Discrete analogue of Boltzmann factor and discrete thermodynamics

W. Chung[a], H. Hassanabadi[b] and A. Boumali[c]

[a]*Department of Physics and Research Institute of Natural Science,*
College of Natural Science, Gyeongsang National University, Jinju 660-701, Korea.
e-mail: mimip44@naver.com
[b]*Faculty of physics, Shahrood University of Technology, Shahrood, Iran.*
e-mail: h.hasanabadi@shahroodut.ac.ir
[c]*Laboratoire de Physique Appliquée et Théorique, Université Larbi-Tébessi- Tébessa, Algeria.*
e-mail: boumali.abdelmalek@gmail.com

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In this paper we present the discrete thermodynamics where the inverse temperature is not continuous but discrete. We construct the discrete analogue of Boltzmann factor based on the discrete inverse temperature lattice. We study the discrete thermodynamics related to the discrete analogue of Boltzmann factor. We also discuss the superstatistics for the discrete inverse temperature.

Keywords: Superstatistics; discrete analogue of Boltzmann.

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1. Introduction

The Boltzmann factor for a state with energy E and equilibrium inverse temperature $\beta = 1/(k_B T)$ is given by

$$B_E(\beta) = e^{-\beta E}, \tag{1}$$

where T and k_B denote the equilibrium temperature and Boltzmann constant, respectively. When we regard the Boltzmann factor as a function in β, we know that it is a solution of the first order differential equation

$$\frac{dy}{d\beta} = -Ey, \tag{2}$$

where $y = B_E(\beta)$.

In the thermal field theory [1-3], the inverse temperature is regarded as an inverse time through the relation

$$\beta = it. \tag{3}$$

Thus, the Boltzmann factor in the thermal field theory corresponds to the time evolution operator in the quantum field theory,

$$B_E(\beta) \to U_E(t) = e^{-itE}, \tag{4}$$

where the time evolution operator obeys the first order differential equation

$$\frac{dU_E(t)}{dt} = -iEU_E(t). \tag{5}$$

Using Eq. (3), we know that the Eq. (5) is equivalent to Eq. (2).

The imaginary-time formalism is just a mathematical tool to represent the partition function as a path integral, which does not mean that the imaginary time is equivalent to temperature.

Use of the discrete time in physics has long history. First use was focussed on the discrete calculus of variations [4,5]. After this, the discrete Nöther theorem was found [6]. The possibility that time could be regarded as a discrete dynamical variable was examined through all phases of mechanics [7]. Some progress has been accomplished in this direction [4-10]. Recently, discrete time is adopted in the study of the stochastic wave equation [11-16].

In the discrete time mechanics, the continuous time t is replaced with a discrete times forming the lattice

$$\mathbb{T} = \{t_n | t_n = t_0 + n\tau, \quad n = 0, 1, 2, \cdots\}. \tag{6}$$

The classical discrete time mechanics was discussed in [10]. Here the derivative with respect to time in the continuous time mechanics was replaced with the finite difference between two adjacent discrete times, which is defined as

$$\Delta x(t_n) = \frac{x(t_{n+1}) - x(t_n)}{\tau}. \tag{7}$$

Thus, the quantum evolution operator in the discrete time lattice obeys the first order finite difference equation,

$$\Delta U_E(t_n) = -iEU_E(t_n), \tag{8}$$

which is solved as

$$U_E(t_n) = (1 - i\tau E)^n. \tag{9}$$

The Eq. (8) becomes Eq. (5) in the continuous time limit $\tau \to 0$ with $t_n = n\tau = t$ fixed.

In this paper we introduce the discrete inverse temperature from the discrete analogue of Eq. (4) and use it to construct the analogue of Boltzmann factor based on the discrete inverse temperature lattice. We investigate the discrete thermodynamics based on the discrete analogue of Boltzmann factor. We also discuss the superstatistics for the discrete inverse temperature. This paper is organized as follows: In Sec. 2 we discuss the discrete analogue of Boltzmann factor. In Sec. 3 we discuss the entropy and internal energy in discrete thermodynamics. In Sec. 4 we discuss some examples. In Sec. 5 we discuss the discrete superstatistics.

2. Discrete analogue of Boltzmann factor

From the discrete analogue of Eq. (3), we can define the discrete inverse temperature corresponding to the discrete time as

$$\beta_n = it_n, \tag{10}$$

which defines the discrete inverse temperature lattice

$$\mathbb{B} = \{\beta_n | \beta_n = \beta_0 + nb, \quad n = 0, 1, 2, \cdots\}. \tag{11}$$

Here we introduce the discrete inverse temperature as a discretization of the continuous inverse temperature. Among possible discrete inverse temperatures, we adopt the discrete inverse temperature with equal spacing for simplicity.

Another motivation of the discrete inverse temperature is to find the origin of Tsallis's q-deformed Boltzmann factor. Thus, the discrete analogue of the inverse temperature is a kind of deformation corresponding to the Tsallis's q-deformed Boltzmann factor, which will be discussed later.

For the discrete inverse temperatures, the discrete temperatures T_n are defined as

$$\beta_n = \frac{1}{k_B T_n}, \tag{12}$$

which implies

$$T_n = \frac{1}{k_B(\beta_0 + nb)}. \tag{13}$$

Thus, the above equation shows that (i) the discrete temperature forms a harmonic sequence, and (ii) it depends on the choice of β_0. In this stage, three cases can be discussed:

Case of $\beta_0 > 0$: In this case, we have non-zero minimum temperature. We have two values:

$$T_0 = \frac{1}{k_B \beta_0} > 0, \tag{14}$$

$$\lim_{n\to\infty} T_n = 0. \tag{15}$$

Case of $\beta_0 = 0$: In this case, we have zero minimum temperature. We have two values:

$$T_0 = \infty, \tag{16}$$

$$\lim_{n\to\infty} T_n = 0. \tag{17}$$

Case of $\beta_0 < 0$: In this case, we have negative temperature [17] for $n < -\beta_0/b$. We have two values:

$$T_0 = \frac{1}{k_B \beta_0} < 0, \tag{18}$$

$$\lim_{n\to\infty} T_n = 0. \tag{19}$$

From now on we refer to the thermodynamics with a discrete Boltzmann factor as the discrete thermodynamics. In the discrete thermodynamics, the thermodynamic equilibrium occurs at the discrete inverse temperature. In this model, the thermodynamic quantities depends on the discrete inverse temperature. Thus, the discrete analogue of Eq. (2) is given by

$$\Delta B_E(\beta_n) = -E B_E(\beta_n), \tag{20}$$

where the finite difference is defined as

$$\Delta F(\beta_n) = \frac{F(\beta_{n+1}) - F(\beta_n)}{b}. \tag{21}$$

Solving Eq. (20), we get

$$B_E(\beta_{n+1}) = (1 - bE)\, B_E(\beta_n), \tag{22}$$

which gives

$$B_E(\beta_n) = (1 - bE)^n\,, \tag{23}$$

where we set

$$B_E(\beta_0) = 1. \tag{24}$$

The continuous version is obtained by setting $\beta_n = \beta_0 + nb = \beta$ and taking the limit $n \to \infty, b \to 0$ with $nb + \beta_0 = \beta$ fixed. In the continuous limit, we have the Boltzmann factor (1). Indeed, we get

$$\lim_{b\to 0, \beta_n = \beta} B_E(\beta_n) = e^{-(\beta - \beta_0)E}. \tag{25}$$

When b is not zero, the Eq. (23) is well defined only for $E \le 1/b$. Thus, we demand that the energy is bounded from above for non-zero b. Thus, the discrete Boltzmann factor takes the form

$$B_E(\beta_n) = \begin{cases} (1 - bE)^n & \left(E \le \frac{1}{b}\right) \\ 0 & \left(E \ge \frac{1}{b}\right) \end{cases}. \tag{26}$$

This equation shows that the discrete Boltzmann factor is a kind of deformed Boltzmann factor. That means the existence of a relationship between the discrete Boltzmann factor and the well-known q-deformed Boltzmann factor appearing in Tsallis's entropy [18].

Now, if we set $\beta_N = \beta =$ finite, we have $b = \beta/N$. The continuous inverse temperature is then obtained by taking the limit $b \to 0$ or $N \to \infty$ with $Nb = \beta$ fixed.

If we identify $q - 1 = -b$, we can express Eq. (26) in terms of q-exponential function [18] as

$$B_E(\beta) = [e_q(E)]^{-\beta}, \tag{27}$$

where q-exponential is defined as

$$e_q(x) = [1 + (1-q)x]_+^{\frac{1}{1-q}}, \tag{28}$$

and $[\;]_+$ denotes the Tsallis cutoff which implies that $[x]_+ = 0$ for $x \leq 0$. Thus, the energy upper bound comes from the Tsallis cutoff. We note here that the Boltzmann factor given in Eq.(27) was introduced in Ref. [19].

In addition, we can see that Eq. (27) is not the same as the Tsallis's q-deformed Boltzmann factor. But, when we identify $N = 1/1-q$, we obtain

$$B_E(\beta) = e_q(-\beta E), \tag{29}$$

which is the Tsallis's q-deformed Boltzmann factor.

From the discrete Boltzmann factor, we know that the probability finding a state with energy E at the equilibrium inverse temperature β_n for a system is proportional to the discrete Boltzmann factor,

$$P_E(\beta_n) = \frac{1}{Z(\beta_n)} B_E(\beta_n) = \frac{1}{Z(\beta_n)}(1-bE)^n, \tag{30}$$

where the partition function $Z(\beta_n)$ is defined as

$$Z(\beta_n) = \sum_E (1-bE)^n, \tag{31}$$

for a discrete energy, and

$$Z(\beta_n) = \int_E dE\,(1-bE)^n, \tag{32}$$

for a continuous energy.

3. Entropy and internal energy in discrete thermodynamics

For a system which is in thermal equilibrium with a reservoir of given discrete inverse temperature β_n we use the canonical ensemble formulation. The probability of finding a state with E_i in this system is given by

$$P_i(\beta_n) = \frac{1}{Z(\beta_n)}\,(1-bE_i)^n, \tag{33}$$

which obeys

$$\sum_i P_i(\beta_n) = 1. \tag{34}$$

Now let us consider the entropy in the form,

$$S = -k_B \sum_i P_i(\beta_n) \ln P_i(\beta_n). \tag{35}$$

For the average, the linear average is not the only one that can be used. In the general theory of averages, for any monotonously increasing and bijective function $\psi(x)$ called deforming map, the Kolmogorov-Nagumo (KN) average [20,21] can be adopted. Now let us define the internal energy U as the KN mean of energy as

$$\sum_i \psi(E_i) P_i(\beta_n) = \psi(U). \tag{36}$$

Based on the variational method for the discrete theory [4,5], we can obtain the maximum entropy probability form the extreme condition of the functional,

$$\Phi = S + \lambda_1 \left(\sum_i \psi(E_i) P_i(\beta_n) - \psi(U) \right) + \lambda_2 \left(\sum_i P_i - 1 \right). \tag{37}$$

Demanding $\partial\Phi/\partial P_i = 0$, we get

$$-k_B(1 + \ln P_i) + \lambda_1 \psi(E_i) + \lambda_2 = 0. \tag{38}$$

Comparing Eq. (32) with Eq. (37), we get

$$\lambda_1 = k_B(\beta_n - \beta_0), \tag{39}$$

$$\lambda_2 = k_B(\ln Z - 1), \tag{40}$$

and

$$\psi(x) = -\frac{1}{b}\ln(1-bx). \tag{41}$$

Thus, we have

$$\psi(U) = -\frac{1}{b}\sum_i P_i(\beta_n)\ln(1-bE_i). \tag{42}$$

The internal energy (or energy expectation value) is then given by

$$\langle E_i \rangle = U(\beta_n) = \frac{1}{b}\left(1 - e^{\sum_i P_i(\beta_n)\ln(1-bE_i)}\right). \tag{43}$$

Using the relation

$$(-\Delta)Z = \sum_i E_i(1-bE_i)^n, \tag{44}$$

we have

$$U = \frac{1}{b}\left(1 - e^{\frac{1}{Z}\ln(1+b\Delta)Z}\right). \tag{45}$$

In the continuum limit, Eq. (44) becomes

$$U = -\frac{1}{Z}\frac{\partial Z}{\partial \beta}. \tag{46}$$

The discrete specific heat for the temperature interval $J_n = [T_{n+1}, T_n]$ is defined as

$$C^{(J_n)} = \frac{U(\beta_{n+1}) - U(\beta_n)}{T_{n+1} - T_n}. \tag{47}$$

Thus, the Boltzmann-Gibbs relation reads

$$S = \left(\frac{1}{T_n} - \frac{1}{T_0}\right)\left(-\frac{1}{b}\ln(1-bU)\right) + k_B \ln Z. \tag{48}$$

4. Some examples

Now let us discuss some examples based on the discrete thermodynamics.

4.1. Classical harmonic oscillator

Let us discuss the classical harmonic oscillator whose Hamiltonian is given by

$$H = \frac{p^2}{2m} + \frac{1}{2}mw^2x^2, \tag{49}$$

where the energy E is continuous and $E \geq 0$. The partition function at discrete inverse temperature β_n is then given by

$$Z(\beta_n) = \int_0^{1/b} dE\,(1-bE)^n = \frac{1}{b(1+n)} = \frac{1}{\beta_n - \beta_0 + b}. \tag{50}$$

The internal energy is then given by

$$U(\beta_n) = \frac{1}{b}\left(1 - e^{-\frac{1}{n+1}}\right) = \frac{n\left(1 - e^{-\frac{1}{n+1}}\right)}{\beta_n - \beta_0}. \tag{51}$$

In the continuum limit, we have

$$U(\beta_n) \to U(\beta) = \frac{1}{\beta - \beta_0} = \frac{k_B T}{1 - \frac{T}{T_0}}. \tag{52}$$

The discrete specific heat for $J_n = [T_{n+1}, T_n]$ is given by

$$C^{(J_n)} = \frac{k_B}{b^2}(\beta_0 + bn)(\beta_0 + b(n+1)) \times \left(e^{-\frac{1}{n+1}} - e^{-\frac{1}{n+2}}\right). \tag{53}$$

In the continuum limit, we have

$$C^{(J_n)} \to k_B. \tag{54}$$

4.2. Maxwell-Boltzmann distribution of molecular speeds in a gas

Now let us apply discrete thermodynamics to the kinetic theory of an ideal gas. First we consider the single particle case. Let us consider the Maxwell-Boltzmann distribution of molecular speeds in a gas which is actually a probability density function of a continuous variable, $v = \sqrt{v_x^2 + v_y^2 + v_z^2}$, the speed of a molecule with a mass μ. The discrete Boltzmann factor is given by

$$B\left(\frac{1}{2}\mu v^2 : \beta_n\right) = \left(1 - \frac{b}{2\mu}v^2\right)^n. \tag{55}$$

The partition function is

$$Z = \int_0^{\sqrt{2\mu/b}} 4\pi v^2 dv \left(1 - \frac{b}{2\mu}v^2\right)^n = \frac{\left(\frac{2\pi\mu}{b}\right)^{3/2}\Gamma(n+1)}{\Gamma\left(n+\frac{5}{2}\right)}. \tag{56}$$

Thus the internal energy

$$U = \left\langle \frac{1}{2}\mu v^2 \right\rangle = \frac{1}{b}\left(1 - e^{H_n - H_{n+\frac{3}{2}}}\right), \tag{57}$$

where H_x denotes the harmonic number. The rms speed is then given by

$$v_{rms} = \sqrt{\frac{2}{\mu b}\left(1 - e^{H_n - H_{n+\frac{3}{2}}}\right)}. \tag{58}$$

In the continuum limit, Eq. (57) becomes the well-known result,

$$v_{rms} \approx \sqrt{\frac{3kT}{\mu}}, \tag{59}$$

where we used the formula

$$H_n \approx \gamma + \ln n + \frac{1}{2n}. \tag{60}$$

for a large n and γ denotes the Euler constant.

Now let us discuss the ideal gas system consisting of N identical particles. The total energy of this system is

$$E = \sum_{i=1}^{3N} \frac{1}{2}\mu v_i^2 = \frac{1}{2}\mu v^2, \tag{61}$$

where we set

$$v_1 = v_{1x},\ v_2 = v_{1y},\ v_3 = v_{1z}, \cdots, \quad v_{3N-2} = v_{Nx}, v_{3N-1} = v_{Ny},\ v_{3N} = v_{Nz}. \tag{62}$$

Using the $3N$-dimensional hyper spherical coordinate, we can write the partition function as

$$Z = \Omega_{3N-1} \int_0^{\sqrt{2\mu/b}} \left(1 - \frac{b}{2\mu}v^2\right)^n v^{3N-1} dv = \frac{\left(\frac{2\pi\mu}{b}\right)^{3N/2}\Gamma(n+1)}{\Gamma\left(n+1+\frac{3}{2}N\right)}, \tag{63}$$

where Ω_{3N-1} is the solid angle of the $3N$-dimensional hyper sphere,

$$\Omega_{3N-1} = \frac{2\pi^{3N/2}}{\Gamma\left(\frac{3N}{2}\right)}. \tag{64}$$

The rms speed is then given by

$$v_{rms} = \sqrt{\frac{2}{\mu b}\left(1 - e^{H_n - H_{n+\frac{3N}{2}}}\right)}. \tag{65}$$

In the continuum limit, Eq.(64) becomes the well-known result,

$$v_{rms} \approx \sqrt{\frac{3NkT}{\mu}}. \tag{66}$$

4.3. Two level system

Now let us consider two level system consisting of $-\epsilon$ and ϵ. The partition function reads

$$Z(\beta_n) = (1 + b\epsilon)^n + (1 - b\epsilon)^n. \tag{67}$$

The internal energy is then given by

$$U(\beta_n) = \frac{1}{b}\Big[1 - (1 + b\epsilon)^{\frac{1}{Z}(1+b\epsilon)^n} - (1 - b\epsilon)^{\frac{1}{Z}(1-b\epsilon)^n}\Big]. \tag{68}$$

In the continuum limit Eq. (67) becomes

$$U(\beta) = \epsilon \tanh(\beta\epsilon). \tag{69}$$

5. Discrete superstatistics

Now let us discuss the superstatistics for the discrete Boltzamnn factor. In this case we regard as the discrete inverse temperatures as random variables $\tilde{\beta}_m$ $(m = 0, 1, 2, \cdots)$ which belongs to $\mathbb{B}$. Besides, we demand that the mean of $\tilde{\beta}_m$ is the equilibrium inverse temperature β_n and set the variance of $\tilde{\beta}_m$ to be σ^2. For the random inverse temperatures, we introduce the probability distribution function $f(\tilde{\beta}_m)$ obeying

$$b\sum_{m=0}^{\infty} f(\tilde{\beta}_m) = 1, \tag{70}$$

and

$$\beta_n = \langle\tilde{\beta}_m\rangle = b\sum_{m=0}^{\infty} \tilde{\beta}_m f(\tilde{\beta}_m), \tag{71}$$

and

$$b^2\sigma^2 = \langle\tilde{\beta}_m^2\rangle - \langle\tilde{\beta}_m\rangle^2. \tag{72}$$

From the superstatistics [22], we define the superstatistical Boltzmann factor as

$$B_E^{(s)}(\beta_n) = b\sum_{m=0}^{\infty} B_E(\tilde{\beta}_m) f(\tilde{\beta}_m). \tag{73}$$

The superstatistical partition function is defined as

$$Z^{(s)} = \sum_{n=0}^{\infty} B_E^{(s)}(\beta_n). \tag{74}$$

As an example, let us consider the following probability distribution function

$$f(\tilde{\beta}_m) = A\delta_{m,n-1} + B\delta_{m,n} + \delta_{m,n+1}. \tag{75}$$

From Eq. (69), Eq. (70) and Eq. (71), we get

$$b(A + B + C) = 1, \tag{76}$$

$$C = A, \tag{77}$$

$$b(C + A) = \sigma^2. \tag{78}$$

Thus, we have

$$f(\tilde{\beta}_m) = \frac{\sigma^2}{2b}\delta_{m,n-1} + \frac{1}{b}(1 - \sigma^2)\delta_{m,n} + \frac{\sigma^2}{2b}\delta_{m,n+1}. \tag{79}$$

From the superstatistics [22], we define the superstatistical discrete Boltzmann factor as

$$B_E^{(s)}(\beta_n) = b\sum_{m=0}^{\infty} B_E(\tilde{\beta}_m) f(\tilde{\beta}_m). \tag{80}$$

In the low-energy asymptotics of superstatistics, the generalized Boltzmann factor is then given by

$$B_E^{(s)}(\beta_n) = (1 - bE)^n \left(1 + \frac{\sigma^2 bE(bE - 4)}{2(1 - bE)}\right), \tag{81}$$

and the superstatistical partition function is given by

$$Z^{(s)} = \frac{1}{\beta_n - \beta_0 + b} + \frac{\sigma^2}{2}\left(\frac{1}{\beta_n - \beta_0} + \frac{1}{\beta_n - \beta_0 + 2b} - \frac{2}{\beta_n - \beta_0 + b}\right). \tag{82}$$

6. Conclusion

Based on the discrete time mechanics and inverse temperature formalism in the thermal field theory, we introduced the discrete inverse temperature and discussed the discrete analogue of the thermodynamics. To do so, we introduced the discrete inverse temperature lattice and defined the discrete analogue of Boltzmann factor. For a general discussion, we considered that there exists a finite minimum inverse temperature corresponding to a finite maximum temperature. We adopted the discrete inverse temperature as having the equal spacing.

Our discrete inverse temperature is different from the discrete inverse temperature [23] appearing in the superstatistics where discrete inverse temperature was regarded as a fluctuation around the equilibrium temperature. But our discrete inverse temperature can be regarded as a discretization of the continuous inverse temperature. The discrete inverse temperature in Eq. (11) is not a unique choice. We can consider more general discrete inverse temperature. For example, we can consider the pseudo discrete inverse temperature through

$$\beta_{n+1} \ominus_f \beta_n = \text{const} = b, \tag{83}$$

or

$$\beta_{n+1} = \beta_n \oplus_f b, \tag{84}$$

where the pseudo-addition and pseudo subtraction [24] are defined as

$$a \oplus_f b = f^{-1}(f(a) + f(b)), \tag{85}$$

and

$$a \ominus_f b = f^{-1}(f(a) - f(b)). \tag{86}$$

For simplicity, in this paper we considered the case of $f = Id$.

We found that discrete Boltzmann factor could be obtained for the maximum entropy principle with a certain KN mean for the energy. We found the formula for the internal energy defined as a KN mean of energy and investigated the relation between the internal energy and partition function. As examples we presented three examples; classical harmonic oscillator, Maxwell-Boltzmann distribution of molecular speeds in a gas, two level system. Finally we discussed the discrete superstatistics for the discrete thermodynamics.

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