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The thermal Green functions in nonextensive quantum statistical mechanics

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Abstract. The thermal Green functions of the quantum-mechanical harmonic oscillator are constructed within the framework of nonextensive statistical mechanics with *normalized q-expectation values*. For the Tsallis index q greater than unity, these functions are found to be expressed analytically in terms of the Hurwitz zeta function. It is found that influence of the nonextensivity on the time-ordered thermal propagator is relevant only at the "on-shell" states. In particular, the finite-temperature contribution to the thermal propagator becomes enhanced for the strong nonextensivity.

PACS. 05.30.-d Quantum statistical mechanics

Thermal field theory is attracting continuous interest in various research areas including solid state physics, particle physics, and cosmology. Among others, quark-gluon plasma (*i.e.*, quantum chromodynamics at finite temperature) and quantum processes in the early Universe may be thought of as typical examples. There is a common important point behind them: the systems treated there include long-range interactions in themselves. In the former example, there is no natural mechanism which shields the chromomagnetic force, in contrast to the chromoelectric component [1]. In the latter one, quantum fields are put under influence of gravitational interaction [2]. Both of them are nonextensive systems.

Nonextensivity is also relevant when a system has long-time memory, (multi)fractal configuration, or quantum group structure. A feature of a nonextensive system is that the total internal energy does not become proportional to the number of microscopic elements of the system in the thermodynamic limit. To treat such a system thermodynamically, suitable generalization of Boltzmann-Gibbs statistical mechanics seems to be essential [3]. Nowadays a possible approach to this problem is known. It was initiated and developed by Tsallis. This formalism [4,5], referred to as nonextensive statistical mechanics (NSM), and related mathematical frameworks have been successfully applied to, *e.g.*, the Ising model with long-range interactions [6], astrophysical and cosmological problems [7], Lévy-type random walks [8], the traveling salesman problem [9], studies of biomolecules [10], and quantum groups [11]. (A comprehensive list of references is currently available at URL [12].)

Unfortunately, nonextensive generalization of thermal field theory is still far out of reach, mainly due to mathematical difficulty of treating infinite degrees of freedom. One should however recall that within the framework of Boltzmann-Gibbs statistical mechanics some important physical properties of thermal field theory can still be found in dynamics of a single quantum-mechanical particle in the heat bath: *e.g.*, the spectral property and the imaginary time periodicity of the thermal Green functions.

In this paper, we study the quantum-mechanical thermal Green functions based on NSM, in hope of giving a step toward nonextensive thermal field theory. In particular, we use NSM with *normalized q-expectation values* [13], which has recently been proposed to remedy some unfamiliar points contained in the former approach in references [4,5]. We derive the closed analytic expressions for the thermal Green functions in the real-time formalism and discuss influence of the nonextensivity on their properties.

We start our discussion with summarizing the basics of NSM with normalized q-expectation values developed in reference [13]. This formalism is based on Tsallis' postulate for the entropy [4]:

$$S_q[\hat{\rho}] = -\frac{k_{\mathrm{B}}}{q-1}\mathrm{Tr}(\hat{\rho}^q - \hat{\rho}), \tag{1}$$

where q is a constant which is referred to as the Tsallis index and $\hat{\rho}$ is the normalized density operator. k_{B} is Boltzmann's constant which is henceforth set equal to unity. In the limit $q \to 1$, $S_q[\hat{\rho}]$ converges on the Shannon-von Neumann entropy: $S[\hat{\rho}] = -\mathrm{Tr}(\hat{\rho}\ln\hat{\rho})$. Regarding the entropic nature of $S_q[\hat{\rho}]$, it has been shown that it satisfies the concavity [4,5] and the generalized H-theorem [14]. In contrast to the Shannon-von Neumann entropy, however, the additivity is modified. Suppose a system be divided into two independent subsystems whose density operators

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are given by $\hat{\rho}^{(1)}$ and $\hat{\rho}^{(2)}$, and the total density operator be the product $\hat{\rho}^{(1)} \otimes \hat{\rho}^{(2)}$. Then the Tsallis entropy satisfies

$$S_q[\hat{\rho}^{(1)} \otimes \hat{\rho}^{(2)}] = S_q[\hat{\rho}^{(1)}] + S_q[\hat{\rho}^{(2)}] + (1-q) S_q[\hat{\rho}^{(1)}] S_q[\hat{\rho}^{(2)}]. \tag{2}$$

Thus $S_q[\hat{\rho}]$ is subextensive (superextensive) for $q > 1$ ($q < 1$) and extensive only in the limit $q \to 1$. The entropy functional in equation (1) should be optimized under the constraints regarding the normalization condition and the normalized q-expectation values of the system Hamiltonian $\hat{H}$ and the total number operator $\hat{N}$:

$$\mathrm{Tr}(\hat{\rho}) = 1, \tag{3}$$

$$\langle \hat{Q} \rangle_q = \mathrm{Tr}(\hat{P}\hat{Q}) \quad (\hat{Q} = \hat{H}, \hat{N}), \tag{4}$$

where $\hat{P}$ in equation (4) denotes the *escort distribution* defined by [15]

$$\hat{P} = \frac{\hat{\rho}^q}{\mathrm{Tr}(\hat{\rho}^q)} \cdot \tag{5}$$

Using the thermodynamic formalism for the entropy functional $S_q[\hat{\rho}]$ under the constraints given in equations (3, 4), the optimal density operator is found to be

$$\hat{\rho} = \frac{1}{Z_q(\beta)} \Big\{ 1 - (1-q)(\beta/c) \times \Big[\hat{H} - \mu\hat{N} - (U_q - \mu N_q) \Big] \Big\}^{1/(1-q)}, \tag{6}$$

which describes a nonextensive grand canonical ensemble, where

$$c = \mathrm{Tr}(\hat{\rho}^q), \tag{7}$$

$$U_q = \langle \hat{H} \rangle_q, \tag{8}$$

$$N_q = \langle \hat{N} \rangle_q. \tag{9}$$

β and μ are the inverse temperature and the chemical potential, respectively. $Z_q(\beta)$ is the generalized grand partition function

$$Z_q(\beta) = \mathrm{Tr} \Big\{ 1 - (1-q)(\beta/c) \times \Big[\hat{H} - \mu\hat{N} - (U_q - \mu N_q) \Big] \Big\}^{1/(1-q)}. \tag{10}$$

From equations (6, 7, 10), follows the identical relation

$$c = [Z_q(\beta)]^{1-q}. \tag{11}$$

In the extensive limit $q \to 1$, $Z_q(\beta)$ converges on the ordinary grand partition function:

$$Z_q(\beta) \to Z_1(\beta) \equiv Z(\beta) = \mathrm{Tr}\exp\Big[-\beta(\hat{H} - \mu\hat{N}) \Big], \tag{12}$$

provided that the prefactor $\exp[\beta(U_q - \mu N_q)]$ has been absorbed into the normalization of $\hat{\rho}$ in this limit. Quite remarkably it can be shown [13] that all of equilibrium thermodynamic relations hold also in NSM in the analogous forms.

In this paper, we restrict ourselves to the range of the Tsallis index greater than unity

$$q > 1. \tag{13}$$

This restriction allows us to use the Mellin transform to express the density operator in a more analytically-tractable exponential form:

$$\begin{aligned} &\Big\{ 1 + (q-1)(\beta/c)[\hat{H} - \mu\hat{N} - (U_q - \mu N_q)] \Big\}^{-1/(q-1)} \\ &= \frac{1}{\Gamma(s)} \int_0^\infty \mathrm{d}\sigma\, \sigma^{s-1} \exp\Big(-\sigma \Big\{ 1 + (\beta/sc) \\ &\quad \times [\hat{H} - \mu\hat{N} - (U_q - \mu N_q)] \Big\} \Big) \\ &= \frac{s^s}{\Gamma(s)} \int_0^\infty \mathrm{d}\tau\, \tau^{s-1} \mathrm{e}^{-s\tau} \exp\Big\{ -\tau(\beta/c) \\ &\quad \times [\hat{H} - \mu\hat{N} - (U_q - \mu N_q)] \Big\}. \end{aligned} \tag{14}$$

$\Gamma(s)$ in this equation is Euler's gamma function and the integration variable is changed as $\sigma \to \tau = \sigma/s$ in the second equality, where s is a positive constant given by

$$s = \frac{1}{q-1} \cdot \tag{15}$$

From equation (14), formally follows the integral representation of $Z_q(\beta)$ [16]

$$Z_q(\beta) = \frac{s^s}{\Gamma(s)} \int_0^\infty \mathrm{d}\tau\, \tau^{s-1} \times \exp\{ -[s - (\beta/c)(U_q - \mu N_q)]\tau \} Z(\tau\beta/c), \tag{16}$$

which manifestly shows how the generalized grand partition function is related to the ordinary grand partition function. We note that to derive this relation the order of the integration and the trace operation is assumed to be commutative. Accordingly care has to be taken to the range of s for convergence of the integral: the range may depend on the system, in general. For later convenience, here we also present the Mellin transform of $\hat{\rho}^q$

$$\begin{aligned} \hat{\rho}^q = &\frac{s^s}{[Z_q(\beta)]^{1+1/s}\Gamma(s)} \int_0^\infty \mathrm{d}\tau\, \tau^s \\ &\times \exp\{ -[s - (\beta/c)(U_q - \mu N_q)]\tau \} \\ &\times \exp[-\tau(\beta/c)(\hat{H} - \mu\hat{N})]. \end{aligned} \tag{17}$$

Let us consider as a simple system the harmonic oscillator with a frequency ω and a unit mass, which can be regarded as a single-mode scalar field. The normal-ordered Hamiltonian reads ($\hbar \equiv 1$)

$$\hat{H} = \omega \hat{a}^\dagger \hat{a}, \tag{18}$$

where $\hat{a}^\dagger$ and $\hat{a}$ are respectively the creation and annihilation operators at initial time $t = 0$ and satisfy the commutation relations: $[\hat{a}, \hat{a}] = [\hat{a}^\dagger, \hat{a}^\dagger] = 0$, $[\hat{a}, \hat{a}^\dagger] = 1$.

The position and momentum operators at $t = 0$, $\hat{x}_0$ and $\hat{p}_0$ are given in terms of $\hat{a}^\dagger$ and $\hat{a}$ as $\hat{x}_0 = (\hat{a}^\dagger + \hat{a})/\sqrt{2\omega}$ and $\hat{p}_0 = i(\hat{a}^\dagger - \hat{a})/\sqrt{\omega/2}$. The eigenvalues of $\hat{H}$ are $E_n = \omega n$ $(n = 0, 1, 2, \ldots)$. The chemical potential is irrelevant in the present case of a single particle and is set equal to zero: $\mu = 0$. The ordinary single-particle partition function is

$$Z(\beta) = \frac{1}{1 - \mathrm{e}^{-\beta\omega}}\cdot \tag{19}$$

On the other hand, the generalized partition function $Z_q(\beta)$ in equation (10) is

$$Z_q(\beta) = \sum_{n=0}^{\infty} \frac{1}{[1 + (\beta/sc)(\omega n - U_q)]^s} = \left(\frac{sc}{\beta\omega}\right)^s \zeta(s, a), \tag{20}$$

where [17]

$$a = \frac{sc}{\beta\omega} - \frac{U_q}{\omega}\cdot \tag{21}$$

$\zeta(s, a)$ in equation (20) is the Hurwitz zeta function [18], which is defined by

$$\zeta(s, a) = \sum_{n=0}^{\infty} \frac{1}{(a + n)^s}, \tag{22}$$

provided that $a + n \neq 0$ for $\forall n$. In this representation, the condition Re $s > 1$ has to be imposed, but it is possible to extend to the cases of the other values of s (except the singularity at $s = 1$) by analytic continuation. One can also use equation (16) to calculate $Z_q(\beta)$ but finds nothing but the integral representation of $\zeta(s, a)$.

Similarly, the generalized internal energy U_q is calculated as follows:

$$\begin{aligned} U_q &= \frac{\omega}{c} \mathrm{Tr}(\hat{a}^\dagger \hat{a} \hat{\rho}^q) \\ &= \frac{\omega}{c[Z_q(\beta)]^q} \left(\frac{sc}{\beta\omega}\right)^{s+1} \sum_{n=0}^{\infty} \frac{n}{(a + n)^{s+1}} \\ &= \omega \left(\frac{s}{\beta\omega}\right)^{s+1} c^{2s+1} \left[\zeta(s, a) - a\zeta(s + 1, a)\right], \end{aligned} \tag{23}$$

where equation (11) has been used.

The quantity c can be calculated in two ways. One is to use equations (11, 20). The other is to evaluate equation (7) directly. The former gives

$$c = \left(\frac{\beta\omega}{s}\right)^{1/2} [\zeta(s, a)]^{-1/2s}, \tag{24}$$

whereas the latter yields

$$c = \left(\frac{s}{\beta\omega}\right)^{-\frac{s+1}{2s+1}} \left[\zeta(s + 1, a)\right]^{-\frac{1}{2s+1}}. \tag{25}$$

Equations (23, 24) [or (25)] determine U_q and c. The consistency between equations (24, 25) leads to the equation for a:

$$\frac{[\zeta(s, a)]^{1+1/2s}}{\zeta(s + 1, a)} = \left(\frac{s}{\beta\omega}\right)^{1/2}. \tag{26}$$

In addition, substitution of equations (24, 25) into equation (23) gives rise to

$$\frac{\zeta(s, a)}{\zeta(s + 1, a)} = \frac{sc}{\beta\omega}\cdot \tag{27}$$

Furthermore, from equations (26, 27), follows:

$$\zeta(s, a) = c^{-2s} \left(\frac{\beta\omega}{s}\right)^s. \tag{28}$$

It is generically a numerical problem to solve equations (23) and (24) [or, (25-28)] with respect to U_q and c.

Now we proceed to study the thermal Green functions within the framework of NSM. Let us define the generalized thermal Green functions as follows:

$$G_q^+(t, t' : \beta) = \langle \hat{x}(t) \hat{x}(t') \rangle_q, \tag{29}$$

$$G_q^-(t, t' : \beta) = \langle \hat{x}(t') \hat{x}(t) \rangle_q. \tag{30}$$

Here $\hat{x}(t)$ is the position operator of the particle in the Heisenberg picture and equations (4, 5) are employed for the normalized q-expectation values.

First we consider the spectral function. Using equations (29, 30), it is given by

$$\rho_q(k_0 : \beta) = \int_{-\infty}^{\infty} \mathrm{d}(t - t') \mathrm{e}^{ik_0(t-t')} \times [G_q^+(t, t' : \beta) - G_q^-(t, t' : \beta)], \tag{31}$$

provided that the temporal translational invariance is assumed, *i.e.*, $G_q^\pm(t, t' : \beta) = G_q^\pm(t - t' : \beta)$. Note that the combination $G_q^+(t, t' : \beta) - G_q^-(t, t' : \beta)$ appearing in the integrand is given by the normalized q-expectation value of $[\hat{x}(t), \hat{x}(t')]$. In the present case of the harmonic oscillator (corresponding to the unperturbed field in perturbative thermal field theory), this commutator is nothing but a c-number. In fact, the position operator in the Heisenberg picture, $\hat{x}(t) = \mathrm{e}^{i\hat{H}t} \hat{x}_0 \mathrm{e}^{-i\hat{H}t} = \hat{x}_0 \cos(\omega t) + (\hat{p}_0/\omega) \sin(\omega t)$, gives $[\hat{x}(t), \hat{x}(t')] = (1/i\omega) \sin[\omega(t - t')]$. Therefore the spectral function is explicitly given by

$$\rho(k_0) = 2\pi\varepsilon(k_0)\delta(k_0^2 - \omega^2) \tag{32}$$

with $\varepsilon(k_0) = -1$ $(k_0 < 0), +1$ $(k_0 > 0)$, which obviously carries no information on the thermal effects. That is, the spectral properties are the same for the system at zero temperature states, Boltzmann-Gibbs thermal states, and thermal states in NSM.

Next we evaluate $G_q^\pm(t, t' : \beta)$ analytically. Using equation (17) with $\mu = 0$, equations (29, 30) can collectively be expressed as

$$G_q^\pm(t, t' : \beta) = \frac{s^s c^{2s+1}}{\beta^{s+1} \Gamma(s)} \int_0^\infty \mathrm{d}\lambda\, \lambda^s \mathrm{e}^{-\omega a \lambda} Z(\lambda) G^\pm(t, t' : \lambda), \tag{33}$$

where a is given in equation (21) and the change is made for the integration variable as $\tau \to \lambda = \tau\beta/c$. $G^{\pm}(t,t':\beta=\lambda)$ appearing in the integrand are the ordinary real-time thermal Green functions calculated using the ordinary thermal density operator $\hat{\rho} = e^{-\beta\hat{H}}/Z(\beta)$. Explicitly, they are given by

$$G^{\pm}(t,t':\beta) = \frac{1}{2\omega}\left[\frac{\mathrm{e}^{\pm i\omega(t-t')}}{\mathrm{e}^{\beta\omega}-1} + \frac{\mathrm{e}^{\mp i\omega(t-t')}}{1-\mathrm{e}^{-\beta\omega}}\right], \tag{34}$$

which manifestly satisfy the celebrated Kubo-Martin-Schwinger condition [1]

$$G^{+}(t,t':\beta) = G^{-}(t+i\beta,t':\beta). \tag{35}$$

Substituting equation (34) into equation (33), we have

$$\begin{aligned} G_q^{\pm}(t,t':\beta) &= \frac{s^s c^{2s+1}}{2\omega\beta^{s+1}\Gamma(s)} \\ &\quad\times\left[\mathrm{e}^{\pm i\omega(t-t')}\int_0^{\infty}\mathrm{d}\lambda\,\lambda^s\mathrm{e}^{-\lambda(a+1)\omega}\frac{1}{(1-\mathrm{e}^{-\lambda\omega})^2}\right. \\ &\quad\left.+\,\mathrm{e}^{\mp i\omega(t-t')}\int_0^{\infty}\mathrm{d}\lambda\,\lambda^s\mathrm{e}^{-\lambda a\omega}\frac{1}{(1-\mathrm{e}^{-\lambda\omega})^2}\right] \\ &= \frac{c^{2s+1}}{2\omega}\left(\frac{s}{\beta\omega}\right)^{s+1} \\ &\quad\times\left[\mathrm{e}^{\pm i\omega(t-t')}\sum_{m,n=0}^{\infty}\frac{1}{(a+1+m+n)^{s+1}}\right. \\ &\quad\left.+\,\mathrm{e}^{\mp i\omega(t-t')}\sum_{m,n=0}^{\infty}\frac{1}{(a+m+n)^{s+1}}\right]. \end{aligned} \tag{36}$$

From the formulas ($b > 0$)

$$\zeta(s,b+1) = \zeta(s,b) - b^{-s}, \tag{37}$$

$$\sum_{m,n=0}^{\infty}\frac{1}{(b+m+n)^s} = \zeta(s-1,b) + (1-b)\zeta(s,b), \tag{38}$$

which can respectively be derived using equation (22) and the Mellin transform, we obtain the following expressions for the generalized thermal Green functions:

$$\begin{aligned} G_q^{\pm}(t,t':\beta) &= \frac{c^{2s+1}}{2\omega}\left(\frac{s}{\beta\omega}\right)^{s+1} \\ &\quad\times\Big\{[\zeta(s,a) - a\zeta(s+1,a)]\mathrm{e}^{\pm i\omega(t-t')} \\ &\quad+ [\zeta(s,a) + (1-a)\zeta(s+1,a)]\,\mathrm{e}^{\mp i\omega(t-t')}\Big\} \\ &= \frac{1}{2\omega}\left\{\left[\frac{\zeta(s,a)}{\zeta(s+1,a)} - a\right]\mathrm{e}^{\pm i\omega(t-t')}\right. \\ &\quad\left.+\left[\frac{\zeta(s,a)}{\zeta(s+1,a)} - a + 1\right]\mathrm{e}^{\mp i\omega(t-t')}\right\}. \end{aligned} \tag{39}$$

These expressions are to be compared with equation (34). The Kubo-Martin-Schwinger condition is no longer satisfied by $G_q^{\pm}(t,t':\beta)$. This is a very result of the nonexponential form of the density operator in NSM. From equations (21, 27), we see that the factors appearing in the square brackets in equation (39) can be rewritten as

$$\frac{\zeta(s,a)}{\zeta(s+1,a)} - a = \frac{U_q}{\omega} = \langle\hat{a}^{\dagger}\hat{a}\rangle_q, \tag{40}$$

$$\frac{\zeta(s,a)}{\zeta(s+1,a)} - a + 1 = \langle\hat{a}\hat{a}^{\dagger}\rangle_q, \tag{41}$$

which are natural nonextensive generalizations of the Planck factors $1/(e^{\beta\omega}-1)$ and $1/(1-e^{-\beta\omega})$ in equation (34), respectively.

Finally let us also calculate the generalized time-ordered thermal propagator, which is defined by

$$D_q(t,t':\beta) = \theta(t-t')G_q^{+}(t,t':\beta) + \theta(t'-t)G_q^{-}(t,t':\beta), \tag{42}$$

where $\theta(t) = 0\ (t<0), 1\ (t>0)$. Like in equation (33), this function is also related to the ordinary thermal propagator in Boltzmann-Gibbs statistical mechanics as follows:

$$D_q(t,t':\beta) = \frac{s^s c^{2s+1}}{\beta^{s+1}\Gamma(s)}\int_0^{\infty}\mathrm{d}\lambda\,\lambda^s\mathrm{e}^{-\omega a\lambda}Z(\lambda)D(t,t':\lambda). \tag{43}$$

The Fourier transform of $D(t,t':\beta)$ has been discussed by Dolan and Jackiw [19] in the context of ordinary thermal field theory. In the present mechanical case, it is given by [1]

$$\begin{aligned} \tilde{D}(k_0:\beta) &= \int_{-\infty}^{\infty}\mathrm{d}(t-t')\mathrm{e}^{ik_0(t-t')}D(t,t':\beta) \\ &= \frac{i}{k_0^2-\omega^2+i\varepsilon} + \frac{2\pi}{\mathrm{e}^{\beta\omega}-1}\delta(k_0^2-\omega^2), \end{aligned} \tag{44}$$

where ε is an infinitesimal positive constant. Substituting this equation into the Fourier transform of equation (42), we find the following generalized thermal propagator:

$$\begin{aligned} \tilde{D}(k_0:\beta) &= \frac{i}{k_0^2-\omega^2+i\varepsilon} \\ &\quad+ 2\pi\left[\frac{\zeta(s,a)}{\zeta(s+1,a)} - a\right]\delta(k_0^2-\omega^2). \end{aligned} \tag{45}$$

From this, we conclude that the effect of the nonextensivity is relevant only at the "on-shell" states $k_0 = \pm\omega$. The behavior of the function $f(s,a) = \zeta(s,a)/\zeta(s+1,a) - a$ is shown in Figure 1. It is seen that this factor monotonically decreases with respect to s at fixed a. Therefore, for the strong nonextensivity [*i.e.*, a large (small) value of q (s)], the thermal effect becomes enhanced.

To summarize, within the framework of nonextensive quantum statistical mechanics with normalized q-expectation values, we have presented the closed analytic expressions of the thermal Green functions of the harmonic oscillator in terms of the Hurwitz zeta function.

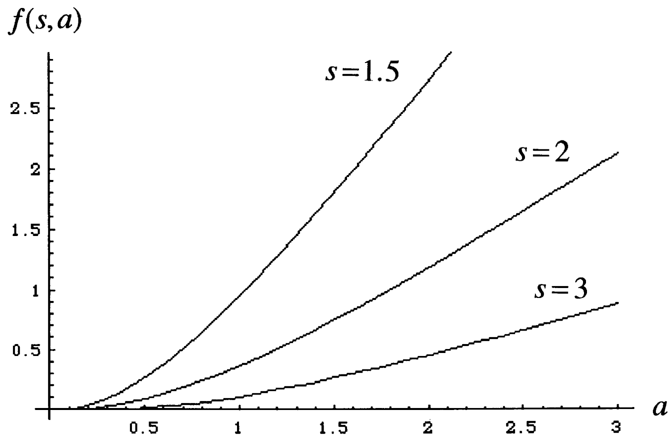

Fig. 1. Plots of $f(s,a) = \zeta(s,a)/\zeta(s+1,a) - a$ with respect to a for $s = 1.5$, 2, 3. All quantities are dimensionless.

It is found that the finite-temperature contribution to the time-ordered thermal propagator is present only at the on-shell states and becomes enhanced for the strong nonextensivity.

Note added in proof

Quite recently, the following two works have come to the author's attention. One is reference [20], which discusses a role of the Hurwitz zeta function in NSM. The other [21] considers the thermal Green functions in NSM, but no explicit formulas are given to them. Both of these works are based on NSM with *unnormalized q-expectation values* and their physical scopes are different from the present work's.

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