Quantum statistical mechanics for nonextensive systems

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(Received 8 September 1998)

The traditional basis of description of many-particle systems in terms of Green functions is here generalized to the case when the system is nonextensive, by incorporating the Tsallis form of the density matrix indexed by a nonextensive parameter q. This is accomplished by expressing the many-particle q Green function in terms of a parametric contour integral over a kernel multiplied by the usual grand canonical Green function which now depends on this parameter. We study one- and two-particle Green functions in detail. From the one-particle Green function, we deduce some experimentally observable quantities such as the one-particle momentum distribution function and the one-particle energy distribution function. Special forms of the two-particle Green functions are related to physical dynamical structure factors, some of which are studied here. We deduce different forms of sum rules in the q formalism. A diagrammatic representation of the q Green functions similar to the traditional ones follows because the equations of motion for both of these are formally similar. Approximation schemes for one-particle q Green functions such as Hartree and Hartree-Fock schemes are given as examples. This extension enables us to predict possible experimental tests for the validity of this framework by expressing some observable quantities in terms of the q averages. [S1063-651X(99)10201-0]

PACS number(s): 05.70.Ce, 05.20.−y, 05.30.Ch

I. INTRODUCTION

Ever since Tsallis [1] (also see Ref. [2]) proposed maximum q entropy for examining nonextensive systems by employing q mean values so as to obtain thermostatistics, it has spawned a large number of investigations on a wide variety of topics in this subject. Here we cite a representative set of such works of current interest in physics along with the values of the nonextensive parameter q associated with some of the phenomena: Lévy superdiffusion [3] and anomalous correlated diffusion [4]; turbulence in a two-dimensional pure electron plasma ($q=\frac{1}{2}$) [5]; dynamic linear response theory [6]; perturbation and variation methods for calculation of thermodynamic quantities [7]; thermalization of an electron-phonon system ($q>1$) [8]; low-dimensional dissipative systems ($q<1$) [9]; and some astrophysical applications [10]. The q values quoted here were either fitted to experiment or obtained from computer simulations or model calculations. In Ref. [9] and, more recently, Ref. [11], the relationship between q and the underlying dynamics has been explored. An important result emerging from this study is that the range of interactions controls the type of sensitivity to initial conditions that a large system will exhibit. Thus the exponential sensitivity ($q=1$) of strong chaos is found for short range interactions, and the power-law sensitivity ($q\neq 1$) of weak chaos for long range interactions. Thus q is a measure of the range and size of the interactions controlling the system behavior. Given these features, it appears expedient to develop methods of dealing with such situations, for which the Green function method is one of the most successful ones. The purpose of this paper is to present an enlarged version of our short communication [12] containing a generalization of the thermodynamic Green function (here in slightly modified form) theory of the quantum statistical mechanics of many-particle systems [13] when they are nonextensive in this q formalism. This modified form is consistent with a recent reformulation of the formalism in Ref. [14], which was put forward to include the invariance property of the ensemble under the choice of origin of the scales of quantities and enables us to develop a diagrammatic theory parallel to the conventional theory. This generalization then leads us to propose possible experimental tests of nonextensive features predicted in such a formalism by calculating measurable quantities such as the momentum distribution function for electrons measurable in positron annihilation and x-ray Compton scattering experiments [15], Bose condensation in confined small numbers of atoms [16], and cross sections for scattering by external probes such as neutrons, photons, etc. [17] in terms of the q mean values. Section II contains the development of the q Green function theory. In Sec. II A, the q one-particle Green function is studied in detail using an integral representation so as to include all values of q. In Sec. II B, after a brief discussion of the q n-particle Green function expression for the q mean value of the Hamiltonian, various important thermodynamic quantities in the q framework are given. We outline a diagrammatic procedure and illustrate it with the Hartree approximation in Sec. II C, and with the Hartree-Fock approximation in Sec. II D. In Sec. II E, we discuss the response functions and their implications in the q framework. This serves as an example of a two-particle Green function. In Sec. III, we develop expressions for various relevant quantities amenable to experimental investigation, with a focus on systems with few particles. We present expressions for an average number of particles obeying Bose and Fermi statistics at low temperatures, and also a typical scattering function, using the q formalism. We also display these in Figs. 2, 3, and 4. We end the paper with a summary and concluding remarks in Sec. IV.

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II. GREEN FUNCTION THEORY

In this section, we develop the thermodynamic Green function theory in describing the properties of nonextensive many-particle systems. This provides a method of discussing properties of nonextensive systems with no more conceptual difficulty than those of the extensive systems. The method is applicable to particles obeying any statistics, and for equilibrium or nonequilibrium situations. We present this development in five subsections.

A. One-particle Green function

We adopt second-quantized particle creation and annihilation operators in the Heisenberg representation, as in the standard book by Kadanoff and Baym [13] (henceforth cited as KB) to describe a many-particle system whose Hamiltonian operator is $\hat{H}$ and whose number operator is $\hat{N}$. In this way we describe nonextensive systems at arbitrary temperatures, and for boson or fermion systems in equilibrium, by maximizing the Tsallis entropy $S_q=(1-\mathrm{Tr}\,\hat{\rho}^q)/(q-1)$. $\mathrm{Tr}\,\hat{\rho}=1$ and $\hat{\rho}$ is the system density matrix, subject to the constraints of fixed q mean values $\langle\hat{H}\rangle_q=\mathrm{Tr}\,\hat{H}\hat{\rho}^q$ and $\langle\hat{N}\rangle_q=\mathrm{Tr}\,\hat{N}\hat{\rho}^q$ (see Ref. [14] for a discussion for these constraints). Thus $\langle 1\rangle_q=\mathrm{Tr}\,\hat{\rho}^q=1+(1-q)S_q$, and we define the one-particle q Green function in a form which is different from that given in Ref. [12]

$$G^{(q)}(1,1';\beta,\mu)=\frac{1}{i\langle 1\rangle_q}\langle T(\Psi(1)\Psi^\dagger(1'))\rangle_q \equiv\frac{1}{i\langle 1\rangle_q}\mathrm{Tr}[\hat{P}(\hat{H},\hat{N};q,\beta,\mu)T(\Psi(1)\Psi^\dagger(1'))], \tag{1}$$

where

$$\hat{P}(\hat{H},\hat{N};q,\beta,\mu)=[1-\beta(1-q)(\hat{H}-\mu\hat{N})]^{q/(1-q)}/(Z_q)^q,$$

$$Z_q=\mathrm{Tr}[1-\beta(1-q)(\hat{H}-\mu\hat{N})]^{1/(1-q)}, \tag{2}$$

$$\mathrm{Tr}\,\hat{P}(\hat{H},\hat{N};q,\beta,\mu)=\frac{\tilde{Z}_q}{Z_q^q},$$

with

$$\tilde{Z}_q=\mathrm{Tr}(1-\beta(1-q)(\hat{H}-\mu\hat{N}))^{q/(1-q)}.$$

Equation (2) is a consequence of the Tsallis entropy maximization stated above. Here β and μ are the Lagrange multipliers associated with the two constraints, and have the same significance as the inverse temperature and chemical potential in the usual description. Equation (1) differs from that in Ref. [12] by the appearance of the factor $\langle 1\rangle_q$. This definition proves to be very useful in developing a diagrammatic analysis as in conventional Green function theory, as will be shown subsequently. Here 1 refers to the space-time of a particle at $(\vec{r}_1,t_1)$, and T is the usual Wick time-ordering symbol:

$$\mathrm{T}\,(\Psi(1)\Psi^\dagger(1'))=\Psi(1)\Psi^\dagger(1') \quad \text{for} \quad t_1>t_{1'}$$
$$=\pm\Psi^\dagger(1')\Psi(1) \quad \text{for} \quad t_1<t_{1'}. \tag{3}$$

The creation $\Psi^\dagger(\vec{r'},t)$ and annihilation $\Psi(\vec{r},t)$ operators obey the canonical commutation rules (CCR's) at equal times:

$$\Psi(\vec{r},t)\Psi(\vec{r'},t)\mp\Psi(\vec{r'},t)\Psi(\vec{r},t)=0,$$

and its Hermitian conjugate, (4)

$$\Psi(\vec{r},t)\Psi^\dagger(\vec{r'},t)\mp\Psi^\dagger(\vec{r'},t)\Psi(\vec{r},t)=\delta(\vec{r}-\vec{r'}).$$

In the above and in subsequent analysis, the upper sign refers to bosons and the lower to fermions. The definitions for other multiparticle q Green functions follow in the same fashion. We may also note that the conventional grand canonical ensemble results given by KB are obtained when we take the limit $q=1$ in these expressions.

There is a useful trick to calculate Z_q in terms of a parametric integral over the usual grand canonical partition function, $Z_1=\mathrm{Tr}\exp(-\beta(\hat{H}-\mu\hat{N}))$, which now depends on the parameter multiplied by a kernel. The first such proposal by Hilhorst (private communication to Tsallis [18]) was valid for $q>1$, which was extended for $q<1$ by Prato [19]. Here we employ a contour integral representation, from which the above representations as well as others are obtained by a suitable deformation of the contour [20]. We express the q Green function in terms of a parametric integral over a different form of the kernel multiplied by the usual grand canonical Green function which now depends on this parameter. The general contour integral form is [21]

$$b^{1-z}\frac{i}{2\pi}\int_C du\,\exp(-ub)(-u)^{-z}=\frac{1}{\Gamma(z)}, \tag{5}$$

with $b>0$ and $\mathrm{Re}\,z>0$, where the contour C starts from $+\infty$ on the real axis, encircles the origin once counterclockwise, and returns to $+\infty$. This representation is very general, from which we can obtain other integral representations. In particular, the results of Hilhorst [18] ($q>1$) and Prato [19] ($q<1$) are just deformations of the contour in Eq. (5). Other representations are possible, such as [20] ($q<1$)

$$\frac{\exp(ab)b^{1-z}}{2\pi}\int_{-\infty}^{\infty}dt\frac{\exp(itb)}{(a+it)^z}=\frac{1}{\Gamma(z)} \quad \text{for} \quad b>0$$
$$=0 \quad \text{for} \quad b<0, \tag{6}$$

with $a>0$, $\mathrm{Re}\,z>0$, and $-\pi/2<\arg(a+it)<\pi/2$, and where the countour was deformed from C to C_1, as shown in Fig. 1 below. These particular representations are useful in several specific calculations, for example, for a classical ideal gas [19] and for blackbody radiation [22] with $q<1$. However, we employ Eq. (5) in this paper because it is very suitable in a general discussion, on the same footing, to all cases $q>1$, $q=1$, and $q<1$.

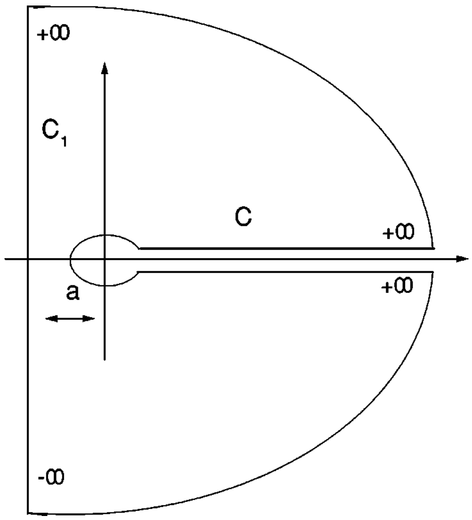

FIG. 1. This figure shows the contour employed to obtain Eq. (6).

By taking $b=1-(1-q)\beta(\hat{H}-\mu\hat{N})$ and $z=1+1/(1-q)$, we obtain the expression for Z_q, and by taking $z=1/(1-q)$ we obtain the corresponding expression for the q Green function:

$$Z_q(\beta,\mu)=\int_C du\, K_q^{(1)}(u) Z_1(-\beta u(1-q),\mu), \tag{7}$$

and

$$G^{(q)}(1,1';\beta,\mu)=\int_C du\, \tilde{K}_q^{(2)}(u) Z_1(-\beta u(1-q),\mu) \times G^{(1)}(1,1';-\beta u(1-q),\mu), \tag{8}$$

$$\tilde{K}_q^{(2)}(u)=\frac{K_q^{(2)}(u)}{\langle 1\rangle_q},$$

where

$$K_q^{(2)}(u)=-\frac{(1-q)u}{(Z_q)^q}K_q^{(1)}(u) = i\frac{\Gamma(1/(1-q))}{2\pi(Z_q)^q}\exp(-u)(-u)^{-1/(1-q)}. \tag{9}$$

$G^{(1)}(1,1';\beta,\mu)$ is the usual grand canonical one-particle Green function given by KB. Similar expressions hold for the multiparticle q Green functions. In addition, the dynamic linear response function derived in Ref. [6] will be re-expressed in terms of the parametric integral over the usual time-response functions [13]. It should be remarked that in all subsequent analysis the choice of the deformations of the contour in the u integration is such that the resulting integrals are all convergent, and this feature gives us the conditions on q mentioned above and discussed in detail by Lenzi [20].

Following KB, we introduce correlation functions

$$G_>^{(q)}(11';\beta,\mu)=\frac{1}{i\langle 1\rangle_q}\langle \Psi(1)\Psi^\dagger(1')\rangle_q,$$
$$G_<^{(q)}(11';\beta,\mu)=\frac{\pm}{i\langle 1\rangle_q}\langle \Psi^\dagger(1')\Psi(1)\rangle_q. \tag{10}$$

The notations $>$ and $<$ are intended to exhibit the feature that $G^{(q)}(1,1';\beta,\mu)=G_>^{(q)}(1,1';\beta,\mu)$ for $t_1>t_{1'}$ and $G^{(q)}(1,1';\beta,\mu)=G_<^{(q)}(1,1';\beta,\mu)$ for $t_1<t_{1'}$. Using Eq. (8), we may similarly express $G_>^{(q)}$ and $G_<^{(q)}$ in terms of the corresponding grand canonical correlation functions. The spectral weight function in frequency space, obtained by taking the Fourier transform with respect to time differences, $A(\vec{r}_1,\vec{r}_{1'};\omega)$, introduced by KB, reflects only the properties of the Hamiltonian $\hat{H}$. The average occupation number in the grand canonical ensemble of a mode with energy ω, $f(\omega,\beta)=[\exp(\beta(\omega-\mu))\mp 1]^{-1}$, takes account of the basic permutation symmetry of the system. We can thus express $G_>^{(q)}$ and $G_<^{(q)}$ in terms of these in the following ways:

$$iG_>^{(q)}(\vec{r}_1,\vec{r}_{1'};\omega;\beta,\mu)=\int_C du\, \tilde{K}_q^{(2)}(u) Z_1(-\beta u(1-q),\mu) iG_>^{(1)}(\vec{r}_1,\vec{r}_{1'};\omega;-\beta u(1-q),\mu)$$
$$=\int_C du\, \tilde{K}_q^{(2)}(u)[1\pm f(\omega,-\beta u(1-q),\mu)]A(\vec{r}_1,\vec{r}_{1'};\omega)Z_1(-\beta u(1-q),\mu), \tag{11}$$

$$iG_<^{(q)}(\vec{r}_1,\vec{r}_{1'};\omega;\beta,\mu)=\int_C du\, \tilde{K}_q^{(2)}(u) Z_1(-\beta u(1-q),\mu) iG_<^{(1)}(\vec{r}_1,\vec{r}_{1'};\omega;-\beta u(1-q),\mu)$$
$$=\pm\int_C du\, \tilde{K}_q^{(2)}(u) f(\omega,-\beta u(1-q))A(\vec{r}_1,\vec{r}_{1'};\omega)Z_1(-\beta u(1-q),\mu). \tag{12}$$

Thus the spectral weight function is found to be

$$A(\vec{r}_1,\vec{r}_{1'};\omega)=i(G_>^{(q)}(\vec{r}_1,\vec{r}_{1'};\omega;\beta,\mu)-G_<^{(q)}(\vec{r}_1,\vec{r}_{1'};\omega;\beta,\mu))=\int_C du\, \tilde{K}_q^{(2)}(u)A(\vec{r}_1,\vec{r}_{1'};\omega)Z_1(-\beta u(1-q),\mu). \tag{13}$$

From this we deduce an important sum rule

$$i\int_{-\infty}^{\infty}\frac{d\omega}{2\pi}(G_{>}^{(q)}(\vec{r}_1,\vec{r}_{1'};\omega;\beta,\mu)-G_{<}^{(q)}(\vec{r}_1,\vec{r}_{1'};\omega;\beta,\mu))=\int_C du\,\tilde{K}_q^{(2)}(u)\,\delta(\vec{r}_1-\vec{r}_{1'})Z_1(-\beta u(1-q),\mu)=\delta(\vec{r}_1-\vec{r}_{1'}). \tag{14}$$

This is just an expression of the equal time CCR of the particle fields. For a uniform system, we can take Fourier transforms with respect to $\vec{r}_1-\vec{r}_{1'}$ in Eq. (12), and express the one-particle momentum distribution function $\langle\hat{N}(\vec{p})\rangle_q$ in terms of the spectral weight function of the N-particle system.

$$\langle\hat{N}(\vec{p})\rangle_q=\pm\int_C du\,K_q^{(2)}(u)\int_{-\infty}^{\infty}\frac{d\omega}{2\pi}\,\frac{A(\vec{p};\omega)Z_1(-\beta(1-q)u,\mu)}{(e^{-\beta(1-q)u(\omega-\mu)}\mp 1)} \tag{15}$$

Similarly the one-particle frequency distribution function $\langle\hat{N}(\omega)\rangle_q$ is given by

$$\langle\hat{N}(\omega)\rangle_q=\pm V\int_C du\,K_q^{(2)}(u)\frac{Z_1(-\beta(1-q)u,\mu)}{(e^{-\beta(1-q)u(\omega-\mu)}\mp 1)}\int\frac{d^Dp}{(2\pi)^D}A(\vec{p};\omega). \tag{16}$$

Here V is the volume of the D-dimensional space in which the particles reside. The chemical potential is determined by the expression for the q mean value of the total number operator $\hat{N}$,

$$\frac{\langle\hat{N}\rangle_q}{V}=\pm\int_C du\,K_q^{(2)}(u)\int_{-\infty}^{\infty}\frac{d\omega}{2\pi}\int\frac{d^Dp}{(2\pi)^D}\,\frac{Z_1(-\beta(1-q)u,\mu)}{(e^{-\beta(1-q)u(\omega-\mu)}\mp 1)}A(\vec{p};\omega). \tag{17}$$

B. $G_n^{(q)}(123\ldots n;1'2'3'\ldots n';\beta,\mu)$

So far we have discussed the one-particle properties. The above development is similarly extended to generalize the many-particle q Green functions. Using the same notations as in KB, we have, in general,

$$G_n^{(q)}(12\ldots n,1'2'\ldots n';\beta,\mu)=\frac{1}{i^n\langle 1\rangle_q}\langle T(\Psi(1)\Psi(2)\ldots\Psi(n)\Psi^{\dagger}(1')\Psi^{\dagger}(2')\ldots\Psi^{\dagger}(n'))\rangle_q$$
$$=\int_C du\,\tilde{K}_q^{(2)}(u)Z_1(-\beta u(1-q),\mu)G_n^{(1)}(12\ldots n,1'2'\ldots n';-\beta(1-q)u,\mu). \tag{18}$$

To illustrate how these higher order Green functions arise, consider, for example, a many-particle system with a Hamiltonian containing the one-body potential $V_1(\vec{r}_1)$ and the instantaneous two-body interaction potential $V_2(\vec{r}_1,\vec{r}_2)$, which is symmetric under interchange of 1 and 2:

$$\hat{H}=\int d\vec{r}\frac{\vec{\nabla}\Psi^{\dagger}(\vec{r},t)\cdot\vec{\nabla}\Psi(\vec{r},t)}{2m}+\int d\vec{r}\,V_1(\vec{r})\Psi^{\dagger}(\vec{r},t)\Psi(\vec{r},t)+\frac{1}{2}\int\int d\vec{r}\,d\vec{r}'\,\Psi^{\dagger}(\vec{r},t)\Psi^{\dagger}(\vec{r}',t)V_2(\vec{r},\vec{r}')\Psi(\vec{r}',t)\Psi(\vec{r},t). \tag{19}$$

The equation of motion obeyed by any operator $\hat{X}(t)$ in the Heisenberg representation is

$$i\frac{\partial}{\partial t}\hat{X}(t)=[\hat{X}(t),\hat{H}(t)], \tag{20}$$

and so the one-particle Green function obeys the equation

$$\left(i\frac{\partial}{\partial t_1}+\frac{\vec{\nabla}_1^2}{2m}-V_1(\vec{r}_1)\right)G^{(q)}(1,1')=\delta(1-1')\pm i\int d\vec{r}_2\,V_2(\vec{r}_1,\vec{r}_2)G_2^{(q)}(12,1'2^+)|_{t_2=t_1}. \tag{21}$$

In a similar fashion we can also write an equation of motion for $G_2^{(q)}$ involving $G_3^{(q)}$, and so on, obtaining a heierarchy of equations for all the Green functions. It should be noted that these equations are of the same form as in KB for $q=1$, and this feature is a consequence of the definition given in Eq. (1) here, in contrast to the one given in Ref. [12]. It is this feature that allows us to employ a diagrammatic analysis of these equations in the same manner as in the conventional theory, thus obtaining the theory in the same form for nonextensive systems as for extensive ones. In addition to the detailed dynamical information, $G^{(q)}$ contains all possible information about the statistical mechanics of the system. We have already given the q expectation value of the density of particle in terms of $G_{<}^{(q)}$ from Eq. (12). Following KB we can express the q expectation value of Hamiltonian (19):

$$\langle \hat{H} \rangle_q = \frac{\pm i}{4} \langle 1 \rangle_q \int d\vec{r} \left[i \left(\frac{\partial}{\partial t} - \frac{\partial}{\partial t'} \right) + \frac{\nabla \cdot \nabla'}{m} - V_1(r) - V_1(r') \right] G_{<}^{(q)}(\vec{r},t;\vec{r}',t') \Big|_{\vec{r}'=\vec{r},t'=t} . \tag{22}$$

For the free-particle case $V_1(r)=0$, as in Eqs. (15) and (16), we have

$$\frac{\langle \hat{H} \rangle_q}{V} = \int_C du \, K_q^{(2)}(u) \int_{-\infty}^{\infty} \frac{d\omega}{2\pi} \int \frac{d^D p}{(2\pi)^D} \left(\frac{\omega + p^2/2m}{2} \right) \frac{Z_1(-\beta(1-q)u,\mu)}{(e^{-\beta(1-q)u(\omega-\mu)} \mp 1)} A(\vec{p};\omega). \tag{23}$$

Following Curado and Tsallis [2], we have the grand canonical potential given by

$$\Xi_q = -\frac{1}{\beta} \frac{Z_q^{1-q}-1}{1-q} = \langle \hat{H} \rangle_q - \frac{1}{\beta} S_q - \mu \langle \hat{N} \rangle_q , \tag{24}$$

where the q thermodynamic quantities, q pressure P_q, q average number $\langle \hat{N} \rangle_q$, and q entropy S_q are,

$$P_q = -\left(\frac{\partial \Xi_q}{\partial V} \right)_{T,\mu}, \quad \langle \hat{N} \rangle_q = -\left(\frac{\partial \Xi_q}{\partial \mu} \right)_{T,V}, \quad S_q = -\left(\frac{\partial \Xi_q}{\partial T} \right)_{V,\mu}. \tag{25}$$

By writing a coupling constant λ in front of the interaction energy, $\hat{H} = \hat{H}_0 + \lambda \hat{V}$ where

$$\hat{H}_0 = \int d\vec{r} \frac{\vec{\nabla} \Psi^\dagger(\vec{r},t) \cdot \vec{\nabla} \Psi(\vec{r},t)}{2m} + \int d\vec{r} \, V_1(\vec{r}) \Psi^\dagger(\vec{r},t) \Psi(\vec{r},t) \tag{26}$$

and

$$\hat{V} = \tfrac{1}{2} \int \int d\vec{r} \, d\vec{r}' \;\; \Psi^\dagger(\vec{r},t) \Psi^\dagger(\vec{r}',t) V_2(\vec{r},\vec{r}') \Psi(\vec{r}',t) \Psi(\vec{r},t). \tag{27}$$

we obtain, for fixed β, μ, and V,

$$\frac{\partial}{\partial \lambda} \frac{Z_q^{1-q}-1}{1-q} = -\beta \langle \hat{V} \rangle_q , \tag{28}$$

from which we deduce

$$\left(\frac{Z_q^{1-q}-1}{1-q} \right)_{\lambda=1} - \left(\frac{Z_q^{1-q}-1}{1-q} \right)_{\lambda=0} = -\beta \int_0^1 \frac{d\lambda}{\lambda} \langle \lambda \hat{V} \rangle_{q,\lambda} . \tag{29}$$

Now $\langle \lambda \hat{V} \rangle_{q,\lambda}$ is the q expectation value of the interaction energy for coupling strength λ. It may be expressed in terms of the spectral weight function,

$$\langle \lambda \hat{V} \rangle_{q,\lambda} = V \int_C du \, K_q^{(2)}(u) \int_{-\infty}^{\infty} \frac{d\omega}{2\pi} \int \frac{d^D p}{(2\pi)^D} \left(\frac{\omega - p^2/2m}{2} \right) \frac{Z_1(-\beta(1-q)u,\mu)}{(e^{-\beta(1-q)u(\omega-\mu)} \mp 1)} A_\lambda(\vec{p};\omega), \tag{30}$$

so that

$$\Xi_q = -\frac{1}{\beta} \left(\frac{Z_q^{1-q}-1}{1-q} \right)_{\lambda=1} = -\frac{1}{\beta} \left(\frac{Z_q^{1-q}-1}{1-q} \right)_{\lambda=0} + V \int_0^1 \frac{d\lambda}{\lambda} \int_C du \, K_q^{(2)}(u)$$
$$\times \int_{-\infty}^{\infty} \frac{d\omega}{2\pi} \int \frac{d^D p}{(2\pi)^D} \left(\frac{\omega - p^2/2m}{2} \right) \frac{Z_1(-\beta(1-q)u,\mu)}{(e^{-\beta(1-q)u(\omega-\mu)} \mp 1)} A_\lambda(\vec{p};\omega). \tag{31}$$

We have the general result for the q pressure,

$$P_q = \frac{1}{\beta} \left(\frac{1}{Z_q^q} \frac{\partial Z_q}{\partial V} \right)_{\lambda=0} - \int_0^1 \frac{d\lambda}{\lambda} \int_C du \, K_q^{(2)}(u) \int_{-\infty}^{\infty} \frac{d\omega}{2\pi} \int \frac{d^D p}{(2\pi)^D} \left(\frac{\omega - p^2/2m}{2} \right) \frac{Z_1(-\beta(1-q)u,\mu)}{(e^{-\beta(1-q)u(\omega-\mu)} \mp 1)} A_\lambda(\vec{p};\omega)$$
$$- V \frac{\partial}{\partial V} \left\{ \int_0^1 \frac{d\lambda}{\lambda} \int_C du \, K_q^{(2)}(u) \int_{-\infty}^{\infty} \frac{d\omega}{2\pi} \int \frac{d^D p}{(2\pi)^D} \left(\frac{\omega - p^2/2m}{2} \right) \frac{Z_1(-\beta(1-q)u,\mu)}{(e^{-\beta(1-q)u(\omega-\mu)} \mp 1)} A_\lambda(\vec{p};\omega) \right\}, \tag{32}$$

from which we obtain, using Eq. (25), that the constant term, $(1/\beta Z_q^q)\partial Z_q/\partial V|_{\lambda=0}$ is just the q pressure P_q for free particles. We may also note that the q isothermal compressibility $\kappa_{T,q}$, which is related to the velocity of sound in the system, is given by

$$\kappa_{T,q}=-\frac{1}{V}\left(\frac{\partial V}{\partial P_q}\right)_T=\frac{1}{V\beta}\left\{\left(\frac{\partial \mu}{\partial P_q}\right)_T\right\}^2\left(\frac{\partial^2}{\partial\mu^2}\frac{Z_q^{1-q}-1}{1-q}\right)_{T,V}$$
$$=q\frac{\beta}{V}\left\{\left(\frac{\partial \mu}{\partial P_q}\right)_T\right\}^2\left(\left\langle \hat{N}\frac{1}{1-\beta(1-q)(\hat{H}-\mu\hat{N})}\hat{N}\right\rangle_q - Z_q^{q-1}\langle\hat{N}\rangle_q^2\right)_{T,V}. \tag{33}$$

The two-particle Green function is often useful in examining certain correlation functions which are just related to one-particle-like functions because the physical operators are appropriate contractions of the operators appearing in its definition. As an example, consider the density fluctuations; here the density operator $\hat{n}(\vec{r},t)$ is given by $\hat{n}(\vec{r},t)=\Psi^{\dagger}(\vec{r},t)\Psi(\vec{r},t)$. Thus the density-density correlation function is given by $\langle T(\hat{n}(\vec{r}_1,t_1)\hat{n}(\vec{r}_2,t_2))\rangle_q=\langle T(\Psi^{\dagger}(1)\Psi(1)\Psi^{\dagger}(2)\Psi(2))\rangle_q$. We now give the results of two of the commonly used approximations in many-particle theory in the q formalism. As in KB, we may develop a diagrammatic analysis of the Green function equation (21). Other schemes follow similarly.

C. Hartree approximation

The Hartree approximation is one of the simplest approximations made in many branches of physics. Thus it would be interesting to find the corresponding result in the Tsallis formalism. In this context we determine $G^{(q)}(1,1')$, when $V(\vec{r}_1)=0$ and $v\neq 0$, with a corresponding approximate $G_2^{(q)}$. This approximation is physically motived as in standard case. Thus, as a first approximation, we take

$$G_2^{(q)}(12;1'2')=G^{(q)}(1,1')G^{(q)}(2,2'), \tag{34}$$

and substitute this into Eq. (21) to obtain the Hartree result. For a translationally invariant system, Eq. (21) becomes simple. Since $\langle\hat{N}(\vec{r}_2)\rangle_q$ is then independent of the position $\vec{r}_2$, the average potential is constant. Then, $\int d\vec{r}_2\, V_2(\vec{r}_1-\vec{r}_2)(\langle\hat{N}\rangle_q/V)=(\langle\hat{N}\rangle_q/V)v$ where $v=\int d\vec{r}\, V_2(\vec{r})$. Thus we obtain a spectral function $A(\vec{p},\omega)=2\pi\delta(\omega-p^2/2m-(\langle N\rangle_q/V)v)$. To find the solution to the Hartree approximation, we solve for the density of the particle [Eq. (17)] using the spectral function obtained above:

$$\frac{\langle\hat{N}\rangle_q}{V}=\int_C du\, K_q^{(2)}(u)\times\int\frac{d^Dp}{(2\pi)^D}\frac{Z_1(-\beta(1-q)u,\mu)}{(e^{-\beta(1-q)u((\langle N\rangle_q/V)v+p^2/2m-\mu)}\mp 1)}. \tag{35}$$

The energy per unit volume form Eq. (23) is then found to be

$$\frac{\langle\hat{H}\rangle_q}{V}=\int_C du\, K_q^{(2)}(u)\int\frac{d^Dp}{(2\pi)^D}\left(\frac{\langle N\rangle_q}{2V}v+\frac{p^2}{2m}\right)\times\frac{Z_1(-\beta(1-q)u,\mu)}{(e^{-\beta(1-q)u((\langle N\rangle_q/V)v+p^2/2m-\mu)}\mp 1)}, \tag{36}$$

$$\frac{\langle\hat{H}\rangle_q}{V}=\frac{1}{2}\left(\frac{\langle N\rangle_q}{V}\right)^2 v+\int_C du\, K_q^{(2)}(u)\int\frac{d^Dp}{(2\pi)^D}\left(\frac{p^2}{2m}\right)\times\frac{Z_1(-\beta(1-q)u,\mu)}{(e^{-\beta(1-q)u((\langle N\rangle_q/V)v+p^2/2m-\mu)}\mp 1)}. \tag{37}$$

D. Hartree-Fock approximation

In the Hartree approximation discussed above, the explicit appearance of the exclusion principle does not appear. This comes about in the Hartree-Fock approximation where the approximation $G_2^{(q)}$ is now

$$G_2^{(q)}(12;1'2')=G^{(q)}(1,1')G^{(q)}(2,2')\pm G^{(q)}(1,2')G^{(q)}(2,1'). \tag{38}$$

Thus we substitute Eq. (38) into Eq. (21), and after some calculation obtain

$$\left(i\frac{\partial}{\partial t_1}+\frac{\vec{\nabla}_1^2}{2m}\right)G^{(q)}(1,1')-i\int d\vec{r}_2\langle r_1|U|r_2\rangle G^{(q)}(2,1')|_{t_2=t_1}=\delta(1-1'), \tag{39}$$

where

$$\langle r_1|U|r_2\rangle=\delta(\vec{r}_2-\vec{r}_1)\int d\vec{r}_3\, V_2(\vec{r}_1-\vec{r}_3)\frac{\langle\hat{N}(\vec{r}_3)\rangle_q}{V}+iV_2(\vec{r}_1-\vec{r}_2)G_<^{(q)}(1,2)\Big|_{t_2=t_1}. \tag{40}$$

Considering a translationally invariant system, we can express Eq. (39) in terms of the Fourier-transform in space to obtain

$$\left[i\frac{\partial}{\partial t_1}-E(p)\right]G^{(q)}(p,t_1-t_{1'})=\delta(t_1-t_{1'}) \tag{41}$$

and

$$E(p)=\frac{p^2}{2m}+\frac{\langle\hat{N}\rangle_q}{V}v\pm\int\frac{d^3\vec{p}}{(2\pi)^3}v(\vec{p}-\vec{p}\,')\frac{\langle N(\vec{p})\rangle_q}{V}, \tag{42}$$

where $v(\vec{p})=\int d\vec{r}\, e^{-i\vec{p}\cdot\vec{r}}V_2(\vec{r})$ is the Fourier transform of the potential $V_2(\vec{r})$, and the spectral function is of the same form as before; $A(\vec{p},\omega)=2\pi\delta(\omega-E(\vec{p}))$. Substituting the spectral function into Eq. (15), we have

$$\frac{\langle\hat{N}(\vec{p})\rangle_q}{V}=\int_C du\, K_q^{(2)}(u)\frac{Z_1(-\beta(1-q)u,\mu)}{e^{-\beta(1-q)u(E(p)-\mu)}\mp 1}. \tag{43}$$

The generalized Hartree-Fock single-particle energy $E(p)$ must then be obtained as the self-consistent solution of Eqs. (42) and (43).

E. Response functions

We now turn our attention to rewriting the dynamic response and the scattering cross section in the q formalism in terms of the integrals over the usual ones, as was done above. From Ref. [6], the dynamic linear response of a quantity $\hat{B}$ to an external probe that generates $\hat{A}$ in the q formalism is

$$\chi_{BA}^{(q)}(\omega,\beta,\mu)=\lim_{\epsilon\to 0}\int_0^\infty dt\, e^{-i\omega t-\epsilon t}\frac{1}{i}\phi_{BA}^{(q)}(t,\beta,\mu), \quad (44)$$

where

$$\phi_{BA}^{(q)}(t,\beta,\mu)=\mathrm{Tr}\{\hat{P}(\hat{H},\hat{N};q,\beta,\mu)[\hat{A}(0),\hat{B}(t)]\}. \quad (45)$$

This, in terms of the integral representation, is

$$\chi_{BA}^{(q)}(\omega,\beta,\mu)=\int_C du\, K_2^q(u)Z_1(-\beta u(1-q),\mu)\times\chi_{BA}^{(1)}(\omega,-\beta(1-q)u,\mu) \quad (46)$$

where $\chi_{BA}^{(1)}(\omega,-\beta(1-q)u,\mu)$ is the usual Kubo dynamical response function evaluated now at a temperature $-\beta u(1-q)$. In Ref. [6], the general fluctuation-dissipation theorem was derived in the q formalism. Here we obtain an equivalent but different form of the same result. Rewriting the q avereges of the anticommutator and commutator expressions, we have

$$\Psi_{BA}^{(q)}(t,\beta,\mu)=\tfrac{1}{2}\mathrm{Tr}\,\hat{P}(\hat{H},\hat{N};q,\beta,\mu)[\hat{A}(0)\hat{B}(t)+\hat{B}(t)\hat{A}(0)]=\tfrac{1}{2}\int_C du\, K_q^{(2)}(u)Z_1(-\beta u(1-q),\mu)\Psi_{BA}^{(1)}(t,-\beta u(1-q),\mu), \quad (47)$$

$$\Phi_{BA}^{(q)}(t,\beta)=\lim_{\epsilon\to 0}\int_t^\infty dt'\, e^{-\epsilon t'}\mathrm{Tr}\{\hat{P}(\hat{H},\hat{N};q,\beta,\mu)[\hat{A}(0),\hat{B}(t)]\}=\int_C du\, K_{(q)}^{(2)}(u)Z_1(-\beta u(1-q),\mu)\Phi_{BA}^{(q=1)}(t',-\beta u(1-q),\mu). \quad (48)$$

The fluctuation-dissipation theorem due to Kubo [23] for the extensive case $(q=1)$ is

$$\Psi_{BA}^{(1)}(\omega,\beta,\mu)=E_\beta(\omega)\Phi_{BA}^{(1)}(\omega,\beta,\mu), \quad (49)$$

with

$$E_\beta(\omega)=\frac{\omega}{2}\coth\left(\frac{\beta\omega}{2}\right). \quad (50)$$

Here we obtain

$$\Psi_{BA}^{(q)}(\omega,\beta,\mu)=\frac{\omega}{4}\int_C du\, K_q^{(2)}(u)Z_1(-\beta u(1-q),\mu)\times\coth\left(\frac{-\beta u(1-q)\omega}{2}\right)\Phi_{BA}^{(1)}(\omega,-\beta u(1-q),\mu)). \quad (51)$$

We now relate the scattering function defined for example, by Lovesey [17] in the q formalism as

$$S^{(q)}(\vec{k},\omega,\beta)=\frac{1}{2\pi}\int_{-\infty}^{\infty}dt\,\exp(-i\omega t)\langle\hat{A}^\dagger(0)\hat{A}(t)\rangle_q^{(c)}, \quad (52)$$

where $\hat{A}$ is the operator which affects the change in the states of the system in a scattering process. Here the superscript (c) denotes a canonical ensemble instead of the grand canonical ensemble used earlier. This is equivalent formally to setting $\mu=0$ in the earlier development. Then, using our transformation, we express this scattering function in terms of the usual $q=1$ scattering function

$$S^{(q)}(\vec{k},\omega,\beta)=\int_C du\, K_q^{(2)}(u)Z_1(-\beta u(1-q))\times S^{(1)}(\vec{k},\omega,-\beta u(1-q)). \quad (53)$$

From Ref. [6], by taking $\hat{B}=\hat{A}^\dagger$, we have that the imaginary part of the q susceptibility, $\chi_{\hat{A}^\dagger\hat{A}}^{(q)}(\omega,\beta)$, can be expressed in terms of the $q=1$ scattering function

$$\mathrm{Im}\,\chi_{\hat{A}^\dagger\hat{A}}^{(q)}(\vec{k},\omega,\beta)=\pi\int_C du\, K_q^{(2)}(u)Z_1(-\beta u(1-q))\times[1-\exp(-\beta u(1-q)\omega)]\times S^{(1)}(\vec{k},\omega,-\beta u(1-q)). \quad (54)$$

We have thus expressed the q scattering function as well as the imaginary part of the associated q susceptibility in terms of the parametric integrals over a kernel multiplied by the usual scattering function which now depends on this parameter, as displayed above. We will now discuss, in Sec. III, three suggestions for a possible experimental investigation of the validity of the q framework for nonextensive systems based on the results obtained here.

III. APPLICATIONS

(*a*) *Electron system*: The momentum distribution for electrons is given by Eq. (15) with a lower sign. This function is directly observable in positron annihilation experiments [15]. We use the free electron spectral weight function $A(\vec{p};\omega) = 2\pi\delta(\omega-\vec{p}^2/2m)$ in this calculation for simplicity of presentation. We first observe that the zero temperature result for the q mean value of the total number has the same form as for the usual $q=1$ case. Details of the actual calculation will be given here. Thus

$$\langle\hat{N}\rangle_q = V\int\int\int \frac{dk_x}{2\pi}\frac{dk_y}{2\pi}\frac{dk_z}{2\pi}\langle\hat{N}(\vec{k})\rangle_q. \tag{55}$$

From this, we have obtained the usual Fermi sphere result for $q<1$, so that, in terms of the Fermi sphere radius $q=1$, the positron annihilation is found to be of the same form but with a q-dependent correction. For small $\langle\hat{N}\rangle_1$ as for the small systems mentioned above, we find $\langle\hat{N}\rangle_q \simeq \langle\hat{N}\rangle_1[1+[(1-q)^2/(2-q)](\pi^2/5)\langle\hat{N}\rangle_1^2]$. In Fig. 2 we display the q dependence of the ratio $\langle\hat{N}\rangle_q/\langle\hat{N}\rangle_1$ for two representative values of $\langle\hat{N}\rangle_1$ to represent the expected change in the number distribution that may be found in either positron annihilation or x-ray Compton scattering experiments [15] for small systems with $\langle\hat{N}\rangle_1=40$ and 60. Other results can be obtained in this context such as $P_q \approx \frac{2}{5}(\langle\hat{N}\rangle_q/V)\epsilon_F$ and $U_q \approx \frac{3}{5}\langle\hat{N}\rangle_q\epsilon_F$ (ϵ_F is the Fermi energy).

(b) Boson system: The recent work on Bose condensation of atoms [16] involves condensation of a small number of atoms of the order of 100–170 confined to a small region of space by magnetic trapping. Here we revisit this problem by calculating the transition temperature and the momentum distribution near the transition temperature to see if one could discern the q dependence. For this purpose, we use Eq. (17) with the upper sign, pertinent to bosons. We also take free-particle spectral weight function, $A(\vec{p};\omega) = 2\pi\delta(\omega-\vec{p}^2/2m)$, and find, for q less than 1,

$$\frac{\langle\hat{N}\rangle_q}{V} = \frac{\Gamma\left(\frac{1}{1-q}\right)}{2\pi Z_q^q}\int_{-\infty}^{\infty}du\frac{e^{1+iu}}{(1+iu)^{1/(1-q)}} \times\int\frac{d^3p}{(2\pi)^3}\frac{Z_1(\beta(1-q)(1+iu),\mu)}{e^{\beta(1-q)(1+iu)(p^2/2m-\mu)}-1}, \tag{56}$$

which, near the Bose condensation, is approximately found to be

$$\frac{\langle\hat{N}\rangle_q}{\langle\hat{N}\rangle_1} \simeq \frac{\Gamma\left(\frac{2-q}{1-q}\right)}{2\pi(1-q)^{1/2}Z_q^q}\left(\frac{\beta_c^{(1)}}{\beta_c^{(q)}}\right)^{3/2} \times\int_{-\infty}^{\infty}du\frac{e^{1+iu}}{(1+iu)^{1/(1-q)+3/2}} \times Z_1(\beta_c^{(q)}(1-q)(1+iu)). \tag{57}$$

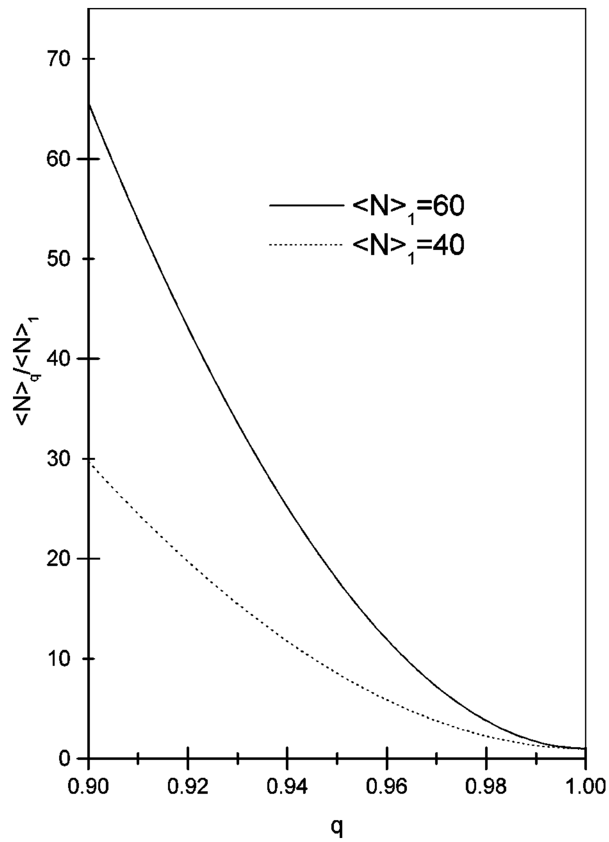

FIG. 2. Plot of $\langle\hat{N}\rangle_q/\langle\hat{N}\rangle_1$ as a function of q for $\langle\hat{N}\rangle_1=40$ and 60 for q near 1.

After some calculations, we obtain

$$\frac{\langle\hat{N}\rangle_q}{\langle\hat{N}\rangle_1} \simeq \left(\frac{T_c^{(q)}}{T_c^{(1)}}\right)^{3/2}\frac{\Gamma\left(\frac{2-q}{1-q}\right)}{(1-q)^{(1/2)}\Gamma\left(\frac{2-q}{1-q}+\frac{1}{2}\right)} \times\left\{1+\frac{\langle\hat{N}\rangle_1}{(1-q)^{(3/2)}}\frac{\zeta(5/2)}{\zeta(3/2)}\left(\frac{T_c^{(q)}}{T_c^{(1)}}\right)^{3/2} \times\left[\frac{\Gamma\left(\frac{2-q}{1-q}+\frac{1}{2}\right)}{\Gamma\left(\frac{2-q}{1-q}+2\right)} - q\frac{\Gamma\left(\frac{2-q}{1-q}\right)}{\Gamma\left(\frac{2-q}{1-q}+\frac{3}{2}\right)}\right]\right\}. \tag{58}$$

In Fig. 3 we display a plot of $\langle\hat{N}\rangle_q/\langle\hat{N}\rangle_1$ versus $\beta_c^{(1)}/\beta_c^{(q)}$ for one representative value of $\langle\hat{N}\rangle_1$ for $q=0.6$ and $q=0.9$. Curilef [24] calculated $T_c^{(q)}/T_c^{(1)}$ for $q\approx1$, and found it to increase for $\langle\hat{N}\rangle_q/\langle\hat{N}\rangle_1$ equal to unity; from our Fig. 3, we see a similar increasing trend as we go from $q=0.6$ to 0.9.

(c) Scattering experiments: The fabrication of quasiperiodic superlattices was successfully realized as early as 1985 [25], and experimentally investigated by x-ray diffraction, neutron diffraction, etc. See Ref. [26]. These systems afford

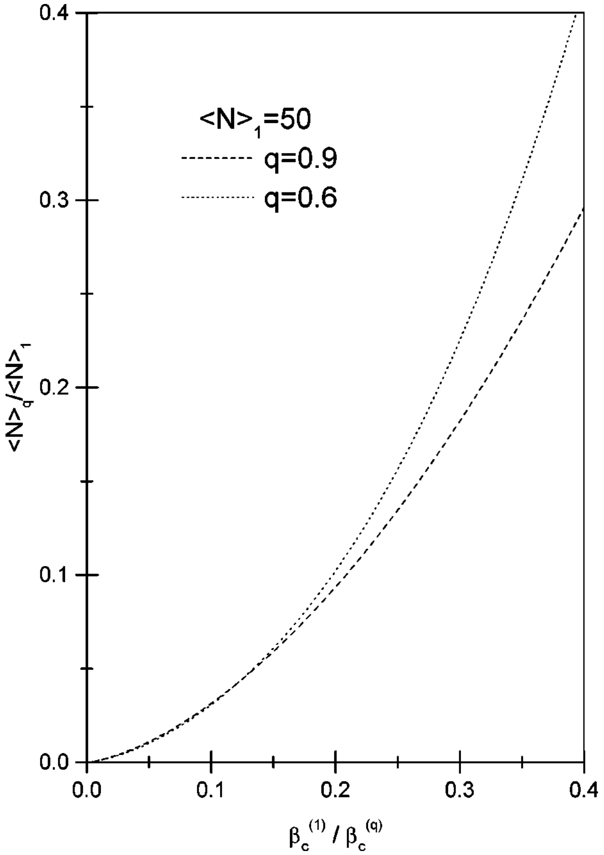

FIG. 3. Plot of $\langle\hat{N}\rangle_q/\langle\hat{N}\rangle_1$ as a function of $\beta_c^{(1)}/\beta_c^{(q)}$ for $\langle\hat{N}\rangle_1=50$, and for $q=0.6$ and 0.9.

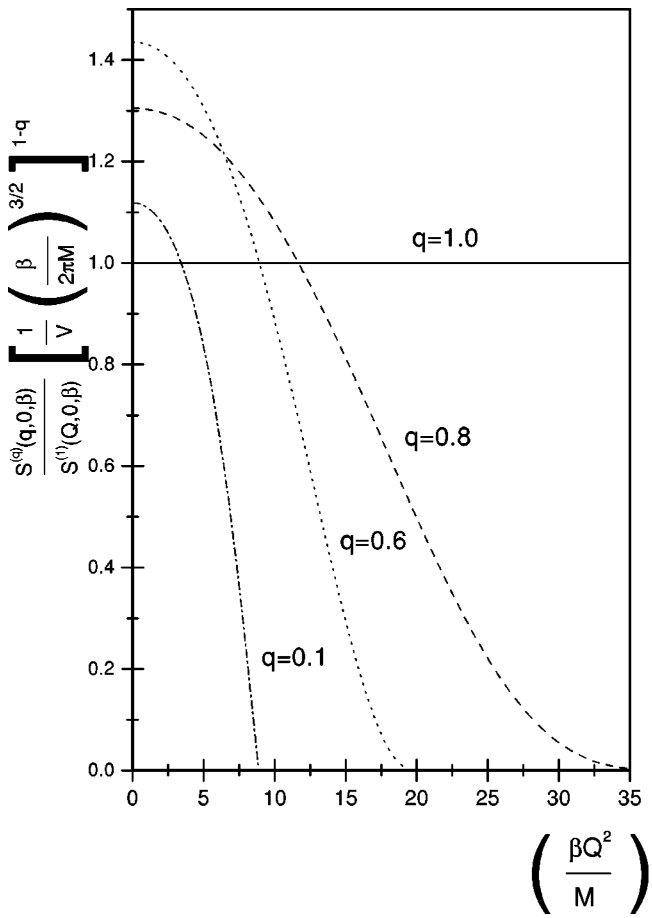

FIG. 4. Plot of the static $(\omega=0)$,$[S^{(q)}(Q,0,\beta)]/[S^{(1)}(Q,0,\beta)][1/V(\beta/2\pi M)^{3/2}]^{1-q}$, for $q=0.1$, 0.6, 0.8, and 1 as a function of $\beta Q^2/M$.

another class of possible experimental avenue to test the q framework when we consider the *finite size effects* they might display. By using some known forms for the structure factor $S^{(1)}$ in Eq. (53), we can calculate $S^{(q)}$ for $q<1$, etc., as was done in the other two calculations. We propose to use our framework for such scattering cross section calculations to investigate these in some model structures. The scattering of a neutron or x ray from a vibrating particle of mass M will be calculated as an example of our framework. For this, the operator $\hat{A}$ is the Fourier transform of the particle density,

$$\hat{A}=\int d\vec{r}\,\exp(i\vec{Q}\cdot\vec{r})\,\delta(\vec{r}-\vec{R}(t))=\exp(i\vec{Q}\cdot\vec{R}(t)), \quad (59)$$

where $\vec{R}$ denotes the atom position, and $\vec{Q}$ is the change of wave vector of the neutron or the x ray. The expression for $\hat{A}(t)$ can be obtained from its equation of motion, with $\hat{H}=\vec{p}^2/(2M)$, where $\vec{p}$ is the conjugate momentum to $\vec{R}$. We obtain

$$\hat{A}(t)=\exp(i\vec{Q}\cdot\vec{R})\exp\left(\frac{it}{2M}(2\vec{Q}\cdot\vec{p})+Q^2\right), \quad (60)$$

and after some algebra, we have

$$S^{(q)}(Q,\omega,\beta)=\left(\frac{2\pi M^2 V}{\beta Q Z_q^q}\right)\times\left(1-(1-q)\frac{M\beta}{2Q^2}\left(\omega-\frac{Q^2}{2M}\right)^2\right)^{1/(1-q)}, \quad (61)$$

where Z_q is given by

$$Z_q=V\left(\frac{2M\pi}{(1-q)\beta}\right)^{3/2}\frac{\Gamma\left(\frac{2-q}{1-q}\right)}{\Gamma\left(\frac{2-q}{1-q}+\frac{3}{2}\right)} \quad (62)$$

for the case $q<1$. In Fig. 4, we display the static $(\omega=0)$ expression

$$[S^{(q)}(Q,0,\beta)]/[S^{(q=1)}(Q,0,\beta)][(1/V)(\beta/2\pi M)^{3/2}]^{1-q}$$

for different q values as a function of $\beta Q^2/M$.

IV. SUMMARY AND CONCLUSIONS

In this paper we have developed in detail a Green function theory for nonextensive systems based on the q ensemble of Tsallis. By means of a contour representation [Eqs. (5) and

(6)], we have made this theory resemble the usual one for extensive systems given by KB, for example, even though, in actual practice, the results are very different, as exemplified by the representative results given in Sec. II for a variety of situations. Before this development, thermodynamic quantities for model systems were computed in the Tsallis ensemble as, for example, in Refs. [19,24]. With the present work, we believe that the theory of many-particle systems for the Tsallis ensemble has been considerably extended and placed on a par with conventional theory based on the Gibbsian ensemble, in that we have been able to compute response functions in addition to thermodynamic quantities. Here we have examined three physical entities which are amenable to experimental investigation, and which we hope give the possibility of a direct verification of the use of Tsallis ensembles. As with the examples cited in Sec. I, the q values will have to be chosen to fit the experimental observation, and thus will indicate the long-range nature of the underlying interactions and other nonextensive features present in the system under investigation. All three examples chosen to display the q dependences in the figures were for $q<1$, because they were all concerned with free-particle systems. In fact, the case of q different from unity is expected to apply for long-range interacting Hamiltonian systems [14]. From a formal point of view, noninteracting and short-range interacting systems are mathematically well posed problems only for $q<1$. In conclusion, here we have developed a formalism associated with Tsallis statistics for describing nonextensive many-particle systems by a suitable generalization of the corresponding Green function techniques, so commonly employed in such studies for extensive systems. As with the usual Green function theory, which has been traditionally successful in explaining experimental observations, the present work enables us to analyze future possible experimental work on nonextensive systems.

ACKNOWLEDGMENTS

Professor C. Tsallis made valuable remarks to improve the presentation of this work, for which many thanks are due. A.K.R. acknowledges the financial support for his travel, and congenial local hospitality from UFRN and CBPF, Brazil, which made this collaborative work possible. He also acknowledges the partial support of his research by the U.S. Office of Naval Research. Partial support from CNPq and PRONEX (Brazilian agencies) is acknowledged as well.

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