

single-sided power spectral densities (PSD) of this signal computed by the Fourier transformation and by the method of maximum entropy. In the ranges of  $a$  corresponding to chaotic dynamics the spectrum has no prominent peaks and is practically continuous, which is one of the landmarks of chaos.

For individual values of  $a$ , compute the auto-correlations

$$R_{xx}(\tau) = \langle x(t)x(\tau+t) \rangle_t - (\langle x(t) \rangle_t)^2$$

of the sequences  $\{x(t)\}_{i=0}^{N-1}$  and determine an approximation of the correlation length  $\xi$  as a function of  $a$ . Choose  $N$  large enough that  $R_{xx}(\tau)/R_{xx}(0)$  will be precise to three digits. Assume that the auto-correlation has the form

$$R_{xx}(\tau) = Ae^{-|\tau|/\xi}.$$

It can be shown that

$$\xi = \log \left( \frac{|S_1^2 - S_2|}{S_1^2 + S_2} \right)^{-1}, \quad S_n = \sum_{t=0}^{\infty} R_{xx}(t)^n.$$

Systems in which all correlations between quantities converge to zero at long times, are said to *mix the space*, which is one of the key properties permitting a statistical analysis of dynamics.

### 6.9.2 Diffusion and Chaos in the Standard Map

In some Hamiltonian systems, continuous dynamics can be translated to discrete dynamics. This applies in particular to systems on which we act with a periodic external force in the form of short pulses. The point  $(p, q)$  of the trajectory of the system (position and momentum) at time  $t+1$  is related to the point at time  $t$  when the system receives the pulse, by the equations

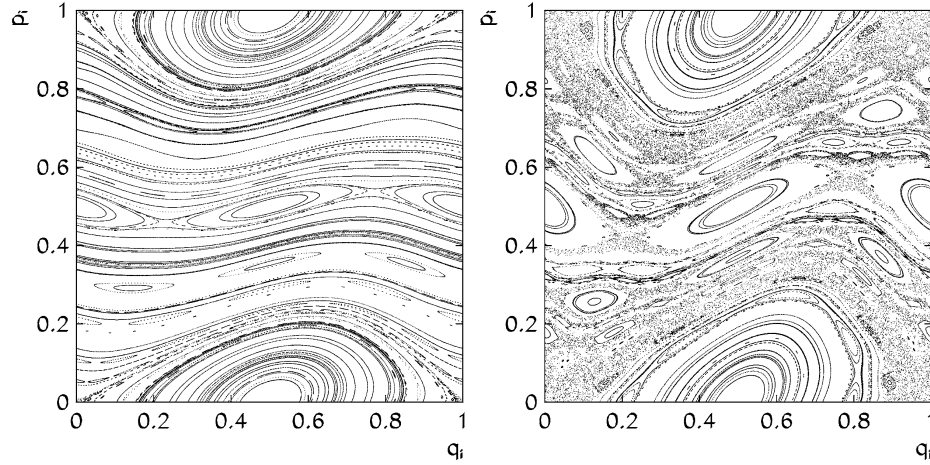
$$\begin{aligned} p(t+1) &= p(t) + F(q(t), p(t)), \\ q(t+1) &= q(t) + G(p(t+1)), \end{aligned}$$

where  $F$  is the force pulse and  $G$  represents the dynamics between the pulses. In such systems a very clear connection between diffusion and auto-correlation exists. The diffusion coefficient is defined as

$$D = \lim_{t \rightarrow \infty} \frac{1}{2t} \langle [q(t) - q(0)]^2 \rangle,$$

where  $\langle \cdot \rangle$  denotes the phase average (average over initial points  $(q(0), p(0))$  distributed uniformly in the region of phase space which is invariant with respect to the dynamics). The time auto-correlation function  $G$  is defined as

$$R_{GG}(\tau) = \langle G(p(\tau))G(p(0)) \rangle - \langle G(p(0)) \rangle^2.$$



**Fig. 6.19** Phase portraits of the standard map for different values of the parameter  $K$ . [Left]  $K = 0.5$ . [Right]  $K = 1.0$

By assuming that this system sufficiently quickly mixes the phase space, a relation between the diffusion coefficient and auto-correlation can be derived:

$$D = R_{GG}(0) + 2 \sum_{k=1}^{\infty} R_{GG}(k). \quad (6.39)$$

⊙ Analyze the dynamical system of the standard (Chirik's) map

$$\begin{aligned} p(t+1) &= p(t) + \frac{K}{2\pi} \sin(2\pi q(t)) \mod 1, \\ q(t+1) &= q(t) + p(t+1) \mod 1, \end{aligned}$$

which is defined on the torus  $(q(t), p(t)) \in [0, 1)^2$ . This map played a major role in the development of the theory of classical and quantum chaos [63]. Examples of phase portraits obtained by propagating a number of uniformly distributed points in the case of  $K = 0.5$  and  $K = 1.0$  are shown in Fig. 6.19. By increasing  $K$  above  $\approx 0.97$  the chaotic region of the phase space, where the points are distributed uniformly, becomes ever larger, until diffusion occurs throughout.

Compute the time auto-correlation  $R_{pp}(\tau) = \langle p(\tau+t)p(t) \rangle_t - \langle p(t) \rangle_t^2$  of the momentum samples  $\{p(t)\}_{t=0}^{N-1}$  for the values  $K = 1, 2, 5$ , and  $10$ , with the initial point  $(q(0), p(0))$  in the chaotic region of the phase space. The expected absolute error of  $R_{pp}(\tau)$  should be less than  $10^{-3}$ . If the auto-correlation decays rapidly, show it in the rescaled form  $R_{pp}(\tau)/R_{pp}(0)$  in logarithmic scale. If you observe an exponential fall-off of the auto-correlation,

$$|R_{pp}(\tau)| \sim e^{-\tau/\xi},$$

estimate the correlation length  $\xi$  which represents the time after which the trajectories become statistically independent. To compute the auto-correlation use the FFT algorithm (Sect. 4.2.5).

⊕ Observe the dependence of the diffusion coefficient  $D$  on the parameter  $K$  from the interval  $[2, 20]$ . Compute  $D$  by summing the auto-correlations of momentum (i.e. by using (6.39) in which  $R_{GG}$  is replaced by  $R_{pp}$ ). The initial points of the map should be located in the chaotic region of the phase space. An analytic approximation for the diffusion coefficient can be found in [63].

### 6.9.3 Phase Transitions in the Two-Dimensional Ising Model

Some properties of systems consisting of magnetic dipoles with local interactions can be nicely explained by the *Ising model*. This model assumes that the dipoles are arranged in the nodes of a two-dimensional mesh and that the spins  $s_i$  are either “up” ( $s_i = 1$ ) or “down” ( $s_i = -1$ ). The Hamiltonian (the energy) of such a system in the presence of an external magnetic field  $H$  can be written in the form

$$E = -J \sum_{\langle i, j \rangle} s_i s_j - H \sum_i s_i, \quad (6.40)$$

where the indices  $i$  and  $j$  represent the coordinates of the spins on the mesh (in two dimensions  $i \in \mathbb{N}_0^2$ ). The first sum in (6.40) runs over neighboring points only. The parameter  $J$  determines how the spins interact. For  $J > 0$  the adjacent dipoles tend to point in the same direction, while for  $J < 0$  they tend in the opposite directions. In the following we set  $J > 0$ . The total magnetization of the system is

$$M = \sum_i s_i.$$

At different temperatures the system may reside in ferromagnetic or paramagnetic phase. The temperature  $T_c$  of the phase transition between these phases in the absence of external field ( $H = 0$ ) is given by the equation  $\sinh(2J/(k_B T_c)) = 1$ , which has the solution  $T_c \approx 2.269185 J/k_B$ .

⊙ At the book’s website you can find the data for the thermodynamic equilibrium state of spins in the two-dimensional Ising model at various temperatures. A few examples are shown in Fig. 6.20. Compute the auto-correlation function of the orientation of spins on a  $N \times N$  mesh,

$$R_{ss}(i, j) = \frac{1}{N^2} \sum_{k, l} s_{k+i, l+j} s_{k, l},$$

where we assume periodic boundary conditions. Average the auto-correlation over the neighborhood of the points with approximately the same radius  $r$ . Assume that the auto-correlation has the form

$$|R_{ss}(i, j)| \sim C e^{-r/L}, \quad r = \sqrt{i^2 + j^2},$$

and estimate the correlation length  $L$ . Show  $L$  as a function of temperature: you should observe a strong increase in  $L$  near the critical temperature  $T_c$ .