Mathematical Statistical Physics – LMU München, summer semester 2012

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Homework sheet 10 – due on 29.06.2012 – and exercises for the class on 22.06.2012

10.1 *DLR condition and conditional probability.* Let $\mu_\Lambda^{\beta,\beta'}(.|\eta)$ denote the grand canonical measure of some system in the box Λ with the boundary condition $\eta \in \Omega_{\Lambda^c}$. Using this, define

$$\gamma_\Lambda^{\beta,\beta'}(.|\eta) := \mu_\Lambda^{\beta,\beta'}(.|\eta \cap \Lambda^c) \otimes \delta_{\eta\cap\Lambda^c}$$

for all $\eta \in \Omega$ as a product measure on $\Omega = \Omega_\Lambda \times \Omega_{\Lambda^c}$.

The Dobrushin-Lanford-Ruelle condition for a measure μ on Ω to be Gibbs is

$$\mu = \mu \otimes \gamma_\Lambda^{\beta,\beta'} \quad \text{for every bounded } \Lambda,$$

where $\gamma_\Lambda^{\beta,\beta'}$ is viewed as a probability kernel from Ω to Ω. Show that this is the same as requiring that

$$\mu_1 = \mu_2 \otimes \mu_\Lambda^{\beta,\beta'},$$

where μ_1 and μ_2 are the two marginals of the measure μ on $\Omega = \Omega_\Lambda \times \Omega_{\Lambda^c}$, and $\mu_\Lambda^{\beta,\beta'}$ is viewed as a probability kernel from Ω_{Λ^c} to Ω_Λ.

10.2 **(homework)** *The partition function and the effect of ignoring the velocity.* Consider a system of interacting point particles in d dimensions with Hamiltonian $H(q,p) = \sum_i \frac{\vec{p}_i^2}{2m} + \sum_{i<j} \Phi(|q_i - q_j|)$. Consider the canonical partition function $Z^{can}(V,N,\beta)$ and the grand canonical partition function $Z^{gr}(V,\beta,\beta')$ (or $Z^{gr}(V,\beta,z)$ if you like), which are integrals of some weight functions on the phase space.

Now define the *configurational partition functions* by "ignoring the velocity". That is, e.g. $Z^{can}_{conf}(V,N,\beta)$ is an integral on the *configuration space only* of the canonical weight function with the kinetic energy omitted.

(a) Find the relation between the partition function and the configurational partition function, both in the canonical and the grand canonical setting.

(b) Calculate the density of the free gas with parameters β, z and m.

Solution:

(a) The integral defining the canonical partition function factorizes into a configurational and a velocity integral:

$$\begin{aligned} Z^{can}(V,N,\beta) &= \frac{1}{N!}\int_{\Lambda^N\times\mathbb{R}^{d\cdot N}} e^{-\beta H(q,p)}\,\mathrm{d}q\,\mathrm{d}p = \\ &= \frac{1}{N!}\int_{\Lambda^N\times\mathbb{R}^{d\cdot N}} e^{-\beta\sum_i \frac{\vec{p}_i^2}{2m}} e^{-\beta\sum_{i<j}\Phi(|q_i-q_j|)}\,\mathrm{d}q\,\mathrm{d}p = \\ &= \frac{1}{N!}\left(\int_{\Lambda^N} e^{-\beta\sum_{i<j}\Phi(|q_i-q_j|)}\,\mathrm{d}q\right)\left(\int_{\mathbb{R}^{d\cdot N}} e^{-\beta\sum_i\frac{\vec{p}_i^2}{2m}}\,\mathrm{d}p\right). \end{aligned}$$

The velocity integral can be computed explicitly, and the rest is exactly the configurational partition function:

$$\int_{\mathbb{R}^{d\cdot N}} e^{-\beta\sum_i\frac{\vec{p}_i^2}{2m}}\,\mathrm{d}p = \left(\int_{-\infty}^{\infty} e^{-\beta\frac{p_{1x}^2}{2m}}\,\mathrm{d}p_{1x}\right)^{d\cdot N} = \sqrt{\frac{2\pi m}{\beta}}^{d\cdot N},$$

so

$$Z^{can}(V,N,\beta) = \sqrt{\frac{2\pi m}{\beta}}^{d\cdot N} \frac{1}{N!}\int_{\Lambda^N} e^{-\beta\sum_{i<j}\Phi(|q_i-q_j|)}\,\mathrm{d}q = \sqrt{\frac{2\pi m}{\beta}}^{d\cdot N} Z^{can}_{conf}(V,N,\beta).$$

In the grand canonical partition function we use $z := e^{-\beta'}$ as the parameter, for convenience only. Now the grand canonical partition function can be expressed with the canonical as

$$\begin{aligned} Z^{gr}(V,\beta,z) &= \sum_{N=0}^{\infty} z^N Z^{can}(V,N,\beta), \\ Z^{gr}_{conf}(V,\beta,z) &= \sum_{N=0}^{\infty} z^N Z^{can}_{conf}(V,N,\beta). \end{aligned}$$

Using the previous result,

$$\begin{aligned} Z^{gr}(V,\beta,z) &= \sum_{N=0}^{\infty} z^N \sqrt{\frac{2\pi m}{\beta}}^{d\cdot N} Z^{can}_{conf}(V,N,\beta) = \\ &= \sum_{N=0}^{\infty} \left(z\sqrt{\frac{2\pi m}{\beta}}^{d}\right)^N Z^{can}_{conf}(V,N,\beta) = \\ &= Z^{gr}_{conf}\left(V,\beta,z\sqrt{\frac{2\pi m}{\beta}}^{d}\right). \end{aligned}$$

(b) In the free gas $\Phi = 0$, so

$$Z^{can}_{conf}(V,N,\beta) = \frac{1}{N!}\int_{\Lambda^N} 1\,\mathrm{d}q = \frac{V^N}{N!}$$

and

$$Z^{gr}_{conf}(V,\beta,z) = \sum_{N=0} z^N \frac{V^N}{N!} = e^{zV},$$

so

$$\log Z^{gr}_{conf}(V,\beta,\beta') = zV = Ve^{-\beta'}.$$

So the density of the "*configuration free gas*" is

$$\rho_{conf} := \frac{\mathbb{E}_{conf}N}{V} = -\frac{1}{V}\frac{\partial}{\partial\beta'}\log Z^{gr}_{conf}(V,\beta,\beta') = \frac{1}{V}Ve^{-\beta'} = z.$$

In particular, this is independent of β. However, if we do not ignore the velocities, we get

$$log Z^{gr}(V,\beta,z) = \log Z^{gr}_{conf}\left(V,\beta,z\sqrt{\frac{2\pi m}{\beta}}^{d}\right) = Vz\sqrt{\frac{2\pi m}{\beta}}^{d},$$

so

$$\log Z^{gr}(V,\beta,\beta') = V\sqrt{\frac{2\pi m}{\beta}}^{d} e^{-\beta'},$$

which gives

$$\rho := \frac{\mathbb{E}N}{V} = -\frac{1}{V}\frac{\partial}{\partial\beta'}\log Z^{gr}(V,\beta,\beta') = \frac{1}{V}V\sqrt{\frac{2\pi m}{\beta}}^{d} e^{-\beta'} = z\sqrt{\frac{2\pi m}{\beta}}^{d}.$$

10.3 **(homework)** *Is the grand canonical ensamble with boundary condition well defined?* Show that the grand canonical measure is well defined with any boundary condition in a system of interacting point particles with a bounded finite range pair interaction. What can we say if the pair interaction is only tempered and stable?

Solution: Forst of all, *sorry for the error in the exercise*, the statement is not true as written. As you will see from the solution, we need to assume that the pair interaction is finite range and *stable* – that is, there exists a $B < \infty$ such that

$$\sum_{1 \le i \le j \le N} \Phi(|q_i - q_j|) \ge -BN \quad \text{for every } N \text{ and } q_1, \dots, q_N \in \mathbb{R}^d.$$

Stability immediately implies that Φ is bounded from below by $-2B$ (just consider stability with $N = 2$.)

We need to show that the grand canonical partition function with boundary

$$Z(\Lambda, \beta, \beta'|\eta) := \sum_{N=1}^{\infty} \frac{1}{N!} \int_{\Lambda^N \times \mathbb{R}^{Nd}} e^{-\beta H_\Lambda(\omega|\eta) - \beta' N} \, \mathrm{d}\omega =$$
$$= \sum_{N=1}^{\infty} e^{-\beta' N} \frac{1}{N!} \int_{\Lambda^N \times \mathbb{R}^{Nd}} e^{-\beta\left(\sum_{i=1}^N \frac{p_i^2}{2m} + \sum_{1 \le i \le j \le N} \Phi(|q_i - q_j|) + \sum_{i=1}^N \sum_{j=1}^\infty \Phi(|q_i - \eta_j|)\right)} \, \mathrm{d}q \, \mathrm{d}p$$

is finite for every boundary configuration $\eta = \{\eta_j\}$. The key observation is that a boundary configuration is by definition *locally finite*, so there are only *finitely many* η_j for which $\Phi(|q_i - \eta_j|)$ can be nonzero – i.e. they are within the range of the interaction from some point of Λ. So the "interaction with the boundary configuration" term

$$\sum_{i=1}^{N} \sum_{j=1}^{\infty} \Phi(|q_i - \eta_j|)$$

is in fact a finite sum, and can be replaced by

$$\sum_{i=1}^{N} \sum_{j=1}^{M} \Phi(|q_i - \eta_j|),$$

where M is the above finite number of particles. This M of course depends on η, but that doesn't matter – we are looking only at a fixed η at a time. So since Φ is bounded from below by $-2B$, the "interaction with the boundary configuration" term satisfies

$$\sum_{i=1}^{N} \sum_{j=1}^{M} \Phi(|q_i - \eta_j|) \ge -2BMN.$$

For Z to be finite, we also need a bound on the "interactions within Λ" term

$$\sum_{1 \le i \le j \le N} \Phi(|q_i - q_j|).$$

This is the place where *we need stability* to get

$$\sum_{1 \le i \le j \le N} \Phi(|q_i - q_j|) \ge -BN.$$

(If we only used that $\Phi \geq -2B$ as before, we would only get $\sum_{1\leq i\leq j\leq N} \Phi(|q_i - q_j|) \geq -BN(N-1)$, which is not enough – the sum w.r.t. N in the definition of Z would not converge, at least for β big. Sorry again.)

All in all, we have

$$Z(\Lambda, \beta, \beta'|\eta) \leq \sum_{N=0}^{\infty} \frac{1}{N!} e^{-\beta' N} e^{\beta(BN+2BMN)} \int_{\Lambda^N \times \mathbb{R}^{Nd}} e^{-\beta \sum_{i=1}^{N} \frac{p_i^2}{2m}} \, \mathrm{d}q \, \mathrm{d}p.$$

The remaining integral is just V^N times the usual Gaussian velocity integral:

$$\int_{\Lambda^N \times \mathbb{R}^{Nd}} e^{-\beta \sum_{i=1}^{N} \frac{p_i^2}{2m}} \, \mathrm{d}q \, \mathrm{d}p = V^N \int_{\mathbb{R}^{Nd}} e^{-\beta \sum_{i=1}^{N} \frac{p_i^2}{2m}} \, \mathrm{d}p = V^N \sqrt{\frac{2\pi m}{\beta}}^{Nd}.$$

Writing this back,

$$Z(\Lambda, \beta, \beta'|\eta) \leq \sum_{N=0}^{\infty} \frac{1}{N!} \left(e^{-\beta' + \beta(B+2BM)} V \sqrt{\frac{2\pi m}{\beta}} \right)^N = \exp\left(e^{-\beta' + \beta(B+2BM)} V \sqrt{\frac{2\pi m}{\beta}} \right) < \infty.$$

Bonus question: What can we say if Φ is only tempered and stable? For a tempered and stable Φ the above Z may very well be infinite even for a locally finite η. Indeed, if $\Phi(r) \nearrow 0$ as $r \to \infty$, but it is not finite range, then – no matter how fast it goes to zero – one can construct a sequence $r_j \to \infty$ (which means that the set $\{r_j\}$ is locally finite) so that $\sum_{j=1}^{\infty} \Phi(r_j) = -\infty$. Similarly, one can construct a locally finite configuration $\eta = \{\eta_j\}$ (even in 1 dimension) such that $\sum_{j=1}^{\infty} \Phi(|q_1 - \eta_j|) = -\infty$ not only for a given q_1, but also for an entire neighbourhood of it, so already for $N = 1$ the factor $e^{-\beta H(\omega|\eta)}$ is infinite for a positive measure set of ω-s, and thus $Z = \infty$.

To avoid such a disaster, one can *impose further restrictions* on the boundary configurations η allowed. In particular, one can *demand* that η satisfy a property stronger than being just locally finite (also ruling out a fast growth of the density at infinity): Let η be such that there exists a $K = K(\eta) < \infty$, for which

$$\sum_{j=1}^{\infty} \Phi(|q - \eta_j|) > -K \text{ for any } q \in \Lambda. \tag{1}$$

For such η, the above argument about the finiteness of Z goes through.

If Φ has some regularity, e.g. it's eventually monotone and goes to zero not faster than exponentially, then it's enough to demand $\sum_{j=1}^{\infty} \Phi(|q - \eta_j|) > -\infty$ for a fixed q, say $q = 0$, and (1) follows automatically for the other $q \in \Lambda$.

10.4 *Consistency property.* Show that $\gamma_{\Lambda'}^{\beta,\beta'} = \gamma_{\Lambda'}^{\beta,\beta'} \otimes \gamma_{\Lambda}^{\beta,\beta'}$ for every bounded $\Lambda \subset \Lambda' \subset \mathbb{R}^d$.

10.5 *Gibbs measures of the free gas.* Find and describe every Gibbs measure of the free gas.

10.6 **(homework)** *Ising model in one dimension.* For the Ising model in one dimension, let the phase space be $\omega = \{-1, 1\}^N$ and the Hamiltonian be $H : \Omega \to \mathbb{R}$ be defined as

$$H(\sigma_1, \ldots, \sigma_N) := \sum_{i=1}^{N} (J\sigma_i\sigma_{i+1} + h\sigma_i).$$

(We use the convention $\sigma_{N+1} := \sigma_1$, which corresponds to periodic boundary conditions.)

(a) Calculate the partition function

$$Z(N,\beta,h) := \sum_{\sigma\in\Omega} e^{-\beta H(\sigma)}.$$

Hint: In the expression definig Z, discover a power of a 2×2 matrix. If you do it well, this matrix will be symmetric. In the end, you only need to calculate the eigenvalues.

(b) Calcualte the entropy in the thermodynamic limit (understand the question well) and show that it is a smooth function of h for every $\beta > 0$.

Solution:

(a) To "do it well", we write H as a sum of terms that are symmetric in the pair $(\sigma_i, \sigma_i + 1)$ (making use of the periodic boundary condition):

$$H(\sigma_1,\ldots,\sigma_N) := \sum_{i=1}^{N}(\frac{h}{2}\sigma_i + J\sigma_i\sigma_{i+1} + \frac{h}{2}\sigma_{i+1}).$$

Introduce the notation

$$P_{s,t} := e^{-\beta(\frac{h}{2}s+Jst+\frac{h}{2}t)},$$

with which

$$Z(N,\beta,h) := \sum_{\sigma\in\Omega} e^{-\beta H(\sigma)} = \sum_{\sigma_1,\ldots,\sigma_N\in\{-1,1\}} \prod_{i=1}^{N} P_{\sigma_i,\sigma_{i+1}} = \sum_{\sigma_1\in\{-1,1\}} P^N_{\sigma_1,\sigma_{N+1}}$$

if we consider P as the 2×2 matrix (indexed by $\{-1,1\}$)

$$P = \begin{pmatrix} P_{-1,-1} & P_{-1,1} \\ P_{1,-1} & P_{1,1} \end{pmatrix} = \begin{pmatrix} e^{\beta(h-J)} & e^{\beta J} \\ e^{\beta J} & e^{\beta(-h-J)} \end{pmatrix}.$$

So, since the periodic boundary condition means $\sigma_1 = \sigma_{N+1}$,

$$Z(N,\beta,h) = \sum_{s\in\{-1,1\}} P^N_{s,s} = \mathbf{Tr}(P^N).$$

Denote the two (different real) eigenvalues of P by λ_1 and λ_2 so that $|\lambda_1| < |\lambda_2|$:

$$\begin{aligned} \lambda_1 &= e^{-\beta J}\left(\cosh(\beta h) - \sqrt{\sinh^2(\beta h) + e^{4\beta J}}\right), \\ \lambda_1 &= e^{-\beta J}\left(\cosh(\beta h) + \sqrt{\sinh^2(\beta h) + e^{4\beta J}}\right). \end{aligned}$$

With these,

$$Z(N,\beta,h) = \lambda_1^N + \lambda_2^N.$$

(b) "understand the question well" means: scale with N appropriately before taking the limit. In our case the "good" thermodynamic limiting quantity is the free energy per particle (times $-\beta$) (also called pressure (times $-\beta$) in the context of the Ising model)

$$B(\beta,h) := \lim_{N\to\infty} \frac{1}{N}\log Z(N,\beta,h) = \log \lim_{N\to\infty} \sqrt[N]{\lambda_1^N + \lambda_2^N} = \log\lambda_2,$$

so

$$B(\beta, h) = -\beta J + \log\left(\cosh(\beta h) + \sqrt{\sinh^2(\beta h) + e^{4\beta J}}\right).$$

This is clearly analytic in both variables since it is a composition of functions that are analytic (in the interiour of their domains) and the argument of both the square root and the logarithm is alwasy positive.

The limiting entropy (per particle) is

$$s(\beta, h) = B(\beta, h) - \beta \frac{\partial}{\partial \beta} B(\beta, h)$$

(see Exercise 5.2), which inherits analiticity from B.