LMU Munich
Summer term 2018

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Exercises on Mathematical Statistical Physics
Sheet 9

Problem 1 (Relative entropy I) Let $E = \{1, ..., r\}$ be a finite set and $\mathcal{M}_{1,+} := \{p \in \mathbb{R}_+^r : p_1 + \cdots + p_r = 1\}$. $\mathcal{M}_{1,+}$ is equipped with the Euclidean metric. Fix a reference measure $q \in \mathcal{M}_{1,+}$; let $q^{\otimes n}(x_1, \ldots x_n) := q(x_1)q(x_2)\cdots q(x_n)$ be the produce measure on E^n.

a) Let $K_n := \{k = (k_1, \ldots k_r) \in \mathbb{N}_0^r : k_1 + \cdots + k_r = n\}$ and for $k \in K_n$,

$A(k_1, ..., k_r) := \{x = (x_1, \ldots x_n) \in E^n : \forall\, s \in \{1, \ldots r\}\, x$ has exactly k_s entries equal to $s\}$.

Provide formulas for $|K_n|$, $|A(k)|$, and $q^{\otimes n}(A(k))$.

b) Let $p \in \mathcal{M}_{1,+}$ and $(k^{(n)})_{n\in\mathbb{N}}$ be a sequence in $\mathbb{N}_0^r$ s.t. $k^{(n)} \in K_n$. Show that if $\frac{1}{n}k^{(n)} \to p$, as $n \to \infty$, then

$$\lim_{n\to\infty} \frac{1}{n} \log q^{\otimes n}(A(k_1^{(n)}, ..., k_r^{(n)}))$$

converges.

c) For $x \in E^n$, define the empirical measure $L_n(\cdot\,; x) \in \mathcal{M}_{1,+}$ by $L_n(s; x) = \frac{1}{n}|\{i : x_i = s\}|$. Show that the following holds true:

(i) For every closed set $F \subset \mathcal{M}_{1,+}$,

$$\limsup_{n\to\infty} \frac{1}{n} \log q^{\otimes n}(L_n(\cdot\,; x) \in F) \leq -\inf_{p\in F} h(p|q).$$

(ii) For every open set $O \subset \mathcal{M}_{1,+}$

$$\liminf_{n\to\infty} \frac{1}{n} \log q^{\otimes n}(\{x \in E : L_n(\cdot\,; x) \in O\}) \geq -\inf_{p\in O} h(p|q).$$

Remark: (i) and (ii) are a way of formalizing the heuristic identity $q^{\otimes n}(L_n(\cdot\,; x) \approx p) \approx e^{-n\,h(p|q)}$. Probabilists would speak of a large deviations principle with speed n and rate function $p \mapsto h(p|q)$.

Problem 2 Consider probability measures p on $\mathbb{N}_0$ and the Shannon entropy

$$S(p) := -\sum_{k=0}^{\infty} p_k \log p_k \ \in [0, \infty) \cup \{\infty\}.$$

Given $m > 0$, compute $\max\{S[p]\,|\, p\,\text{prob. meas. on}\ \mathbb{N}_0,\ \sum_{k=0}^{\infty} k\, p_k = m\}$. Show that the maximizer is unique.

Problem 3 (1D jellium) $V(x) = -\frac{1}{2}|x|$ 1D Coulomb potential. $\mathscr{U}_n : \left[-\frac{L}{2}, \frac{L}{2}\right]^n \to \mathbb{R}$, $\rho := \frac{n}{L}$,

$$\mathscr{U}_n(x_1, ..., x_n) := \sum_{1 \le i < j \le n} V(x_i - x_j) - \rho \sum_{i=1}^n \int_{-L/2}^{L/2} V(x_i - y)\, \mathrm{d}y + \frac{\rho^2}{2} \iint_{\left[-\frac{L}{2}, \frac{L}{2}\right]^2} V(y - y')\, \mathrm{d}y \mathrm{d}y'.$$

n particles of charge 1 embedded in a homogeneous neutralizing background of charge density ρ.

a) Split $\left[-\frac{L}{2}, \frac{L}{2}\right]$ into n intervals of identical length $\frac{L}{n}$, and let $x_1^\circ \le \cdots \le x_n^\circ$ be the midpoints of the intervals. Show that for all $-\frac{L}{2} \le x_1 \le \cdots \le x_n \le \frac{L}{2}$ and some constant $C_{n,L} \ge 0$,

$$\mathscr{U}_n(x_1, ..., x_n) = \frac{\rho}{2} \sum_{i=1}^n (x_i - x_i^\circ)^2 + C_{n,L}. \tag{1}$$

b) For $a > 0$, consider the energy cost of translating particle no k of the ground state

$$\mathscr{E}_{k,n}(a) := \inf\{\mathscr{U}_n(x_1, ... x_n) \mid -\frac{L}{2} \le x_1 \le \cdots \le x_n \le \frac{L}{2},\ x_k = x_k^\circ + a\} - \min \mathscr{U}_n.$$

Prove or disprove for each a and k, the energy cost goes to 0 as $n \to \infty$.

c) Give a heuristic answer to the following question: in the infinite-volume limit $L, n \to \infty$ at fixed ρ, do you expect that the translational symmetry is broken? Explain why your understanding is consistent with the understanding of the Mermin-Wagner theorem.

d) Consider a the energy $\mathscr{U}_n$ of a chain of harmonic oscillators: $\ell > 0$ fixed rest length of the springs,

$$\mathscr{U}_n(x_1, ..., x_n) = \frac{1}{2} \sum_{k=1}^{n+1} (x_k - x_{k-1} - \ell)^2, \quad x_1 \le \cdots \le x_n$$

with "pinned" boundary conditions $x_0 = 0$, $x_{n+1} = (n+1)\ell$. Suppose that n is even. Let $x_1^\star \le \cdots \le x_n^\star$ be the minimizer of $\mathscr{U}_n$. Show that

$$\lim_{n \to \infty} \left(\min \left\{ \mathscr{U}_n(x_1, ..., x_n) \,:\, x_{n/2} = x_{n/2}^\star + a \right\} - \min \mathscr{U}_n \right) = 0,$$

for every fixed $a \in \mathbb{R}$.

The solutions to these exercises will be discussed on Monday, 18.06.