Don't let these slip through the net!

Handbook of Graphs and Networks: From the Genome to the Internet

Editors *Stefan Bornholdt* and *Heinz Georg Schuster*

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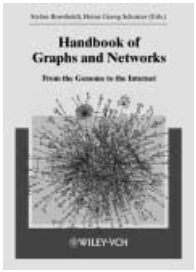
This edited volume covers the statistical mechanics, the mathematics and numerous applications of a rapidly growing new scientific discipline: the physics of networks. This metaphor relates to the description of the structure and the dynamics of complex interacting systems occurring in such diverse areas as physics, biology, economics, ecology, sociology, and computer science, to name but a few.



The volume grew out of an international conference on dynamical networks in complex systems held in Kiel in summer 2001. The book contains 16 chapters written by the active players in the field. The various chapters present a compilation of up-to-date, timely minireviews covering the rich and multifaceted diversity of this area of complexity research. The first four chapters focus on the structure of networks and introduce the reader to the different tools and methods borrowed from statistical physics and mathematics and being put to work for this new discipline. The following five chapters address specific themes of biological networks, and the remaining ones cover a variety of interdisciplinary applications such as traffic, economics, food webs, social networks, the Internet, evolution of human language or the problem of the origin of life. This list alone demonstrates the fascinating character of this new area of complexity research.

Although some well written and very useful recent reviews on special aspects of the field do already exist (see: R. Albert, A. L. Barabasi, *Rev. Mod. Phys.* **2002**, *74*, 47 – 97; S. N. Dorogovtsev, J. F. F. Mendes, *Adv. Phys.* **2002**, *51*, 1079 – 1187) this volume offers a rather broad view on the rich diversity of the field; indeed it provides the reader with an excellent introduction into the science of networks, namely the interplay of *nodes* (*vertices*), *links* (*edges*) and corresponding *degrees* of nodes (i.e., the number of links connected to that node). This reviewer recommends the interested reader to skip the very first chapter in the book—which mainly lists several mathematical results—but to start directly with the instructively written exposition by M. E. J. Newman in chapter 2 on "Random graphs as models of networks". Here, the author introduces the reader in a tutorial style to the network jargon, does list the main results and also discusses the main differences among different classes of networks. Starting from the pioneering work in the fifties and sixties on *random* graph models by Erdős and Rényi, which are characterized by a Poisson degree distribution $p(k)$ for the degree k, recent studies of real-world networks such as the internet exhibit quite a different behavior, namely power-law degree distribution $P(k) \sim k^{-\gamma}$; that is, so-termed scale-free networks (Barabási and Albert). Such a power law has seemingly been observed much earlier: As early as in 1926, A. J. Lotka observed that the number of citations in the academic literature follows a power-law. Other differences with random networks relate to the phenomenon of *clustering*, that is, the probability of two nodes being connected by a link is higher when the nodes in question have a common neighbor (Watts and Strogatz). Loosely speaking, it accounts for the phenomenon that the "friend of your friend is likely also your friend". Moreover, the node – node distance increases rather slowly with the number of nodes n, generally logarithmically, as is also the case for random graphs, (small-world effect).

Clearly, the physics of real-world networks impacts several prominent issues such as the spread of a contagious disease (or a virus) in population and in computer networks. In this context, it is particular interesting to learn from chapter 4, by S. Havlin and his collaborators, and from chapter 5, by R. Pastor-Satorras and A. Vespignani, that there exists a lack of epidemic threshold (a percolation transition does not take place) in scale-free networks with an exponent $\gamma < 3$, such as is the case for the Internet and the web of sexual contacts. Put differently, these scale-free networks are prone to the persistence of diseases, whatever infective rate they may have. Thus, a computer virus can practically never be totally eliminated (unless one destroys essentially all the nodes). Likewise, this branch of networks constitutes a new class for percolation theory with interesting applications for mankind.

I personally find it fascinating to learn from S. Havlin and his collaborators that scale-free networks with $2 < \gamma < 3$ are resilient to random breakdown; on the other hand, intentional attacks of the most highly connected nodes easily disrupt the network (for all values of γ).

Naturally, all of this insight is essential for devising efficient immunization strategies, or to understand in greater detail the complexity of interactions among

genes (the genome network), or the interactions among proteins (the proteome), as exemplified in chapter 7 by R. V. Sole and R. Pastor-Satorras. Other interesting applications of network theory involve the study of interacting neural networks for which W. Kinzel, in chapter 9, provides an essay covering novel phenomena relating to synchronization by mutual learning, together with its application to a novel classical scheme for cryptography.

Overall, this reviewer highly recommends this "Handbook of Graphs and Networks", both for the nonspecialist students and researchers and the experts as well. It serves as a good source of reference for both communities. As mentioned above, I find chapter 1 on the collection of the various network-related, mathematical results misplaced by the editors; moreover, statements by the authors of chapter 1 of the type: "As it happens, from a mathematical point of view, the experimental results of [D.J. Watts and S.H. Strogatz, 1998] were far from surprising", do not please this reviewer either. Likewise, I find chapter 15, entitled "Social Percolators and Self Organized Criticality" to be of somewhat marginal research content. All the remaining chapters, however, are very informative and well-written: I am convinced that an interested reader does profit from this collection of minireviews and likely becomes invigorated to do his/her own research in this fascinating field. Being so, this book belongs on the desk of any practitioner of this new and exciting research area.

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An Introduction to Theoretical Chemistry

by *Jack Simons*

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A Swiss-Army Knife for the Theoretical Chemistry Apprentice

Jack Simons' "An Introduction to Theoretical Chemistry" (ITC) is one of the rare books about everything in theoretical chemistry. Of course, this verdict depends a lot on what you define theoretical chemistry to be. I was a little bit surprised that Jack Simons, in his definition, also includes statistical mechanics, which is typically part of the physical chemistry curriculum. At this point, one may suspect that theoretical chemistry may be redefined as everything a chemist may do without actually performing experiments. But in his foreword, Jack Simons explicitly steps back from such a definition, by warning the reader that he will put more emphasis on analytical theory rather than on computational applications.

In any case, the breadth of coverage is quite striking indeed: An introductory section of the book treats the foundations of quantum mechanics, all the way from its pedagogically very important differences from classical mechanics to the obligatory textbook topics of angular-momentum coupling and the full solution of the hydrogen atom problem.

Perturbation and variation theory as well as point group symmetry (including projection operators and direct products) are also covered. The three main, advanced parts of the book treat electronic structure theory, statistical mechanics, and reaction dynamics. In the electronic structure theory section, we find not only basic Hartree – Fock and density functional theory, but also glimpses at various high-level treatments of electron correlation, such as configuration interaction, coupled-cluster, r1,2-approaches and Quantum Monte Carlo; even time-dependent methods are mentioned (propagator methods for electronic excited states). The statistical mechanics section presents not only the partition function and its connection to thermodynamic quantities, but also basics of Monte Carlo and molecular dynamics simulations, as well as lattice theories. The reaction dynamics part not only treats standard topics such as transition state theory, but also its exact quantum mechanical counterpart (evaluation of the rate constant $k(T)$ by flux – flux correlation function expressions), and not only classical trajectories but also wavepacket propagation and surface hopping.

In addition to this all-encompassing catalogue of topics, Jack Simons also throws in two other useful additions: At several places in the book, he includes brief treatments of various kinds of spectroscopy, to supply a link from theory to experiment. And a full quarter of the book is devoted to problems (sometimes standard, more often refreshingly nonstandard) and their detailed solutions.

At this point of my description, you may well ask how it is possible to fit all this into a standard-size, single-volume textbook. Obviously, if each of those many topics were treated to full depth, Jack Simons would have ended up with a many-volume monument.

So, he had to make severe cuts, in scope and substance. Therefore, the ultimate question I have to answer as reviewer is this: Is there enough material left for each of those many topics to make this book useful? From the standpoint of a practicing professional, my personal answer is no, the cuts are too deep for my needs. Just to give two examples: Quantum-mechanical wave-packet propagation is laudably mentioned, and even the Fourier-transform relation between time-correlation functions and spectra is discussed—but the wave-packet propagation is performed by semiclassical Gaussian packets only, almost as if there were nothing else, creating the false impression that wave packet propagation necessarily is a short-time approximative treatment of dynamics. In the electronic structure section, configuration interaction, Møller – Plesset perturbation theory, and coupled-cluster are all discussed on less than five pages, obviously only scratching the surface.

The author softens his cuts by naming advanced undergraduates and beginning graduates as his target readership, and by repeatedly pointing to other sources throughout the book—mostly to his own earlier textbook "Quantum Mechanics in Chemistry" (QMIC) and to additional material on his web site, but occasionally also to several other, more specialized textbooks. This raises two follow-up questions for this target readership: Instead of ITC, should we better buy QMIC directly? Or should we better buy several more specialized textbooks?

In some way, ITC does look like a watered-down and shortened version of QMIC. But there are enough differences

