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Microcanonical foundation for systems with power-law distributions

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Abstract. Starting from a microcanonical basis with the principle of equal *a priori* probability, it is shown using the method of steepest descents that besides ordinary Boltzmann–Gibbs theory with the exponential distribution a theory describing systems with power-law distributions can also be derived.

Systems exhibiting power-law behaviour in their probability distributions are quite ubiquitous in nature. Examples are statistical properties of fully developed turbulence [1], anomalous diffusion [2], the velocity distributions of vibrating powders [3], thermalization of heavy quarks in collisional processes [4], the transverse-momentum distributions of hadron jets in e^+e^- collisions [5] and molecular line-shape cumulants in low-temperature glasses [6]. Many such systems are typically in non-equilibrium. However, the structures of statistical power-law distributions persist for remarkably long periods or over wide regimes. Therefore, it is natural to imagine that they reside in certain kinds of maximum-entropy states. It is an interesting problem to understand the properties of such systems based on the principles of statistical mechanics, because these systems can hardly be described by ordinary Boltzmann–Gibbs canonical ensemble theory, whose distribution contains the exponential factor. In this paper, we show that it is actually possible to derive non-Boltzmann–Gibbs theory from the microcanonical basis with the principle of equal *a priori* probability and the resulting distribution may be of the required power law.

We first recall the Gibbs theorem [7, 8], which states that a subsystem of a microcanonical ensemble with large degrees of freedom is *uniquely* characterized by the standard canonical distribution. Historically, this theorem has repeatedly been proved in various ways, such as the method of counting and the method of steepest descents. Starting from the microcanonical basis with the principle of equal *a priori* probability, the exponential distribution is obtained for the canonical ensemble. Therefore, if the Gibbs theorem were universal, then any of the equilibrium theories other than Boltzmann–Gibbs theory could not exist and consequently power-law distributions would be excluded, as long as microcanonical ensemble theory is the basis. Here, we show that a route to canonical ensemble theory for systems with power-law distributions is actually allowed within the microcanonical ensemble theory.

To exhibit this route, we begin with the standard discussion [9] concerning the Gibbs theorem by considering a classical system s and take its N replicas $s_1, s_2, \ldots, s_N$. The collection $\boldsymbol{S} = \{s_\alpha\}_{\alpha=1,2,\ldots,N}$ is referred to as a supersystem. Let A_α be a physical quantity (e.g. the energy) associated with the system s_α. It is a statistical random variable and its value denoted by $a(m_\alpha)$ is assumed to be bounded from below, where m_α labels the allowed configurations of s_α. The quantity of physical interest is the average of $\{A_\alpha\}_{\alpha=1,2,\ldots,N}$ over the supersystem: $(1/N)\sum_{\alpha=1}^{N} A_\alpha$. According to microcanonical ensemble theory, the probabilities of finding $\boldsymbol{S}$ in the configurations in which the values of the average quantity lies around a certain value $\bar{a}$, i.e.

$$\left|\frac{1}{N}\sum_{\alpha=1}^{N} a(m_\alpha) - \bar{a}\right| < \varepsilon \tag{1}$$

are all equal. ε is assumed to be

$$\varepsilon \sim \mathrm{O}(N^{-1-\delta}) \qquad (\delta > 0). \tag{2}$$

In the ordinary discussion [9] of deriving the Boltzmann–Gibbs exponential distribution, ε is taken to be of $\mathrm{O}\big(1/\sqrt{N}\big)$, which comes from the law of large numbers in the central-limit theorem. However, in the present discussion, what we are interested in is the power-law distributions of the Lévy type. Therefore, the relevant mathematical principle is the Lévy–Gnedenko generalized central-limit theorem in the half-space [10] (due to the boundedness of $a(m_\alpha)$ from below), from which the condition in equation (2) arises. More precisely, the generalized law of large numbers in the generalized central-limit theorem indicates that ε is of $\mathrm{O}(N^{-1/\alpha})$, where α is the characteristic exponent of the Lévy-stable distributions (see equation (29)). Since α is in the range (0, 1) for the half-space problem [10], consequently equation (2) follows with δ being an arbitrary positive number. In this respect, we should recall the fact that at this level $\alpha \to 1$–0 is the singular limit and so the ordinary law of large numbers is not reproduced in such a naive limiting procedure.

The equiprobability $\boldsymbol{P}(m_1, m_2, \ldots, m_N)$ associated with this condition is

$$P(m_1, m_2, \ldots, m_N) \propto \theta(\varepsilon - |M|) \tag{3}$$

$$M \equiv \frac{1}{N}\sum_{\alpha=1}^{N} a(m_\alpha) - \bar{a} = \frac{1}{N}[a(m_1) - \bar{a}] + \frac{1}{N}[a(m_2) - \bar{a}] + \cdots + \frac{1}{N}[a(m_N) - \bar{a}] \tag{4}$$

where $\theta(x)$ in equation (3) denotes the Heaviside unit-step function. To shift from microcanonical ensemble theory to canonical ensemble theory, we fix the objective system and eliminate the others. The probability of finding the objective system, say s_1, in the configuration $m_1 = m$ is given by

$$p(m) = \sum_{m_2,\ldots,m_N} P(m, m_2, \ldots, m_N) \tag{5}$$

which characterizes the canonical ensemble.

To prove the Gibbs theorem, the following integral representation of the step function is employed:

$$\theta(x) = \int_{\beta-\mathrm{i}\infty}^{\beta+\mathrm{i}\infty} \mathrm{d}\phi\, \frac{\mathrm{e}^{\phi x}}{2\pi \mathrm{i}\phi} \tag{6}$$

where β is an arbitrary positive constant. Then, in the large-N limit, one applies the method of steepest descents to evaluate the integration over ϕ. Contextually, it is clear that the exponential distribution in Boltzmann–Gibbs canonical ensemble theory has its origin in this integral representation of $\theta(x)$ using the exponential function. As long as the exact step function is used without any approximation, the exponential distribution can never be realized. The steepest-descent approximation plays an essential role in the derivation of the exponential distribution. A crucial point here is that the result obtained by the steepest-descent approximation depends on the choice of the representation of the step function, in general.

To examine the possibility of obtaining the power-law-type distribution, we consider the 'q-exponential function', which is defined by

$$e_q(x) \equiv \begin{cases} [1+(1-q)x]^{1/(1-q)} & (1+(1-q)x > 0) \\ 0 & (1+(1-q)x \leqslant 0) \end{cases} \tag{7}$$

where q is a real parameter satisfying the condition

$$q > 1. \tag{8}$$

In the limit $q \to 1+0$, $e_q(x)$ converges to the ordinary exponential function. An important point is that even if the exponential function in the integrand in equation (6) is replaced by the q-exponential function, still the equality

$$\theta(x) = \int_{\beta-\mathrm{i}\infty}^{\beta+\mathrm{i}\infty} \mathrm{d}\phi \, \frac{e_q(\phi x)}{2\pi \mathrm{i}\phi} \tag{9}$$

holds, as long as β is taken to satisfy

$$1-(q-1)\beta x_{\max} > 0. \tag{10}$$

Here, $x_{\max}$ is the fixed maximum value of x in its range of interest, and it turns out to be possible to let it become arbitrarily large in the subsequent discussion of the steepest-descent approximation. (We shall return to this point later.) In equation (9), there is a branch point in the integrand, and therefore a cut has to be introduced in the complex ϕ-plane. However, such analytic complication can easily be overcome if the following integral representation is employed:

$$e_q(\phi x) = \frac{1}{\Gamma(1/(q-1))} \int_0^\infty \mathrm{d}t \, t^{1/(q-1)-1} \exp\{-[1+(1-q)\phi x]t\} \tag{11}$$

where $\Gamma(s)$ is the gamma function. Using this representation in equation (9) and changing the order of integration, one finds the right-hand side to be

$$\frac{1}{\Gamma(1/(q-1))} \int_0^\infty \mathrm{d}t \, t^{1/(q-1)-1} \mathrm{e}^{-t} \int_{\beta-\mathrm{i}\infty}^{\beta+\mathrm{i}\infty} \mathrm{d}\phi \, \frac{\mathrm{e}^{(q-1)tx\phi}}{2\pi \mathrm{i}\phi}$$
$$= \frac{1}{\Gamma(1/(q-1))} \int_0^\infty \mathrm{d}t \, t^{1/(q-1)-1} \mathrm{e}^{-t} \theta((q-1)tx). \tag{12}$$

Since $q > 1$, $\theta((q-1)tx) = \theta(x)$ and therefore one sees that equation (9) in fact holds. This non-uniqueness of the representation of the step function thus turns out to lead to non-uniqueness of canonical ensemble theory.

Equation (9) may be understood from the viewpoint that the step function is of discrete topology and therefore can remain invariant under continuous deformation of the exponential function in the integrand in equation (6). In this respect, it is clear that the use of the q-exponential function is nothing but one particular choice of deformation.

Now, we wish to evaluate the integral of the form

$$\theta(\varepsilon - M) = \int_{\beta-\mathrm{i}\infty}^{\beta+\mathrm{i}\infty} \frac{\mathrm{d}\phi}{2\pi \mathrm{i}\phi} e_q((\varepsilon - M)\phi) \tag{13}$$

with M in equation (4), using the method of steepest descents for large N. What is essential here is that in the method of steepest descents the large-N approximation is performed inside the integral. This is also a crucial point, from which non-uniqueness of canonical ensemble theory arises.

Let us recall the following property of the q-exponential function:

$$e_q(a)\, e_q(b) = e_q(a + b + (1 - q)ab). \tag{14}$$

If the quantities a and b are of $\mathrm{O}(1/N)$, for example, then

$$e_q(a + b) \approx e_q(a)\, e_q(b) \tag{15}$$

up to $\mathrm{O}(1/N^2)$. Therefore, recalling that ε is of $\mathrm{O}(N^{-1-\delta})$ and each term in the sum in equation (4) is of $\mathrm{O}(1/N)$, we can approximate equation (13) as follows:

$$\theta(\varepsilon - M) \approx \int_{\beta-\mathrm{i}\infty}^{\beta+\mathrm{i}\infty} \frac{\mathrm{d}\phi}{2\pi\mathrm{i}\phi} e_q(\phi\varepsilon) \prod_{\alpha=1}^{N} e_q\left(-\phi\frac{1}{N}[a(m_\alpha) - \bar{a}]\right). \tag{16}$$

Noting that $\theta(\varepsilon - |M|) = \theta(\varepsilon - M) - \theta(-\varepsilon - M)$ and changing the integration variable as $\phi \to N\phi$, we obtain

$$\theta(\varepsilon - |M|) \approx \int_{\beta^*-\mathrm{i}\infty}^{\beta^*+\mathrm{i}\infty} \mathrm{d}\phi\, \frac{\sinh_q(N\phi\varepsilon)}{\pi\mathrm{i}\phi} \prod_{\alpha=1}^{N} e_q(-\phi[a(m_\alpha) - \bar{a}]) \tag{17}$$

where $\sinh_q(x) \equiv [e_q(x) - e_q(-x)]/2$ and

$$\beta^* = \frac{\beta}{N}. \tag{18}$$

Let us examine the condition in equation (10). In the present context, it is written as

$$1 - (q - 1)\beta^* N|\pm\varepsilon - M|_{\max} > 0. \tag{19}$$

The rectangular distribution function we are considering here has a very narrow support with the width 2ε. On the other hand, $|\pm\varepsilon - M|_{\max}$ is of $\mathrm{O}(N^{-1-\delta})$ with $\delta > 0$. Therefore, in the large-N limit, β^* can be an arbitrary positive constant.

Thus, working out to the leading order in N, we can express the probability as follows:

$$\begin{aligned} p_q(m) &= \sum_{m_2,\ldots,m_N} \boldsymbol{P}(m, m_2, \ldots, \ldots m_N) \\ &\approx \frac{1}{W} \int_{\beta^*-\mathrm{i}\infty}^{\beta^*+\mathrm{i}\infty} \mathrm{d}\phi\, \frac{\sinh_q(N\phi\varepsilon)}{\pi\mathrm{i}\phi} e_q(-\phi[a(m) - \bar{a}]) \\ &\quad\times \sum_{m_2,\ldots,\ldots m_N} \prod_{\alpha=2}^{N} e_q(-\phi[a(m_\alpha) - \bar{a}]) \\ &= \frac{1}{W} \int_{\beta^*-\mathrm{i}\infty}^{\beta^*+\mathrm{i}\infty} \mathrm{d}\phi\, \frac{\sinh_q(N\phi\varepsilon)}{\pi\mathrm{i}\phi} \frac{e_q(-\phi[a(m) - \bar{a}])}{\tilde{Z}_q(\phi)} \exp\left[N \ln \tilde{Z}_q(\phi)\right] \end{aligned} \tag{20}$$

where

$$\tilde{Z}_q(\phi) = \sum_m e_q(-\phi[a(m) - \bar{a}]) \tag{21}$$

and W is the number of possible configurations satisfying equation (1) and is given by

$$W = \int_{\beta^*-\mathrm{i}\infty}^{\beta^*+\mathrm{i}\infty} \mathrm{d}\phi\, \frac{\sinh_q(N\phi\varepsilon)}{\pi\mathrm{i}\phi} \exp\left[N \ln \tilde{Z}_q(\phi)\right] \tag{22}$$

which ensures the normalization for $p_q(m)$. Now, using the real part β^* of ϕ, the steepest-descent condition reads

$$\frac{\partial \tilde{Z}_q}{\partial \beta^*} = 0 \tag{23}$$

which leads to

$$p_q(m) = \frac{1}{\tilde{Z}_q(\beta^*)} e_q\big(-\beta^*[a(m) - \bar{a}]\big) \tag{24}$$

$$\bar{a} = \sum_m P_q(m)\, a(m) \tag{25}$$

simultaneously, where $P_q(m)$ is given by

$$P_q(m) = \frac{[p_q(m)]^q}{\sum_m [p_q(m)]^q}. \tag{26}$$

These results follow from equation (7) and the relation

$$\frac{\mathrm{d}e_q(x)}{\mathrm{d}x} = [e_q(x)]^q. \tag{27}$$

We emphasize that the above steepest-descent approximation is mathematically well justified, since the last factor in the integrand in equation (20) is the ordinary exponential function.

The distribution function in equation (24) is seen to asymptotically exhibit the power-law behaviour

$$p_q(m) \sim \frac{1}{[a(m)]^{1/(q-1)}} \tag{28}$$

as desired. Here, let us recall the exact Lévy-stable distribution with characteristic exponent α in the half-space [10]:

$$L_\alpha(a(m)) = \frac{1}{2\pi}\int_{-\infty}^{\infty} \mathrm{d}k\, \exp\left\{-\mathrm{i}ka(m) - \lambda|k|^\alpha \exp\left[\mathrm{i}\varepsilon(k)\frac{\eta\pi}{2}\right]\right\} \qquad (0 < \alpha < 1) \tag{29}$$

where λ is a positive constant, η a constant satisfying $|\eta| \leqslant \alpha$ and $\varepsilon(k) = k/|k|$ the sign function of k. $L_\alpha(a(m))$ has the following asymptotic form for large values of $a(m)$:

$$L_\alpha(a(m)) \sim [a(m)]^{-1-\alpha}. \tag{30}$$

Comparing equation (28) with equation (30), we find that q and α are related to each other as

$$q = \frac{\alpha + 2}{\alpha + 1}. \tag{31}$$

From this, we also find that δ in equation (2) satisfies

$$\delta = \frac{2q - 3}{2 - q}. \tag{32}$$

In addition, it has recently been shown [11] that the distribution in equation (24), in fact, converges to the exact Lévy-stable distribution in equation (29) by many-fold convolutions in accordance with the generalized central-limit theorem. On the other hand, it is evident that in the limit $q \to 1 + 0$ all the discussions become reduced to the ordinary ones in Boltzmann–Gibbs theory with the familiar canonical distribution of the exponential form.

In the field of thermodynamics of chaotic systems [12], $P_q(m)$ in equation (26) is referred to as the escort distribution, which is also a probability distribution associated with the original distribution $p_q(m)$. The steepest-descent condition yields the fact that the arithmetic mean of $\{A_\alpha\}_{\alpha=1,2,\ldots,N}$ coincides with the generalized expectation value with respect to the escort distribution as in equation (25).

To interpret β^* in equation (24) as the inverse temperature, it is necessary to consider the zeroth law of thermodynamics. This is a non-trivial problem for systems obeying power-law distributions. However, it has recently been found [13] that, by considering macroscopic thermodynamics of equilibrium of such systems in contact with each other, β^* can indeed be regarded as the physical inverse temperature.

In conclusion, we have shown that not only ordinary Boltzmann–Gibbs canonical ensemble theory but also a theory for systems with power-law distributions can be obtained from microcanonical basis with the principle of equal *a priori* probability. It is worth pointing out that the structure in equations (24)–(26) is the characteristic of non-extensive statistical mechanics [14]. It is known that the generalized canonical ensemble theory derived from the maximum entropy principle based on the Tsallis entropy [15] with equation (25) as the constraint gives rise to the distribution in equation (24). However, it is essential to recall that here we made no initial assumptions on the definition of the statistical expectation value and the form of the entropy. Also, we may mention that the same result as the present one can also be obtained by three other independent methods: the counting algorithm [16], the generalized central-limit theorem [17] and the macroscopic thermodynamics of equilibrium of systems in contact with each other [13].

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