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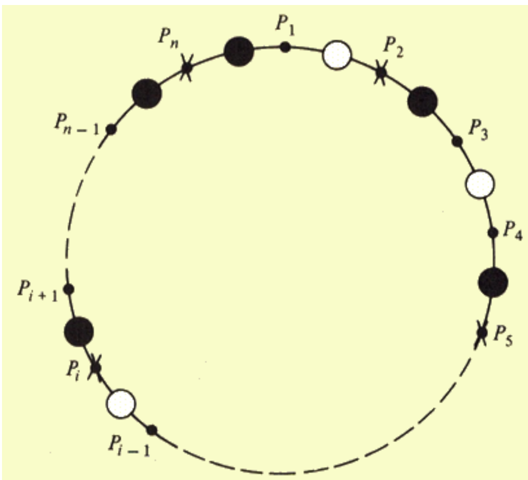
Mathematical Statistical Physics: Assignment 9

Problem 40: *Grand-canonical distribution as a marginal* (hand in, 35 points)
We consider an ideal gas in a container $\Lambda \subset \mathbb{R}^3$ subdivided into a region Λ_A and its complement $\Lambda_B = \Lambda \setminus \Lambda_A$. There are no walls between Λ_A and Λ_B, so particles can pass freely. We write $A := \Lambda_A \times \mathbb{R}^3$ and $B := \Lambda_B \times \mathbb{R}^3$ for the corresponding subsets of Γ_1; the total phase space is $\Gamma = {}^N\Gamma_1$; the phase space of system A is now a phase space of a variable number of particles, $\Gamma_A = \cup_{n=0}^{N} {}^nA$. For $x \in \Gamma$ let $x_A = x \cap A$ and $x_B = x \cap B$, so $x = x_A \cup x_B$; correspondingly, Γ can be regarded as a subset of $\Gamma_A \times \Gamma_B$. We have that $H(x_1, \ldots, x_N) = \sum_{j=1}^{N} H_1(x_j)$ and $H_A(x_1, \ldots, x_n) = \sum_{j=1}^{n} H_1(x_j)$ for $n = 0 \ldots N$. For simplicity, we start from a canonical (rather than micro-canonical) distribution ρ_{can} on Γ, i.e., (ideal gas): N points in Γ_1 are chosen i.i.d. according to the Maxwell-Boltzmann distribution $\rho_1 = Z_1^{-1} e^{-\beta H_1}$. The marginal ρ_A of ρ_{can} on Γ_A ranges over different particle numbers; so does $Z_A^{-1} e^{-\beta H_A}$, but it is not the same distribution! Show that instead in the limit $\Lambda \to \infty$, $N \to \infty$, Λ_A fixed, H_1 fixed, $N \int_A \rho_1 \to c > 0$ (with suitable constant c),

$$\rho_A(x_1, \ldots, x_n) = \frac{1}{Z} \exp\Big[-\beta\big(H_A(x_1 \ldots x_n) - \mu n\big)\Big] \tag{1}$$

with suitable constant $\mu \in \mathbb{R}$. This is the grand-canonical distribution. (If we write phase points in Γ_A as ordered, then a further factor $1/n!$ appears in (1).)

Problem 41: *The Kac ring model*[1] (hand in, 65 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" 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

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

[1] 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 solution

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

(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 $p \in \Delta p\mathbb{N}_0$,

$$\Gamma_\nu = \Gamma_p = \Big\{(X,Y) \in \Gamma : N_b \in \Big[(p-\Delta p/2)N, (p+\Delta p/2)N\Big)\Big\}\,. \tag{4}$$

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

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

(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

$$D(t+1) = D(t) + 2(\tilde{N}_w - \tilde{N}_b)\,. \tag{6}$$

(d) Without knowing the micro state, we cannot determine $\tilde{N}_b$, so the macro evolution equation (6) is "not autonomous." However, for typical Y the *hypothesis of molecular chaos*

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

applies, stating that the balls are unrelated 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.

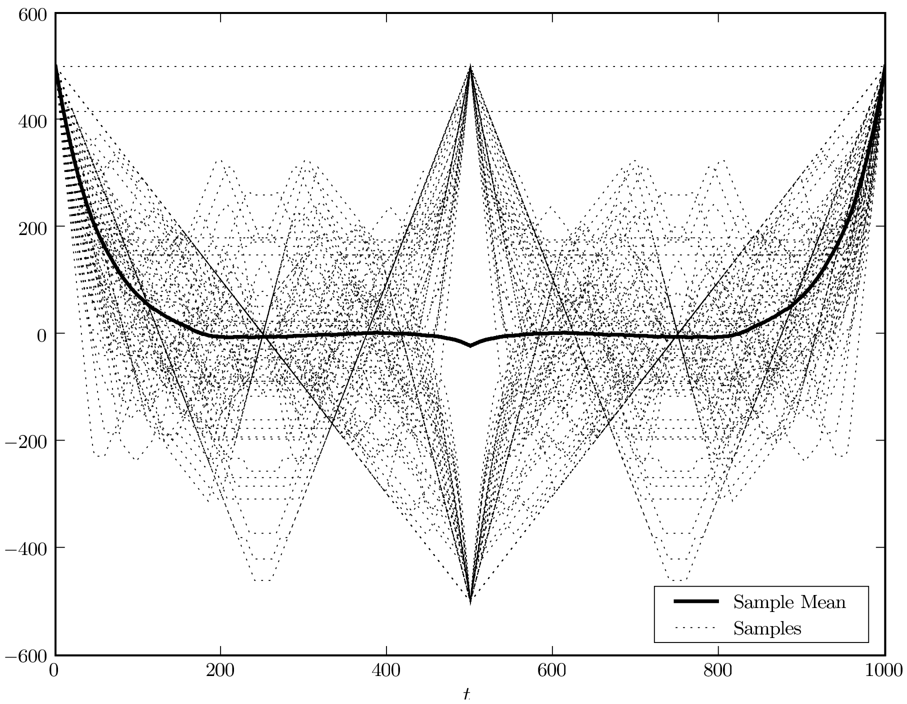


Figure (for illustration only): Numerical simulation of $D(t)$ for 400 realizations of Y with $\mu = 0.009$ on a Kac ring with $N = 500$ balls, initially all black, over a full period $t = 2N$. Thick curve: $D(t)$ averaged over the 400 runs. From Gottwald and Oliver.[1]

Hand in: By 8:15am on Tuesday, June 28, 2022 via `urm.math.uni-tuebingen.de`