Tutorial 1, Statistical Mechanics: Concepts and applications 2017/18 ICFP Master (first year)

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Tutorial

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1. General properties of the characteristic functions.

- (a) [EASY] Prove the following properties:
 - $\Phi_{\xi}(0) = 1$.

The total probability is normalized to 1.

- $\Phi_{\xi}(-t) = \Phi_{\xi}^{*}(t)$.

The probability distribution is real.

- $|\Phi_{\mathcal{E}}(t)| \leq 1$.

The absolute value of the integral is bounded from above by the integral of the absolute value, which is $\Phi_{\xi}(0)$.

- $\Phi_{a\xi+b}(t) = e^{ibt}\Phi_{\xi}(at)$.

Under a change of variables $\xi' = f(\xi)$, with $f(\xi)$ monotonous, the probability distribution transforms as follows

$$\pi_{\xi'}(x) = \frac{\pi_{\xi}(f^{-1}(x))}{|f'(f^{-1}(x))|}.$$
 (1)

In particular, under a linear transformation we have

$$\pi_{a\xi+b}(x) = |a|^{-1}\pi_{\xi}((x-b)/a)$$
 (2)

and hence

$$\Phi_{a\xi+b}(t) = \int dx \ e^{ixt} |a|^{-1} \pi_{\xi}((x-b)/a) = e^{ibt} \Phi_{\xi}(at).$$
 (3)

(b) [EASY] Let ξ_1 and ξ_2 two independent random variables, what is the characteristic function of their sum? What about the sum of n independent random variables?

Since ξ_1 and ξ_2 are independent, so are $e^{it\xi_1}$ and $e^{it\xi_2}$.

$$\Phi_{\xi_1 + \xi_2}(t) = \mathbb{E}(e^{it(x_1 + x_2)}) = \mathbb{E}(e^{itx_1}e^{itx_2}) = \mathbb{E}(e^{itx_1})\mathbb{E}(e^{itx_2}) = \Phi_{\xi_1}(t)\Phi_{\xi_2}(t)$$

This can be readily generalized to N variables

$$\Phi_{\sum_{i}^{N} \xi_{i}}(t) = \prod_{i=1}^{N} \Phi_{\xi_{i}}(t).$$
 (4)

(c) [EASY] Name the first two cumulants. What is the variance of the sum of two independent random variables?

The first cumulant κ_1 is the mean. The second cumulant is the variance. The cumulants are proportional to the coefficients of the series expansion of the logarithm of the characteristic function. Since the logarithm of a product is the sum of the logarithms, the n-th cumulant of the sum of two independent random variables is the sum of the n-th cumulant of the random variables. In particular, this applies to n = 2, i.e. to the variance.

2. Sum of random variables with uniform distribution.

(a) [EASY] Compute the characteristic function of the sum of n random variables ξ_j with uniform distribution $\pi_{\xi_j}(x) = \frac{1}{2a}\theta_H(x+a)\theta_H(a-x)$, where $\theta_H(x+a)$ is the Heaviside theta function.

The characteristic function of π_{ξ_j} is simply given by $\frac{\sin(at)}{at}$, therefore the characteristic function of the sum of n uniform variables is $(\frac{\sin(at)}{at})^n$.

(b) [EASY-MEDIUM] Show that the characteristic function of $\xi^{(n)} = \sum_{j=1}^{n} \xi_j$ can be written in the following form:

$$\Phi_{\xi^{(n)}} = \frac{1}{(2ia)^n} t^{-n} \sum_{k=0}^n \binom{n}{k} (-1)^k e^{i(n-2k)at}$$
(5)

Hint 1: Express the sin functions using complex exponentials $(\sin x = \frac{e^{ix} - e^{-ix}}{2i})$ and use the binomial theorem $(a+b)^j = \sum_{k=0}^j \binom{j}{k} a^j b^{j-k}$.

$$\left(\frac{\sin(at)}{at}\right)^n = \frac{t^{-n}}{(2ia)^n} (e^{iat} - e^{-iat})^n = \frac{t^{-n}}{(2ia)^n} \sum_{k=0}^n \binom{n}{k} [e^{iat}]^{n-k} [-e^{-iat}]^k = \frac{t^{-n}}{(2ia)^n} \sum_{k=0}^n \binom{n}{k} (-1)^k e^{i(n-2k)at} \quad (6)$$

(c) [HARD] Compute the inverse Fourier transform of the characteristic function and show that the distribution of $\xi^{(n)}$ can be written as²

$$\pi_{\xi^{(n)}} = \frac{1}{(n-1)!(2a)^n} \sum_{k=0}^n \binom{n}{k} (-1)^k \max((n-2k)a - x, 0)^{n-1}.$$
 (7)

Hint 1: Move the sum outside of the integral of the inverse Fourier transform. Warning: the resulting integrals are divergent, but the divergencies have to simplify, so don't worry too much! The finite part of the integrals can be extracted using the Cauchy principal value, usually denoted by P.V., which, in the case of a singularity at zero, reads as

P.V.
$$\int_{-\infty}^{\infty} f(t) = \lim_{\epsilon \to 0^{+}} \left[\int_{-\infty}^{-\epsilon} f(t) + \int_{\epsilon}^{\infty} f(t) \right].$$
 (8)

Hint 2: Compute the (finite part of the) integrals by integrating by parts n-1 times (note that the original product of sin functions has a zero of order n at t=0).

Hint 3: P.V. $\int_{-\infty}^{\infty} dt t^{-1} e^{itb} = i\pi \operatorname{sgn}(b)$.

Hint 4: $\sum_{k=0}^{n} {n \choose k} (-1)^k (x+k)^j = 0$ for any x and integer j = 1, ..., n-1.

We must compute

$$\pi_{\xi^{(n)}}(x) = \frac{1}{2\pi} \int dt e^{-ixt} \frac{1}{(2ia)^n} t^{-n} \sum_{k=0}^n \binom{n}{k} (-1)^k e^{i(n-2k)at}. \tag{9}$$

First, we move the sum outside of the integral and take the principal value

$$\pi_{\xi^{(n)}}(x) = \frac{1}{2\pi} \sum_{k=0}^{n} P.V. \int dt \frac{1}{(2ia)^n} t^{-n} \binom{n}{k} (-1)^k e^{i((n-2k)a-x)t}.$$
 (10)

Since $(\sin(at))^n$ has a zero of order n at t=0, the boundary parts which come from the integration by parts (taking the integral of t^{-n} and the derivative of the rest) and which could have given contribution from t=0 are in fact zero for n-1 consecutive integration by parts. Thus we find

$$\pi_{\xi^{(n)}}(x) = \frac{1}{2\pi} \sum_{k=0}^{n} \binom{n}{k} (-1)^k \frac{((n-2k)a-x)^{n-1}}{(2a)^n (n-1)!} \text{P.V.} \int dt \ t^{-1} e^{i((n-2k)a-x)t} \,. \tag{11}$$

The integral can be easily evaluated and gives

$$\pi_{\xi^{(n)}}(x) = \sum_{k=0}^{n} \binom{n}{k} (-1)^{k} \frac{((n-2k)a-x)^{n-1}}{2(2a)^{n}(n-1)!} \operatorname{sgn}((n-2k)a-x) =$$

$$\sum_{k=0}^{n} \binom{n}{k} (-1)^{k} \frac{((n-2k)a-x)^{n-1}}{2(2a)^{n}(n-1)!} [2\theta_{H}((n-2k)a-x)-1] =$$

$$\sum_{k=0}^{n} \binom{n}{k} (-1)^{k} \frac{((n-2k)a-x)^{n-1}}{(2a)^{n}(n-1)!} \theta_{H}((n-2k)a-x), \quad (12)$$

where in the last step we used the identity in Hint 4 to keep only the term multiplied by the step function. The proof is concluded noting that $x\theta_H(x) = \max(x, 0)$.

(d) [MEDIUM] Verify the validity of the central limit theorem for the sum of variables with uniform distribution (you can work with the characteristic function).

Hint 1: $\log \frac{\sin t}{t} = \sum_{n=1}^{\infty} \frac{(-1)^n B_{2n}}{2n(2n)!} (2t)^{2n}$, where the coefficients B_n are known as "Bernoulli numbers", $B_0 = 1$, $B_2 = \frac{1}{6}$, $B_4 = -\frac{1}{30}$, et cetera.

The characteristic function of $\tilde{\xi} = \frac{\xi^{(n)}}{\sqrt{n}} = \frac{1}{\sqrt{n}} \sum_{j=1}^{n} \xi_j$ is given by

$$\phi_{\tilde{\xi}}(t) = \phi_{\xi^{(j)}}(t/\sqrt{n}) = \left(\sqrt{n} \frac{\sin(at/\sqrt{n})}{at}\right)^n = \exp\left(n\log\left(\sqrt{n} \frac{\sin(at/\sqrt{n})}{at}\right)\right) = \exp\left(\sum_{j=1}^{\infty} n^{1-j} \frac{(-1)^j B_{2j}}{2j(2j)!} (2at)^{2j}\right) = \exp\left(-\frac{(at)^2}{6} + O(1/n)\right).$$
(13)

In the limit $n \to \infty$ this approaches the characteristic function of a Gaussian with mean zero and variance $a^2/3$.

- 3. **Stable distributions. Definition**: A non-degenerate distribution π_{ξ} is a stable distribution if it satisfies: let ξ_1 and ξ_2 be independent copies of a random variable ξ (they have the same distribution π_{ξ}). Then π_{ξ} is said to be stable if for any constants a > 0 and b > 0 the random variable $a\xi_1 + b\xi_2$ has the distribution $\pi_{c\xi+d}$ for some constants c > 0 and d.
 - (a) [MEDIUM] Prove that the Gaussian $\pi_{\xi}(x) = \frac{1}{\sqrt{2\pi}\sigma}e^{-\frac{(x-\mu)^2}{2\sigma^2}}$ is a stable distribution.

Remember the propriety of the generating functions

$$\Phi_{a\xi+b}(t) = e^{ibt}\Phi_{\xi}(at) \tag{14}$$

The generating function $\phi^{(G)}(t)$ of a Gaussian distribution is given by

$$\Phi^{(G)}(t) = e^{-(2\sigma^2)t^2} \tag{15}$$

We consider the characteristic function of the sum of the two random variables $a\xi + b\xi$, which we know to be given by the product of the characteristic functions of the single (Gaussian) distributions

$$\Phi_{a\xi+b\xi}(t) = \Phi_{a\xi}^{(G)}(t)\Phi_{b\xi}^{(G)}(t) = e^{-(2\sigma^2)t^2(a^2+b^2)} = \Phi_{\sqrt{a^2+b^2}\xi}^{(G)}(t)$$
(16)

We have then shown that the distribution of the sum of the two Gaussian random variables $a\xi + b\xi$ is a Gaussian distribution of the variable $c\xi$ with $c = \sqrt{a^2 + b^2}$. Therefore the Gaussian distribution is stable.

(b) [EASY] Consider a characteristic function of the form

$$\Phi_{\xi}(t) = \exp(it\mu - (c_0 + ic_1 f_{\alpha}(t))|t|^{\alpha}), \qquad (17)$$

with $1 \le \alpha < 2$. Show that $f_{\alpha}(t) = \operatorname{sgn}(t)$, for $\alpha \ne 1$, and $f_1(t) = \operatorname{sgn}(t) \log |t|$ produce stable distributions. These are also known as $L\acute{e}vy$ distributions, after Paul Lévy, the first mathematician who studied them.

As before we consider the conbination of two random variables with a Lévi distribution has the characteristic function

$$\Phi_{a\xi_1 + b\xi_2}(t) = \exp(it(a+b)\mu - (c_0 + ic_1f_\alpha(t))|(a+b)^{1/\alpha}t|^\alpha).)$$
 (18)

If $\alpha \neq 1$ this is mapped into the same distribution by the transformation $t \rightarrow (a+b)^{-1/\alpha}t$ and $\mu \rightarrow (a+b)^{1/\alpha-1}\mu$. For $\alpha = 1$ the transformation is $t \rightarrow (a+b)^{-1}t$ and $\mu \rightarrow \mu - \frac{c_1}{\alpha}\log(a+b)$.

(c) [EASY] Find a distinctive feature of the Lévy distributions.

The second cumulant

$$\kappa_2 = (-i)^2 \partial_t^2 \log \Phi(t) \Big|_{t=0} \sim \operatorname{sign}(t) |t|^{\alpha-2} + \dots \Big|_{t=0} = \infty$$
 (19)

as $\alpha < 2$, it diverges.

- (d) [EASY] Assumes $\alpha \neq 1$ and show that, in order to be $\Phi_{\xi}(t)$ the Fourier transform of a probability distribution, the coefficient c_1 can not be arbitrarily large; determine its maximal value.
 - **Hint 1:** One can show (MEDIUM-HARD) that the inverse Fourier transform of (??) has the tails

$$\pi_{\xi}(x) \xrightarrow{|x| \gg 1} \frac{\Gamma(1+\alpha)}{2\pi |x|^{1+\alpha}} \left(c_0 \sin \frac{\pi \alpha}{2} - c_1 \operatorname{sgn}(x) \cos \frac{\pi \alpha}{2} \right). \tag{20}$$

The probability distribution must be positive or equal to zero, therefore the coefficients of the tails of the Lévi distributions must be positive. Since

$$\pi_{\xi}(x) \xrightarrow{|x| \gg 1} \frac{\Gamma(1+\alpha)}{2\pi|x|^{1+\alpha}} \left(c_0 \sin \frac{\pi\alpha}{2} - c_1 \operatorname{sgn}(x) \cos \frac{\pi\alpha}{2} \right) \tag{21}$$

we find

$$|c_1| < c_0 \left| \tan \frac{\pi \alpha}{2} \right| \tag{22}$$