3 Approach to Equilibrium : Worked Examples

(3.1) Consider the matrix

$$M = \begin{pmatrix} 4 & 4 \\ -1 & 9 \end{pmatrix} \quad .$$

(a) Find the characteristic polynomial $P(\lambda) = \det(\lambda \mathbb{I} - M)$ and the eigenvalues.

(b) For each eigenvalue λ_α, find the associated right eigenvector R_i^α and left eigenvector L_i^α. Normalize your eigenvectors so that $\langle\, L^\alpha \,|\, R^\beta \,\rangle = \delta_{\alpha\beta}$.

(c) Show explicitly that $M_{ij} = \sum_\alpha \lambda_\alpha \, R_i^\alpha \, L_j^\alpha$.

Solution :

(a) The characteristic polynomial is

$$P(\lambda) = \det \begin{pmatrix} \lambda - 4 & -4 \\ 1 & \lambda - 9 \end{pmatrix} = \lambda^2 - 13\,\lambda + 40 = (\lambda - 5)(\lambda - 8) \quad ,$$

so the two eigenvalues are $\lambda_1 = 5$ and $\lambda_2 = 8$.

(b) Let us write the right eigenvectors as $\vec{R}^\alpha = \begin{pmatrix} R_1^\alpha \\ R_2^\alpha \end{pmatrix}$ and the left eigenvectors as $\vec{L}^\alpha = \begin{pmatrix} L_1^\alpha & L_2^\alpha \end{pmatrix}$. Having found the eigenvalues, we only need to solve four equations:

$$4R_1^1 + 4R_2^1 = 5R_1^1 \quad , \quad 4R_1^2 + 4R_2^2 = 8R_1^2 \quad , \quad 4L_1^1 - L_2^1 = 5L_1^1 \quad , \quad 4L_1^2 - L_2^2 = 8L_1^2 \quad .$$

We are free to choose $R_1^\alpha = 1$ when possible. We must also satisfy the normalizations $\langle\, L^\alpha \,|\, R^\beta \,\rangle = L_i^\alpha R_i^\beta = \delta^{\alpha\beta}$. We then find

$$\vec{R}^1 = \begin{pmatrix} 1 \\ \frac{1}{4} \end{pmatrix} \quad , \quad \vec{R}^2 = \begin{pmatrix} 1 \\ 1 \end{pmatrix} \quad , \quad \vec{L}^1 = \begin{pmatrix} \frac{4}{3} & -\frac{4}{3} \end{pmatrix} \quad , \quad \vec{L}^2 = \begin{pmatrix} -\frac{1}{3} & \frac{4}{3} \end{pmatrix} \quad .$$

(c) The projectors onto the two eigendirections are

$$P_1 = |\, R^1 \,\rangle\langle\, L^1 \,| = \begin{pmatrix} \frac{4}{3} & -\frac{4}{3} \\ \frac{1}{3} & -\frac{1}{3} \end{pmatrix} \quad , \quad P_2 = |\, R^2 \,\rangle\langle\, L^2 \,| = \begin{pmatrix} -\frac{1}{3} & \frac{4}{3} \\ -\frac{1}{3} & \frac{4}{3} \end{pmatrix} \quad .$$

Note that $P_1 + P_2 = \mathbb{I}$. Now construct

$$\lambda_1 \, P_1 + \lambda_2 \, P_2 = \begin{pmatrix} 4 & 4 \\ -1 & 9 \end{pmatrix} \quad ,$$

as expected.

(3.2) Consider a three-state system with the following transition rates:

$$W_{12} = 0 \quad , \quad W_{21} = \gamma \quad , \quad W_{23} = 0 \quad , \quad W_{32} = 3\gamma \quad , \quad W_{13} = \gamma \quad , \quad W_{31} = \gamma \quad .$$

(a) Find the matrix Γ such that $\dot{P}_i = -\Gamma_{ij} P_j$.

(b) Find the equilibrium distribution $P_i^{\rm eq}$.

(c) Does this system satisfy detailed balance? Why or why not?

Solution :

(a) Following the prescription in the lecture notes, we have

$$\Gamma = \gamma \begin{pmatrix} 2 & 0 & -1 \\ -1 & 3 & 0 \\ -1 & -3 & 1 \end{pmatrix} \quad .$$

(b) Note that summing on the row index yields $\sum_i \Gamma_{ij} = 0$ for any j, hence $(1, 1, 1)$ is a left eigenvector of Γ with eigenvalue zero. It is quite simple to find the corresponding right eigenvector. Writing $\vec{\psi}^{\,\rm t} = (a, b, c)$, we obtain the equations $c = 2a$, $a = 3b$, and $a + 3b = c$, the solution of which, with $a + b + c = 1$ for normalization, is $a = \frac{3}{10}$, $b = \frac{1}{10}$, and $c = \frac{6}{10}$. Thus,

$$P^{\rm eq} = \begin{pmatrix} 0.3 \\ 0.1 \\ 0.6 \end{pmatrix} \quad .$$

(c) The equilibrium distribution does not satisfy detailed balance. Consider for example the ratio $P_1^{\rm eq}/P_2^{\rm eq} = 3$. According to detailed balance, this should be the same as W_{12}/W_{21}, which is zero for the given set of transition rates.

(3.3) A *Markov chain* is a process which describes transitions of a discrete stochastic variable occurring at discrete times. Let $P_i(t)$ be the probability that the system is in state i at time t. The evolution equation is

$$P_i(t+1) = \sum_j Q_{ij}\, P_j(t) \quad .$$

The *transition matrix* Q_{ij} satisfies $\sum_i Q_{ij} = 1$ so that the total probability $\sum_i P_i(t)$ is conserved. The element Q_{ij} is the *conditional probability* that for the system to evolve to state i at time $t+1$ given that it was in state j at time t. Now consider a group of Physics graduate students consisting of three theorists and four experimentalists. Within each group, the students are to be regarded as indistinguishable. Together, the students rent two apartments, A and B. Initially the three theorists live in A and the four experimentalists live in B. Each month, a random occupant of A and a random occupant of B exchange domiciles. Compute the transition matrix Q_{ij} for this Markov chain, and compute the average fraction of the time that B contains two theorists and two experimentalists, averaged over the effectively infinite time it takes the students to get their degrees. *Hint:* Q is a 4×4 matrix.

Solution:

There are four states available, and they are listed together with their degeneracies in Table 2.

$\vert\, j \,\rangle$	room A	room B	$g_j^{\rm A}$	$g_j^{\rm B}$	$g_j^{\rm TOT}$
$\vert\, 1 \,\rangle$	TTT	EEEE	1	1	1
$\vert\, 2 \,\rangle$	TTE	EEET	3	4	12
$\vert\, 3 \,\rangle$	TEE	EETT	3	6	18
$\vert\, 4 \,\rangle$	EEE	ETTT	1	4	4

Table 1: States and their degeneracies.

Let's compute the transition probabilities. First, we compute the transition probabilities out of state $\vert\, 1 \,\rangle$, *i.e.* the matrix elements Q_{j1}. Clearly $Q_{21} = 1$ since we must exchange a theorist (T) for an experimentalist (E). All the other probabilities are zero: $Q_{11} = Q_{31} = Q_{41} = 0$. For transitions out of state $\vert\, 2 \,\rangle$, the nonzero elements are

$$Q_{12} = \tfrac{1}{4} \times \tfrac{1}{3} = \tfrac{1}{12} \quad , \quad Q_{22} = \tfrac{3}{4} \times \tfrac{1}{3} + \tfrac{1}{4} \times \tfrac{2}{3} = \tfrac{5}{12} \quad , \quad Q_{32} = \tfrac{1}{2} \quad .$$

To compute Q_{12}, we must choose the experimentalist from room A (probability $\frac{1}{3}$) with the theorist from room B (probability $\frac{1}{4}$). For Q_{22}, we can either choose E from A and one of the E's from B, or one of the T's from A and the T from B. This explains the intermediate steps written above. For transitions out of state $\vert\, 3 \,\rangle$, the nonzero elements are then

$$Q_{23} = \tfrac{1}{3} \quad , \quad Q_{33} = \tfrac{1}{2} \quad , \quad Q_{43} = \tfrac{1}{6} \quad .$$

Finally, for transitions out of state $\vert\, 4 \,\rangle$, the nonzero elements are

$$Q_{34} = \tfrac{3}{4} \quad , \quad Q_{44} = \tfrac{1}{4} \quad .$$

The full transition matrix is then

$$Q = \begin{pmatrix} 0 & \frac{1}{12} & 0 & 0 \\ 1 & \frac{5}{12} & \frac{1}{3} & 0 \\ 0 & \frac{1}{2} & \frac{1}{2} & \frac{3}{4} \\ 0 & 0 & \frac{1}{6} & \frac{1}{4} \end{pmatrix} \quad .$$

Note that $\sum_i Q_{ij} = 1$ for all $j = 1, 2, 3, 4$. This guarantees that $\phi^{(1)} = (1\,,\,1\,,\,1\,,\,1)$ is a left eigenvector of Q with eigenvalue 1. The corresponding right eigenvector is obtained by setting $Q_{ij}\, \psi_j^{(1)} = \psi_i^{(1)}$. Simultaneously solving

these four equations and normalizing so that $\sum_j \psi_j^{(1)} = 1$, we easily obtain

$$\psi^{(1)} = \frac{1}{35}\begin{pmatrix} 1 \\ 12 \\ 18 \\ 4 \end{pmatrix} \quad .$$

This is the state we converge to after repeated application of the transition matrix Q. If we decompose $Q = \sum_{\alpha=1}^{4} \lambda_\alpha \, | \, \psi^{(\alpha)} \, \rangle \langle \, \phi^{(\alpha)} \, |$, then in the limit $t \to \infty$ we have $Q^t \approx | \, \psi^{(1)} \, \rangle \langle \, \phi^{(1)} \, |$, where $\lambda_1 = 1$, since the remaining eigenvalues are all less than 1 in magnitude[1]. Thus, Q^t acts as a *projector* onto the state $| \, \psi^{(1)} \, \rangle$. Whatever the initial set of probabilities $P_j(t=0)$, we must have $\langle \, \phi^{(1)} \, | \, P(0) \, \rangle = \sum_j P_j(0) = 1$. Therefore, $\lim_{t\to\infty} P_j(t) = \psi_j^{(1)}$, and we find $P_3(\infty) = \frac{18}{35}$. Note that the equilibrium distribution satisfies detailed balance:

$$\psi_j^{(1)} = \frac{g_j^{\rm TOT}}{\sum_l g_l^{\rm TOT}} \quad .$$

[1] One can check that $\lambda_1 = 1$, $\lambda_2 = \frac{5}{12}$, $\lambda_3 = -\frac{1}{4}$. and $\lambda_4 = 0$.

(3.4) Suppose I have three bags containing among them four coins. Initially, bag #1 contains a quarter, bag #2 contains a dime, and bag #3 contains two nickels. At each time step, I choose two bags randomly and randomly exchange one coin from each bag. The time evolution satisfies $P_i(t+1) = \sum_j Q_{ij}\, P_j(t)$, where Q_{ij} is the conditional probability $Q_{ij} = P(i\,,\, t+1\,|\,j\,,\, t)$ that the system is in state i at time $t+1$ given that it was in state j at time t.

(a) How many configurations are there for this system?

(b) Construct the transition matrix Q_{ij} and verify that $\sum_i Q_{ij} = 1$.

(c) Find the eigenvalues of Q (you may want to use something like `Mathematica`).

(d) Find the equilibrium distribution $P_i^{\rm eq}$.

Solution :

(a) There are seven possible configurations for this system, shown in Table 2 below.

	1	2	3	4	5	6	7
bag 1	Q	Q	D	D	N	N	N
bag 2	D	N	Q	N	Q	D	N
bag 3	NN	DN	NN	QN	DN	QN	DQ
g	1	2	1	2	2	2	2

Table 2: Configurations and their degeneracies for problem 3.

(b) The transition matrix is

$$Q = \begin{pmatrix} 0 & \frac{1}{6} & \frac{1}{3} & 0 & 0 & \frac{1}{6} & 0 \\ \frac{1}{3} & \frac{1}{6} & 0 & \frac{1}{6} & \frac{1}{3} & 0 & \frac{1}{6} \\ \frac{1}{3} & 0 & 0 & \frac{1}{6} & \frac{1}{6} & 0 & 0 \\ 0 & \frac{1}{6} & \frac{1}{3} & \frac{1}{6} & 0 & \frac{1}{3} & \frac{1}{6} \\ 0 & \frac{1}{3} & \frac{1}{3} & 0 & \frac{1}{6} & \frac{1}{6} & \frac{1}{6} \\ \frac{1}{3} & 0 & 0 & \frac{1}{3} & \frac{1}{6} & \frac{1}{6} & \frac{1}{6} \\ 0 & \frac{1}{6} & 0 & \frac{1}{6} & \frac{1}{6} & \frac{1}{6} & \frac{1}{3} \end{pmatrix}$$

(c) Interrogating `Mathematica`, I find the eigenvalues are

$$\lambda_1 = 1 \quad , \quad \lambda_2 = -\tfrac{2}{3} \quad , \quad \lambda_3 = \tfrac{1}{3} \quad , \quad \lambda_4 = \tfrac{1}{3} \quad , \quad \lambda_5 = \lambda_6 = \lambda_7 = 0 \quad .$$

(d) We may decompose Q into its left and right eigenvectors, writing

$$Q = \sum_{a=1}^{7} \lambda_a \,|\, R^a \,\rangle\langle\, L^a \,|$$

$$Q_{ij} = \sum_{a=1}^{7} \lambda_a \, R_i^a \, L_j^a$$

The full matrix of left (row) eigenvectors is

$$L = \begin{pmatrix} 1 & 1 & 1 & 1 & 1 & 1 & 1 \\ -2 & 1 & 2 & -1 & -1 & 1 & 0 \\ -1 & 0 & -1 & 0 & 0 & 0 & 1 \\ 0 & -1 & 0 & 1 & -1 & 1 & 0 \\ 1 & -1 & 1 & -1 & 0 & 0 & 1 \\ 1 & 0 & -1 & -1 & 0 & 1 & 0 \\ -1 & -1 & 1 & 0 & 1 & 0 & 0 \end{pmatrix}$$

The corresponding matrix of right (column) eigenvectors is

$$R = \frac{1}{24} \begin{pmatrix} 2 & -3 & -6 & 0 & 4 & 1 & -5 \\ 4 & 3 & 0 & -6 & -4 & -1 & -7 \\ 2 & 3 & -6 & 0 & 4 & -5 & 1 \\ 4 & -3 & 0 & 6 & -4 & -7 & -1 \\ 4 & -3 & 0 & -6 & -4 & 5 & 11 \\ 4 & 3 & 0 & 6 & -4 & 11 & 5 \\ 4 & 0 & 12 & 0 & 8 & -4 & -4 \end{pmatrix}$$

Thus, we have $RL = LR = \mathbb{I}$, *i.e.* $R = L^{-1}$, and

$$Q = R\,\Lambda\,L \quad ,$$

with $\Lambda = \mathsf{diag}\big(1\,,\,-\frac{2}{3}\,,\,\frac{1}{3}\,,\,\frac{1}{3}\,,\,0\,,\,0\,,\,0\big)$.

The right eigenvector corresponding to the $\lambda = 1$ eigenvalue is the equilibrium distribution. We therefore read off the first column of the R matrix:

$$(P^{\rm eq})^{\rm t} = \big(\tfrac{1}{12} \quad \tfrac{1}{6} \quad \tfrac{1}{12} \quad \tfrac{1}{6} \quad \tfrac{1}{6} \quad \tfrac{1}{6} \quad \tfrac{1}{6}\big) \quad .$$

Note that

$$P_i^{\rm eq} = \frac{g_i}{\sum_j g_j} \quad ,$$

where g_j is the degeneracy of state j (see Tab. 2). Why is this so? It is because our random choices guarantee that $Q_{ij}\,g_j = Q_{ji}\,g_i$ for each i and j (*i.e.* no sum on repeated indices). Now sum this equation on j, and use $\sum_j Q_{ji} = 1$. We obtain $\sum_j Q_{ij}\,g_j = g_i$, which says that the $|\,g\,\rangle$ is a right eigenvector of Q with eigenvalue 1. To obtain the equilibrium probability distribution, we just have to normalize by dividing by $\sum_j g_j$.

(3.5) A ball of mass m executes perfect one-dimensional motion along the symmetry axis of a piston. Above the ball lies a mobile piston head of mass M which slides frictionlessly inside the piston. Both the ball and piston head execute ballistic motion, with two types of collision possible: (i) the ball may bounce off the floor, which is assumed to be infinitely massive and fixed in space, and (ii) the ball and piston head may engage in a one-dimensional elastic collision. The Hamiltonian is

$$H = \frac{P^2}{2M} + \frac{p^2}{2m} + MgX + mgx \quad ,$$

where X is the height of the piston head and x the height of the ball. Another quantity is conserved by the dynamics: $\Theta(X - x)$. *I.e.*, the ball always is below the piston head.

(a) Choose an arbitrary length scale L, and then energy scale $E_0 = MgL$, momentum scale $P_0 = M\sqrt{gL}$, and time scale $\tau_0 = \sqrt{L/g}$. Show that the dimensionless Hamiltonian becomes

$$\bar{H} = \tfrac{1}{2}\bar{P}^2 + \bar{X} + \frac{\bar{p}^2}{2r} + r\bar{x} \quad ,$$

with $r = m/M$, and with equations of motion $d\bar{X}/dt = \partial\bar{H}/\partial\bar{P}$, *etc.* (Here the bar indicates dimensionless variables: $\bar{P} = P/P_0$, $\bar{t} = t/\tau_0$, *etc.*) What special dynamical consequences hold for $r = 1$?

(b) Compute the microcanonical average piston height $\langle X \rangle$. The analogous dynamical average is

$$\langle X \rangle_T = \lim_{T\to\infty} \frac{1}{T} \int_0^T dt\, X(t) \quad .$$

When computing microcanonical averages, it is helpful to use the Laplace transform, discussed in ch. 3 of the lecture notes. (It is possible to compute the microcanonical average by more brute force methods as well.)

(c) Compute the microcanonical average of the rate of collisions between the ball and the floor. Show that this is given by

$$\Big\langle \sum_i \delta(t - t_i) \Big\rangle = \big\langle \Theta(v)\, v\, \delta(x - 0^+) \big\rangle \quad .$$

The analogous dynamical average is

$$\langle \gamma \rangle_T = \lim_{T\to\infty} \frac{1}{T} \int_0^T dt\, \sum_i \delta(t - t_i) \quad ,$$

where $\{t_i\}$ is the set of times at which the ball hits the floor.

(d) How do your results change if you do not enforce the dynamical constraint $X \geq x$?

(e) Write a computer program to simulate this system. The only input should be the mass ratio r (set $\bar{E} = 10$ to fix the energy). You also may wish to input the initial conditions, or perhaps to choose the initial conditions randomly (all satisfying energy conservation, of course!). Have your program compute the microcanonical as well as dynamical averages in parts (b) and (c). Plot out the Poincaré section of P *vs.* X for those times when the ball hits the floor. Investigate this for several values of r. Just to show you that this is interesting, I've plotted some of my own numerical results in fig. 1.

Solution:

(a) Once we choose a length scale L (arbitrary), we may define $E_0 = M\,g\,L$, $P_0 = M\sqrt{gL}$, $V_0 = \sqrt{gL}$, and $\tau_0 = \sqrt{L/g}$ as energy, momentum, velocity, and time scales, respectively, the result follows directly. Rather than write $\bar{P} = P/P_0$ *etc.*, we will drop the bar notation and write

$$H = \tfrac{1}{2}P^2 + X + \frac{p^2}{2r} + rx \quad .$$

(b) What is missing from the Hamiltonian of course is the interaction potential between the ball and the piston head. We assume that both objects are impenetrable, so the potential energy is infinite when the two overlap. We further assume that the ball is a point particle (otherwise reset ground level to minus the diameter of the ball). We can eliminate the interaction potential from H if we enforce that each time $X = x$ the ball and the piston head undergo an elastic collision. From energy and momentum conservation, it is easy to derive the elastic collision formulae

$$P' = \frac{1-r}{1+r}\,P + \frac{2}{1+r}\,p$$

$$p' = \frac{2r}{1+r}\,P - \frac{1-r}{1+r}\,p \quad .$$

We can now answer the last question from part (a). When $r = 1$, we have that $P' = p$ and $p' = P$, *i.e.* the ball and piston simply exchange momenta. The problem is then equivalent to two identical particles elastically bouncing off the bottom of the piston, and moving through each other as if they were completely transparent. When the trajectories cross, however, the particles exchange identities.

Averages within the microcanonical ensemble are normally performed with respect to the phase space distribution

$$\varrho(\boldsymbol{\varphi}) = \frac{\delta\big(E - H(\boldsymbol{\varphi})\big)}{\mathsf{Tr}\;\delta\big(E - H(\boldsymbol{\varphi})\big)} \quad ,$$

where $\boldsymbol{\varphi} = (P, X, p, x)$, and

$$\mathsf{Tr}\;F(\boldsymbol{\varphi}) = \int\limits_{-\infty}^{\infty} dP \int\limits_{0}^{\infty} dX \int\limits_{-\infty}^{\infty} dp \int\limits_{0}^{\infty} dx\; F(P, X, p, x) \quad .$$

Since $X \geq x$ is a dynamical constraint, we should define an appropriately restricted microcanonical average:

$$\big\langle F(\boldsymbol{\varphi})\big\rangle_{\mu\mathrm{ce}} \equiv \widetilde{\mathsf{Tr}}\,\Big[F(\boldsymbol{\varphi})\,\delta\big(E - H(\boldsymbol{\varphi})\big)\Big] \Big/ \widetilde{\mathsf{Tr}}\,\delta\big(E - H(\boldsymbol{\varphi})\big)$$

where

$$\widetilde{\mathsf{Tr}}\,F(\boldsymbol{\varphi}) \equiv \int\limits_{-\infty}^{\infty} dP \int\limits_{0}^{\infty} dX \int\limits_{-\infty}^{\infty} dp \int\limits_{0}^{X} dx\; F(P, X, p, x)$$

is the modified trace. Note that the integral over x has an upper limit of X rather than ∞, since the region of phase space with $x > X$ is *dynamically inaccessible*.

When computing the traces, we shall make use of the following result from the theory of Laplace transforms. The Laplace transform of a function $K(E)$ is

$$\widehat{K}(\beta) = \int\limits_{0}^{\infty} dE\; K(E)\, e^{-\beta E} \quad .$$

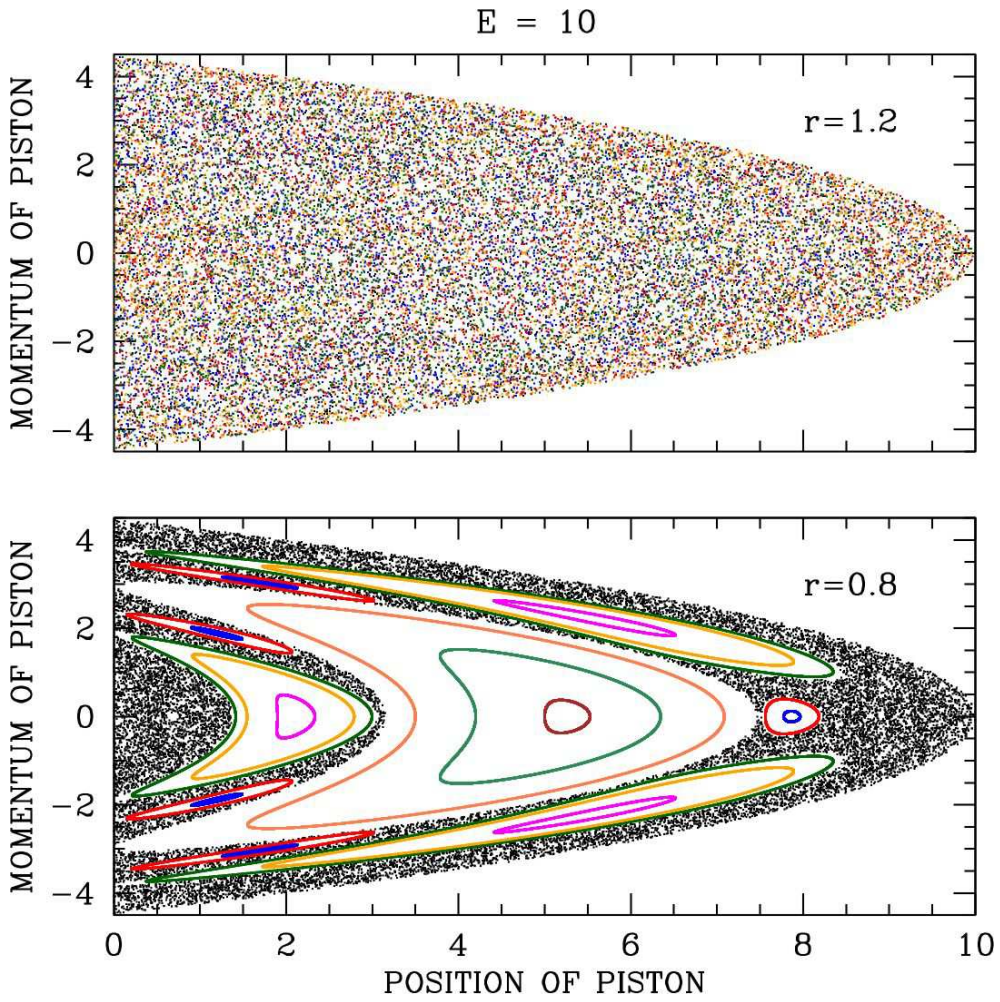

Figure 1: Poincaré sections for the ball and piston head problem. Each color corresponds to a different initial condition. When the mass ratio $r = m/M$ exceeds unity, the system apparently becomes ergodic.

The inverse Laplace transform is given by

$$K(E) = \int\limits_{c-i\infty}^{c+i\infty} \frac{d\beta}{2\pi i}\, \widehat{K}(\beta)\, e^{\beta E} \quad ,$$

where the integration contour, which is a line extending from $\beta = c - i\infty$ to $\beta = c + i\infty$, lies to the right of any singularities of $\widehat{K}(\beta)$ in the complex β-plane. For this problem, all we shall need is the following:

$$K(E) = \frac{E^{t-1}}{\Gamma(t)} \quad \Longleftrightarrow \quad \widehat{K}(\beta) = \beta^{-t} \quad .$$

For a proof, see ch. 4 of the lecture notes.

We're now ready to compute the microcanonical average of X. We have

$$\langle X \rangle = \frac{N(E)}{D(E)} \quad ,$$

where

$$N(E) = \widetilde{\mathsf{Tr}}\left[X\,\delta(E-H)\right]$$
$$D(E) = \widetilde{\mathsf{Tr}}\,\delta(E-H) \quad .$$

Let's first compute $D(E)$. To do this, we compute the Laplace transform $\widehat{D}(\beta)$:

$$\begin{aligned}\widehat{D}(\beta) &= \widetilde{\mathsf{Tr}}\,e^{-\beta H} \\ &= \int\limits_{-\infty}^{\infty} dP\,e^{-\beta P^2/2} \int\limits_{-\infty}^{\infty} dp\,e^{-\beta p^2/2r} \int\limits_{0}^{\infty} dX\,e^{-\beta X} \int\limits_{0}^{X} dx\,e^{-\beta r x} \\ &= \frac{2\pi\sqrt{r}}{\beta} \int\limits_{0}^{\infty} dX\,e^{-\beta X}\left(\frac{1-e^{-\beta r X}}{\beta r}\right) = \frac{\sqrt{r}}{1+r}\cdot\frac{2\pi}{\beta^3} \quad .\end{aligned}$$

Similarly for $\widehat{N}(\beta)$ we have

$$\begin{aligned}\widehat{N}(\beta) &= \widetilde{\mathsf{Tr}}\,X\,e^{-\beta H} \\ &= \int\limits_{-\infty}^{\infty} dP\,e^{-\beta P^2/2} \int\limits_{-\infty}^{\infty} dp\,e^{-\beta p^2/2r} \int\limits_{0}^{\infty} dX\,X\,e^{-\beta X} \int\limits_{0}^{X} dx\,e^{-\beta r x} \\ &= \frac{2\pi\sqrt{r}}{\beta} \int\limits_{0}^{\infty} dX\,X\,e^{-\beta X}\left(\frac{1-e^{-\beta r X}}{\beta r}\right) = \frac{(2+r)\,r^{3/2}}{(1+r)^2}\cdot\frac{2\pi}{\beta^4} \quad .\end{aligned}$$

Taking the inverse Laplace transform, we then have

$$D(E) = \frac{\sqrt{r}}{1+r}\cdot\pi E^2 \qquad , \qquad N(E) = \frac{(2+r)\,\sqrt{r}}{(1+r)^2}\cdot\tfrac{1}{3}\pi E^3 \quad .$$

We then have

$$\langle X\rangle = \frac{N(E)}{D(E)} = \left(\frac{2+r}{1+r}\right)\cdot\tfrac{1}{3}E \quad .$$

The 'brute force' evaluation of the integrals isn't so bad either. We have

$$D(E) = \int\limits_{-\infty}^{\infty} dP \int\limits_{0}^{\infty} dX \int\limits_{-\infty}^{\infty} dp \int\limits_{0}^{X} dx\,\delta\big(\tfrac{1}{2}P^2 + \tfrac{1}{2r}p^2 + X + rx - E\big) \quad .$$

To evaluate, define $P = \sqrt{2}\,u_x$ and $p = \sqrt{2r}\,u_y$. Then we have $dP\,dp = 2\sqrt{r}\,du_x\,du_y$ and $\frac{1}{2}P^2 + \frac{1}{2r}\,p^2 = u_x^2 + u_y^2$. Now convert to 2D polar coordinates with $w \equiv u_x^2 + u_y^2$. Thus,

$$\begin{aligned}D(E) &= 2\pi\sqrt{r}\int\limits_{0}^{\infty} dw \int\limits_{0}^{\infty} dX \int\limits_{0}^{X} dx\,\delta\big(w + X + rx - E\big) \\ &= \frac{2\pi}{\sqrt{r}}\int\limits_{0}^{\infty} dw \int\limits_{0}^{\infty} dX \int\limits_{0}^{X} dx\;\Theta(E-w-X)\,\Theta(X+rX-E+w) \\ &= \frac{2\pi}{\sqrt{r}}\int\limits_{0}^{E} dw \int\limits_{\frac{E-w}{1+r}}^{E-w} dX = \frac{2\pi\sqrt{r}}{1+r}\int\limits_{0}^{E} dq\,q = \frac{\sqrt{r}}{1+r}\cdot\pi E^2 \quad ,\end{aligned}$$

with $q = E - w$. Similarly,

$$\begin{aligned} N(E) &= 2\pi\sqrt{r}\int_0^\infty dw \int_0^\infty dX\, X \int_0^X dx\, \delta\big(w + X + rx - E\big) \\ &= \frac{2\pi}{\sqrt{r}} \int_0^\infty dw \int_0^\infty dX\, X \int_0^X dx\ \Theta(E - w - X)\,\Theta(X + rX - E + w) \\ &= \frac{2\pi}{\sqrt{r}} \int_0^E dw \int_{\frac{E-w}{1+r}}^{E-w} dX\, X = \frac{2\pi}{\sqrt{r}} \int_0^E dq \left(1 - \frac{1}{(1+r)^2}\right) \cdot \tfrac{1}{2} q^2 = \left(\frac{2+r}{1+r}\right) \cdot \frac{\sqrt{r}}{1+r} \cdot \tfrac{1}{3}\pi E^3 \quad . \end{aligned}$$

(c) Using the general result

$$\delta\big(F(x) - A\big) = \sum_i \frac{\delta(x - x_i)}{\big|F'(x_i)\big|} \quad ,$$

where $F(x_i) = A$, we recover the desired expression. We should be careful not to double count, so to avoid this difficulty we can evaluate $\delta(t - t_i^+)$, where $t_i^+ = t_i + 0^+$ is infinitesimally later than t_i. The point here is that when $t = t_i^+$ we have $p = r\,v > 0$ (*i.e.* just after hitting the bottom). Similarly, at times $t = t_i^-$ we have $p < 0$ (*i.e.* just prior to hitting the bottom). Note $v = p/r$. Again we write $\gamma(E) = N(E)/D(E)$, this time with

$$N(E) = \widetilde{\mathsf{Tr}}\left[\Theta(p)\, r^{-1} p\, \delta(x - 0^+)\, \delta(E - H)\right] \quad .$$

The Laplace transform is

$$\begin{aligned} \widehat{N}(\beta) &= \int_{-\infty}^\infty dP\, e^{-\beta P^2/2} \int_0^\infty dp\, r^{-1}\, p\, e^{-\beta p^2/2r} \int_0^\infty dX\, e^{-\beta X} \\ &= \sqrt{\frac{2\pi}{\beta}} \cdot \frac{1}{\beta} \cdot \frac{1}{\beta} = \sqrt{2\pi}\,\beta^{-5/2} \quad . \end{aligned}$$

Thus,

$$N(E) = \tfrac{4\sqrt{2}}{3}\, E^{3/2}$$

and

$$\langle\gamma\rangle = \frac{N(E)}{D(E)} = \tfrac{4\sqrt{2}}{3\pi}\left(\frac{1+r}{\sqrt{r}}\right) E^{-1/2} \quad .$$

(d) When the constraint $X \geq x$ is removed, we integrate over all phase space. We then have

$$\begin{aligned} \widehat{D}(\beta) &= \mathsf{Tr}\ e^{-\beta H} \\ &= \int_{-\infty}^\infty dP\, e^{-\beta P^2/2} \int_{-\infty}^\infty dp\, e^{-\beta p^2/2r} \int_0^\infty dX\, e^{-\beta X} \int_0^\infty dx\, e^{-\beta r x} = \frac{2\pi\sqrt{r}}{\beta^3} \quad . \end{aligned}$$

For part (b) we would then have

$$\begin{aligned} \widehat{N}(\beta) &= \mathsf{Tr}\ X\, e^{-\beta H} \\ &= \int_{-\infty}^\infty dP\, e^{-\beta P^2/2} \int_{-\infty}^\infty dp\, e^{-\beta p^2/2r} \int_0^\infty dX\, X\, e^{-\beta X} \int_0^\infty dx\, e^{-\beta r x} = \frac{2\pi\sqrt{r}}{\beta^4} \quad . \end{aligned}$$

The respective inverse Laplace transforms are $D(E) = \pi\sqrt{r}\,E^2$ and $N(E) = \frac{1}{3}\pi\sqrt{r}\,E^3$. The microcanonical average of X would then be

$$\langle X\rangle = \tfrac{1}{3}E \quad .$$

Using the restricted phase space, we obtained a value which is greater than this by a factor of $(2+r)/(1+r)$. That the restricted average gives a larger value makes good sense, since X is not allowed to descend below x in that case. For part (c), we would obtain the same result for $N(E)$ since $x = 0$ in the average. We would then obtain

$$\langle\gamma\rangle = \tfrac{4\sqrt{2}}{3\pi}\,r^{-1/2}\,E^{-1/2} \quad .$$

The restricted microcanonical average yields a rate which is larger by a factor $1 + r$. Again, it makes good sense that the restricted average should yield a higher rate, since the ball is not allowed to attain a height greater than the instantaneous value of X.

(e) It is straightforward to simulate the dynamics. So long as $0 < x(t) < X(t)$, we have

$$\dot X = P \quad , \quad \dot P = -1 \quad , \quad \dot x = \frac{p}{r} \quad , \quad \dot p = -r \quad .$$

Starting at an arbitrary time t_0, these equations are integrated to yield

$$\begin{aligned} X(t) &= X(t_0) + P(t_0)\,(t-t_0) - \tfrac{1}{2}(t-t_0)^2 \\ P(t) &= P(t_0) - (t-t_0) \\ x(t) &= x(t_0) + \frac{p(t_0)}{r}\,(t-t_0) - \tfrac{1}{2}(t-t_0)^2 \\ p(t) &= p(t_0) - r(t-t_0) \quad . \end{aligned}$$

We must stop the evolution when one of two things happens. The first possibility is a bounce at $t = t_{\rm b}$, meaning $x(t_{\rm b}) = 0$. The momentum $p(t)$ changes discontinuously at the bounce, with $p(t_{\rm b}^+) = -p(t_{\rm b}^-)$, and where $p(t_{\rm b}^-) < 0$ necessarily. The second possibility is a collision at $t = t_{\rm c}$, meaning $X(t_{\rm c}) = x(t_{\rm c})$. Integrating across the collision, we must conserve both energy and momentum. This means

$$P(t_{\rm c}^+) = \frac{1-r}{1+r}\,P(t_{\rm c}^-) + \frac{2}{1+r}\,p(t_{\rm c}^-)$$

$$p(t_{\rm c}^+) = \frac{2r}{1+r}\,P(t_{\rm c}^-) - \frac{1-r}{1+r}\,p(t_{\rm c}^-) \quad .$$

r	$X(0)$	$\langle X(t)\rangle$	$\langle X\rangle_{\mu\rm ce}$	$\langle\gamma(t)\rangle$	$\langle\gamma\rangle_{\mu\rm ce}$	r	$X(0)$	$\langle X(t)\rangle$	$\langle X\rangle_{\mu\rm ce}$	$\langle\gamma(t)\rangle$	$\langle\gamma\rangle_{\mu\rm ce}$
0.3	0.1	6.1743	5.8974	0.5283	0.4505	1.2	0.1	4.8509	4.8545	0.3816	0.3812
0.3	1.0	5.7303	5.8974	0.4170	0.4505	1.2	1.0	4.8479	4.8545	0.3811	0.3812
0.3	3.0	5.7876	5.8974	0.4217	0.4505	1.2	3.0	4.8493	4.8545	0.3813	0.3812
0.3	5.0	5.8231	5.8974	0.4228	0.4505	1.2	5.0	4.8482	4.8545	0.3813	0.3812
0.3	7.0	5.8227	5.8974	0.4228	0.4505	1.2	7.0	4.8472	4.8545	0.3808	0.3812
0.3	9.0	5.8016	5.8974	0.4234	0.4505	1.2	9.0	4.8466	4.8545	0.3808	0.3812
0.3	9.9	6.1539	5.8974	0.5249	0.4505	1.2	9.9	4.8444	4.8545	0.3807	0.3812

Table 3: Comparison of time averages and microcanonical ensemble averages for $r = 0.3$ and $r = 1.2$. Initial conditions are $P(0) = x(0) = 0$, with $X(0)$ given in the table and $E = 10$. Averages were performed over a period extending for $N_{\rm b} = 10^7$ bounces.

In the following tables I report on the results of numerical simulations, comparing dynamical averages with (restricted) phase space averages within the microcanonical ensemble. For $r = 0.3$ the microcanonical averages

poorly approximate the dynamical averages, and the dynamical averages are dependent on the initial conditions, indicating that the system is not ergodic. For $r = 1.2$, the agreement between dynamical and microcanonical averages generally improves with averaging time. Indeed, it has been shown by N. I. Chernov, *Physica D* **53**, 233 (1991), building on the work of M. P. Wojtkowski, *Comm. Math. Phys.* **126**, 507 (1990) that this system is ergodic for $r > 1$. Wojtkowski also showed that this system is equivalent to the *wedge billiard*, in which a single point particle of mass m bounces inside a two-dimensional wedge-shaped region $\{(\mathrm{x},\mathrm{y}) \,|\, \mathrm{x} \geq 0\ ,\ \mathrm{y} \geq \mathrm{x}\,\mathrm{ctn}\,\phi\}$ for some fixed angle $\phi = \tan^{-1}\sqrt{\frac{m}{M}}$. To see this, pass to relative ($\mathcal{X}$) and center-of-mass ($\mathcal{Y}$) coordinates,

$$\mathcal{X} = X - x \qquad\qquad \mathcal{P}_x = \frac{mP - Mp}{M+m}$$
$$\mathcal{Y} = \frac{MX + mx}{M+m} \qquad\qquad \mathcal{P}_y = P + p \quad .$$

Then

$$H = \frac{(M+m)\,\mathcal{P}_x^2}{2Mm} + \frac{\mathcal{P}_y^2}{2(M+m)} + (M+m)\,g\mathcal{Y} \quad .$$

There are two constraints. One requires $X \geq x$, *i.e.* $\mathcal{X} \geq 0$. The second requires $x > 0$, *i.e.*

$$x = \mathcal{Y} - \frac{M}{M+m}\,\mathcal{X} \geq 0 \quad .$$

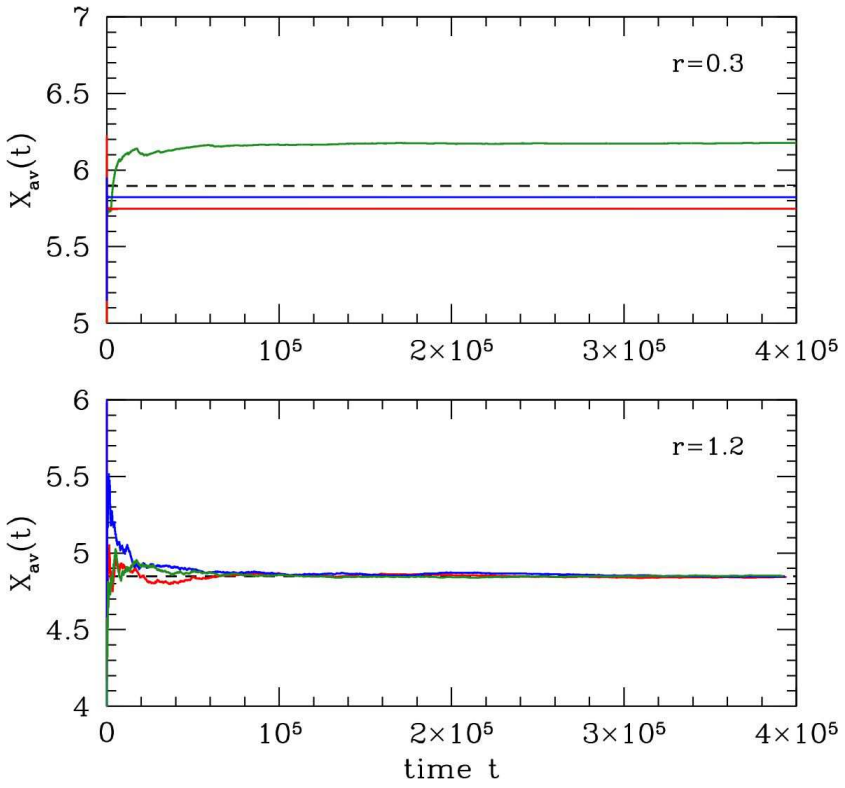

Figure 2: Long time running numerical averages $X_{\rm av}(t) \equiv t^{-1}\int_0^t dt'\ X(t')$ for $r = 0.3$ (top) and $r = 1.2$ (bottom), each for three different initial conditions, with $E = 10$ in all cases. Note how in the $r = 0.3$ case the long time average is dependent on the initial condition, while the $r = 1.2$ case is ergodic and hence independent of initial conditions. The dashed black line shows the restricted microcanonical average, $\langle X\rangle_{\mu\rm ce} = \frac{(2+r)}{(1+r)}\cdot\frac{1}{3}E$.

Now define $\mathsf{x} \equiv \mathcal{X}$, $\mathsf{p}_x \equiv \mathcal{P}_x$, and rescale $\mathsf{y} \equiv \frac{M+m}{\sqrt{Mm}}\,\mathcal{Y}$ and $\mathsf{p}_y \equiv \frac{\sqrt{Mm}}{M+m}\,\mathcal{P}_y$ to obtain

$$H = \frac{1}{2\mu}\left(\mathsf{p}_x^2 + \mathsf{p}_y^2\right) + \mathsf{M}\, g\, \mathsf{y}$$

with $\mu = \frac{Mm}{M+m}$ the familiar reduced mass and $\mathsf{M} = \sqrt{Mm}$. The constraints are then $\mathsf{x} \geq 0$ and $\mathsf{y} \geq \sqrt{\frac{M}{m}}\,\mathsf{x}$.

r	$X(0)$	$N_{\rm b}$	$\langle X(t)\rangle$	$\langle X\rangle_{\mu{\rm ce}}$	$\langle \gamma(t)\rangle$	$\langle \gamma\rangle_{\mu{\rm ce}}$
1.2	7.0	10^4	4.8054892	4.8484848	0.37560388	0.38118510
1.2	7.0	10^5	4.8436969	4.8484848	0.38120356	0.38118510
1.2	7.0	10^6	4.8479414	4.8484848	0.38122778	0.38118510
1.2	7.0	10^7	4.8471686	4.8484848	0.38083749	0.38118510
1.2	7.0	10^8	4.8485825	4.8484848	0.38116282	0.38118510
1.2	7.0	10^9	4.8486682	4.8484848	0.38120259	0.38118510
1.2	1.0	10^9	4.8485381	4.8484848	0.38118069	0.38118510
1.2	9.9	10^9	4.8484886	4.8484848	0.38116295	0.38118510

Table 4: Comparison of time averages and microcanonical ensemble averages for $r = 1.2$, with $N_{\rm b}$ ranging from 10^4 to 10^9.

(3.6) Consider a toroidal phase space $(x, p) \in \mathbb{T}^2$. You can describe the torus as a square $[0, 1] \times [0, 1]$ with opposite sides identified. Design your own modified Arnold cat map acting on this phase space, *i.e.* a 2×2 matrix with integer coefficients and determinant 1.

(a) Start with an initial distribution localized around the center – say a disc centered at $(\frac{1}{2}, \frac{1}{2})$. Show how these initial conditions evolve under your map. Can you tell whether your dynamics are mixing?

(b) Now take a pixelated image. For reasons discussed in the lecture notes, this image should exhibit Poincaré recurrence. Can you see this happening?

Solution :

(a) Any map

$$\begin{pmatrix} x' \\ p' \end{pmatrix} = \overbrace{\begin{pmatrix} a & b \\ c & d \end{pmatrix}}^{M} \begin{pmatrix} x \\ p \end{pmatrix} \quad ,$$

will do, provided $a, b, c, d \in \mathbb{Z}$ and $\det M = ad - bc = 1$. Such matrices are said to be elements of the *modular group*: $M \in \mathsf{SL}(2, \mathbb{Z})$. Arnold's cat map $M = \begin{pmatrix} 1 & 1 \\ 1 & 2 \end{pmatrix}$ and its generalizations $M = \begin{pmatrix} 1 & 1 \\ p & p+1 \end{pmatrix}$ are modular transformations. Starting from an initial square distribution, we iterate the map up to three times and show the results in Fig. 3. The numerical results are consistent with a mixing flow. (With just a few further interations, almost the entire torus is covered.)

(c) A pixelated image exhibits Poincaré recurrence, as we see in Fig. 4.

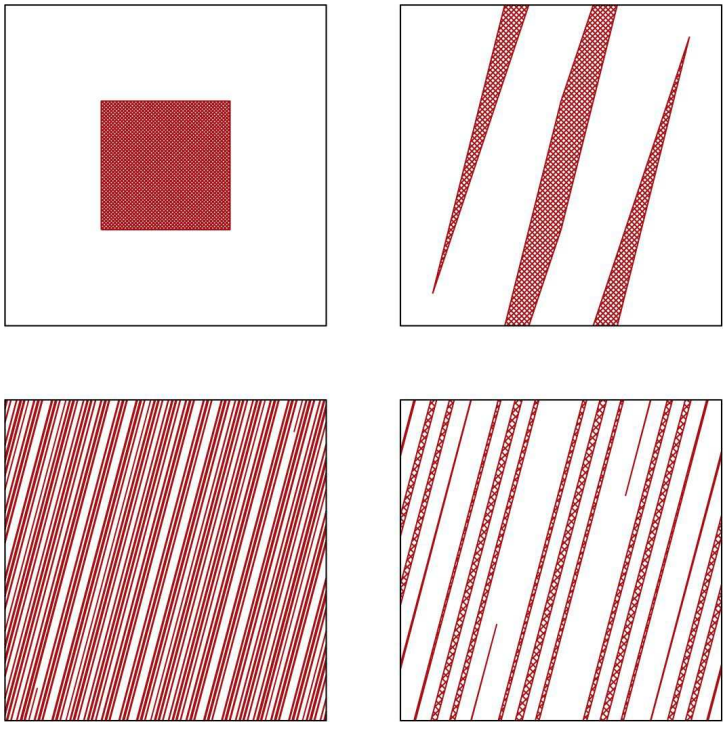

Figure 3: Zeroth, first, second, and third iterates of the generalized cat map with $p = 2$, acting on an initial square distribution (clockwise from upper left).

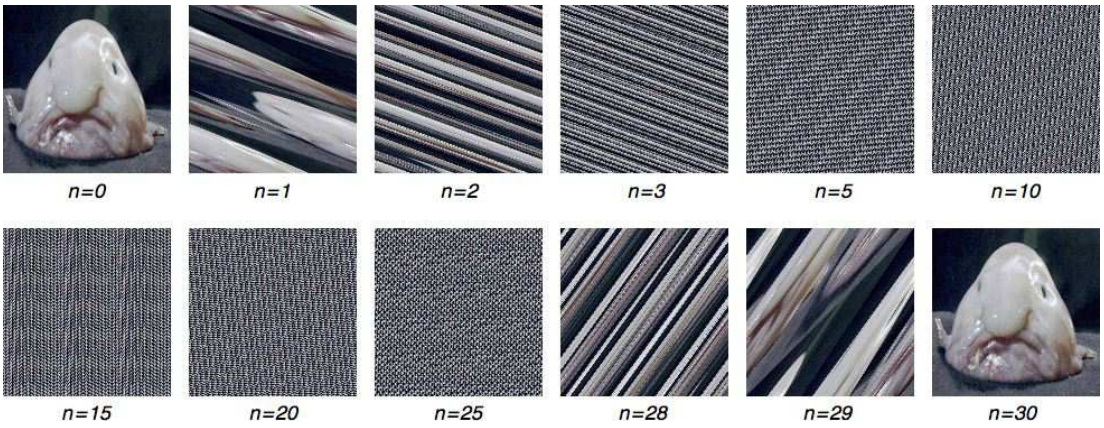

Figure 4: Evolution of a pixelated blobfish under the $p = 2$ generalized cat map.

(3.7) Consider a modified version of the Kac ring model where each spin exists in one of three states: A, B, or C. The flippers rotate the internal states cyclically: A→B→C→A.

(a) What is the Poincaré recurrence time for this system? *Hint:* the answer depends on whether or not the total number of flippers is a multiple of 3.

(b) Simulate the system numerically. Choose a ring size on the order of $N = 10,000$ and investigate a few flipper densities: $x = 0.001$, $x = 0.01$, $x = 0.1$, $x = 0.99$. Remember that the flippers are located randomly at the start, but do not move as the spins evolve. Starting from a configuration where all the spins are in the A state, plot the probabilities $p_{\rm A}(t)$, $p_{\rm B}(t)$, and $p_{\rm C}(t)$ *versus* the discrete time coordinate t, with t ranging from 0 to the recurrence time. If you can, for each value of x, plot the three probabilities in different colors or line characteristics (*e.g.* solid, dotted, dashed) on the same graph.

(c) Let's call $a_t = p_{\rm A}(t)$, *etc.* Explain in words why the *Stosszahlansatz* results in the equations

$$\begin{aligned} a_{t+1} &= (1-x)\,a_t + x\,c_t \\ b_{t+1} &= (1-x)\,b_t + x\,a_t \\ c_{t+1} &= (1-x)\,c_t + x\,b_t \quad . \end{aligned}$$

This describes what is known as a *Markov process*, which is governed by coupled equations of the form $P_i(t+1) = \sum_j Q_{ij}\,P_j(t)$, where Q is the *transition matrix*. Find the 3×3 transition matrix for this Markov process.

(d) Show that the total probability is conserved by a Markov process if $\sum_i Q_{ij} = 1$ and verify this is the case for the equations in `(c)`.

(e) One can then eliminate $c_t = 1 - a_t - b_t$ and write these as two coupled equations. Show that if we define

$$\tilde{a}_t \equiv a_t - \tfrac{1}{3} \qquad , \qquad \tilde{b}_t \equiv b_t - \tfrac{1}{3} \qquad , \qquad \tilde{c}_t \equiv c_t - \tfrac{1}{3}$$

that we can write

$$\begin{pmatrix} \tilde{a}_{t+1} \\ \tilde{b}_{t+1} \end{pmatrix} = R \begin{pmatrix} \tilde{a}_t \\ \tilde{b}_t \end{pmatrix} \quad ,$$

and find the 2×2 matrix R. Note that this is *not* a Markov process in A and B, since total probability for the A and B states is not itself conserved. Show that the eigenvalues of R form a complex conjugate pair. Find the amplitude and phase of these eigenvalues. Show that the amplitude never exceeds unity.

(f) The fact that the eigenvalues of R are complex means that the probabilities should *oscillate* as they decay to their equilibrium values $p_{\rm A} = p_{\rm B} = p_{\rm C} = \frac{1}{3}$. Can you see this in your simulations?

Solution :

(a) If the number of flippers $N_{\rm f}$ is a multiple of 3, then each spin will have made an integer number of complete cyclic changes A→B→C→A after one complete passage around the ring. The recurrence time is then N, where N is the number of sites. If the number of flippers $N_{\rm f}$ is not a multiple of 3, then the recurrence time is simply $3N$.

(b) See figs. 5, 6, 7.

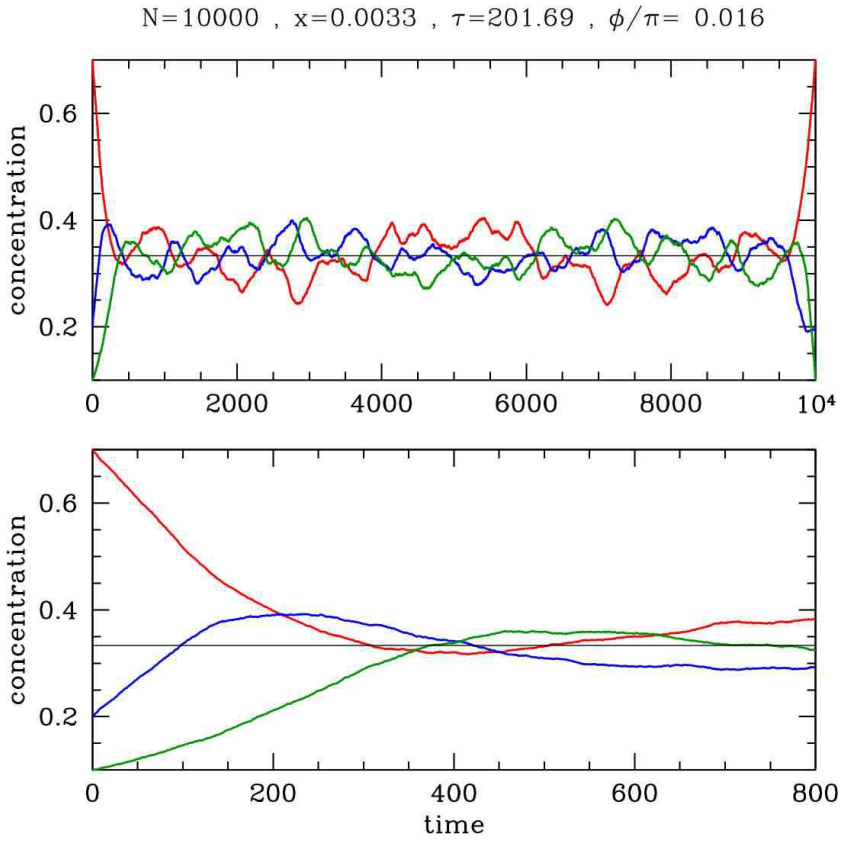

Figure 5: Simulation of three state Kac ring model with initial conditions $a_{t=0} = 0.7$, $b_{t=0} = 0.2$, $c_{t=0} = 0.1$. Note the oscillations as equilibrium is approached.

(c) According to the *Stosszahlansatz*, the probability a_{t+1} that a given spin will be in state A at time $(t+1)$ is the probability a_t it was in A at time t times the probability $(1-x)$ that it did not encounter a flipper, plus the probability c_t it was in state C at time t times the probability x that it did encounter a flipper. This explains the first equation. The others follow by cyclic permutation. The transition matrix is

$$Q = \begin{pmatrix} 1-x & 0 & x \\ x & 1-x & 0 \\ 0 & x & 1-x \end{pmatrix} \quad .$$

(d) The total probability is $\sum_i P_i$. Assuming $\sum_i Q_{ij} = 1$, we have

$$\sum_i P_i(t+1) = \sum_i \sum_j Q_{ij}\, P_j(t) = \sum_j \left(\sum_i Q_{ij} \right) P_j(t) = \sum_j P_j(t)$$

and the total probability is conserved. That's a Good Thing.

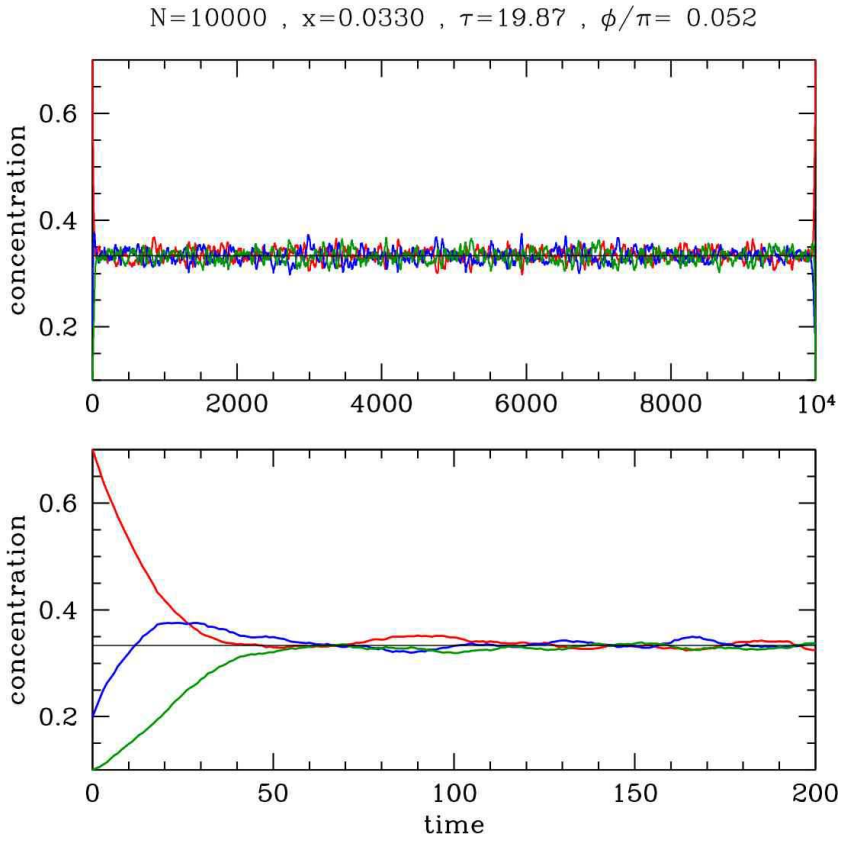

Figure 6: Simulation of three state Kac ring model with initial conditions $a_{t=0} = 0.7$, $b_{t=0} = 0.2$, $c_{t=0} = 0.1$.

(e) Substituting $a_t = \tilde{a}_t + \frac{1}{3}$, *etc.* into the Markov process and eliminating $\tilde{c}_t = -\big(\tilde{a}_t + \tilde{b}_t\big)$, we obtain

$$R = \begin{pmatrix} 1-2x & -x \\ x & 1-x \end{pmatrix} \quad .$$

The characteristic polynomial for R is

$$\begin{aligned} P(\lambda) = \det\,\big(\lambda\cdot 1 - R\big) &= (\lambda - 1 + 2x)(\lambda - 1 + x) + x^2 \\ &= \lambda^2 - (2-3x)\,\lambda + (1 - 3x + 3x^2) \quad . \end{aligned}$$

The eigenvalues are the two roots of $P(\lambda)$:

$$\lambda_\pm = 1 - \tfrac{3}{2}\,x \pm i\tfrac{\sqrt{3}}{2}\,x \quad .$$

Note that we can write

$$\lambda_\pm(x) = e^{-1/\tau(x)}\ e^{\pm i\phi(x)}$$

where

$$\tau(x) = -\frac{2}{\ln\big(1 - 3x + 3x^2\big)} \qquad , \qquad \phi(x) = \tan^{-1}\left(\frac{\sqrt{3}\,x}{2-3x}\right) \quad .$$

Since $x(1-x)$ achieves its maximum volume on the unit interval $x \in [0,1]$ at $x = \frac{1}{2}$, where $x(1-x) = \frac{1}{4}$, we see that $\frac{1}{2} \le |\lambda(x)| \le 1$, hence $0 \le \tau(x) \le \ln 2$. We plot $\tau(x)$ and $\phi(x)$ in fig. 7.

If you managed to get this far, then you've done all that was asked. However, one can go farther and analytically solve the equations for the Markov chain. In so doing, we will discuss the linear algebraic aspects of the problem.

The matrix R is real but not symmetric. For such a matrix, the characteristic polynomial satisfies $\big[P(\lambda)\big]^* = P(\lambda^*)$, hence if λ is a root of $P(\lambda = 0)$, which is to say λ is an eigenvalue, then so is λ^*. Accordingly, the eigenvalues of a real asymmetric matrix are either real or come in complex conjugate pairs. We can decompose such a matrix R as a sum over its eigenvectors,

$$R_{ij} = \sum_\alpha \lambda_\alpha \, \psi_i^\alpha \, \phi_j^\alpha \quad ,$$

where

$$\sum_j R_{ij} \, \psi_j^\alpha = \lambda_\alpha \, \psi_i^\alpha$$
$$\sum_i \phi_i^\alpha \, R_{ij} = \lambda_\alpha \, \phi_j^\alpha \quad .$$

Thus, ψ_j^α is the $j^{\rm th}$ component of the $\alpha^{\rm th}$ *right eigenvector* of R, while ϕ_i^α is the $i^{\rm th}$ component of the $\alpha^{\rm th}$ *left eigenvector* of R. Note that ϕ^α is a right eigenvector for the transposed matrix $R^{\rm t}$. We can further impose the normalization condition,

$$\big\langle \, \phi^\alpha \, \big| \, \psi^\beta \, \big\rangle = \sum_i \psi_i^\alpha \, \phi_i^\beta = \delta^{\alpha\beta} \quad .$$

One can check that the following assignment of eigenvectors is valid for our $R(x)$ matrix:

$$\vec\psi_+ = \begin{pmatrix} 1 \\ -e^{i\pi/3} \end{pmatrix}$$
$$\vec\phi_+ = \tfrac{1}{\sqrt{3}} \, e^{i\pi/6} \begin{pmatrix} 1 & e^{i\pi/3} \end{pmatrix} \quad .$$

and

$$\vec\psi_- = \begin{pmatrix} 1 \\ -e^{-i\pi/3} \end{pmatrix}$$
$$\vec\phi_+ = \tfrac{1}{\sqrt{3}} \, e^{-i\pi/6} \begin{pmatrix} 1 & e^{-i\pi/3} \end{pmatrix} \quad .$$

Let us write the vector

$$\vec\eta_t = \begin{pmatrix} \tilde a_t \\ \tilde b_t \end{pmatrix} \quad .$$

We then may expand $\vec\eta_t$ in the right eigenvectors of R, writing

$$\vec\eta_t = \sum_\alpha C_\alpha \, \lambda_\alpha^t \, \vec\psi^\alpha \quad .$$

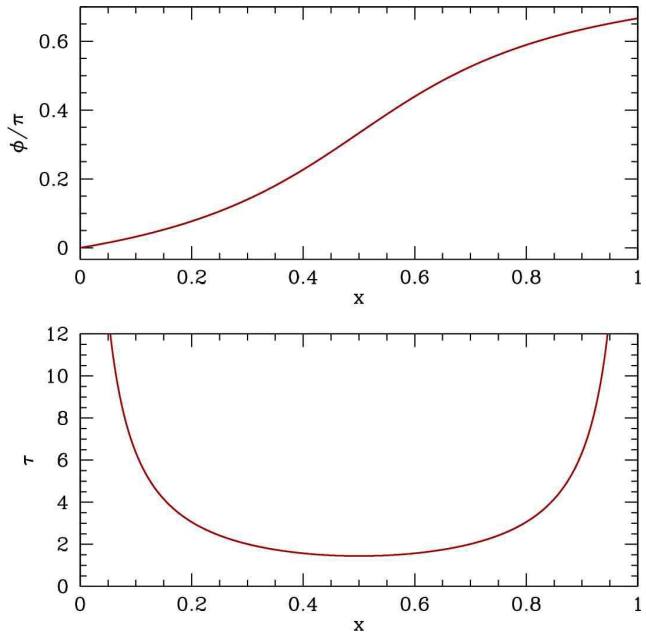

Figure 7: Phase angle and relaxation time for the three state Kac ring model with *Stosszahlansatz*.

Suppose we begin in a state where $a_{t=0} = 1$ and $b_{t=0} = c_{t=0} = 0$. Then we have $\tilde a_{t=0} = \frac{2}{3}$ and $\tilde b_{t=0} = -\frac{1}{3}$, hence

$$C_\alpha = \big\langle \, \vec\phi^\alpha \, \big| \begin{pmatrix} +2/3 \\ -1/3 \end{pmatrix} \big\rangle \quad .$$

We thereby find $C_+ = C_- = \frac{1}{3}$, and

$$\tilde a_t = \tfrac{2}{3} \, e^{-t/\tau} \, \cos\big(t\,\phi\big)$$
$$\tilde b_t = \tfrac{2}{3} \, e^{-t/\tau} \, \sin\big(t\,\phi - \tfrac{\pi}{6}\big) \quad ,$$

with $\tilde c_t = -\big(\tilde a_t + \tilde b_t\big)$.

(f) Yes! The oscillation is particularly clear in the lower panel of fig. 5.

(3.8) Consider a spin singlet formed by two $S = \frac{1}{2}$ particles, $|\,\Psi\,\rangle = \frac{1}{\sqrt{2}}\big(|\uparrow_A \downarrow_B\rangle - |\downarrow_A \uparrow_B\rangle\big)$. Find the reduced density matrix, $\rho_A = \mathrm{Tr}_B |\,\Psi\,\rangle\langle\,\Psi\,|$.

Solution :

We have

$$|\,\Psi\,\rangle\langle\,\Psi\,| = \tfrac{1}{2}|\uparrow_A\downarrow_B\rangle\langle\uparrow_A\downarrow_B| + \tfrac{1}{2}|\downarrow_A\uparrow_B\rangle\langle\downarrow_A\uparrow_B| - \tfrac{1}{2}|\uparrow_A\downarrow_B\rangle\langle\downarrow_A\uparrow_B| - \tfrac{1}{2}|\downarrow_A\uparrow_B\rangle\langle\uparrow_A\downarrow_B| \quad .$$

Now take the trace over the spin degrees of freedom on site B. Only the first two terms contribute, resulting in the reduced density matrix

$$\rho_A = \mathrm{Tr}_B |\,\Psi\,\rangle\langle\,\Psi\,| = \tfrac{1}{2}|\uparrow_A\rangle\langle\uparrow_A| + \tfrac{1}{2}|\downarrow_A\rangle\langle\downarrow_A| \quad .$$

Note that $\mathrm{Tr}\,\rho_A = 1$, but whereas the full density matrix $\rho = \mathrm{Tr}_B |\,\Psi\,\rangle\langle\,\Psi\,|$ had one eigenvalue of 1, corresponding to eigenvector $|\,\Psi\,\rangle$, and three eigenvalues of 0, corresponding to any state orthogonal to $|\,\Psi\,\rangle$, the reduced density matrix ρ_A does not correspond to a 'pure state' in that it is not a projector. It has two degenerate eigenvalues at $\lambda = \frac{1}{2}$. The quantity $S_A = -\,\mathrm{Tr}\,\rho_A \ln \rho_A = \ln 2$ is the *quantum entanglement entropy* for the spin singlet.