Statistical Physics Summer 2019

Shannon entropy and fluctuations of energy — 01.04, 2019

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1 Overview

In the last lecture we talked about canonical distribution.

In this lecture we covered: Shannon entropy, fluctuations of energy and fluctuations of magnetisation.

2 Reminder

As we remember we have a system in equilibrium. It can have one of r states. Each state is associated with energy ε_r and probability of being in this state is p_r equal to:

$$p_r = \frac{1}{z}e^{-\beta\varepsilon_r} \quad \beta = \frac{1}{k_B T} \quad z = \sum_r e^{-\beta\varepsilon_r} \tag{1}$$

For n particles z will be equal to

$$z = \frac{1}{N!h^{3N}} \int dq_1...dq_N dp_1...dp_N e^{-\beta\varepsilon(\{q\},\{p\})} \tag{2}$$

We have also shown that internal energy at different time is different. It is a random variable, so we use average energy, defined as follows

$$U =< \varepsilon >= \sum_r \varepsilon_r P_r p_r = \frac{1}{z}\sum_r \varepsilon_r e^{-\beta\varepsilon_r} = \frac{\partial}{\partial\beta}\ln z = U \tag{3}$$

2.1 Scheme

Having energy, we can calculate partition function, using which we can calculate internal energy, which is our connection to thermodynamics. Or given as a diagram:

$$\varepsilon \to Z \to U \to \text{thermodynamics} \tag{4}$$

Using p_r we calculated ε_r. Bur let's say we have another variable depending on state. Then p_r averages A (which is state of a system), eg. magnetism

$$< A >= \sum_r A_r p_r \tag{5}$$

3 Relation to thermodynamics

Assume $F = -k_B T \ln z^*$ where F is free energy ($F = U - TS$). Let's recall we discussed

$$U = -T^2 (\frac{\partial}{\partial T} \frac{F}{T})_V {}^{**} \tag{6}$$

Now, insert * into ** and calculate, so you'll get

$$-\frac{\partial}{\partial \beta} \ln z = U \tag{7}$$

4 Shannon Entropy & Canonical Distribution

Let's define new probability $\{p_r\} : S_H = - < \ln p >= - \sum_r p_r \ln p_r$

When there are few paths, system will choose the one which will result in max entropy.

Question Search maxima of S_H

We have to cases
case a $\sum_r = 1$
We then use Lagrange multiplier:

$$L = - \sum_l p_l \ln(p_l) - \lambda \sum_l p_l \tag{8}$$

Now let's calculate it:

$$\frac{\partial L}{\partial p_r} = \sum_l \frac{\partial}{\partial p_r} (p_l \ln p_l) - \lambda \sum_l \frac{\partial}{\partial p_r} p_l = - \frac{\partial}{\partial p_r} (p_r \ln p_r) - \lambda = \tag{9}$$

$$= -\{\ln p_r + p_r \frac{1}{p_r}\} - \lambda = - \ln p_r - 1 - \lambda = 0 \tag{10}$$

So we see that

$$\ln p_r = 1 - \lambda = const \implies p_r = const \tag{11}$$

And because all probabilities sum up to 1, then biggest entropy is for states with equal probability ($\frac{1}{N}$). We can also see, that

$$S_H = - \sum_l p_l \ln p_l = - \sum_{l-1}^{N} \frac{1}{N} \ln \frac{1}{N} = -(\frac{1}{N} \ln \frac{1}{N}) \sum_{l-1}^{N} -1 = -ln \frac{1}{N} \tag{12}$$

and thus Shannon entropy is given by

$$S_H = \ln N \tag{13}$$

where N is number of states for a given system. This means Shannon entropy for equal states gives **Boltzman entropy**.

case b $\sum_l p_l = 1$ and $\sum p_l \varepsilon_l = const$
In this example we use Laplace multiplier again, this time in form

$$L = -\sum_l p_l \ln(p_l) - \lambda \sum_l p_l - \beta \sum_l p_l \varepsilon_l \tag{14}$$

Where λ, and β are Laplace multipliers. Calculation was left as homework. Expected result follows

$$p_r \sim e^{-\beta \varepsilon_r} \tag{15}$$

5 Fluctuations of energy

Imagine we have a system exchanging energy with the environment. Average energy of such system is equal to

$$< \varepsilon >= U \tag{16}$$

Variance of such random variable ε is given

$$< (\varepsilon - < \varepsilon >)^2 > \tag{17}$$

Using the integral from 2 we obtain

$$< (\varepsilon - < \varepsilon >)^2 >= C_v k_B T^2 \tag{18}$$

where C stands for heat capacity.

6 Fluctuations of magnetisation

Similar thing goes for magnetisation, with exception we have

$$M = \sum_l S_i \tag{19}$$

and

$$< (M - < M >)^2 >= N k_B T \chi \tag{20}$$

where χ is magnetic susceptibility denoted as

$$\chi = \frac{\partial m}{\partial B}(T, B = 0); \quad m = \frac{< M >}{N} \tag{21}$$