Math 254A Lecture 11 Notes

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1 Mathematical Setup for Statistical Mechanics

1.1 Relationship to type counting

Our goal is to set up some mathematical models of physical systems with large numbers of degrees of freedom and see whether "most microstates look the same" after fixing a few macroscopic parameters.

To begin with, we will focus on n classical[1] non-interacting, identical point particles moving around in a potential. Non-interacting particles can be thought of as particles where the energies of interaction are negligible compared to the total energy of the system.

We will describe the particles via their positions $r_1, \dots, r_n \in \mathbb{R}^3$ and velocities $v_1, \dots, v_n \in \mathbb{R}^3$. Newton's law says

$$m \frac{dv_i}{dt} = m \frac{d^2 r_i}{dt} = F_i = -\nabla V(r_i).$$

We will assume the mass m equals 1, so $v_i = p_i$, the momentum. The total energy is

$$\Phi(r_1, \dots, r_n, p_1, \dots, p_n) = \sum_{i=1}^n \varphi(r_i, p_i), \qquad \varphi(r_i, p_i) = v(r_i) + \frac{1}{2}|p_i|^2.$$

We want to study averages over the set

$$\Omega(n, I) = \{(r_1, \dots, p_n) \in (\mathbb{R}^3)^n \times (\mathbb{R}^3)^n : \frac{1}{n}\Phi(r_1, \dots, p_n) \in I = (E - \varepsilon, E + \varepsilon)\}$$

for some desired total energy E and error tolerance ε.

The first step is to ask: How big is $\Omega(n, I)$ in the sense of Lebesgue measure? This is just an instance of generalized type counting: $M = \mathbb{R}^3 \times \mathbb{R}^3$, $\lambda = m_3 \times m_3$, and $\varphi : M \to [0, \infty)$. Note that we are assuming V is lower bounded, and we are adjusting it by a constant to assume its minimum equals 0. Now the asymptotic behavior of

$$\lambda^{\times n}\left(\left\{(r_1, \dots, p_n) : \frac{1}{n}\Phi \in I\right\}\right) = \exp\left(n \cdot \sup_{E \in I} s(E) + o(n)\right).$$

[1] Here, classical means not quantum. You can do this with quantum physics, but it requires making use of the full machinery of Hilbert spaces.

To go further, we need to know more about s in the present situation.[2]

1.2 Assumptions of the model and properties of the entropy

Here are the salient features of the present situation and a necessary assumption:

- (M, λ) is σ-finite but not finite.
- $\min \varphi = 0 = \text{ess } \min \varphi$, i.e. $\lambda(\{(r,p) : \varphi(r,p) < a\}) > 0$ for all $a > 0$.
- We need V to confine particles strongly enough to bounded regions of space. Mathematically, we will ask that $\int e^{-\beta\varphi}\, d\lambda < \infty$ for all $\beta > 0$. [Note that $\int e^{-\beta\varphi}\, d\lambda = \iint_{\mathbb{R}^3 \times \mathbb{R}^3} e^{-\beta V} e^{-(\beta/2)|p|^2}\, dm_3(r)\, dm_3(p)$.][3]

Under these assumptions, we know that $s(E)$ exists, is upper semicontinuous, concave, and is $s : \mathbb{R} \to [-\infty, \infty)$. In fact, we also know that $s \equiv -\infty$ on $[-\infty, 0)$, so we can focus on $s|_{[0,\infty)}$. In this case, we have our variational formula

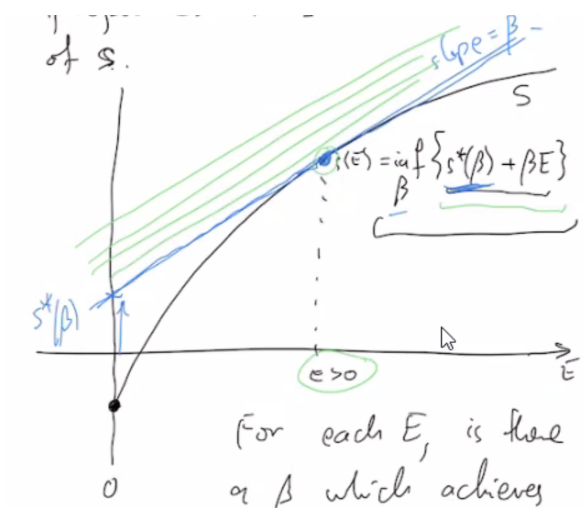
$$s(E) = \inf_{\beta} \{s^*(\beta) + \langle \beta, E \rangle\},$$

where

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

Note that we have switched y with $-\beta$, as β has a physical interpretation.

We will use the formula for s^* to derive more qualitative features of s. We will set up ways of translating properties of s^* into those of s. Here is a picture of s and s^*:



[2]In this situation, s is $\frac{1}{n}$ times the **Boltzman entropy**/

[3]Notably, gravity does not satisfy this assumption, but gravity operates on different scales than we are working with, so we will ignore it.

For each E, is there a β which achieves the equality $s(E) = s^*(\beta) + \beta(E)$? The answer is yes, if and only if s has finite one-sided derivative on at least one side, and then you can use any $D_-s(E) \leq \beta \leq D_+s(E)$. In particular, if $s'(E)$ exists, then the unique choice is $\beta = s'(E)$.