PHYSICS 200B : CLASSICAL MECHANICS
SOLUTION SET #3

[**1**] Consider the matrix

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

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

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

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.

[**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 $\mathit{\Gamma}$ such that $\dot{P}_i = -\mathit{\Gamma}_{ij} P_j$.

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

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

Solution :

(a) Following the prescription in Eq. 3.3 of the Lecture Notes, we have

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

(b) Note that summing on the row index yields $\sum_i \mathit{\Gamma}_{ij} = 0$ for any j, hence $(1,1,1)$ is a left eigenvector of $\mathit{\Gamma}$ with eigenvalue zero. It is quite simple to find the corresponding right eigenvector. Writing $\vec{\psi}^{\,\text{t}} = (a,b,c)$, 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,

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

(c) The equilibrium distribution does not satisfy detailed balance. Consider for example the ratio $P_1^{\text{eq}}/P_2^{\text{eq}} = 3$. 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] 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^{A}	g_j^{B}	g_j^{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 $|\,1\,\rangle$, *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 $|\,2\,\rangle$, 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 $|\,3\,\rangle$, 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 $|\,4\,\rangle$, 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:

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

[4] 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

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

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

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. 1, 2, 3.

(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

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

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

(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

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

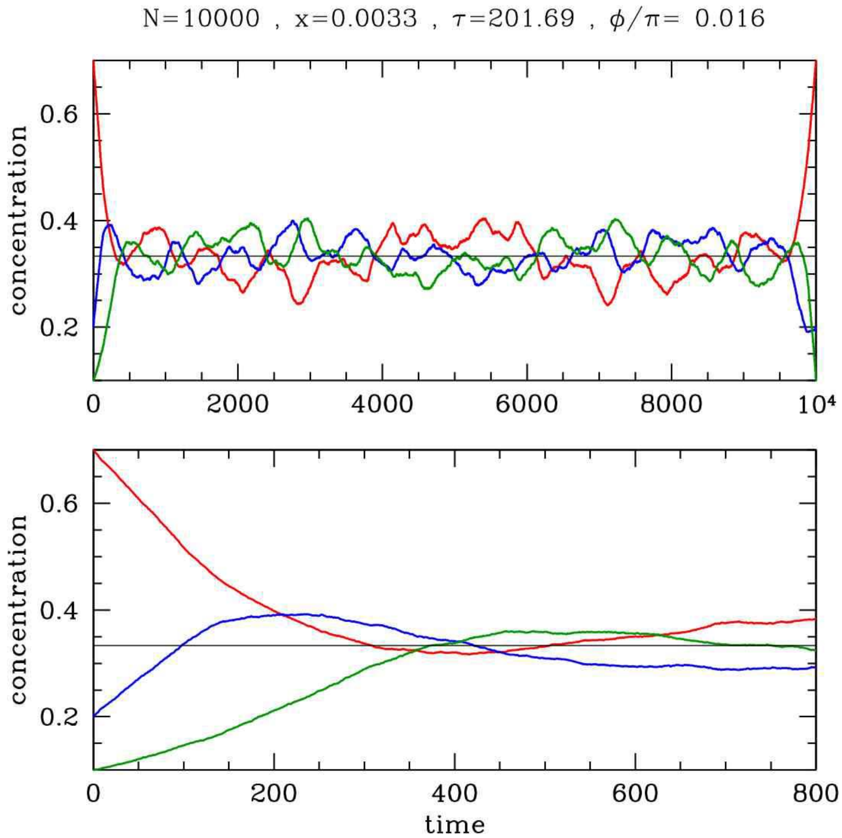

Figure 1: Simulation of three state Kac ring model with initial conditions $a_{t=0} = 0.7$, $b_{t=0} = 0.2$, $c_{t=0} = 0.1$. Note the oscillations as equilibrium is approached.

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. 3.

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,

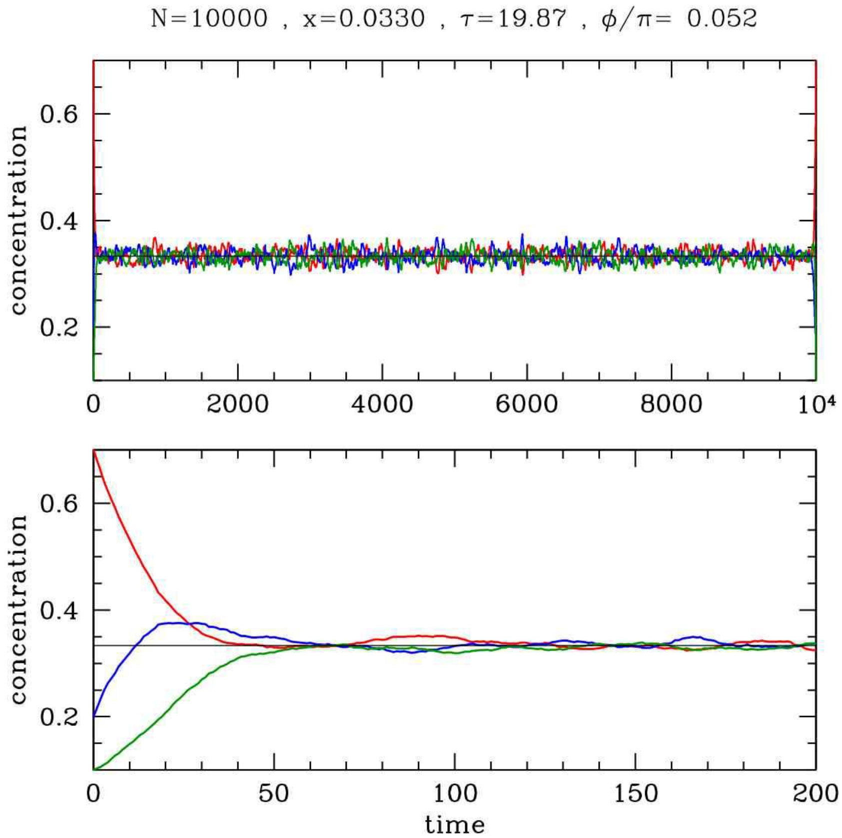

Figure 2: Simulation of three state Kac ring model with initial conditions $a_{t=0} = 0.7$, $b_{t=0} = 0.2$, $c_{t=0} = 0.1$.

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,

$$R_{ij} = \sum_\alpha \lambda_\alpha\, \psi^\alpha_i\, \phi^\alpha_j \quad ,$$

where

$$\sum_j R_{ij}\, \psi^\alpha_j = \lambda_\alpha\, \psi^\alpha_i$$

$$\sum_i \phi^\alpha_i\, R_{ij} = \lambda_\alpha\, \phi^\alpha_j \quad .$$

Thus, ψ^α_j is the $j^{\rm th}$ component of the $\alpha^{\rm th}$ *right eigenvector* of R, while ϕ^α_i 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,

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

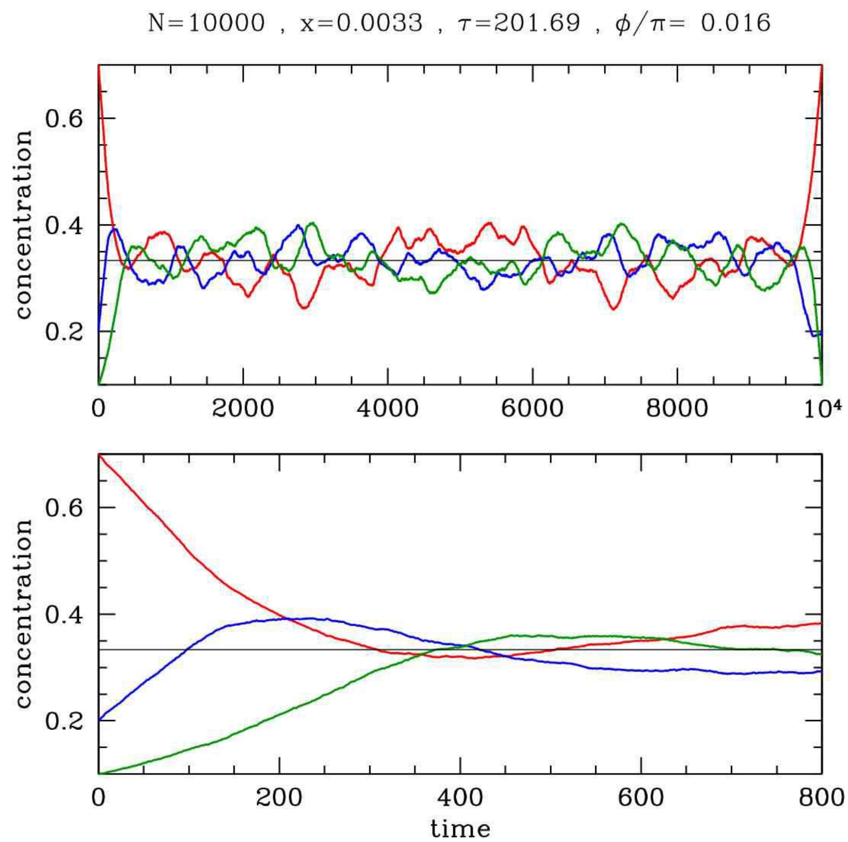

Figure 3: Phase angle and relaxation time for the three state Kac ring model with *Stosszahlansatz*.

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

$$\vec{\psi}_+ = \begin{pmatrix} 1 \\ -e^{i\pi/3} \end{pmatrix}$$
$$\vec{\phi}_+ = \frac{1}{\sqrt{3}}\, e^{i\pi/6} \begin{pmatrix} 1 & e^{i\pi/3} \end{pmatrix} \quad .$$

and

$$\vec{\psi}_- = \begin{pmatrix} 1 \\ -e^{-i\pi/3} \end{pmatrix}$$
$$\vec{\phi}_+ = \frac{1}{\sqrt{3}}\, e^{-i\pi/6} \begin{pmatrix} 1 & e^{-i\pi/3} \end{pmatrix} \quad .$$

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

$$\vec{\eta}_t = \sum_\alpha C_\alpha \, \lambda_\alpha^t \, \vec{\psi}^\alpha \quad .$$

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

$$\begin{aligned} \tilde{a}_t &= \tfrac{2}{3}\, e^{-t/\tau} \cos\big(t\,\phi\big) \\ \tilde{b}_t &= \tfrac{2}{3}\, e^{-t/\tau} \sin\big(t\,\phi - \tfrac{\pi}{6}\big) \quad , \end{aligned}$$

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. 1.