Mathematical Statistical Physics – LMU München, summer semester 2012

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Homework sheet 9 – due on 22.06.2012 – and exercises for the class on 15.06.2012

9.1 **(homework)** *Canonical partition function and density of states.* As you all know, the canonical ensamble (or canonical distribution) has the density $f_{\alpha,\beta}(\omega) = \frac{1}{Z(\alpha,\beta)} e^{-\beta H(\omega)}$ w.r.t. an approriate reference measure μ_{ref} on the phase space $\Omega = \{\omega\}$. Here β is the inverse temperature, and α denotes all the possibles other parameters (e.g. volume, particle number, etc.) which influence the shape of Ω, μ_{ref} and the Hamiltonian $H : \Omega \to \mathbb{R}$. The normalizing factor $Z(\alpha, \beta)$ is called the partition function (we suppose that it is finite).

Denote by μ_E the push-forward of μ_{ref} from Ω to $\mathbb{R}$ by H – which means that

$$\mu_E(B) := \mu_{ref}(\{\omega : H(\omega) \in B\})$$

for any Borel $B \subset \mathbb{R}$. This could vaguely be called the "distribution of H w.r.t. μ_{ref}". (Only vaguely, because μ_{ref} is usually not a probability measure, so $H : \Omega \to \mathbb{R}$ cannot be called a random variable if we consider Ω equipped with μ_{ref}.) Suppose (for simplicity only) that this μ_E is absolutely continuous w.r.t. Lebesgue measure on $\mathbb{R}$, and denote its density by $\rho = \rho_\alpha(E)$. This ρ_α can be called the **density of states**.

(a) When Ω is equipped with the canonical measure, the energy is a random variable. Show that under the above condition (that μ_E is absolutely continuous w.r.t. Lebesgue measure) this random variable is absolutely continuous (w.r.t Lebesgue measure), and calculate the density in terms of ρ, Z and β.

(b) Express $Z(\alpha, \beta)$ with the help of β and ρ_α (or β and μ_E, if you want to be more general), and be happy that this is possible.

9.2 **(homework)** *Energy fluctuations for the free gas.* Consider the free gas in the canonical ensamble, and keep the density fixed by setting $V = Nv$ with $v = const.$ Also fix the temperature by setting $\beta = const.$ Now for every N the energy density H/V is a random variable.

(a) Calculate the expectation and the variance of this H/V as a function of N. What can we say about the weak convergence of H/V in the limit $N \to \infty$?

(b) Set $N = 10^{23}$. Estimate the probability that H/V deviates from its expectation with at least 0.000001%.

9.3 *Density fluctuations for the free gas.* Consider the free gas in the grand canonical ensamble. Keeping β and β' fixed, the density N/V is a random variable parametrized by V.

(a) Calculate the expectation and the variance of this N/V as a function of V. What can we say about the weak convergence of N/V in the limit $V \to \infty$?

(b) Set the parameters so that $\mathbb{E}N = 10^{23}$. Estimate the probability that N/V deviates from its expectation with at least 0.000001%.

9.4 *Tempered and stable pair interactions.* Let $\Phi : \mathbb{R}^+ \to \mathbb{R} \cup \{\infty\}$ be a pair interaction potential which satisfies the following:

(a) Φ is bounded from below,

(b) There is an $R_1 > 0$ such that $\Phi(r) = \infty$ for all $r \le R_1$,

(c) There is an $R_2 < \infty$ such that $\Phi(r) = 0$ for all $r \geq R_2$.

Show that Φ is tempered and stable.

9.5 *Tempered and stable pair interactions II.* Let $\Phi : \mathbb{R}^+ \to \mathbb{R} \cup \{\infty\}$ be a pair interaction potential which satisfies the following:

(a) Φ is bounded from below,

(b) There is an $R_1 > 0$ such that $\Phi(r) = \infty$ for all $r \leq R_1$,

(c) There is an $R_2 < \infty$ such that $\Phi(r) \leq 0$ for all $r \geq R_2$,

(d) $\Phi(r) \to 0$ exponentially fast as $r \to \infty$.

Show that Φ is tempered and stable.

9.6 *Basics of convex functions.* If a and b are elements of a linear space V over $\mathbb{R}$, then their **convex combinations** are the elements $\alpha a + \beta b$ where $0 \leq \alpha \in \mathbb{R}$, $0 \leq \beta \in \mathbb{R}$ and $\alpha + \beta = 1$. A **set** $A \subset V$ is called **convex** if it contains every convex combination of its elements. For a convex $A \subset V$, the **function** $f : A \to \mathbb{R} \cup \{\infty\}$ is called **convex** if

$$f(\alpha a + \beta b) \leq \alpha f(a) + \beta f(b)$$

for any $a, b \in A$, $0 \leq \alpha \in \mathbb{R}$, $0 \leq \beta \in \mathbb{R}$ and $\alpha + \beta = 1$. Show that convexity is a very strong regularity property by proving the following statements: Suppose $f : I \to \mathbb{R} \cup \{\infty\}$ is convex and finite on the open (but possibly infinite) interval $I \subset \mathbb{R}$. Then

(a) it is necessarily continuous,

(b) it has one-sided derivatives everywhere on I,

(c) These one-sided derivatives are monotonically non-decreasing,

(d) f is differentiable in all but at most countably many points.

9.7 *Midpoint convexity.* Let $I \subset \mathbb{R}$ be a (possibly infinite) interval. The function $f : I \to \mathbb{R} \cup \{\infty\}$ is called **midpoint convex**, if $f(\frac{a+b}{2}) \leq \frac{f(a)+f(b)}{2}$ for every $a, b \in I$. Show that if $f : I \to \mathbb{R} \cup \{\infty\}$ is finite, midpoint convex and bounded on a subinterval $\emptyset \neq J \subset I$, then it is bounded on any bounded interval, (continuous) and convex.

9.8 **(homework)** *Jensen's inequality.* If $a_1, \ldots, a_n$ are elements of a linear space V over $\mathbb{R}$, then their convex combinations are the elements $\sum_{i=1}^n \alpha_i a_i$ where $0 \leq \alpha_1, \ldots, \alpha_n \in \mathbb{R}$ and $\sum_{i=1}^n \alpha_i = 1$.

(a) Show that if $A \subset V$ is convex and $a_1, \ldots, a_n \in A$, then any convex combination $\sum_{i=1}^n \alpha_i a_i$ is also in A.

(b) Show that if $A \subset V$ is convex, $f : A \to \mathbb{R} \cup \{\infty\}$ is convex and $a_1, \ldots, a_n \in A$, $0 \leq \alpha_1, \ldots, \alpha_n \in \mathbb{R}$ and $\sum_{i=1}^n \alpha_i = 1$, then

$$f\left(\sum_{i=1}^n \alpha_i a_i\right) \leq \sum_{i=1}^n \alpha_i f(a_i).$$

This is the simplest form of Jensen's inequality.