Math 254A Lecture 13 Notes

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1 Observing Macroscopic Quantities From Microscopic States

1.1 Recap

We have a phase space (M, λ) which is a σ finite but not finite measure space. The energy of one particle is $\varphi : M \to [0, \infty)$, where $\min \varphi = \operatorname{ess\,min} \varphi = 0$. Then we know that

$$\lambda^{\times n}\left(\left\{(p_1, \dots, p_n) \in M^n : \frac{1}{n}\Phi_n(p_1, \dots, p_n) := \frac{1}{n}\sum_{i=1}^n \varphi(p_i) \in I\right\}\right)$$
$$= \exp\left(n \cdot \sup_{x \in I} s(x) + o(n)\right),$$

where

$$s(x) = \inf_{\beta > 0}\{s^*(\beta) + \beta x\}.$$

We also have the Fenchel-Legendre transform

$$s^*(\beta) = \log \int e^{-\beta\varphi}.$$

β achieves equality in the definition of s

$$\begin{aligned}
&\iff s \text{ has a tangent of slope } \beta \text{ at } x \\
&\iff D_+ s(x) \le \beta \le D_- s(x) \\
&\iff s^*(\beta + (-s(x)) = -\beta x \\
&\iff D_- s^*(\beta) \le -x \le D_+ s^*(\beta) \\
&\iff s^* \text{ has a tangent of slope } -x \text{ at } \beta.
\end{aligned}$$

Using s^*, we can prove:

- $$s^*(\beta) \to \begin{cases} \log \lambda(\{\varphi = 0\}) & \beta \to \infty \\ \infty & \beta \downarrow 0. \end{cases}$$

- s^* is strictly decreasing and strictly convex.
- s^* is differentiable on $(0, \infty)$.
- $$s(x) \to \begin{cases} \log \lambda(\{\varphi = 0\}) & x \downarrow 0 \\ \infty & x \to \infty. \end{cases}$$
- s is strictly increasing and strictly concave.
- s is differentiable on $(0, \infty)$.

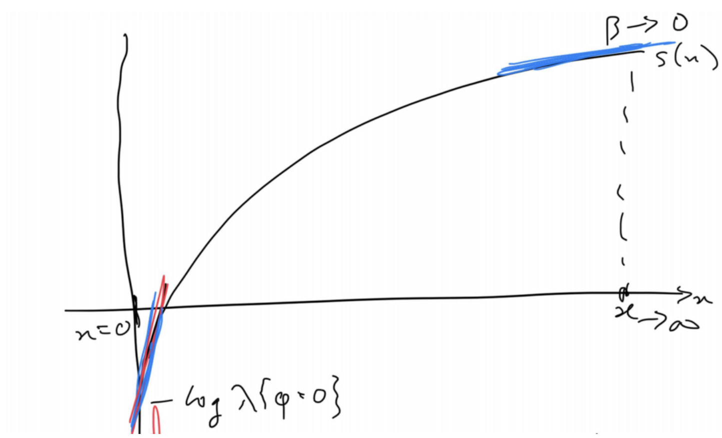
1.2 Behavior of s'

Let's analyze the behavior of s':

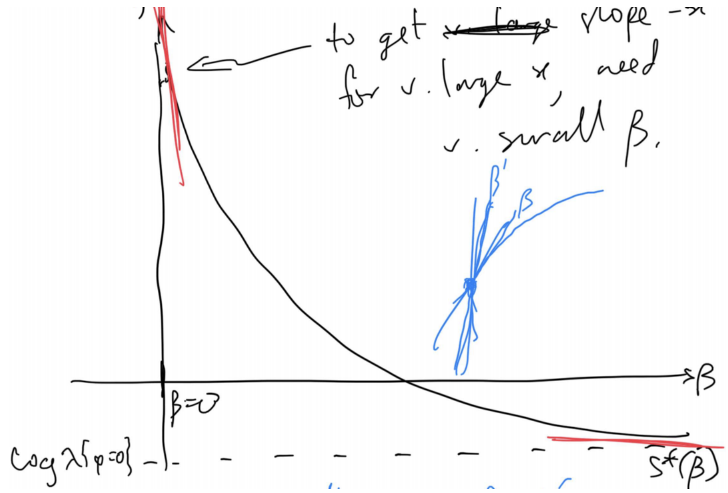
Proposition 1.1.

$$s'(x) \to \begin{cases} 0 & x \to \infty \\ \infty & x \to 0. \end{cases}$$

Instead of a formal proof, here are some pictures. Look at the possible slopes we can get for points on the graph of s and how they correspond to slopes for points on the graph for s^*.



To get slope $-x$ for very large x in the graph of s^*, we need very small β.



1.3 Observing macroscopic quantities froms microscopic states

Now imagine we are looking at some other macroscopic observable quantity of the microscopic state $(p_1, \ldots, p_n) \in M^n$. We will study functions for the form

$$\Psi_n(p_1, \ldots, p_n) = \sum_{i=1}^{n} \psi(p_i).$$

If $M = \mathbb{R}^3 \times \mathbb{R}^3$, we could take $\psi(r, p) = \mathbb{1}_D(r)$, which indicates whether a particle is in D or not in D; then Ψ_n would be the total number of particles in D.

We need some regularity. A simple sufficient condition is that ψ is bounded. A weaker but still sufficient condition is that for every $\beta > 0$, there is an $\varepsilon > 0$ such that $\int e^{-\beta\varphi} e^{-\gamma\psi}\, d\lambda < \infty$ for all $\gamma \in (-\varepsilon, \varepsilon)$.

Let's assume ψ is bounded, and we'll ask about the distribution of Ψ_n on the approximate level set $\{\frac{1}{n}\Phi_n \in I\}$, where I is a small interval. We need to compare $\lambda^{\times n}(\{\frac{1}{n}\Phi_n \in I\})$ and $\lambda^{\times n}(\{\frac{1}{n}\Phi_n \in I, \frac{1}{n}\Psi_n \in J\})$. We use the generalized type-counting machinery with $\mathbb{R}^2$ to get an asymptotic for this:

$$\begin{aligned}\lambda^{\times n}\left(\left\{\frac{1}{n}\Phi_n \in I, \frac{1}{n}\Psi_n \in J\right\}\right) &= \lambda^{\times n}\left(\left\{(p_1, \ldots, p_n) \in M^n : \frac{1}{n}\sum_{i=1}^{n}(\varphi(p_i), \psi(p_i)) \in I \times J\right\}\right) \\ &= \exp\left(n \cdot \sup_{(x,y)\in I\times J} \widetilde{s}(x, y) + o(n)\right),\end{aligned}$$

where $\widetilde{s}(x, y) : \mathbb{R}^2 \to [-\infty, \infty)$ is an upper semicontinuous, concave function with

$$\widetilde{s}(x, y) = \inf_{\beta,\gamma}\{\widetilde{s}^*(\beta, \gamma) + \beta x + \gamma y\}.$$

and Fenchel-Legendre transform

$$\widetilde{s}^*(\beta, \gamma) = \log \int e^{-\beta\varphi} e^{-\gamma\psi} \, d\lambda.$$

Here, we assume ψ is bounded, $|\psi| \le M$, so

$$\widetilde{s}^*(\beta, \gamma) = \begin{cases} \infty & \beta = 0 \\ < \infty & \beta > 0. \end{cases}$$

Here, $\widetilde{s}(x, y) \le s(x)$ for all $y \in \mathbb{R}$. We want to find a y_0 such that $\widetilde{s}(x, y_0) = s(x)$ and $\widetilde{s}(x, y) < s(x)$ for any other y. This will tell us that conditioned on Φ being x, we are likely to have Ψ be y_0 and not likely to have any other y. We have

$$s(x) = \inf_{\beta > 0} \left\{ \log \int e^{-\beta\varphi} \, d\lambda + \beta x \right\},$$

which is greater than or equal to

$$\widetilde{s}(x, y) = \inf_{\beta > 0, \gamma \in \mathbb{R}} \left\{ \log \int e^{-\beta\varphi} e^{-\gamma\psi} \, d\lambda + \beta x + \gamma y \right\}.$$

Lemma 1.1. *$\widetilde{s}(x, y_0) = s(x)$ and $\widetilde{s}(x, y) < s(x)$ for any other y, where*

$$y_0 = \int \psi e^{-\beta\varphi} \, d\lambda = \langle \psi, \mu_\beta \rangle$$

and

$$d\mu_\beta(p) = \frac{e^{-\beta\varphi(p) \, d\lambda(p)}}{\int e^{-\beta\varphi} \, d\lambda}$$

is the ***Gibbs measure*** *obtained from λ, φ, β.*

Proof. First, s is differentiable, so for every $x > 0$, there is a unique $\beta > 0$ such that $s(x) = \log \int e^{-\beta\varphi} \, d\lambda + \beta x$. To achieve $\widetilde{s}(x, y_0) = s(x)$, we must have that the function $\gamma \mapsto \log \int e^{-\beta\varphi} e^{-\gamma\psi} \, d\lambda + \beta x + \gamma y_0$ achieves its minimum uniquely at $\gamma = 0$. This function of γ is convex (by Hölder), strictly convex if ψ is not a.s. constant, and differentiable. Assuming ψ is not a.s. constant, we need y_0 such that

$$\frac{\partial}{\partial\gamma} \left\{ \log \int e^{-\beta\varphi} e^{-\gamma\psi} \, d\lambda + \beta x + \gamma y_0 \right\} = 0$$

at $\gamma = 0$. This is the derivative of the log of the moment generating function. Differentiate under the integral to get

$$\frac{\partial}{\partial\gamma} \log \int e^{-\beta\varphi} e^{-\gamma\psi} \, d\lambda = \left. \frac{\int -\psi e^{-\beta\varphi} e^{-\gamma\psi} \, d\lambda}{\int e^{-\beta\varphi} e^{\gamma\psi} \, d\lambda} \right|_{\gamma=0} = -\langle \psi, \mu_\beta \rangle.$$

So $\frac{\partial}{\partial\gamma}[\cdots]|_{\gamma=0} = -\langle \psi, \mu_\beta \rangle + y_0$, and this equals 0 iff $y_0 = \langle \psi, \mu_\beta \rangle$. $\square$

Corollary 1.1.

$$\lambda^{\times n}\left(\left\{\left|\frac{1}{n}\Psi_n - \langle\psi,\mu_\beta\rangle\right| > \varepsilon\right\} \;\middle|\; \left\{\frac{1}{n}\Phi_n \in I\right\}\right) \leq e^{-c\cdot n + o(n)},$$

where c is a constant, I is a short enough interval containing x, and we are using conditional probability notation.

Remark 1.1. Given $\frac{1}{n}\Phi_n \approx x$, we found that

$$\begin{aligned}\Psi_n &\approx n(\text{its average over } \{\tfrac{1}{n}\Phi_n \approx n\}^{1}) \\ &\approx n\langle\psi,\mu_\beta\rangle \\ &= \langle\psi(p_1)+\cdots+\psi(p_n), \mu_\beta^{\times n}\rangle \\ &= \int \Psi_n \, d\mu_{\beta,n},\end{aligned}$$

where

$$d\mu_{\beta,n}(p_1,\ldots,p_n) = \frac{e^{-\beta\Psi_n(p_1,\ldots,p_n)}\, d\lambda^{\times n}(p)}{\int e^{-\beta\Psi_n}\, d\lambda^{\times n}} = \mu_\beta \times \cdots \times \mu_\beta$$

is called the **canonical ensemble measure**.

[1] This is called the **microcanonical ensemble**.