

1.7 From chaos to statistical mechanics

Under heaven, all is chaos. The situation is excellent!

— Chairman Mao Zedong, a letter to Jiang Qing

The replacement of individual trajectories by evolution operators which propagate densities feels like a bit of mathematical voodoo. Indeed, something very radical and deeply foundational has taken place. Consider a chaotic flow, such as the stirring of red and white paint by some deterministic machine. *If* we were able to track individual trajectories, the fluid would forever remain a striated combination of pure white and pure red; there would be no pink. What is more, if we reversed the stirring, we would return to the perfect white/red separation. However, that cannot be—in a very few turns of the stirring stick the thickness of the layers goes from centimeters to Ångströms, and the result is irreversibly pink.

Understanding the distinction between evolution of individual trajectories and the evolution of the densities of trajectories is key to understanding statistical mechanics—this is the conceptual basis of the second law of thermodynamics, and the origin of irreversibility of the arrow of time for deterministic systems with time-reversible equations of motion: reversibility is attainable for distributions whose measure in the space of density functions goes exponentially to zero with time.

By going to a description in terms of the asymptotic time evolution operators we give up tracking individual trajectories for long times, but trade the

to the trace as it vanishes smoothly at the leading eigenvalue, while the trace formula diverges.

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uncontrollable trajectories in for a powerful description of the asymptotic trajectory densities. This will enable us, for example, to give exact formulas for transport coefficients such as the diffusion constants without *any* probabilistic assumptions. The classical Boltzmann equation for evolution of 1-particle density is based on *stosszahlansatz*, neglect of particle correlations prior to, or after a 2-particle collision. It is a very good approximate description of dilute gas dynamics, but a difficult starting point for inclusion of systematic corrections. In the theory developed here, no correlations are neglected - they are all included in the cycle averaging formulas such as the cycle expansion for the diffusion constant $2dD = \lim_{T \rightarrow \infty} \langle x(T)^2 \rangle / T$ of a particle diffusing chaotically across a spatially-periodic array,

$$D = \frac{1}{2d} \frac{1}{\langle T \rangle_{\zeta}} \sum' (-1)^{k+1} \frac{(\hat{n}_{p_1} + \dots + \hat{n}_{p_k})^2}{|\Lambda_{p_1} \dots \Lambda_{p_k}|}, \quad (1.18)$$

where \hat{n}_p is a translation along one period of a spatially periodic ‘runaway’ trajectory p . Such formulas are *exact*; the issue in their applications is what are the most effective schemes of estimating the infinite cycle sums required for their evaluation. Unlike most statistical mechanics, here there are no phenomenological macroscopic parameters; quantities such as transport coefficients are calculable to any desired accuracy from the microscopic dynamics.

A century ago it seemed reasonable to assume that statistical mechanics applies only to systems with very many degrees of freedom. More recent is the realization that much of statistical mechanics follows from chaotic dynamics, and already at the level of a few degrees of freedom the evolution of densities is irreversible. Furthermore, the theory that we shall develop here generalizes notions of ‘measure’ and ‘averaging’ to systems far from equilibrium, and transports us into regions hitherto inaccessible with the tools of equilibrium statistical mechanics.

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The concepts of equilibrium statistical mechanics do help us, however, to understand the ways in which the simple-minded periodic orbit theory falters. A non-hyperbolicity of the dynamics manifests itself in power-law correlations and even ‘phase transitions.’

1.8 Chaos: what is it good for?

With initial data accuracy $\delta x = |\delta \mathbf{x}(0)|$ and system size L , a trajectory is predictable only up to the *finite* Lyapunov time (1.1), $T_{\text{Lyap}} \approx \lambda^{-1} \ln |L/\delta x|$. Beyond that, chaos rules. And so the most successful applications of ‘chaos theory’ have so far been to problems where observation time is much longer than a typical ‘turnover’ time, such as statistical mechanics, quantum mechanics, and questions of long term stability in celestial mechanics, where the notion of tracking accurately a given state of the system is nonsensical.

So what is chaos good for? *Transport!* Though superficially indistinguishable from the probabilistic random walk diffusion, in low dimensional settings the deterministic diffusion is quite recognizable, through the fractal dependence of the diffusion constant on the system parameters, and perhaps through non-Gaussian relaxation to equilibrium (non-vanishing Burnett coefficients).

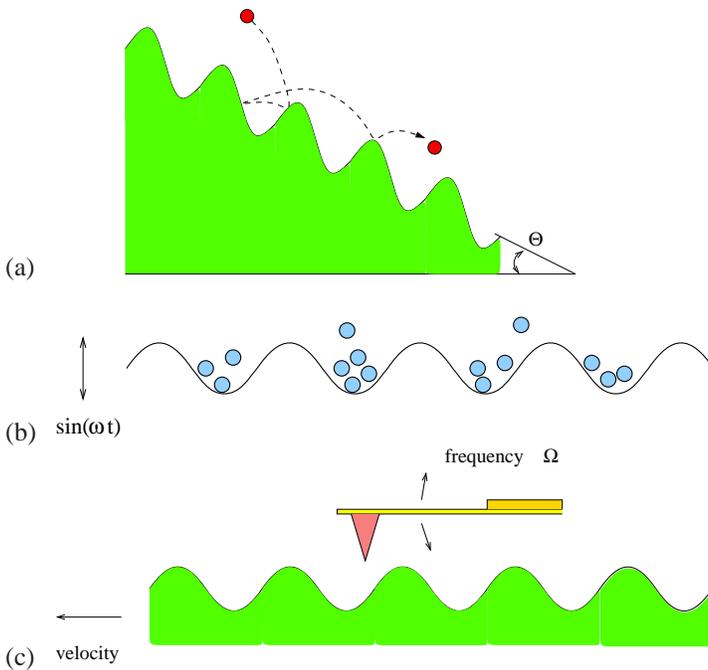


Fig. 1.14 (a) Washboard mean velocity, (b) cold atom lattice diffusion, and (c) AFM tip drag force. (Y. Lan)

Several tabletop experiments that could measure transport on macroscopic scales are sketched in Fig. 1.14 (each a tabletop, but an expensive tabletop). Figure 1.14 (a) depicts a ‘slanted washboard;’ a particle in a gravity field bouncing down the washboard, losing some energy at each bounce, or a charged particle in a constant electric field trickling across a periodic condensed-matter device. The interplay between chaotic dynamics and energy loss results in a terminal mean velocity/conductance, a function of the washboard slant or external electric field that the periodic theory can predict accurately. Figure 1.14 (b) depicts a ‘cold atom lattice’ of very accurate spatial periodicity, with a dilute cloud of atoms placed onto a standing wave established by strong laser fields. Interaction of gravity with gentle time-periodic jiggling of the EM fields induces a diffusion of the atomic cloud, with a diffusion constant predicted by the periodic orbit theory. Figure 1.14 (c) depicts a tip of an atomic force microscope (AFM) bouncing against a periodic atomic surface moving at a constant velocity. The frictional drag experienced is the interplay of the chaotic bouncing of the tip and the energy loss at each tip/surface collision, accurately predicted by the periodic orbit theory. None of these experiments have actually been carried out, (save for some numerical experimentation), but are within reach of what can be measured today.

ChaosBook.org/projects

Given microscopic dynamics, periodic orbit theory predicts observable macroscopic transport quantities such as the washboard mean velocity, cold atom lattice diffusion constant, and AFM tip drag force. But the experimental proposal is sexier than that, and goes into the heart of dynamical systems theory.

Smale 1960s theory of the hyperbolic structure of the non-wandering set (AKA ‘horseshoe’) was motivated by his ‘structural stability’ conjecture, which

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- in non-technical terms - asserts that all trajectories of a chaotic dynamical system deform smoothly under small variations of system parameters.

Why this cannot be true for a system like the washboard in Fig. 1.14(a) is easy to see for a cyclist. Take a trajectory which barely grazes the tip of one of the grooves. An arbitrarily small change in the washboard slope can result in loss of this collision, change a forward scattering into a backward scattering, and lead to a discontinuous contribution to the mean velocity. You might hold out hope that such events are rare and average out, but not so - a loss of a short cycle leads to a significant change in the cycle-expansion formula for a transport coefficient, such as (1.18).

That the structural stability conjecture turned out to be badly wrong is, however, not a blow for chaotic dynamics. Quite to the contrary, it is actually a virtue, perhaps the most dramatic experimentally measurable prediction of chaotic dynamics. As long as microscopic periodicity is exact, the prediction is counterintuitive for a physicist - transport coefficients are *not* smooth functions of system parameters, rather they are non-monotonic, *nowhere differentiable* functions. Conversely, if the macroscopic measurement yields a smooth dependence of the transport on system parameters, the periodicity of the microscopic lattice is degraded by impurities, and probabilistic assumptions of traditional statistical mechanics apply. So the proposal is to –by measuring *macroscopic transport*– conductance, diffusion, drag –observe determinism on *nanoscales*, and –for example– determine whether an atomic surface is clean.

The signatures of deterministic chaos are even more baffling to an engineer: a small increase of pressure across a pipe exhibiting turbulent flow does not necessarily lead to an increase in the mean velocity; mean velocity dependence on pressure drop across the pipe is also a fractal function.

Is this in contradiction with the traditional statistical mechanics? No - deterministic chaos predictions are valid in settings where a few degrees of freedom are important, and chaotic motion time and space scales are commensurate with the external driving and spatial scales. Further degrees of freedom act as noise that smooths out the above fractal effects and restores smooth functional dependence of transport coefficients on external parameters.