Prof. Dr. Roderich Tumulka
Eberhard Karls University Tübingen

Summer semester 2019
June 18, 2019

# Mathematical Statistical Physics: Assignment 8

**Problem 37:** *Addendum to Problem 33* (hand in, 50 points)
Let us revisit Problem 33 in more detail:

(a) Let $M : \mathbb{R}^d \to \mathbb{R}^d$ be a diffeomorphism with Jacobian determinant $|\det DM(\boldsymbol{x})| = 1$ at all $\boldsymbol{x} \in \mathbb{R}^d$. Explain why $M$ preserve volumes, $\mathrm{vol}(M(A)) = \mathrm{vol}(A)$.

(b) Suppose the point $X_0$ in $\mathbb{R}^d$ is chosen randomly with (smooth) probability density $\rho_0 : \mathbb{R}^d \to [0, \infty)$. Show that $M(X_0)$ has density $\rho_1(\boldsymbol{x}) = \rho_0(M^{-1}(\boldsymbol{x}))$.

(c) Now consider a Hamiltonian system on $\mathbb{R}^d$, suppose for simplicity that for each $t \in \mathbb{R}$ the flow map $T^t$ is a diffeomorphism $\mathbb{R}^d \to \mathbb{R}^d$, and recall that $T^t$ has Jacobian determinant 1 (Liouville's theorem). Let $\rho_t$ be the density of $X_t = T^t(X_0)$. Use the transformation formula for integrals to rewrite the integral

$$S_{\mathrm{Gibbs}}(\rho_t) = -k \int_{\mathbb{R}^d} d\boldsymbol{x}\, \rho_t(\boldsymbol{x}) \, \log \rho_t(\boldsymbol{x}) \,, \qquad (1)$$

then conclude that it equals $S_{\mathrm{Gibbs}}(\rho_0)$.

**Problem 38:** *Grand-canonical distribution* (hand in, 50 points)
As the canonical distribution of $\mathscr{S}$ arose as the marginal of the micro-canonical distribution for $\mathscr{S} \cup \mathscr{B}$, so does the grand-canonical distribution; we consider an ideal gas in a container $\Lambda \subset \mathbb{R}^3$ subdivided into a region $\Lambda_A$ and its complement $\Lambda_B = \Lambda \setminus \Lambda_A$. There are no walls between $\Lambda_A$ and $\Lambda_B$, 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 $\Gamma_1$; 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, $\Gamma$ 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 $\rho_{\mathrm{can}}$ on $\Gamma$, i.e., (ideal gas): $N$ points in $\Gamma_1$ are chosen i.i.d. according to the Maxwell-Boltzmann distribution $\rho_1 = Z_1^{-1} e^{-\beta H_1}$. The marginal $\rho_A$ of $\rho_{\mathrm{can}}$ on $\Gamma_A$ 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 $\Lambda \to \infty$, $N \to \infty$, $\Lambda_A$ fixed, $N \int_A \rho_1 \to c > 0$ (with suitable constant $c$),

$$\rho_A(x_1, \ldots, x_n) = \frac{1}{Z} \exp -\beta(H_A(x_1 \ldots x_n) - \mu n) \qquad (2)$$

with suitable constant $\mu \in \mathbb{R}$. This is the grand-canonical distribution. (If we write phase points in $\Gamma_A$ as ordered, then a further factor $1/n!$ appears in (2).)

**Hand in:** Wednesday, June 26, 2019, in the exercise class.