Mathematical Statistical Physics – LMU München, summer semester 2012

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Homework sheet 5 – due on 25.05.2012 – and exercises for the class on 18.05.2012

5.1 *Grand canonical reference measure and identical particles.* In the grand canonical description of a particle system in the container $\Lambda \subset \mathbb{R}^d$, we "try to" use the phase space

$$\Omega^\Lambda := \dot{\cup}_{n\geq 0}\Omega^\Lambda_n,$$

where Ω^Λ_n is the phase space of an n-particle system, so

$$\Omega^\Lambda_n = (\lambda \times \mathbb{R}^d)^n.$$

We "try to" equip this phase space with the reference measure

$$\lambda^\Lambda = \sum_{n\geq 0} \lambda_{\Omega^\Lambda_n},$$

where $\lambda_{\Omega^\Lambda_n}$ is the Lebesgue measure on Ω^Λ_n, that is $\lambda_{\Omega^\Lambda_n} = (\lambda_\Lambda \otimes \lambda_{\mathbb{R}^d})^{\otimes n}$. Now the Liouville theorem ensures that this measure is invariant under any Hamiltonian dynamics.

(a) Show that the choice of the phase space is consistent in the sense that if $\Lambda = \Lambda_1 \dot{\cup} \Lambda_2$, then $\Omega^\Lambda = \Omega^{\Lambda_1} \times \Omega^{\Lambda_2}$ (with suitable natural identifications).

(b) However, show that the choice of λ^Λ is inconsistent: $\lambda^\Lambda \neq \lambda^{\Lambda_1} \otimes \lambda^{\Lambda_2}$.

(c) Notice that in our choice of the measure we have some "freedom": If we want the Liouville theorem to ensure that the measure is invariant, then any measure of the form

$$\lambda^\Lambda = \sum_{n\geq 0} c_n \lambda_{\Omega^\Lambda_n}$$

will do, with $0 < c_n \in R$. How should we choose the sequence c_n, if we want to ensure also that $\lambda^\Lambda = \lambda^{\Lambda_1} \otimes \lambda^{\Lambda_2}$?

(d) What has this got to do with indistinguishability of the particles?

5.2 *Canonical entropy and patrition function.* The canonical measures $\mu_{\Lambda,\beta,N}$ describing a Hamiltonian particle system (with Hamiltonian $\mathcal{H}$) of N particles in the container $\Lambda \subset \mathbb{R}^d$ are probability measures on the phase space Ω^Λ_N which are absolutely continuous w.r.t. $\lambda_{\Omega^\Lambda_N}$ (see footnote [1]), and have density

$$\rho_{\Lambda,\beta,N}(x) = \frac{1}{Z(\Lambda,\beta,N)} e^{-\beta\mathcal{H}(x)}.$$

See the first exercise for notation. β is a parameter and $Z(\Lambda,\beta,N)$ is the suitable normalizing factor called the "partition function". The canonical entropy S^{can} is defined as the relative entropy

$$S^{can}(\Lambda,\beta,N) = H(\mu_{\Lambda,\beta,N}; \lambda_{\Omega^\Lambda_N}),$$

where H stands for relative entropy (not to be mixed with the Hamiltonian $\mathcal{H}$).

[1] If we want to get "correct dependence on N", we better use $c_N \lambda_{\Omega^\Lambda_N} = \frac{1}{N!}\lambda_{\Omega^\Lambda_N}$ as the reference measure, as we learned from Exercise 5.1 and 4.7

(a) Let E denote the expectation of $\mathcal{H}$ w.r.t. $\mu_{\Lambda,\beta,N}$. Express S^{can} in terms of β, E and Z

i. using the definition of relative entropy,

ii. using the maximum entropy principle.

(b) What is the physical meaning of $\log Z$?

5.3 **(homework)** *Grand canonical entropy and patrition function.* The grand canonical measures $\mu_{\Lambda,\beta,\beta'}$ describing a Hamiltonian particle system (with Hamiltonian $\mathcal{H}$) in the container $\Lambda \subset \mathbb{R}^d$ are probability measures on the phase space Ω^Λ which are absolutely continuous w.r.t. λ^Λ, and have density

$$\rho_{\Lambda,\beta,\beta'}(x) = \frac{1}{Z(\Lambda,\beta,\beta')} e^{-\beta\mathcal{H}(x)-\beta' N(x)}.$$

See the first exercise for notation. Here N denotes the particle counting function $N : \Omega^\Lambda \to \mathbb{N}$, $N(x) = n$ if $x \in \Omega^\Lambda_n$. β and β' are parameters and $Z(\Lambda,\beta,\beta')$ is the suitable normalizing factor called the "partition function". The grand canonical entropy S^{gr} is defined as the relative entropy

$$S^{gr}(\Lambda,\beta,\beta') = H(\mu_{\Lambda,\beta,\beta'};\lambda^\Lambda),$$

where H again stands for relative entropy (not to be mixed with the Hamiltonian $\mathcal{H}$).

(a) Let E denote the expectation of $\mathcal{H}$ and $\bar{N}$ denote the expectation of N w.r.t. $\mu_{\Lambda,\beta,\beta'}$. Express S^{gr} in terms of β, E, β', $\bar{N}$ and Z

i. using the definition of relative entropy,

ii. using the maximum entropy principle.

(b) What is the physical meaning of $\log Z$?

5.4 **(homework)** *Canonical description of the free gas.* Consider the free gas with the Hamiltonian given in Exercise 4.7.

(a) Describe the canonical distribution.

(b) Calculate the canonical partition function. Keep the footnote in mind.

(c) Calculate the canonical entropy.

(d) Set $V = Nv$ where V is the volume of Λ, so $S^{can}(\Lambda,\beta,N)$ becomes $S^{can}_{\beta,v}(N)$. How does $S^{can}_{\beta,v}(N)$ scale with N? Compare with the result of Exercise 4.7.

5.5 *Grand canonical description of the free gas.* Consider the free gas with the Hamiltonian given in Exercise 4.7.

(a) Describe the grand canonical distribution.

(b) Calculate the grand canonical partition function. Keep the footnote in mind.

(c) Calculate the grand canonical entropy.

(d) Let V be the volume of Λ. How does $S^{gr}(V,\beta,\beta')$ scale with V? Compare with the result of Exercise 4.7. and the previous exercise.

5.6 **(homework)** *Free gas with several types of particles.* Consider a container which is devided into k parts, separated by thin walls. Each part has volume V_k and contains N_k identical particles of a free gas, which, however, differ from the particles in other compartments. The system is in equilibrium as much as it can be: exchange of energy is allowed. Now we remove the walls, and wait for equilibrium to be reached again. How much does the entropy change?

5.7 *Grand canonical description of the free gas and the Poisson process.* Consider the grand canonical ensamble of the free gas in a container Λ with parameters β, β'.

(a) Let $\Lambda_1 \subset \Lambda$. What is the distribution of the (random) number N_1 of particles that are in Λ_1?

(b) Let Λ_1 and Λ_2 be two *disjoint* subsets of Λ. (That is, $\Lambda_1, \Lambda_2 \subset \Lambda$, $\Lambda_1 \cap \Lambda_2 = \emptyset$.) Let N_i denote the (random) number of particles in Λ_i ($i = 1, 2$). What is the *joint distribution* of N_1 and N_2?