

KOSTAS GAVROGLU and ANA SIMÕES, *Neither Physics nor Chemistry. A History of Quantum Chemistry*. MIT: Cambridge, MA. 2012. 351 pp., illus., index. £27.95. ISBN: 978-0-262-01618-6.

*By José Ramón Bertomeu Sánchez**

After two decades of research and joint projects around the history of quantum chemistry, Kostas Gavroglu and Ana Simões have written an excellent synthesis that will remain the reference book on this topic for a long time. The volume relies on the analysis of a large number of different sources (from published papers and textbooks to personal archives) and the critical reading of the past and present scholarship on these topics. The narrative is organized in four chapters, each one dealing with both the emergence of a particular approach to quantum chemistry and the prominence of a selected group of biographies in a loosely defined geographical setting. The first chapter reviews the contribution of German physicists, starting by the famous paper published by Walter Heitler and Fritz London in 1927. The second one deals with the “chemically-oriented” and “pragmatic” approach of American scientists such as Robert Mulliken and Linus Pauling, while the following chapter offers a similar account of the works of their British colleagues, who enlarged the domain of applied mathematics so as to include quantum chemistry, in the decades after the Second World War. In the last chapter, which is organized around several international conferences, the authors discuss the diverse impact of the advent of the new computers in the different cultures of quantum chemistry during the 1960s. While the geographical focus is centered on Germany, Britain and USA, the last chapter introduces new scenarios in France, Sweden and Japan, so capturing the transnational aspects of the history of quantum chemistry, notably in the account of the decisive international conferences and summer schools which took place in Paris, Shelter Island, Nikko, Valadalen, Boulder or Bethesda. All the chapters include detailed biographical information of the main protagonists with a critical discussion of their relevant scientific contributions. On this later point, the authors heroically face the challenge of many historians of twentieth-century science: how to get out of the “Sisyphean deadlock” (p. xi) of presenting important technical details to a broad and diverse readership, from chemists and

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other scientists to historians and philosophers of science, and also general readers without previous training in science.

Although the history of quantum chemistry is the main motif which connects many general issues in the book the spectrum of topics discussed by the authors make this book interesting to a broad readership. Apart from the biographies and works of the main protagonists, the discussion is organized around what the authors call “six clusters” of issues: epistemic aspects (concepts, methods, approaches), social framework (university politics, teaching, conferences, networking), contingencies (different choices and parallel research agendas), the role of electronic computers (the changing meanings of calculations and experiments after the 1960s), philosophy of science (particularly, the issue of reductionism in chemistry but also the role of theories, semi-empirical methods, virtual experiments and visual models), and the complex but productive coexistence of different styles of reasoning in the emergence of a new subfield such as quantum chemistry.

All these aspects are intermingled in the general narrative and discussed in different ways in each chapter. By describing the different styles of reasoning developed by the main protagonists, the authors show the distinct choices available for the development of quantum chemistry, and not only the famous, but questionable, opposition between the Heitler-London school and the molecular orbital approach promoted by Mulliken. By building up a complex story, Gavroglu and Simões analyse the contributions of many other scientists to the discussion of hybrid concepts and methods (the work of Charles A. Coulson is largely discussed in this sense). The authors also claim that the success of the diverse approaches depended not only on the inherent epistemological virtues, but mostly on the capacity to gain legitimacy inside different academic communities, for instance, how the required numerical techniques were presented in a both meaningful and accessible way to the chemists. From this perspective, the role of pedagogy is highlighted in different parts of the book, for instance, in the sections on the first textbooks on quantum chemistry. The authors show how these books contributed to consolidate keywords, leading concepts and fruitful methodologies, while conveying general views on issues such as the relations between chemistry and physics or the extent and nature of the mathematical methods which could be profitably applied in chemistry. Another important subject discussed in the book is the different institutional settings, which encouraged, constrained or discouraged ties and

exchanges between physics, chemistry and mathematics. These different institutional settings largely contributed to generate sharp contrasts between the different national styles, for instance, the physically oriented approaches of German physicists, whose pioneering work was so important for the origins of quantum chemistry, and the chemically oriented methods of American scientists, whose contributions proved to be more successful in the long run.

The authors brilliantly show how the emergence of an “in-between” discipline was shaped by all these intermingled social issues, epistemic aspects, contingent factors, biographical profiles, styles of reasoning and pedagogical practices. They claim that quantum chemistry is an amazing area for analyzing these issues but one can wonder whether a similar approach could be adopted (and similar or contrasting conclusions reached) when writing the history of other “in-between” twentieth-century fields such as biochemistry, chemical engineering or material science. The crossing of disciplinary borders being so important in the narrative, maybe other studies on trade zones in twentieth-century fields such as microphysics (Peter Gallison) could also provide productive angles to further explorations on questions raised in this book such as the uses of chemical images vs. mathematical equations. Likewise, the book is also a departing point for studies on related topics such as the accommodation of quantum chemistry in other local settings (for instance, the so-called “European Periphery”), its impact on popular culture (departing from the interesting analysis of Coulson’s talks on the interface between science and religion) or the “shock of the old” methods and images, for instance, the long persistence of Lewis’ models in the pedagogical realm. All these issues are mentioned in the book but the authors know that the devil in the details can hardly be encountered in such a general overview without losing balance and coherence. With such an excellent road map at hand, further studies on reduced scales could also displace the focus of the book from innovations to uses, enlarging the examples of appropriation of concepts, methods and images of quantum chemistry in new academic and non-academic contexts.

The main conclusion, that success in quantum chemistry largely depended on the ability of coping with diverging trends and reasoning styles, also applies to the “in-between” area of history and philosophy of science. The book is a convincing proof of the creative power of crossing national and methodological borders, arranging unexpected meetings (such as Cavafy and Pessoa, a good choice in the opening quotations) and venturing in risky explorations at the

disciplinary frontiers. This long historiographical trip of Ana Simões and Kostas Gavroglu has produced a brilliant history of quantum chemistry which will become the reference book for post-graduate students, scientists and historians, while providing a source of creative debates and further research in history and philosophy of science.