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Quantum Chemistry: Classic Scientific Papers

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can sometimes lead to more confusion. One of his candidate misconceptions is the notion that a derivative is "just a rate of change." His solution is to assert (in a statement enclosed in a box for emphasis) that a derivative is just "the ratio of two physical quantities which are defined locally." This may work if the quantities are functionally related, but it does not quite exclude the possibility of trying to define a derivative in the absence of a function.

The book contains numerous unwarranted generalizations ("in all cases of physical interest the separation of variables works"). It also has too many footnotes (18 in chapter 3, 31 in chapter 8—I find them distracting), too many acronyms (PDE, ODE, FODE, SODE, HSOLDE). Additionally, considering the large number of historical notes, some people are bound to take exception to one or another of them. My list includes such things as stopping at Julian Schwinger and Richard Feynman in a list that should have included Sin-Itiro Tomonaga, or describing a positron as a particle with negative energy—which, as P. A. M. Dirac himself cautioned, "would make the dynamical relations all wrong."

I would find the book more attractive if the first couple of chapters were shorter, or had avoided "exorcisms," or were omitted altogether. Then Hassani might have made room for some discussion of probabilities, tensors, and integral transforms. Furthermore, at a time when the physics community is becoming more aware that linear, or separable, or exactly soluble problems do not exhaust the complexity of the physical universe, and the use of computers is more ubiquitous, some discussion of the use of computers for numerical analysis would have been welcome. All in all, however, this book could provide Boas with some serious competition, especially if her forthcoming third edition, scheduled for January 2002, does not come forth soon.

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Quantum Chemistry: Classic Scientific Papers

Hinne Hettema
World Scientific, River Edge, N.J., 2000. $90.00 (478 pp.). ISBN 981-02-2771-X

Hinne Hettema's *Quantum Chemistry* is a finely produced, useful, and highly thought-provoking book. Hettema is a chemist turned philosopher, and he has credentials in both disciplines.

The body of the book consists of 26 German-language papers by 18 authors, written between 1926 and 1934, all expertly translated into English. Of the papers, 21 are from the journal *Zeitshrift für Physik*. Given the importance of these papers, teachers of quantum chemistry or molecular physics well might require their students to read this book at the time they are treating the theory of molecules and molecular spectra. What more valuable experience could there be than to study the magnificent paper by Max Born and J. Robert Oppenheimer, or several of the astounding papers of Fritz London, or those of Friedrich Hund, Egil Hylleraas, John Charles Polanyi, or Eugene Wigner? By 1934, there were many classic papers in English as well as in German, and so "Classic German Scientific Papers" would have been a better subtitle for the book.

At the start of the book is a provoking 23-page essay by Hettema entitled "Philosophical and Historical Introduction." This includes an analysis of the shift of the center of research in quantum chemistry away from Germany and to the English-speaking countries. The author concludes that "the smooth transition of quantum chemistry to the USA, as it took place in the 1930s, had to do with the embedding of the quantum chemistry community in the wider environment in Weimar Germany, and the manner in which the applications of quantum mechanics were ill-suited to the Weimar intellectual environment."

To the contrary, I would rather claim that this transition was due quite simply to the Gilbert N. Lewis–Linus Pauling tradition in the US, plus the distinguished leadership, through the transition period in the English-speaking countries, of Robert Mulliken, John Slater, John Van Vleck, Henry Eyring, John Lennard-Jones (England), and Gerhard Herzberg (Canada). Of these, only Herzberg was an immigrant, although other immigrants played central roles. In particular, one should mention Maria Goeppert-Mayer, whose 1938 paper (with Alfred Sklar) in the *Journal of Chemical Physics* was her only contribution to quantum chemistry but perhaps was the most farsighted electronic-structure paper before World War II. Karl Herzfeld also made important contributions (of which few people know).

When I began research in the 1940s,

superior English sources were available to me. There was the wonderful review on valence theory by Van Vleck and Albert Sherman in *Reviews of Modern Physics* (1935) volume 7, page 167, a little book by W. G. Penney *The Quantum Theory of Valence* (Methuen, 1935), the text *Introduction to Quantum Mechanics* (McGraw-Hill, 1935) by Pauling and E. Bright Wilson, and the monograph by Pauling, *The Nature of the Chemical Bond* (Cornell, 1942). Most important, because it did not eschew mathematics and was up to date, was the great text *Quantum Chemistry* (Wiley, 1944) by Henry Eyring, John Walter, and George Kimball. The masterpieces by Herzberg on atomic and molecular spectroscopy were important because understanding of spectra was a primary goal. I felt no need to consult German sources, save for Wigner's *Gruppentheorie* (Vieweg, 1931). I note in passing, however, that German quantum chemistry became world-class both in quality and quantity by the 1950s.

Hettema states that relations between the physics and chemistry communities have been important in the evolution of quantum chemistry. True! These relations have been particularly supportive of quantum chemistry in the US. Several pioneers from the old days, notably Mulliken (trained as a chemist but professor of physics for most of his career), Slater (physicist), and Lennard-Jones (theoretical chemist) maintained positions of strong leadership through their individual publications as well as schools they established. Theoreticians from all over the world—physicists and chemists alike—flocked to their laboratories, and there soon existed a worldwide network of lifelong friends with common interests. Harold Urey and Joe Mayer in 1932 established the *Journal of Chemical Physics*, which has remained unrivaled. Mulliken led the formation of the division of chemical physics of the American Physical Society. And the educational system quickly responded, with the whole chemical professoriate in the US recognizing that the chemistry undergraduate curriculum should be strong in physical chemistry and should include substantial mathematics and physics.

There is, however a barrier between physics and chemistry, illustrated well by the differences between molecules as viewed by Lewis and as treated in the 26 papers in Hettema's collection. On the one hand (physics), one has a quantum-mechanical many-body problem to be solved; on the other hand (chemistry), there is the vast universe of molecular fact and reigning old chemical theories. Bonds exist and are often transferable; molecules have functional groups that are much the same from molecule to molecule; molecules are composed of atoms, but these atoms are not trivially the same as the atoms of atomic physics.

So, there is the Schrödinger equation, yes; but to achieve full understanding, the molecular theory must be developed carefully, mixing in extensive, quantitative, variegated chemical knowledge. In my opinion, the quantum chemistry of today has been driven not just by solution of the molecular Schrödinger equation begun by the 26 papers in the Hettema collection. It is a more complex subject, born out of decades of work by physical organic chemists, physical inorganic chemists, computational chemists, and theoreticians, effectively interacting.

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Psychoacoustics: Facts and Models

Eberhard Zwicker and Hugo Fastl
Springer-Verlag, New York, 1999 [1990]. 2nd edition. $64.95 (416 pp.). ISBN 3-540-65063-6

Upon his retirement, Eberhard Zwicker wrote *Psychoacoustics: Facts and Models* in collaboration with Hugo Fastl, his colleague of many years. The book was published as 1990 began. Later that year, on 22 November 1990, Zwicker died at his home near Munich, Germany—a great loss to the hearing research community.

Psychoacoustics: Facts and Models was Zwicker's last statement—a summary of the things that had interested him and had been studied in his labs over the years. The list is long: psychoacoustical measures of masking as related to excitation patterns, tuning curves, and temporal effects, in addition to loudness, roughness, subjective duration, nonlinear distortion, binaural effects, and pitch perception for pure and complex tones—including the unusual topic of pitch strength.

The second edition of *Psychoacoustics: Facts and Models* is very similar to the first. A modest amount of new data and references has been added on pitch strength and roughness and on applications. The number of figures has increased by 5%. The greater number of pages in the second edition results mainly from larger type.

The book's introductory chapters include the standard auditory physiology, emphasizing the active cochlea and supplemented with a useful, and still current, introduction to Zwicker's last passion, otoacoustic emissions. The book ends with applications to noise control, audiology, and sound quality—areas in which Fastl is an acknowledged world authority.

Psychoacoustics: Facts and Models is a unique book. It makes no attempt to provide a balanced approach to its subject matter. Essentially 100% of the literature cited in the 42 pages of references is from the Zwicker labs in Stuttgart and Munich. For American readers, this is not necessarily a bad thing; it serves to focus a spotlight on much work that is not well known. German titles are given English translations in the list of references.

Like other books on the topic, *Psychoacoustics: Facts and Models* is filled with data on human hearing. However, it is often difficult for the reader to know what these data represent. Some data appear to come from only one or two experienced listeners. Other results that appear to be data may be only the predictions of models. For instance, it would be impossible actually to measure the highly-structured plot of direct masking by a complex periodic tone as shown in chapter 4, but an inexperienced reader would not know that. Sometimes the presentation misses interesting effects because it relies on inadequate experiments. For instance, the treatment of the pitch of noise band edges somehow missed the pitch shift in the direction of higher spectral density.

The difficulty in interpretation is compounded by a referencing technique that gives all the references at the end of the book in blocks that correspond to chapters or major sections. No specific connections are made between the facts and models in the chapters and the references.

The other side of this coin is that *Psychoacoustics: Facts and Models* never presents data without a great deal of thought and sense of purpose. Data are chosen to demonstrate the operation of basic perceptual models. The models are based on a few elementary principles such as critical-band filtering, critical-band independence, specific loudness, and modulation transfer functions. It is of great value to see how far a rigorous and systematic application of these fundamental ideas can go in explaining the richness of human auditory experience, and this is the special significance of *Psychoacoustics: Facts*