Prof. Dr. Roderich Tumulka
Eberhard Karls University Tübingen

Summer semester 2025
June 5, 2025

Mathematical Statistical Physics: Assignment 8

Problem 36: *Properties of the collision transformation* (hand in, 50 points)
At a collision of two billiard balls with collision parameter $\boldsymbol{\omega} = (\boldsymbol{q}_2 - \boldsymbol{q}_1)/2a$, the velocities change from $\boldsymbol{v} = \boldsymbol{v}_1$ and $\boldsymbol{v}_* = \boldsymbol{v}_2$ to

$$\boldsymbol{v}' = \boldsymbol{v} - [(\boldsymbol{v} - \boldsymbol{v}_*) \cdot \boldsymbol{\omega}]\boldsymbol{\omega} \tag{1}$$
$$\boldsymbol{v}'_* = \boldsymbol{v}_* + [(\boldsymbol{v} - \boldsymbol{v}_*) \cdot \boldsymbol{\omega}]\boldsymbol{\omega}\,. \tag{2}$$

Let $R_{\boldsymbol{\omega}}$ be the linear mapping $\mathbb{R}^6 \to \mathbb{R}^6$ with $R_{\boldsymbol{\omega}}(\boldsymbol{v}, \boldsymbol{v}_*) = (\boldsymbol{v}', \boldsymbol{v}'_*)$. Show that

(a) $R_{\boldsymbol{\omega}}$ is orthogonal, $R_{\boldsymbol{\omega}} \in O(6)$. (*Hint*: By the polarization identity $\boldsymbol{u} \cdot \boldsymbol{v} = \frac{1}{4}\big(|\boldsymbol{u} + \boldsymbol{v}|^2 - |\boldsymbol{u} - \boldsymbol{v}|^2\big)$, it suffices for orthogonality of a linear mapping A that $|A\boldsymbol{u}| = |\boldsymbol{u}|$ for all $\boldsymbol{u}$.)

(b) $\det R_{\boldsymbol{\omega}} = -1$. (You may use without proof that the determinant of a block matrix $\left(\begin{smallmatrix} A & B \\ C & D \end{smallmatrix}\right)$, where A, B, C, D all commute with each other, is[1] $\det(AD - BC)$.)

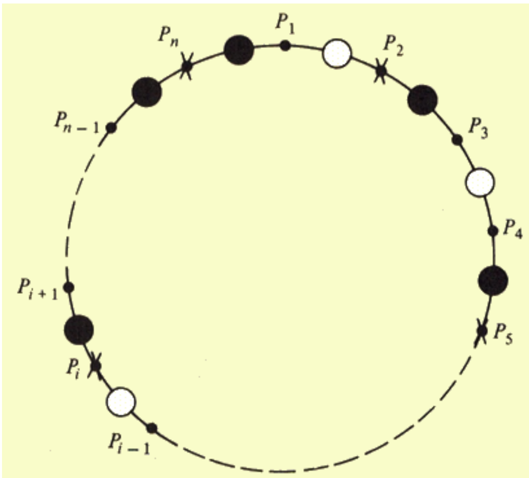
(c) $R_{\boldsymbol{\omega}}^2 = I_6$

(d) $R_{-\boldsymbol{\omega}} = R_{\boldsymbol{\omega}}$

(e) $\boldsymbol{\omega} \cdot (\boldsymbol{v}' - \boldsymbol{v}'_*) = -\boldsymbol{\omega} \cdot (\boldsymbol{v} - \boldsymbol{v}_*)$.

Problem 37: *The Kac ring model*[2] (hand in, 50 points)

This model is a toy version of the Boltzmann equation. Of $N \gg 1$ dots $P_1, \ldots, P_N$ along a circle, L are marked with a cross; let $Y_k = -1$ if P_k is marked, otherwise $Y_k = 1$. Between neighboring points there is always a ball which is either black ($X_k = -1$) or white ($X_k = 1$). In each time step, every ball moves to the next site clockwise and changes its color if it passes a cross. Initially, all balls are black, while crosses are chosen randomly with fixed density $\mu = L/N$. We ask what the distribution of colors is like after many steps.



The balls represent molecules, the color velocity (which here does not affect the motion), collisions

[1] J. R. Silvester: Determinants of Block Matrices. *The Mathematical Gazette* **84(501)**: 460–467 (2000)

[2] M. Kac: Some remarks on the use of probability in classical statistical mechanics. *Acad. Roy. Belg. Bull. Cl. Sci. (5)* **42**: 356–361 (1956)

G. A. Gottwald and M. Oliver: Boltzmann's Dilemma: An Introduction to Statistical Mechanics via the Kac Ring. *SIAM Review* **51**: 613–635 (2009) with each other are replaced by collisions with fixed obstacles ("scatterers"). The dynamics is reversible in the sense that counterclockwise rotation will restore the initial state, and a recurrence theorem holds (with the unrealistic trait that the recurrence time is the same for all states): after $2N$ steps, every ball has passed every scatterer twice and thus regained the original color, so the dynamics is $2N$-periodic.

"Phase space" Γ corresponds to all X_k and Y_k values, $\#\Gamma = 2^{2N}$. The "micro-canonical" distribution is uniform (1/number of phase points). The "equation of motion" reads

$$X_k(t) = Y_{k-1}\, X_{k-1}(t-1) \tag{3}$$

with solution

$$X_k(t) = Y_{k-1} Y_{k-2} \cdots Y_{k-t}\, X_{k-t}(0) \tag{4}$$

(with subtraction modulo N); the Y_k are conserved. The macro variable is $p = N_b/N$ (N_b = number of black balls), coarse-grained with resolution Δp; that is, for $p \in \Delta p \mathbb{N}_0$,

$$\Gamma_\nu = \Gamma_p = \Big\{ (X,Y) \in \Gamma : N_b \in \Big[(p - \Delta p/2)N, (p + \Delta p/2)N \Big) \Big\} . \tag{5}$$

(a) Show that for $S(p) = \log \#\Gamma_p$,

$$\lim_{\Delta p \to 0} \lim_{N \to \infty} \frac{1}{N} S(p) = \log 2 - p \log p - (1-p)\log(1-p) =: s(p) . \tag{6}$$

(b) Show that $\Gamma_{1/2}$ is a dominant macro state for fixed $\Delta p > 0$ and sufficiently large N.

(c) Consider $D(t) = N_b(t) - N_w(t)$ (N_w = number of white balls). Let $\tilde{N}_b$ be the number of black balls that will change color in the next step. Explain why

$$D(t+1) = D(t) + 2(\tilde{N}_w - \tilde{N}_b) . \tag{7}$$

(d) Without knowing the micro state, we cannot determine $\tilde{N}_b$, so the macro evolution equation (7) is "not autonomous." However, for typical Y the *hypothesis of molecular chaos*

$$\tilde{N}_b(t) = \mu N_b(t) , \quad \tilde{N}_w(t) = \mu N_w(t) \tag{8}$$

applies, stating that the balls are unrelated with the crosses. Assume (8) to find a difference equation that provides a closed evolution equation for $D(t)$; it is the analog to the Boltzmann equation. Find the general solution and verify that for $0 < \mu < 1/2$ the solution converges monotonically to 0 (i.e., to the dominant macro state) as $t \to \infty$.

(e) Express p through D and show that the macro evolution of part (d) obeys an H-theorem: $s(p(t))$ increases.

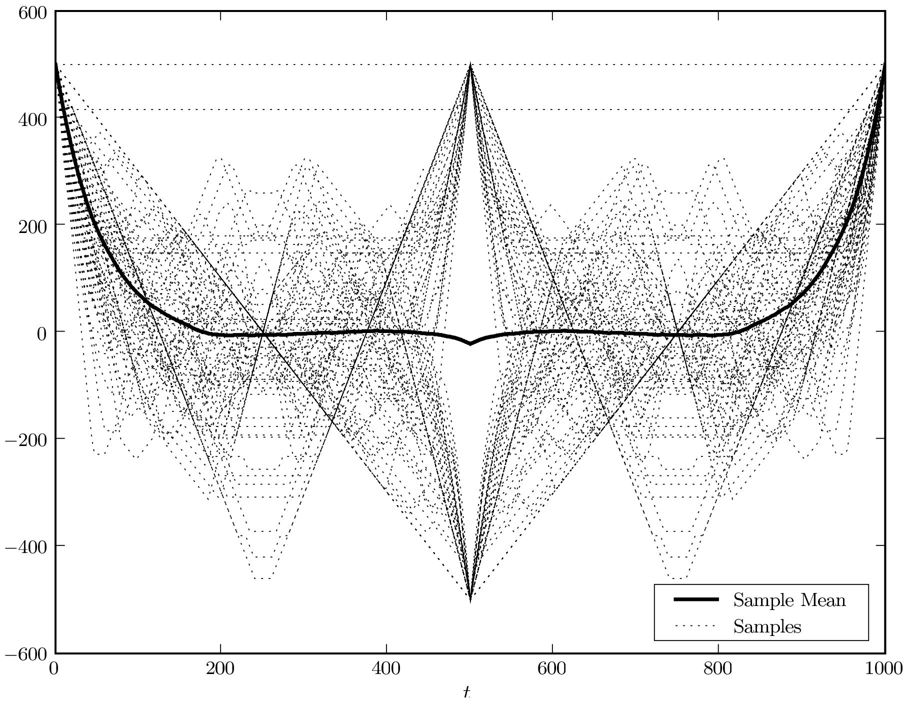


Figure (for illustration only): Numerical simulation of $D(t)$ for 400 realizations of Y with $\mu = 0.009$ on a Kac ring with $N = 500$ balls, initially all black, over a full period $t = 2N$. Thick curve: $D(t)$ averaged over the 400 runs. From Gottwald and Oliver.[1]

Hand in: By 23:59 on Monday, June 30, 2025 via `urm.math.uni-tuebingen.de`