum mechanics. I imagine that they are thinking of discussions about the use of particular methods like the valence-bond or the molecular orbital method and I am sure that they are correct in this observa-

tion. They also are correct, in my opinion, when they say that those who were involved in the pioneering work, were concerned with "legitimizing the epistemological status of various concepts in order to be able to articulate the characteristic discourse of quantum chemistry" (*ibid*.). I think, however, that one can be a bit more specific than that. When Lewis introduced the electron into chemistry he did so in a way that used electrons to allow the nuclei to remain fixed to provide the molecular structure that had, historically, been provided by chemical atoms. When Heitler and London used Schrödinger's equation to look at the Hydrogen molecule, they kept the nuclei fixed and used quantum mechanics on the electrons. With this background I think that it must have seemed natural for chemists to treat the nuclei as distinguishable particles, disposable in space, while the electrons set about the job of holding them together. In that way, molecular structure ideas could be preserved. If quantum mechanics was necessary to describe the electronic motion, then chemists could accommodate it and they would regard the clamped-nuclei electronic Hamiltonian as being quantum mechanics for their purposes.

Although the authors say that they do not want to articulate the philosophical considerations of reductionism, they do recognize that reductionism "has marked the culture of quantum chemists" and "in naive philosophical terms – permeated their practices" but not as a "paralyzing factor" (p. 257). They do however note the work of Woolley which is addressed to quantum chemists and not to philosophers. Woolley's arguments imply that, if it proves possible to get a good approximate solution to Schrödinger's equation describing a polyatomic molecule, treating both electrons and nuclei on an equal footing, then molecular structure will not be apparent in such solutions. Will chemists be able to accommodate this outcome too? My guess is that chemists will continue to ignore it, as at present they ignore it, even though it is an outcome required by the full theory. It seems to me that the book relates the history of the incorporation of quantum mechanics into chemistry rather than the incorporation of chemistry into quantum mechanics. There is no doubt that the dominant disciplinary scheme is chemistry, and I think that this is the idea that readers will come away with.

I very much enjoyed reading the book. I find it to be an honest and thoughtful account of the development of the field. I do hope that its readership goes wider than the science-studies courses that I guess that it is aimed at and that some working chemists read the book too and think about it.

Brian T Sutcliffe:
Lab. de Chimie quantique et Photophysique, Univ. Libre de Bruxelles, 1050 Bruxelles, Belgium; bsutclif@ulb.ac.be