

An Introduction to Chaos in Nonequilibrium Statistical Mechanics

► Jay R. Dorfman
Cambridge U. Press, New York,
1999. \$34.95 paper (287 pp.).
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Until recently, kinetic and nonequilibrium theories looked to many to be a somewhat dense and technical subject. The pieces fell into place following a series of breakthroughs culminating with Lars Onsager's work, but researchers seemed to shrink from attempting any further "corrections." A rekindling of interest was generated by the discovery of transport coefficient divergences by Jay R. Dorfman and E. G. D. Cohen. Interest subsided rather quickly, however, at least from the viewpoint of those not directly involved in kinetics.

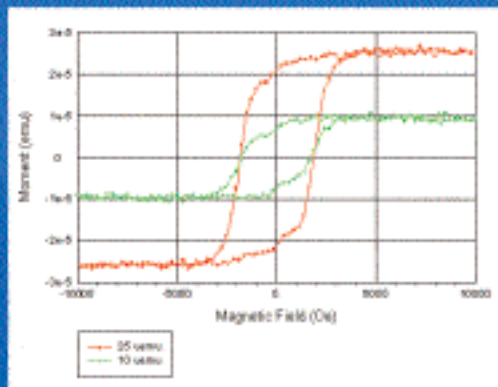
Yet in the 1970s, new ideas emerged quite abruptly, often from David Ruelle's work on turbulence, and percolated into statistical mechanics. In *An Introduction to Chaos in Nonequilibrium Statistical Mechanics*, Dorfman endeavors to write a book ambitiously touching all the relevant work of the past 20 years. No balking at using notions that will sound esoteric to most physicists!

Most physicists, after all, are still too bound to the ancient concept of motion as a composition of uniform rotations (which still permeate the non-posthumous editions of Landau-Lifschitz fluids) and feel little inclined to pay attention to the theoretical work of Yakov G. Sinai, Ruelle, and others, which they find too demanding. They are not convinced that such work carries deep physical meaning, contains applicable ideas, or provides tools for a rational understanding of chaotic motions.

The paradigms of motions were, until very recently, integrable systems. But chaotic-motion paradigms are quite different: The familiar harmonic oscillators are replaced by the "Arnold cat map" or, as Dorfman prefers in this book, the "baker's map." The difficulty is knowing how to apply the paradigms and how to understand certain phenomena based on the abused "back of the envelope" calculation.

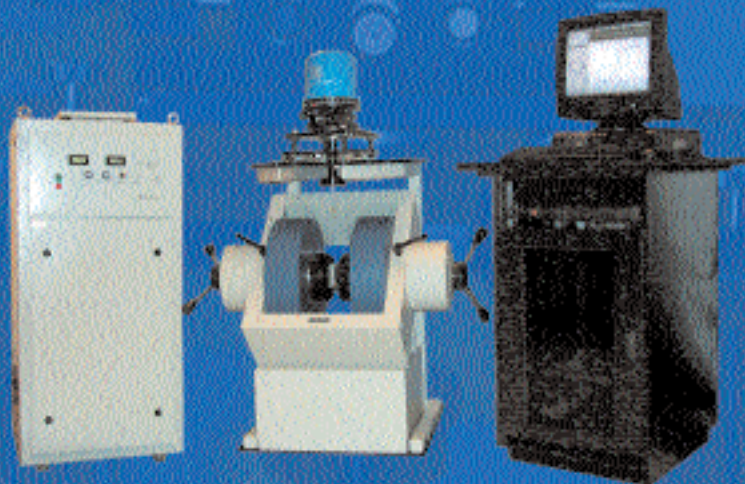
Dorfman begins from classical kinetic theory. Curiously, he presents the ergodic hypothesis, still apparently drawing his inspiration from a well-known footnote (ref. 98/99) of the

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Paul and Tatiana Ehrenfest book *Conceptual Foundations of the Statistical Approach in Mechanics* (Dover, 1990) involving “hypothetical functions as constants of the motion.” He stops short of saying that such functions are nonmeasurable, a mathematical notion denoting the impossibility of writing tables of values. (“Nonmeasurable” is equivalent to a physicist’s “nonexistent.”) Since considering such hypothetical functions as observables had a pernicious influence, and because of the prestige of the Ehrenfests’ treatment, this section could have been a good place for a few more critical details.

A concise analysis of the classical kinetic theory follows. The theory derives and illustrates the Boltzmann equation from a critical perspective. To students, it will be inspiring to find here topics that must otherwise be pursued through the literature, (such as Mark Kac’s ring model or Paul Ehrenfest’s urn model). Dorfman continues with a physical discussion of the meaning of recurrence, ergodicity, or mixing, concepts that are not yet in the cultural heritage of most physicists (chapters 3–6). The Green–Kubo formulae are discussed in chapter 7, in which the van Kampen objections are exposed carefully and in some detail.

Then Dorfman attempts to link the “classical” and the more recent views on chaos. His choice of the baker’s maps to illustrate chaotic motion properties is motivated by their mathematical simplicity. However, “simplicity” is very subjective, and it is not entirely clear that he has made the best choice. The possibility of “computing everything” may induce some readers to lose sight of conceptual difficulties and understandings and to think that everything boils down to technicalities, despite Dorfman’s repeated warnings.

Symbolic dynamics, Lyapunov exponents, and Kolmogorov–Sinai (KS) entropy are introduced mostly from the viewpoint of the corresponding properties of the baker’s map. The SRB (Sinai–Ruelle–Bowen) distributions, the nonequilibrium extension of the Boltzmann–Gibbs distribution, are the central theme of the second half of the book, and Dorfman makes an effort to clarify their meaning via relatively simple calculations. He briefly discusses the “escape rate formalism” that played an important part in showing that something as concrete as a transport coefficient could come out of the “new” ideas and be useful at interpreting simulations. He makes the basic ideas of the “ther-

modynamic formalism” accessible, stressing clearly its surprising relationship to one-dimensional lattice gas statistical mechanics; the “triviality” of the latter renders feasible the apparently intractable analysis of certain chaotic motions.

Dorfman’s pace is fast, at places a bit too fast; it leads to, as he says, “combining almost everything discussed” into the exposition of the Lorentz–Boltzmann equation for Lyapunov exponents and KS entropy of the Lorentz gas—a remarkable novelty in kinetic theory, in which everyone hoped, but hardly expected, to see something new.

It is far from clear that the approach displayed in this book will maintain the rate of development shown so far, as Dorfman implies throughout. In any event, this will remain a first and needed step toward a systematic simple presentation of a developing methodology.

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Introduction to Quantum Mechanics in Chemistry

▶ Mark A. Ratner and
George C. Schatz
*Prentice Hall, Upper Saddle
River, N.J., 2001. \$86.00*
(305 pp.). ISBN 0-13-895491-7

The 1998 Nobel Prize in Chemistry, awarded to Walter Kohn and John A. Pople, demonstrated the influence that computational quantum chemistry has had on the entire field of chemistry. This influence is likely to grow and spill into other active research areas in the near future. An introductory text bridging the gap between the basics of quantum mechanics and the application of ab initio and semi-empirical quantum chemistry theories to problems of chemical interest is thus highly desirable. The textbook, *Introduction to Quantum Mechanics in Chemistry* by Mark A. Ratner and George C. Schatz, which is aimed at nontheoretical chemists and undergraduate students, effectively provides this link. It is a concise, easily readable, and understandable introduction to quantum chemistry and the methods currently used in chemical applications.

After a brief review of the laws of classical mechanics and wave theory, the reader is introduced to the quantum mechanical treatment of the par-