## MATHEMATICAL STATISTICAL PHYSICS: ASSIGNMENT 10

**Problem 43:** An inequality we use (hand in, 30 points) Let (as in the proof of Proposition 8)

$$g(z) = \begin{cases} z & \text{for } 0 \le z \le 1\\ 1 & \text{for } z \ge 1 \end{cases}.$$

Show that for all  $x \ge 0$ ,

 $r(x) := x \log x + 1 - x \ge \frac{1}{4} g(|x - 1|) |x - 1|.$ (1)

(*Hint*: As a start, use r' and r'' to show r is convex and to find its minimum.) For x = f/M we obtain the relation (8.73) used in the proof of Proposition 8.

## **Problem 44:** The Kac ring model<sup>1</sup> (hand in, 70 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 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"  $\Gamma$  corresponds to all  $X_k$  and  $Y_k$  values,  $\#\Gamma = 2^{2N}$ . The "micro-canonical" distribution is the uniform one (number of phase points). The "equation of motion" reads

$$X_k(t) = Y_{k-1} X_{k-1}(t-1)$$
(2)

with solution

$$X_k(t) = Y_{k-1} Y_{k-2} \cdots Y_{k-t} X_{k-t}(0)$$
(3)

<sup>&</sup>lt;sup>1</sup>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 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  $\Delta p$ ; that is, for  $p \in \Delta p \mathbb{N}_0$ ,

$$\Gamma_p = \left\{ (X, Y) \in \Gamma : N_b \in \left[ (p - \Delta p/2)N, (p + \Delta p/2)N \right] \right\}.$$
(4)

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

$$\lim_{\Delta p \to 0} \lim_{N \to \infty} \frac{1}{N} S(p) = \log 2 - p \log p - (1-p) \log(1-p) =: s(p).$$
(5)

(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

$$D(t+1) = D(t) + 2(N_w - N_b).$$
(6)

(d) Without knowing the micro states, we cannot determine  $N_b$ , so the macro evolution equation (6) is "not autonomous." However, for typical Y the hypothesis of molecular chaos

$$\tilde{N}_b(t) = \mu N_b(t), \quad \tilde{N}_w(t) = \mu N_w(t)$$
(7)

applies, stating that the balls are "uncorrelated" with the crosses. Assume (7) 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.



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.<sup>1</sup>

Hand in: Wednesday, July 10, 2019, in the exercise class.