

From normal to anomalous deterministic diffusion

Rainer Klages

Queen Mary University of London
School of Mathematical Sciences, London, UK
<http://www.maths.qmul.ac.uk/~klages>

My three lectures will review how both normal and anomalous diffusion can be understood on the basis of microscopic deterministic chaos [1,2]. The first lecture is about ‘normal’ deterministic diffusion in chaotic dynamical systems, where the mean square displacement of an ensemble of particles grows linearly in time. Starting from the paradigmatic Bernoulli shift I will remind of some fundamental chaos quantities and their relation to each other. I will then consider diffusion in a simple deterministic random walk model constructed by using this map. By applying the escape rate approach to this model, I will derive an exact formula expressing the diffusion coefficient in terms of chaos quantities. Interestingly, the diffusion coefficient turns out to be a fractal function of control parameters, where random walk behavior is only recovered on coarse parameter scales. Computer simulations predict analogous results for Hamiltonian particle billiards like the periodic Lorentz gas, which can be related to single-molecule diffusion in zeolite nanopores.

My second lecture will start with the concept of deterministic thermostats which, applied to systems under external forces, generate time-reversible dissipative chaotic dynamics exhibiting nonequilibrium steady states. As an example, the driven periodic Lorentz gas will be considered. Starting from the chaotic hypothesis, I will talk about nonequilibrium fluctuation relations for thermostated systems, a principle that has important applications to nanosystems. Weakly chaotic dynamical systems like polygonal billiards and a simple nonlinear generalization of the Bernoulli shift displaying intermittency then lead from normal to anomalous diffusion. For the latter map, crosslinks to the new mathematical field of infinite ergodic theory will be outlined.

Lecture three will introduce to stochastic continuous time random walk theory by applying this basic method to a deterministic random walk version of the same map. Analytical results predict subdiffusion, that is, anomalous diffusion with a mean square displacement that grows less than linearly in time [2,3], as is confirmed by computer simulations. In a scaling limit a fractional diffusion equation will be derived. However, as in case of normal diffusion there are complicated fractal, possibly discontinuous parameter dependencies deviating from the predictions of stochastic theory. By applying the escape rate approach to another map model exhibiting Lévy flights, I will derive an example of an escape rate formula for anomalous diffusion. I will then explore the validity of fluctuation relations for anomalous dynamics by considering generalized Langevin equations. My lectures will conclude with outlining applications of these anomalous ideas to theory and experiments on biological cell migration [2].

[1] R.Klages, *Microscopic Chaos, Fractals and Transport in Nonequilibrium Statistical Mechanics* (World Scientific, Singapore, 2007).

[2] R.Klages, *From Deterministic Chaos to Anomalous Diffusion* (book chapter for *Reviews of Non-linear Dynamics and Complexity Vol. 3*, H.G.Schuster (Ed.), Wiley-VCH, Weinheim, 2010).

[3] R. Klages, G.Radons, I.M.Sokolov (Eds.), *Anomalous transport* (Wiley-VCH, Weinheim, 2008).