Tutorial 1, Statistical Mechanics: Concepts and applications

2016/17 ICFP Master (first year)

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Tutorial, with solutions

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I. WORKSHEET

1. **General properties of the characteristic functions.**

Reminder: Let ξ be a random variable with distribution $\pi_\xi(x)$, the expectation value of e^{itx}, *i.e.* the Fourier transform of $\pi_\xi(x)$, is called *characteristic function*

$$\Phi_\xi(t) = \int_{-\infty}^{\infty} \mathrm{d}x \pi_\xi(x) e^{itx} \,. \tag{1}$$

The cumulants κ_n are given by $\kappa_n = (-i)^n \frac{\partial^n}{\partial t^n}\Big|_{t=0} \log \Phi_\xi(t)$

(a) [EASY] Prove the following properties:

- $\Phi_\xi(0) = 1$.
- $\Phi_\xi(-t) = \Phi^*_\xi(t)$.
- $|\Phi_\xi(t)| \le 1$.
- $\Phi_{a\xi+b}(t) = e^{ibt}\Phi_\xi(at)$.

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

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

2. **Sum of random variables with uniform distribution.**

This problem has been solved more than 60 years ago, and a solution, obtained via convolution formulae, can be found in the Rényi's book[1] of 1970.

(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.

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

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

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

(c) [HARD] Calculate the inverse Fourier transform of the characteristic function and show that the distribution of $\xi^{(n)}$ can be written as[2,3]

$$\pi_{\xi^{(n)}} = \frac{1}{(n-1)!(2a)^n} \sum_{k=0}^{n} \binom{n}{k} (-1)^k \max\Big((n-2k)a - x, 0\Big)^{n-1}. \tag{3}$$

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

$$\text{P.V.} \int_{-\infty}^{\infty} f(t) = \lim_{\epsilon \to 0^+} \Big[\int_{-\infty}^{-\epsilon} f(t) + \int_{\epsilon}^{\infty} f(t) \Big]. \tag{4}$$

Hint 2: Try to 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: $\text{P.V.} \int_{-\infty}^{\infty} \mathrm{d}t t^{-1} e^{itb} = i\pi \mathrm{sgn}(b)$.

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

(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.

3. **Stable distributions.**

Reminder: A distribution is called *stable* if a linear combination of two independent random variables has the same distribution, up to mean and scale parameters.

(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.

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

$$\Phi_\xi(t) = \exp\big(it\mu - (c_0 + ic_1 f_\alpha(t))|t|^\alpha\big)\,, \tag{5}$$

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

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

(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 (21) has the tails

$$\pi_\xi(x) \xrightarrow{|x|\gg 1} \frac{\Gamma(1+\alpha)}{2\pi|x|^{1+\alpha}}\Big(c_0 \sin\frac{\pi\alpha}{2} - c_1 \mathrm{sgn}(x)\cos\frac{\pi\alpha}{2}\Big)\,. \tag{6}$$

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[1] A. Rényi, *Probability Theory*, North-Holland Publishing, Amsterdam (1970).

[2] D. M. Bradley and R. C. Gupta, *On the Distribution of the Sum of n Non-Identically Distributed Uniform Random Variables*, Annals of the Institute of Statistical Mathematics (2002) 54: 689 [arXiv:0411298]

[3] W. Feller, *An Introduction to Probability Theory and its Applications*, Vol. II, John Wiley & Sons, New York (1966).

II. SOLUTIONS

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.

- $|\Phi_\xi(t)| \le 1$.

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

$$\pi_{\xi'}(x) = \frac{\pi_\xi(f^{-1}(x)}{|f'(f^{-1}(x))|}\,. \tag{7}$$

In particular, under a linear transformation we have

$$\pi_{a\xi+b}(t) = |a|^{-1}\pi_\xi((x-b)/a) \tag{8}$$

and hence

$$\Phi_{a\xi+b}(t) = \int \mathrm{d}t\; e^{ixt}|a|^{-1}\pi_\xi((x-b)/a) = e^{ibt}\Phi_\xi(at)\,. \tag{9}$$

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

Two random variables ξ_1 and ξ_2 are called independent if $\pi_{\xi_1,\xi_2}(x_1,x_2) = \pi_{\xi_1}(x_1)\pi_{\xi_2}(x_2)$. The probability distribution of $\xi_1+\xi_2$ can be obtained by a weighted integration over all the possible values of the variables with a given sum:

$$\pi_{\xi_1+\xi_2}(x) = \int \mathrm{d}x_2 \pi_{\xi_1,\xi_2}(x-x_2,x_2) = [\pi_{\xi_1} * \pi_{\xi_2}](x)\,. \tag{10}$$

The Fourier transform is then given by

$$\Phi_{\xi_1+\xi_2}(t) = \int_{-\infty}^{\infty} \mathrm{d}x e^{itx}[\pi_{\xi_1} * \pi_{\xi_2}](x) = \int_{-\infty}^{\infty} \mathrm{d}x e^{itx} \int_{-\infty}^{\infty} \mathrm{d}y \pi_{\xi_1}(y)\pi_{\xi_2}(x-y) =$$
$$\int_{-\infty}^{\infty} \mathrm{d}x e^{it(x+y)} \int_{-\infty}^{\infty} \mathrm{d}y \pi_{\xi_1}(y)\pi_{\xi_2}(x) = \Phi_{\xi_1}(t)\Phi_{\xi_2}(t)\,. \tag{11}$$

This can be readily generalized to N variables

$$\Phi_{\sum_i^N \xi_i}(t) = \prod_{i=1}^{N} \Phi_{\xi_i}(t)\,. \tag{12}$$

(c) [EASY] Name the first two cumulants. Which 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] Cast the characteristic function of $\xi^{(n)} = \sum_{j=1}^{n} \xi_j$ in the following form:

$$\Phi_{\xi^{(n)}} = \frac{1}{(2ia)^n} t^{-n} \sum_{k=0}^{n} \binom{n}{k} (-1)^k e^{i(n-2k)at} \tag{13}$$

$$\left(\frac{\sin(at)}{at}\right)^n = \frac{t^{-n}}{(2ia)^n}(e^{iat} - e^{-iat})^n = \frac{t^{-n}}{(2ia)^n} \sum_{k=0}^{n} \binom{n}{k} [e^{iat}]^{n-k} [-e^{-iat}]^k = \frac{t^{-n}}{(2ia)^n} \sum_{k=0}^{n} \binom{n}{k} (-1)^k e^{i(n-2k)at} \tag{14}$$

(c) [HARD] Calculate the inverse Fourier transform of the characteristic function and show that the distribution of $\xi^{(n)}$ can be written as[2]

$$\pi_{\xi^{(n)}} = \frac{1}{(n-1)!(2a)^n} \sum_{k=0}^{n} \binom{n}{k} (-1)^k \max\Big((n-2k)a - x, 0\Big)^{n-1}. \tag{15}$$

We must compute

$$\pi_{\xi^{(n)}}(x) = \frac{1}{2\pi}\int \mathrm{d}t e^{-ixt}\frac{1}{(2ia)^n}t^{-n}\sum_{k=0}^{n}\binom{n}{k}(-1)^k e^{i(n-2k)at}\,. \qquad (16)$$

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

$$\pi_{\xi^{(n)}}(x) = \frac{1}{2\pi}\sum_{k=0}^{n}\mathrm{P.V.}\int \mathrm{d}t\frac{1}{(2ia)^n}t^{-n}\binom{n}{k}(-1)^k e^{i((n-2k)a-x)t}\,. \qquad (17)$$

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*

$$\pi_{\xi^{(n)}}(x) = \frac{1}{2\pi}\sum_{k=0}^{n}\binom{n}{k}(-1)^k\frac{((n-2k)a-x)^{n-1}}{(2a)^n(n-1)!}\mathrm{P.V.}\int \mathrm{d}t\ t^{-1}e^{i((n-2k)a-x)t}\,. \quad (18)$$

The integral can be easily evaluated and gives

$$\begin{aligned}\pi_{\xi^{(n)}}(x) = \sum_{k=0}^{n}\binom{n}{k}(-1)^k\frac{((n-2k)a-x)^{n-1}}{2(2a)^n(n-1)!}\mathrm{sgn}((n-2k)a-x) = \\ \sum_{k=0}^{n}\binom{n}{k}(-1)^k\frac{((n-2k)a-x)^{n-1}}{2(2a)^n(n-1)!}[2\theta_H((n-2k)a-x)-1] = \\ \sum_{k=0}^{n}\binom{n}{k}(-1)^k\frac{((n-2k)a-x)^{n-1}}{(2a)^n(n-1)!}\theta_H((n-2k)a-x)\,,\end{aligned} \quad (19)$$

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).

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

$$\begin{aligned}\phi_{\tilde{\xi}}(t) = \phi_{\xi^{(j)}}(t/\sqrt{n}) = \Big(\sqrt{n}\frac{\sin(at/\sqrt{n})}{at}\Big)^n = \exp\Big(n\log\Big(\sqrt{n}\frac{\sin(at/\sqrt{n})}{at}\Big)\Big) = \\ \exp\Big(\sum_{j=1}^{\infty}n^{1-j}\frac{(-1)^j B_{2j}}{2j(2j)!}(2at)^{2j}\Big) = \exp\Big(-\frac{(at)^2}{6}+O(1/n)\Big)\,.\end{aligned} \quad (20)$$

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.**

(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.

One can easily show that the convolution of two Gaussians is a Gaussian. Since any Gaussian can be transformed to any other Gaussian by means of a translation and a change in scale, the Gaussian is a stable distribution.

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

$$\Phi_\xi(t) = \exp\bigl(it\mu - (c_0 + ic_1 f_\alpha(t))|t|^\alpha)\bigr)\,, \tag{21}$$

with $1 \leq \alpha < 2$. Show that $f_\alpha(t) = \mathrm{sgn}(t)$, for $\alpha \neq 1$, and $f_1(t) = \mathrm{sgn}(t)\log|t|$ produce stable distributions. These are also known as *Lévy distributions*, after Paul Lévy, the first mathematician who studied them.

The sum of two random variables with a Lévi distribution has the characteristic function

$$\Phi_{\xi_1+\xi_2}(t) = \exp\bigl(2it\mu - (c_0 + ic_1 f_\alpha(t))|2^{1/\alpha}t|^\alpha\bigr)\,.) \tag{22}$$

If $\alpha \neq 1$ this is mapped into the same distribution by the transformation $t \to 2^{-1/\alpha}t$ and $\mu \to 2^{1/\alpha - 1}\mu$. For $\alpha = 1$ the transformation is $t \to 2^{-1}t$ and $\mu \to \mu - c_1 \log 2$.

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

The second cumulant (the variance) 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.

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

$$\pi_\xi(x) \xrightarrow{|x|\gg 1} \frac{\Gamma(1+\alpha)}{2\pi|x|^{1+\alpha}}\Bigl(c_0 \sin\frac{\pi\alpha}{2} - c_1 \mathrm{sgn}(x)\cos\frac{\pi\alpha}{2}\Bigr) \tag{23}$$

we find

$$|c_1| < c_0\Bigl|\tan\frac{\pi\alpha}{2}\Bigr| \tag{24}$$