

BOOK REVIEW

Chaotic transport in dynamical systems, by Stephen Wiggins. Springer-Verlag, New York, 1992, 301 pp., \$39.95. ISBN 0-387-97522-5

This is a pioneering book about a fascinating new field of research. In the preface Wiggins indicates the range of applications that will be discussed and defines his use of the word *transport*.

Some explanation of the meaning and context of the title of this book is needed, since the term “transport theory” is ubiquitous throughout science and engineering. For example, fluid mechanicians may be interested in the transport of a “passive scalar” such as heat or dye in a fluid. Chemists might be concerned with the problem of energy transport between different “modes” of oscillation of a molecule in the phase space of some mathematical model. Plasma physicists or accelerator physicists might study escape or trapping of particles in regions of phase space representing motion of a specific type in configuration space. Researchers in celestial mechanics might investigate the capture or passage through resonances in the phase space of some system of masses interacting gravitationally. Control theorists might be concerned with stability questions in nonlinear systems that involve an understanding of the geometry of the regions of phase space of the system corresponding to bounded and unbounded motions. Thus by “transport” I mean motion between regions describing qualitatively different types of motion in the phase space of some dynamical system.

Wiggins gives an interesting introduction to potential applications with emphasis on fluid flow. I will focus on one area: the theory of molecular dynamics. With the recent development of lasers capable of generating ultrashort pulses, experimental chemists now have a tool to probe chemical bonds and to watch molecular dynamics. Recent experiments involving the use of femto-second laser pulses to activate and probe the dynamics of chemical reactions are reviewed in [7]. A new laser catalyzed chemical reaction process is envisioned, where specific chemical bonds are broken and others formed.

The first crude model of the bound dynamics of a molecule describes the nuclei as a collection of point masses connected by springs. By external forcing one wants to excite certain vibrations and suppress others. A more accurate model is given by the Born-Oppenheimer approximation. For each configuration of nuclei, the lowest

energy state of the electron cloud is calculated using quantum mechanics. This value is assigned as the potential energy of the nuclear configuration. The nuclei are assumed to move according to Hamilton's equations of motion.

To model a chemical reaction involving, for example, three atoms A , B , C , suppose that A collides with $B-C$. The goal is to compute the probability that the bond between B and C is broken and the products of the reaction are now $A-B$ and C . One has an ensemble R of (reactant) initial states in phase space corresponding to configurations of the nuclei of the form A together with $B-C$. Each trajectory starting in R scatters past the invariant set (collision complex) of bounded orbits and exits (forming product states). The shape of the triangle formed by the nuclei determines which possible outcome occurs: $A-B$ with C , or A with $B-C$, or $A-C$ with B , or A with B with C .

One may formulate this problem from another point of view by defining a set of near collision states CS . Assume there are four distinct ways to exit from the set CS which lead to the four outcomes defined above. In the terminology of the chemists such states are called "transition states". The problem is to calculate the probabilities of the four outcomes assuming that each collision state is equally probable.

Chemical reaction problems have striking similarities to problems in celestial mechanics. A large variety of potential energy functions are relevant to different chemical reactions. There is intense interest and an extensive literature dating back to an article by Wigner in 1937 [13]. In the chemists terminology "transition states" correspond to the regions around saddle points of the potential function. For a recent discussion of transition states see [12, 10]. For a review of chemical reactions viewed as problems in nonlinear dynamics see [2, 9].

Full quantum mechanical computations of molecular dynamics are still impractical with current computing resources. Semiclassical approximations to the dynamics have been and continue to be very interesting and important (see, e.g., [8, 14]). The associated transport problems (computing the scattering matrix) for most reactions have been little studied.

Many physical problems can be reduced to the study of Hamiltonian systems of differential equations having the form

$$(1) \quad \dot{x} = \frac{\partial H(x, y, t)}{\partial y}, \quad \dot{y} = -\frac{\partial H(x, y, t)}{\partial x}, \quad \dot{t} = 1$$

where $H: R^3 \rightarrow R^1$ is a smooth function which is periodic of period one in t .

The Poincaré map $(x, y, 0) \rightarrow (x(1), y(1), 1)$ associated with (1) may be viewed as an area-preserving map of the x - y -plane. One is lead to study smooth area preserving maps of the plane and the way ensembles of points are transported when such maps are iterated. Invariant curves associated with elliptic fixed points form absolute barriers to transport and are the subject of KAM theory. Partial barriers to transport are formed by "cantori" and also by alternating segments of stable and unstable manifolds of hyperbolic periodic points [11].

A *resonance zone* is a connected region of the plane bounded by alternating initial segments of stable and unstable manifolds of hyperbolic periodic points. The segments must intersect only at their end points. Wiggins refers to resonance zones as regions.

FIGURE 1.

For example, the standard map family is a one-parameter family of area-preserving maps of the plane defined by

$$T : \begin{aligned} y &\rightarrow y - \frac{k}{2\pi} \sin(2\pi x) \\ x &\rightarrow x + y - \frac{k}{2\pi} \sin(2\pi x). \end{aligned}$$

Fix the parameter $k = 3$. There are hyperbolic fixed points $p = (-0.5, 0)$ and $q = (0.5, 0)$. A resonance zone R is formed by four segments of their stable and unstable manifolds. A segment of stable manifold between points c and d will be denoted by $S[c, d]$, and a segment of unstable manifold between points c and d will be denoted by $U[c, d]$. Thus the boundary of R consists of the segments $U[p, a]$, $S[a, q]$, $U[q, b]$, $S[b, p]$ (see Figure 1). R contains an elliptic fixed point e located at $(0, 0)$.

Points enter and exit the resonance zone through “turnstyles”. A turnstyle is the region enclosed by segments of stable and unstable manifolds with common end points z and $T(z)$ where z is a (primary) heteroclinic point. Wiggins calls the region bounded by segments of stable and unstable manifolds which intersect only in their common end points a “lobe”. Thus a turnstyle may consist of several lobes. His approach to the study of transport is based on tracking iterates of lobes. The homoclinic tangle associated with the fixed points p and q is obtained by forward and backward iteration of turnstyle boundaries. Thus the geometry of the homoclinic tangle dictates the shape of iterates of lobes.

In my opinion, the notation for various intersections and unions of lobes is awkward, and there is a practical problem when computing the areas of various lobes and their intersections. Wiggins does not present a good way to do this. He uses Melnikov’s method to approximate the distance between stable and unstable manifolds and thereby to approximate the area of a lobe; however, areas of lobe intersections cannot be conveniently calculated.

Another way to think about transport through a region is in terms of exit time functions [5].

Given a compact set N , define the *exit time function*

$$t(a) = \left\{ \begin{array}{l} \infty \text{ if } T^j(a) \in N \text{ for all } j > 0 \\ \text{the least } j \text{ such that } T^j(a) \notin N \text{ otherwise} \end{array} \right\}.$$

If z is a discontinuity point of the exit time, then the orbit of z must land on the boundary of the resonance zone. Thus z must belong to a stable manifold segment. Discontinuities of the exit time function display stable manifolds localized in the resonance zone.

An alternate way to calculate areas is to use the action principle of MacKay, Meiss, and Percival [11, 5]. The area of any region bounded by alternating segments of stable and unstable manifolds (disjoint except at their end points) can be computed by calculating an action function along the orbits of each heteroclinic point where adjacent segments intersect. A numerical method to locate accurately heteroclinic points of various types is necessary to implement this method.

Rather than constructing a resonance zone, one can approximate the zone by a simple region which contains the zone. For example, replace the resonance of Figure 1 with the square

$$N = \{(x, y): -0.5 \leq x \leq 0.5, -0.5 \leq y \leq 0.5\}.$$

Cover N with a fine grid dividing it into “pixels”. Iterate each pixel until it exits or until some maximum number of iterates is reached. Color the pixel accordingly. This leads to beautiful and amazingly complex pictures. Experimental results for the standard map and for coupled standard maps in four dimensions can be found in [3].

Wiggins presents a theory of transport for Hamiltonian systems with several degrees of freedom in Chapter 6. The key difficulty is to define what is meant by a resonance zone. Wiggins proposes a fairly natural generalization. Periodic orbits are replaced by normally hyperbolic invariant manifolds with codimension one stable or unstable manifolds in an energy surface. In some cases, appropriately chosen alternating pieces of stable and unstable manifolds may bound a region. The practical difficulty of finding such invariant manifolds and approximately constructing a high-dimensional resonance zone will most probably make this construction more trouble than it is worth; however, it has value for theoretical results and for weakly coupled systems.

In any case [6], the maximal invariant set in a resonance zone (in low or in high dimensions) is isolated. Consequently it can be approximated nicely with an isolating block either for a flow [1] or for a discrete dynamical system [4]. One can show that asymptotic properties of the transport rate depend only on the isolated invariant set and are the same for any region which isolates this set. Thus the method of estimating transport through simple regions which approximate resonance zones may work very well. However, as the dimension of phase space increases, the number of pixels necessary to cover a region grows rapidly. Perhaps a Monte Carlo method of randomly choosing points in a region and calculating their exit times may be the best way to proceed.

Researchers concerned with transport problems can learn a lot from Wiggins’s book. His style is energetic. He presents ideas, raises questions, discusses examples, and gives applications. I suggest, however, that you consult the research literature in order to gain a wider perspective on this developing field.

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