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Math Stat Phys: Some In-Class Problems

Problem 1: *Boltzmann equation with external potential*
In an external potential V_1, the Boltzmann equation reads

$$\left(\frac{\partial}{\partial t} + \boldsymbol{v}\cdot\nabla_{\boldsymbol{q}} - \frac{1}{m}\nabla V_1(\boldsymbol{q})\cdot\nabla_{\boldsymbol{v}}\right) f(\boldsymbol{q},\boldsymbol{v},t) = Q(\boldsymbol{q},\boldsymbol{v},t) \tag{1}$$

with the same collision term as given in the lectures,

$$Q(\boldsymbol{q},\boldsymbol{v},t) = \lambda \int_{\mathbb{R}^3} d^3\boldsymbol{v}_* \int_{\mathbb{S}^2} d^2\boldsymbol{\omega}\, 1_{\boldsymbol{\omega}\cdot(\boldsymbol{v}-\boldsymbol{v}_*)>0}\, \boldsymbol{\omega}\cdot(\boldsymbol{v}-\boldsymbol{v}_*) \times \Big[f(\boldsymbol{q},\boldsymbol{v}',t)\, f(\boldsymbol{q},\boldsymbol{v}'_*,t) - f(\boldsymbol{q},\boldsymbol{v},t)\, f(\boldsymbol{q},\boldsymbol{v}_*,t)\Big]\,, \tag{2}$$

and boundary condition

$$f(\boldsymbol{q},\boldsymbol{v},t) = f\big(\boldsymbol{q},\boldsymbol{v}-2[\boldsymbol{v}\cdot\boldsymbol{n}]\boldsymbol{n},t\big) \tag{3}$$

for $\boldsymbol{q}\in\partial\Lambda$ and $\boldsymbol{n}=\boldsymbol{n}(q)$ the outward unit normal vector. Show that the Maxwell-Boltzmann distribution is a stationary solution.

Problem 2: *Grand-canonical distribution as a marginal*
We consider an ideal gas in a container $\Lambda\subset\mathbb{R}^3$ subdivided into a region Λ_A and its complement $\Lambda_B=\Lambda\setminus\Lambda_A$. There are no walls between Λ_A and Λ_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 Γ_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, Γ 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 ρ_{can} on Γ, i.e., (ideal gas): N points in Γ_1 are chosen i.i.d. according to the Maxwell-Boltzmann distribution $\rho_1=Z_1^{-1}e^{-\beta H_1}$. The marginal ρ_A of ρ_{can} on Γ_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 $\Lambda\to\infty$, $N\to\infty$, Λ_A fixed, H_1 fixed, $N\int_A\rho_1\to c>0$ (with suitable constant c),

$$\rho_A(x_1,\ldots,x_n) = \frac{1}{Z}\exp\Big[-\beta(H_A(x_1\ldots x_n)-\mu n)\Big] \tag{4}$$

with suitable constant $\mu\in\mathbb{R}$. This is the grand-canonical distribution. (If we write phase points in Γ_A as ordered, then a further factor $1/n!$ appears in (4).)

Problem 3: *Stirling formula via Laplace's method*

The Stirling formula says that

$$n! \approx n^n e^{-n} \sqrt{2\pi n}. \tag{5}$$

We will derive it non-rigorously by means of Laplace's method: if a (sufficiently smooth) function $f(x)$ has a global maximum at $x = x_m$ and only there, then for $n \gg 1$,

$$\int_{\mathbb{R}} \mathrm{d}x\, e^{nf(x)} \approx e^{nf(x_m)} \sqrt{\frac{2\pi}{n|f''(x_m)|}}. \tag{6}$$

In order to derive (5), follow these steps:

(a) From earlier assignments we know that $n!$ can be expressed by the Gamma function,

$$n! = \Gamma(n+1) = \int_0^\infty \mathrm{d}t\, t^{n+1} e^{-t}. \tag{7}$$

Find a substitution to bring the integrand in the form $e^{nf(x)}$.

(b) The integral

$$\int_{\mathbb{R}} \mathrm{d}x\, e^{nf(x)} \tag{8}$$

is dominated by those x that are in the neighbourhood of the global maximum x_m. Perform a Taylor expansion of $f(x)$ around x_m up to second order (neglecting terms of third order and beyond) to show that

$$\int_{\mathbb{R}} \mathrm{d}x\, e^{nf(x)} \approx e^{nf(x_m)} \int_{\mathbb{R}} \mathrm{d}x\, e^{-\frac{n}{2}|f''(x_m)|(x-x_m)^2}. \tag{9}$$

(c) Evaluate the integral

$$e^{nf(x_m)} \int_{\mathbb{R}} \mathrm{d}x\, e^{-\frac{n}{2}|f''(x_m)|(x-x_m)^2} \tag{10}$$

and deduce (5).

Problem 4: *Dominance of Thermal Equilibrium*
In the lecture, we discussed the fact that the thermal equilibrium macro set Γ_{eq} is almost as huge as the corresponding energy shell Γ_{mc}, a fact known as *dominance of thermal equilibrium.* The goal of this exercise is to obtain the estimate[1]

$$\frac{\mathrm{vol}\,\Gamma_{\mathrm{eq}}}{\mathrm{vol}\,\Gamma_{\mathrm{mc}}} \approx 1 - \exp(-10^{-15}N). \tag{11}$$

To this end, we focus on positions only, i.e., we consider configuration space Λ^N, where $\Lambda \subset \mathbb{R}^3$ has finite volume. Divide Λ into m cells Λ_j of equal volume. We use the

[1] following the lecture notes, p.66-67.

uniform distribution over Λ^N and take the macro variables to be $M_j = [N_j/N\Delta M_j]\Delta M_j$, $j = 1, \ldots, m$, where N_j is the number of particles in Λ_j, meaning that M_j is the rounded relative occupation number of Λ_j.

(a) Under these assumptions, argue that the equilibrium value of M_j is $\nu_j^{\text{eq}} = 1/m$.

(b) Explain that the distribution of N_j is binomial with parameters N and $1/m$. [2]

(c) Use the theorem of de Moivre-Laplace to see that approximately $N_j \sim \mathcal{N}(Nm^{-1}, N(m-1)m^{-2})$.

(d) A deviation of M_j from its equilibrium values requires that N_j deviates from $1/m$ by more than $N\Delta M_j$, i.e., by more that $\sqrt{mN}\Delta M_j$ standard deviations. Use the fact that for $Z \sim \mathcal{N}(0,1)$ and for all $z > 0$

$$\mathbb{P}(|Z| > z) \leq e^{-z^2/2} \tag{12}$$

to show that the probability that any M_j deviates from its equilibrium value $1/m$ is given by

$$\mathbb{P}\left(\exists j : M_j \neq \nu_j^{\text{eq}}\right) \leq mp_0 \tag{13}$$

where $p_0 = \exp(-mN\Delta M_j^2/2)$. Conclude that for $\Delta M_j = 10^{-12}$ and a reasonable choice of m, (11) holds.

[2] Recall: the binomial distribution with parameters n and p is the distribution of the number X of successes among n independent trials of a random experiment that succeeds with probability p. It has expectation np and variance $np(1-p)$.