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Spectral density method in quantum nonextensive thermostatistics and magnetic systems with long-range interactions

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Abstract. Motived by the necessity of explicit and reliable calculations, as a valid contribution to clarify the effectiveness and, possibly, the limits of the Tsallis thermostatistics, we formulate the Two-Time Green Functions Method in nonextensive quantum statistical mechanics within the optimal Lagrange multiplier framework, focusing on the basic ingredients of the related Spectral Density Method (SDM). Besides, to show how the SDM works, we have performed, to the lowest order of approximation, explicit calculations of the low-temperature properties for a quantum d-dimensional spin-1/2 Heisenberg ferromagnet with long-range interactions decaying as $1/r^p$ (r is the distance between spins in the lattice).

PACS. 05.30.-d Quantum statistical mechanics – 05.70.-a Thermodynamics – 75.10.Jm Quantized spin models

1 Introduction

Green's functions (GF's) are currently used in many-body physics and their power and success are widely recognized [1]. There exists at present a large variety of methods and techniques for calculation of the GF's both in classical and quantum thermostatistics [1–5]. In particular, the related *spectral density method* (SDM), originally formulated by Kalashnikov and Fradkin [4] for quantum many-body systems, is a powerful nonperturbative tool which allows a direct study of the macroscopic properties of interacting quantum and classical many-body systems [4–8] also involving phase transitions.

Recently, the increasing interest in Tsallis' nonextensive thermostatistics [9], has stimulated a lot of works [10,11] on the extension of the GF formalism also to this Tsallis' generalized framework of the statistical mechanics with the aim to provide new and effective methods for dealing with realistic nonextensive problems. Along this direction, the two-time GF technique and SDM have been formulated in classical nonextensive thermostatistics in two our papers [11] with application to the Heisenberg spin chain with short-range interactions. Here we wish to present the extension of the same formalism in quantum nonextensive thermostatistics by using the *optimal Lagrange multiplier* (OLM) representation [12], focusing on the spectral density (SD) and its spectral decomposition for their relevance in explicit calculations. Then, in order to show how the method works in the nonextensive context, we apply the extended SDM to a quantum d-dimensional spin-1/2 Heisenberg ferromagnet with long-range interactions decaying as r^{-p} (r is the spin distance and p the decay exponent) and explore, to the lowest order of approximation, the nonextensivity effects on the low-temperature magnetic properties of the model.

In Section 2 we summarize some basic ingredients of the nonextensive quantum thermostatistics in the OLM representation for next utility. Sections 3 and 4 are devoted to the extension of the GF formalism and of the SDM in the nonextensive context, respectively. In Section 5 the extended SDM is applied to the above mentioned spin model. Finally, some concluding remarks are drawn in Section 6.

2 The OLM representation of quantum nonextensive statistical mechanics

The Tsallis' quantum thermostatistics [9] is essentially based on the so called q-entropy (with $k_B = \hbar = 1$)

$$S_q = \frac{1 - \mathrm{Tr}\rho_q^q}{q-1}, \tag{1}$$

where ρ_q is the generalized density operator satisfying the normalization condition $\mathrm{Tr}\rho_q = 1$. In this framework,

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the generalization of the statistical average (referred as *q-expectation value* or *q-mean value*) for the observable O is given by

$$\langle O\rangle_q = \frac{\mathrm{Tr}\left[\rho_q^q O\right]}{\mathrm{Tr}\left[\rho_q^q\right]}. \quad (2)$$

Here, q is a real parameter (called the *nonextensivity index*) which measures the degree of nonextensivity.

Working in the canonical ensemble, the statistical operator ρ_q can be determined adopting the OLM constraint prescriptions in the extremization procedure of S_q [9,12]. Then, assuming the Hamiltonian H of the system to have a complete orthonormal set of eigenvectors $\{|n\rangle\}$ with eigenvalues $\{\varepsilon_n\}$, the normalized probability $p_n = \langle n|\,\rho_q\,|n\rangle$ associated with the n^{th} eigenstate is given by

$$p_n = Z_q^{-1}\left[1-\beta(1-q)\left(\varepsilon_n - U_q\right)\right]^{\frac{1}{1-q}}, \quad (3)$$

where

$$Z_q = \sum_n \left[1-\beta(1-q)\left(\varepsilon_n - U_q\right)\right]^{\frac{1}{1-q}}, \quad (4)$$

and the q-internal energy $U_q = \langle H\rangle_q$ is given by

$$U_q = \overline{Z}_q^{-1}\sum_n p_n^q \varepsilon_n. \quad (5)$$

Here $\langle n|\,\rho_q^q\,|m\rangle = p_n^q\delta_{nm}$ are the matrix elements of the operator ρ_q^q in the $\{|n\rangle\}$ representation and $\overline{Z}_q = \mathrm{Tr}\left[\rho_q^q\right] = \sum_n p_n^q$ denotes the pseudo-partition function in the normalized OLM framework ($\overline{Z}_1$ is not merely the extensive partition function but contains an extra factor). In the previous equations, $\beta = 1/T$ and T is the thermodynamic temperature. It is worth mentioning that, for $q < 1$, the formalism imposes a high-energy cutoff, i.e. $p_n = 0$ whenever the argument of the power function in equations (3), (4) becomes negative [9].

3 Two-time q-Green functions and q-spectral density

In the quantum nonextensive thermostatistics, we define the two-time *retarded* and *advanced* GF's (q-GF's) for two arbitrary operators A and B as

$$G_{qAB}^{(\nu)}\left(t,t'\right) = -i\theta_\nu\left(t-t'\right)\left\langle [A(t),B(t')]_\eta\right\rangle_q, \quad (6)$$

where $\nu = r, a$ stands for "retarded" and "advanced", respectively. Here, $\theta_a(t-t') = -\theta(t'-t)$ and $\theta_r(t-t') = \theta(t-t')$, being $\theta(x)$ the step function; $[...,...]_\eta$ denotes a commutator ($\eta = -1$) or anticommutator ($\eta = +1$); $X(t)$ (with $X = A, B$) is the usual Heisenberg representation of operator X at time t. Of course, for $q = 1$, the conventional formalism is reproduced. It is worth nothing that, for general operators A and B, one can develop the q-GF's framework equivalently with commutators or anticommutators. However, for fermionic or bosonic operators it is of course convenient to use in equation (6) $\eta = -1$ or $\eta = +1$, respectively.

It is now relatively simple generalize most of the basic properties of the conventional two-time GF properties [1,2] in nonextensive context [11].

Within equilibrium ensembles, the functions $G_{qAB}^{(\nu)}\left(t,t'\right)$ depend on times only through the difference $\tau = t - t'$ and hence one can introduce the Fourier transform

$$G_{qAB}^{(\nu)}(\omega) = \int_{-\infty}^{+\infty} d\tau G_{qAB}^{(\nu)}(\tau)\, e^{i\omega\tau}. \quad (7)$$

Besides, in strict analogy with the GF extensive formalism [2,4], the generalized spectral density (q-SD) in the ω-representation is defined by

$$\Lambda_{qAB}(\omega) = \int_{-\infty}^{+\infty} dt e^{i\omega\tau}\left\langle [A(\tau),B]_\eta\right\rangle_q, \quad (8)$$

in terms of which it is easy to write the spectral representation of the associated q-GF's

$$G_{qAB}^{(\nu)}(\omega) = \int_{-\infty}^{+\infty}\frac{d\omega'}{2\pi}\frac{\Lambda_{qAB}(\omega')}{\omega-\omega'+(-1)^\nu i\varepsilon}, \quad \varepsilon\to 0^+, \quad (9)$$

where $(-1)^\nu$ stands for $+1$ if $\nu = r$ and -1 if $\nu = a$. These functions can be analytically continued in the complex ω-plane and combined to construct the single q-GF $G_{qAB}(\omega) = \int_{-\infty}^{+\infty}\frac{d\omega'}{2\pi}\frac{\Lambda_{qAB}(\omega')}{\omega-\omega'}$ of complex ω with a cut along the real axis.

As a next step, one can immediately obtain the spectral decomposition of the q-SD. Indeed, by using equations (3)–(5), from the definition (8) we have the exact representation:

$$\Lambda_{qAB}(\omega) = \frac{2\pi}{\overline{Z}_q}\sum_{nm} p_n^q\left[1+\eta\left(\frac{p_m}{p_n}\right)^q\right] \times A_{nm}B_{mn}\delta\left(\omega-\omega_{mn}\right), \quad (10)$$

with $\omega_{mn} = \varepsilon_m - \varepsilon_n$. Then, the spectral decomposition for $G_{qAB}^{(\nu)}(\omega)$ follows directly from the ω-representation (9). In particular, for $G_{qAB}(\omega)$ we have

$$G_{qAB}(\omega) = \frac{1}{\overline{Z}_q}\sum_{nm}\left[p_n^q + \eta p_m^q\right]\frac{A_{nm}B_{mn}}{\omega-\omega_{mn}}. \quad (11)$$

In strict analogy with the extensive case [4,6,8], equation (11) suggests that the real poles ω_{mn} of $G_{qAB}(\omega)$ represent the exact energy spectrum of undamped excitations in the system.

A comparison of the previous relations with the corresponding extensive ones [4,6] suggests that the Tsallis' statistics does not influence the meaning of GF singularities, but drastically modifies the structure of the spectral weights introducing a mixing of energy levels.

4 The q-spectral density method (q-SDM)

Now we have all the necessary ingredients to extend the SDM in the Tsallis' formalism. By successive derivatives of $\Lambda_{qAB}(\tau) = \langle [A(\tau), B]_\eta \rangle_q = \int_{-\infty}^{+\infty} d\omega \Lambda_{qAB}(\omega) e^{-i\omega\tau}/2\pi$ with respect to τ and then setting $\tau = 0$, one obtains the infinite set of exact equations of motion or *sum rules* for $\Lambda_{qAB}(\omega)$

$$\int_{-\infty}^{+\infty} \frac{d\omega}{2\pi} \omega^m \Lambda_{qAB}(\omega) = \langle [L_H^m A, B]_\eta \rangle_q, \quad (m = 0, 1, 2, ...), \tag{12}$$

where the quantity on the left-hand side of equation (12) is called the *m-moment* of $\Lambda_{qAB}(\omega)$ and L_H^m $(m = 0, 1, 2, ...)$ acts as $L_H^0 A = A$, $L_H^1 A = [A, H]_-$, $L_H^2 A = \left[[A, H]_-, H\right]_-$ and so on.

The set of integral equations (12) represents a typical *moment problem* which should determine exactly the unknown q-SD. Of course, in practical calculations we must look for an approximated solution of $\Lambda_{qAB}(\omega)$, which captures the essential physics of the system under study, truncating the set (12) at a given order.

Suggested by the exact spectral decomposition (10), as a suitable approximation for $\Lambda_{qAB}(\omega)$, one can assume a finite sum of properly weighted δ-functions (the so called *polar ansatz*)

$$\Lambda_{qAB}(\omega) = 2\pi \sum_{k=1}^{n} \lambda_{qAB}^{(k)} \delta(\omega - \omega_{qAB}^{(k)}), \tag{13}$$

where n is a finite integer number and the unknown parameters $\lambda_{qAB}^{(k)}$ and $\omega_{qAB}^{(k)}$ are to be determined self-consistently solving the first $2n$ moment equations in the set (12).

In several situations of experimental interest, also the damping of excitations may be quite relevant so that the polar approximation (13) is inadequate. In this case, to take properly into account the finite life-time of quasi-particles, one can assume, as in the extensive case [6,8], the so called *modified Gaussian ansatz*

$$\Lambda_{qAB}(\omega) = 2\pi\omega \sum_{k=1}^{n} \lambda_{qAB}^{(k)} \frac{\exp\left[-\left(\omega - \omega_{qAB}^{(k)}\right)^2 / \Gamma_{qAB}^{(k)}\right]}{\sqrt{\pi \Gamma_{qAB}^{(k)}}}, \tag{14}$$

where $\Gamma_{qAB}^{(k)}$ represents the width of the peak at $\omega = \omega_{qAB}^{(k)}$ and the life-time of the excitations with frequency $\omega_{qAB}^{(k)}$ is given by $\tau_{qAB}^{(k)} = \sqrt{\Gamma_{qAB}^{(k)}}$ under the condition $\Gamma_{qAB}^{(k)} / \left[\omega_{qAB}^{(k)}\right]^2 \ll 1$. It is worth noting that, the q-SDM is quite general and can be easily applied to different models by introducing the appropriate q-SD.

5 The quantum spin-1/2 Heisenberg ferromagnet with long-range interactions: a q-SDM approach to the lowest order of approximation

The quantum d-dimensional spin-1/2 Heisenberg ferromagnet with long-range interactions [13] is described in the $\mathbf{k}$-space by the Hamiltonian

$$H = -\frac{1}{2N} \sum_{\mathbf{k}} J(\mathbf{k}) \left(S_{\mathbf{k}}^+ S_{-\mathbf{k}}^- + S_{\mathbf{k}}^z S_{-\mathbf{k}}^z\right) - h S_0^z. \tag{15}$$

Here h is the external magnetic field, N is the number of sites $\{j\}$ of a hypercubic lattice with unitary spacing; $\mathbf{S_k}$, $S_{\mathbf{k}}^{\pm}$ and $J(\mathbf{k})$ are the Fourier transforms of the spin operators $\mathbf{S}_j$, $S_j^{\pm} = S_j^x \pm i S_j^y$ and the exchange interaction $J_{ij} = J / |\mathbf{r}_i - \mathbf{r}_j|^p$ $(p > 0,\ J > 0)$, respectively, and the $\mathbf{k}$-sum is restricted over the first Brillouin zone $(1BZ)$.

For spin model (15), the q-expectation value of the magnetization per site is given by

$$m_q = \frac{1}{N} \sum_{j=1}^{N} \left\langle S_j^z \right\rangle_q = \frac{1}{2} - \frac{1}{N^2} \sum_{\mathbf{k}} \left\langle S_{-\mathbf{k}}^- S_{\mathbf{k}}^+ \right\rangle_q. \tag{16}$$

Due to the operatorial representation (15)–(16), in the framework of the q-SDM it is convenient to introduce the q-SD

$$\Lambda_{q\mathbf{k}}(\omega) = \int_{-\infty}^{\infty} dt e^{i\omega\tau} \left\langle \left[S_{\mathbf{k}}^+(\tau), S_{-\mathbf{k}}^-\right]_- \right\rangle_q, \tag{17}$$

which satisfy the infinite hierarchy of moment equations

$$\int_{-\infty}^{+\infty} \frac{d\omega}{2\pi} \omega^m \Lambda_{q\mathbf{k}}(\omega) = \left\langle [L_H^m S_{\mathbf{k}}^+, S_{-\mathbf{k}}^-]_- \right\rangle_q, \quad (m = 0, 1, 2, ...). \tag{18}$$

To the lowest order of approximation, we can assume for $\Lambda_{q\mathbf{k}}(\omega)$ the one δ-function polar ansatz

$$\Lambda_{q\mathbf{k}}(\omega) = 2\pi \lambda_{q\mathbf{k}} \delta(\omega - \omega_{q\mathbf{k}}), \tag{19}$$

where the unknown parameters $\lambda_{q\mathbf{k}}$ and $\omega_{q\mathbf{k}}$ can be determined by solving the first 2 moment equations of the set (18). Then, working close to $q = 1$ and with the near saturation condition $\left\langle S_{\mathbf{k}}^z S_{-\mathbf{k}}^z \right\rangle \approx \left\langle S_{\mathbf{k}}^z \right\rangle \left\langle S_{-\mathbf{k}}^z \right\rangle = N^2 m_q^2 \delta_{\mathbf{k},0}$ [7], we obtain for $\omega_{q\mathbf{k}}$ and m_q the set of self-consistent equations (with $\lambda_{q\mathbf{k}} = 2N m_q$)

$$\omega_{q\mathbf{k}} = h + J \Omega_p(\mathbf{k}) m_q + \frac{J}{N} \sum_{\mathbf{k}'} \frac{[\Omega_p(\mathbf{k} - \mathbf{k}') - \Omega_p(\mathbf{k}')]}{1 - [1 - \beta(1 - q)\omega_{q\mathbf{k}'}]^{\frac{q}{1-q}}}, \tag{20}$$

$$m_q = \frac{1}{2} - \frac{1}{N} \sum_{\mathbf{k}} \frac{2m_q}{[1 - \beta(1 - q)\omega_{q\mathbf{k}}]^{\frac{q}{q-1}} - 1}, \tag{21}$$

where

$$\Omega_p(\mathbf{k}) = \frac{J(0) - J(\mathbf{k})}{J} = \sum_{\mathbf{r}} \frac{1 - \cos \mathbf{k} \cdot \mathbf{r}}{|\mathbf{r}|^p}. \tag{22}$$

It is worth noting that in equation (20), which determines the q-excitation spectrum $\omega_{q\mathbf{k}}$, the contribution $h+J\Omega_p(\mathbf{k})m_q$ is formally identical to the known Tyablikov dispersion relation [1,2] for the corresponding extensive problem.

The solution of the self-consistent problem (20)–(22) is rather complicate and one must consider asymptotic regimes for obtaining explicit analytical results. For instance, in the low-temperature ferromagnetic phase, we can resort to the Tyablikov-like approximation

$$\omega_{q\mathbf{k}} \approx \omega_{\mathbf{k}}^{(T)} = h + \frac{1}{2} J\Omega_p(\mathbf{k}), \quad (23)$$

as a zero order in equations (20), (21). So, in the thermodynamic limit $N \to \infty$, equation (21) yields a cumbersome expression for the q-magnetization $m_q(\beta, h)$ which, for $q = 1$, reproduces the extensive counterpart [13] and can be used to obtain explicit expansion as $q \to 1$.

Interesting representation for $m_q(\beta, h)$ and the q-susceptibility $\chi_q(\beta, h) = \partial m_q(\beta, h)/\partial h$ in the nearly saturation regime can be obtained, for $d < p < 2d$, under condition $\beta h(q-1) > 1$. Assuming the low-k expansion $\Omega_p(\mathbf{k}) \approx A_d(p)k^{p-d}$ [13], where $A_d(p) = \pi^d d^{d-p}\left[\Gamma(p)\right]^{-d}/\sin[\pi(p-d)/2]$ and $\Gamma(z)$ the gamma function, we find indeed

$$m_q(\beta, h) \simeq \frac{1}{2} - \frac{K_d \Lambda^d}{d\,(1+\beta h(q-1))^{\frac{q}{q-1}}} \times {}_2F_1\left(\frac{d}{p-d}, \frac{q}{q-1}; \frac{p}{p-d}; -\frac{JA_d(p)\beta(q-1)\Lambda^{p-d}}{2\,(1+\beta h(q-1))}\right), \quad (24)$$

$$\chi_q(\beta, h) \simeq \frac{K_d \Lambda^d \beta}{(p-d)\,(1+\beta h(q-1))^{\frac{2q-1}{q-1}}} \times \left\{ \frac{q-1}{\left[1+\frac{JA_d(p)\beta(q-1)\Lambda^{p-d}}{2(1+\beta h(q-1))}\right]^{\frac{q}{q-1}}} + \left[1-(2-\frac{p}{d})q\right]\, {}_2F_1\left(\frac{d}{p-d}, \frac{q}{q-1}; \frac{p}{p-d}; -\frac{JA_d(p)\beta(q-1)\Lambda^{p-d}}{2\,(1+\beta h(q-1))}\right) \right\}. \quad (25)$$

Here, ${}_2F_1(a, b; c; z)$ is the hypergeometric function, $K_d = 2^{1-d}\pi^{-d/2}/\Gamma(d/2)$ and Λ is a wave vector cut-off related to the $1BZ$ of the spin lattice.

If, additionally, we assume $\beta h(q-1) \gg 1$ as $T = \beta^{-1} \to 0$, equations (24) and (25) yield $m_q(\beta, h) \simeq 1/2 - \mathcal{A}_d^{(q)}(h)T^{\frac{q}{q-1}}$ and $\chi_q(\beta, h) \simeq \mathcal{B}_d^{(q)}(h)T^{\frac{q}{q-1}}$, where the explicit expressions of $\mathcal{A}_d^{(q)}(h)$ and $\mathcal{B}_d^{(q)}(h)$ (with $h \neq 0$) are inessential for our purposes.

The intrinsically nonextensive region ($p \leq d$), which is not of primary interest in this short contribution, requires a more delicate analysis which will be the subject of a future work.

6 Concluding remarks

In this short note we have extended, in nonextensive quantum thermostatistics, the two-time GF formalism and the related SDM already developed for quantum [4,6] and classical [5,7,8] extensive systems. This offers the possibility to explore, at least in principle, the properties of realistic systems by using the big amount of experiences acquired in extensive problems. In case of the Heisenberg model (15), the polar ansatz (19) yields reasonable results for the excitation spectrum and the relevant thermodynamic q-quantities in the low temperature regime. For describing other thermodynamic regimes in a wider range of temperatures, one could to adopt a new set of approximations involving additional decoupling procedures and higher order moment equations, consistently with the spirit of the SDM [4–8].

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