Mathematical Statistical Physics: Assignment 4

Problem 18: *Equivalence of ensembles* (hand in, 50 points)
An "ideal gas" is one whose molecules do not interact with each other. For an ideal gas without external field in a box Λ, the Hamiltonian is $H(\boldsymbol{q}_1, \boldsymbol{p}_1, \ldots, \boldsymbol{q}_N, \boldsymbol{p}_N) = \sum_{j=1}^N \boldsymbol{p}_j^2/2m$ on the phase space $\Gamma = (\Lambda \times \mathbb{R}^3)^N$. For large N, the micro-canonical distribution μ_{mc} [if you wish with "density" $\rho_{\mathrm{mc}}(x) = \mathscr{N}\,\delta(E - H(x))$] and the canonical distribution μ_{can} [with density $\rho_{\mathrm{can}}(x) = Z^{-1}\exp(-\beta H(x))$] are not very different, provided $E = E(\beta)$ [or $\beta = \beta(E)$] is suitably chosen: Both are constant on every energy surface, and both are narrowly concentrated around a certain energy value. To see this, proceed as follows.

(a) Show that $Z = \frac{1}{2}\,\mathrm{vol}(\Lambda)^N A_{3N} (2m/\beta)^{3N/2}\Gamma(3N/2)$.

(b) For $X \sim \mu_{\mathrm{can}}$, determine $\mathbb{E}H(X)$ and $\mathrm{Var}\,H(X)$. [*Hint*: $\Gamma(x+1) = x\Gamma(x)$.]

(c) Which relation $E(\beta)$ is required to ensure that μ_{mc} and μ_{can} have the same expected energy?

(d) How large is $\mathrm{Var}\,H(X)$ compared to $[\mathbb{E}H(X)]^2$?

Problem 19: *Heat capacity* (hand in, 25 points)
The heat capacity C of a physical body in thermal equilibrium at temperature T is defined to be dE/dT, where dE is the amount of energy that must be supplied to the body to increase its temperature by dT. Heat capacity is an extensive property of matter, meaning that it is additive when disjoined systems get combined. Thus, it is proportional to the size of the object, and the heat capacity per mass is a constant called the specific heat capacity or simply the specific heat c.

(a) From the relation $\overline{e} = \frac{3}{2}kT$, derive a formula for the specific heat of the ideal gas.

(b) Let us consider systems for which, as for the ideal gas, $E = CT$ with temperature independent C. Suppose that system $\mathscr{S}_1$ is isolated and in thermal equilibrium at temperature T_1, $\mathscr{S}_2$ likewise at $T_2 < T_1$. Now we bring $\mathscr{S}_1$ and $\mathscr{S}_2$ in thermal contact and wait for $\mathscr{S}_1 \cup \mathscr{S}_2$ to reach thermal equilibrium. Determine the resulting temperature of $\mathscr{S}_1 \cup \mathscr{S}_2$. (*Hint*: Since $\mathscr{S}_1 \cup \mathscr{S}_2$ is isolated, its energy is conserved.)

Problem 20: *Net force exerted by pressure* (hand in, 25 points)
Show that in the absence of external fields, the net force exerted by the pressure of a gas according to the Maxwellian distribution on the walls of the container vanishes. (As a consequence, the center of mass of the container does not move if it was at rest initially.)
Instructions: Our derivation of the equation of state of an ideal gas, $pV = NkT$, shows, among other things, that the pressure is constant along the wall. The shape $\Lambda \subset \mathbb{R}^3$ of the container can be arbitrary, but we may assume that the boundary $\partial\Lambda$ is piecewise smooth. The force on the surface element $d^2x \subset \partial\Lambda$ has magnitude $p\,d^2x$ and direction outward normal to the wall $\partial\Lambda$. We want to show that the total force is $\mathbf{0}$.

Problem 21: *Alternative proof of Theorem 7* (optional extra credit, 50 points)
We only aim at a weaker version of Theorem 7 that claims, instead of L^1 convergence, merely setwise convergence. A sequence μ_n of measures is said to *converge setwise* (or *strongly*) to μ iff $\mu_n(A) \to \mu(A)$ for every measurable set A. It is clear that convergence in the total variation distance implies setwise convergence; the converse is not true.

Now let $\boldsymbol{Z} = (Z_1, \ldots, Z_d) \sim \mathcal{N}^d(0, I)$, set $X_j = \sqrt{d} Z_j / |\boldsymbol{Z}|$, and let $\varepsilon, \delta \in (0,1)$ be arbitrary.

(a) Show that for sufficiently large d,

$$\mathbb{P}\Big(1 - \delta < \frac{|\boldsymbol{Z}|^2}{d} < 1 + \delta\Big) > 1 - \varepsilon\,. \tag{1}$$

Hint: Clearly, $\mathbb{E}Z_j^2 = \mathrm{Var}(Z_j) = 1$. Use without proof that $\mathrm{Var}(Z_j^2) = 3$.

(b) Show that if μ is a probability measure on $(\Omega, \mathscr{F})$ and $\mu(E) > 1 - \varepsilon$ for some event $E \in \mathscr{F}$, then the total variation distance between μ and the conditional distribution $\mu(\cdot|E) = \mu(\cdot \cap E)/\mu(E)$ is at most 2ε.

(c) Let μ, ν be probability measures on $\Omega_1 \times \Omega_2$ and μ_1, ν_1 their marginals on Ω_1 (i.e., after integrating out Ω_2). Let dist denote the total variation distance. Show that

$$\mathrm{dist}(\mu_1, \nu_1) \leq \mathrm{dist}(\mu, \nu)\,. \tag{2}$$

(d) It is known that for every probability measure μ and every decreasing sequence $A_1 \supseteq A_2 \supseteq \ldots$, $\mu(A_n) \to \mu(\bigcap_m A_m)$ decreasingly as $n \to \infty$. For $C \subseteq \mathbb{R}^k$, let

$$C_\delta := \Big\{\lambda \boldsymbol{x} : \boldsymbol{x} \in C, \lambda \in \Big[\sqrt{1-\delta}, \sqrt{1+\delta}\Big]\Big\}\,. \tag{3}$$

Show that for every probability measure μ, $\mu(C_\delta) \to \mu(C)$ as $\delta \to 0$.

(e) In order to prove Theorem 7 for $\sigma = 1$ and setwise convergence, compare the distribution μ_X of $X_1, \ldots, X_k$ to the conditional distribution μ_{ZE} of $Z_1, \ldots, Z_k$ given the event $E = \{1 - \delta < |\boldsymbol{Z}|^2/d < 1 + \delta\}$, and that in turn to the distribution μ_Z of $Z_1, \ldots, Z_k$.

Hand in: Wednesday, May 22, 2019, in the exercise class.