Quantum Statistical Mechanics for Nonextensive Systems: Prediction for Possible Experimental Tests

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The traditional basis of description of the many-particle systems in terms of the Green functions is here generalized when the system is nonextensive by incorporating the Tsallis form of the density matrix, indexed by a nonextensive parameter, q. 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. [S0031-9007(98)05936-5]

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Ever since Tsallis [1,2] proposed his maximum q entropy for examining nonextensive systems by employing q-mean values so as to obtain thermostatistics about a decade ago, 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: Lévy superdiffusion [3] and anomalous correlated diffusion [4], turbulence in two-dimensional pure electron plasma ($q = 1/2$) [5], dynamic linear response theory [6], perturbation and variation methods for calculation of thermodynamic quantities [7], thermalization of electron-phonon system ($q > 1$) [8], low-dimensional dissipative systems ($q < 1$) [9], and some astrophysical applications [10]. In this list given here, the q values were either fitted to experiment or obtained from computer simulation or from theoretical model calculation. The purpose of this paper is to generalize the thermodynamic Green function theory of the quantum statistical mechanics of many-particle systems [11] when they are nonextensive in this q formalism. This generalization then leads us to propose possible experimental tests of nonextensive features predicted in such a formalism by calculating measurable quantities such as momentum distribution function for electrons measurable in a positron annihilation and x-ray Compton scattering experiments [12], Bose condensation in confined small number of atoms [13], and cross sections for scattering by external probes, such as neutrons, photons, etc. [14], in terms of the q-mean values.

We adopt the second-quantized particle-creation and annihilation operators in the Heisenberg representation as in Kadanoff and Baym (KB) [11] to describe a many-particle system whose Hamiltonian operator is $\hat{H}$ and whose number operator is $\hat{N}$. In this way we describe the nonextensive systems at arbitrary temperatures, and for boson or fermion systems in equilibrium by maximizing the Tsallis entropy $S_q = (1 - \mathrm{Tr}\hat{\rho}^q)/(q - 1)$, $\mathrm{Tr}\hat{\rho} = 1$, $\hat{\rho}$ is the system density matrix, subject to the constraints of fixed q-mean values $\langle\hat{H}\rangle_q = \mathrm{Tr}\hat{H}\hat{\rho}^q$, $\langle\hat{N}\rangle_q = \mathrm{Tr}\hat{N}\hat{\rho}^q$. Thus, we define the one-particle q-Green function,

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

where

$$\begin{aligned} \hat{P}(\hat{H},\hat{N};q,\beta,\mu) &= [1 - \beta(1-q) \\ &\quad \times (\hat{H} - \mu\hat{N})]^{q/(1-q)}/(Z_q)^q, \end{aligned} \tag{2}$$

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

Equation (2) is the 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 inverse temperature and chemical potential in the usual description. 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 $\mathrm{T}[\Psi(1)\Psi^\dagger(1')] = \Psi(1)\Psi^\dagger(1')$ for $t_1 > t_1'$ and $\pm\Psi^\dagger(1')\Psi(1)$ for $t_1 < t_1'$. The creation $\Psi^\dagger(\vec{r}', t')$ and annihilation $\Psi(\vec{r}, t)$ operators obey the canonical commutation rules (CCR) at equal times: $[\Psi(\vec{r},t),\Psi(\vec{r}',t)]_\mp = [\Psi^\dagger(\vec{r}',t),\Psi^\dagger(\vec{r},t)]_\mp = 0$, and $[\Psi(\vec{r},t),\Psi^\dagger(\vec{r}',t)]_\mp = \delta(\vec{r} - \vec{r}')$, where $[\hat{A},\hat{B}]_\mp \equiv \hat{A}\hat{B} \mp \hat{B}\hat{A}$. 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 in 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 [15]) was valid for $q > 1$, which was extended for $q < 1$ by Prato [16]. We employ here a contour integral representation from which the above representations as well as others are obtained by suitable deformation of the contour [17]. 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 [18] $ib^{1-z}\int_C (du/2\pi)e^{-ub}(-u)^{-z} = 1/\Gamma(z)$, where the contour C starts from $+\infty$ on the real axis, encircles the origin once counterclockwise and returns to $+\infty$, and here $\mathrm{Re}\, z > 0$. 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,

$$Z_q(\beta,\mu) = \int_C du\, K_q^{(1)}(u) Z_1(-\beta u(1-q),\mu), \quad (3)$$

$$G^{(q)}(1,1';\beta,\mu) = \int_C du\, K_q^{(2)}(u) Z_1(-\beta u(1-q),\mu) \times G^{(1)}(1,1';-\beta u(1-q),\mu), \quad (4)$$

$$K_q^{(2)}(u) = -\frac{(1-q)u}{(Z_q)^q} K_q^{(1)}(u) = i\frac{\Gamma(1/(1-q))}{2\pi(Z_q)^q} e^{-u}(-u)^{-1/(1-q)}. \quad (5)$$

$G^{(1)}(1,1';\beta,\mu)$ is the usual grand canonical one-particle Green function given in KB. Similar expressions hold for the multiparticle q-Green functions. Also the dynamic linear response function derived in [6] will be reexpressed in terms of the parametric integral over the usual time-response functions [11]. It should be noted 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 discussed in detail by Lenzi [17].

Following KB, introduce correlation functions $G_>^{(q)}(1,1';\beta,\mu) = (-i/\hbar)\langle\Psi(1)\Psi^\dagger(1')\rangle_q$ and $G_<^{(q)}(1,1';\beta,\mu) = (\mp i/\hbar)\langle\Psi^\dagger(1')\Psi(1)\rangle_q$. The notation $>$ and $<$ is 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 (4), 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 by taking the Fourier transform with respect to time differences $A(\vec{r}_1,\vec{r}_1';\omega)$ introduced in 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 the following:

$$i\hbar G_>^{(q)}(\vec{r}_1,\vec{r}_1';\omega;\beta,\mu) = \int_C du\, K_q^{(2)}(u)[1 \pm f(\omega,-\beta u(1-q),\mu)]A(\vec{r}_1,\vec{r}_1';\omega)Z_1(-\beta u(1-q),\mu), \quad (6)$$

$$i\hbar G_<^{(q)}(\vec{r}_1,\vec{r}_1';\omega;\beta,\mu) = \pm\int_C du\, K_q^{(2)}(u) f(\omega,-\beta u(1-q),\mu)A(\vec{r}_1,\vec{r}_1';\omega)Z_1(-\beta u(1-q),\mu), \quad (7)$$

$$i\hbar[G_>^{(q)}(\vec{r}_1,\vec{r}_1';\omega;\beta,\mu) - G_<^{(q)}(\vec{r}_1,\vec{r}_1';\omega;\beta,\mu)] = \int_C du\, K_q^{(2)}(u)A(\vec{r}_1,\vec{r}_1';\omega)Z_1(-\beta u(1-q),\mu). \quad (8)$$

We deduce from (8) an important sum rule

$$i\hbar\int_{-\infty}^{\infty}\frac{d\omega}{2\pi}[G_>^{(q)}(\vec{r}_1,\vec{r}_1';\omega;\beta,\mu) - G_<^{(q)}(\vec{r}_1,\vec{r}_1';\omega;\beta,\mu)] = \delta(\vec{r}_1-\vec{r}_1')\langle 1\rangle_q \equiv \delta(\vec{r}_1-\vec{r}_1')[1 + (1-q)S_q], \quad (9)$$

where we have made use of the sum rule for the spectral weight given in KB and expressed $\langle 1\rangle_q$ in terms of the Tsallis entropy, $S_q = [1 - \mathrm{Tr}\hat{P}(\hat{H},\hat{N};q,\beta,\mu)]/(q-1)$. 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. (7) 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,

$$\langle\hat{N}(\vec{p})\rangle_q = \pm\int_C du\, K_q^{(2)}(u)\int_{-\infty}^{\infty}\frac{d\omega}{2\pi} \times \frac{A(\vec{p};\omega)Z_1(-\beta(1-q)u,\mu)}{e^{-\beta(1-q)u(\omega-u)} \mp 1}. \quad (10)$$

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

$$\langle\hat{N}(\omega)\rangle_q = \pm V\int_C du\, K_q^{(2)}(u)\frac{Z_1(-\beta(1-q)u,\mu)}{e^{-\beta(1-q)u(\omega-\mu)} \mp 1} \times \int \frac{d^D p}{(2\pi)^D}A(\vec{p};\omega). \quad (11)$$

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 $\hat{N}$,

$$\frac{\langle\hat{N}\rangle_q}{V} = \pm\int_C du\, K_q^{(2)}(u)\int_{-\infty}^{\infty}\frac{d\omega}{2\pi}\int\frac{d^D p}{(2\pi)^D} \times \frac{Z_1(-\beta(1-q)u,\mu)}{e^{-\beta(1-q)u(\omega-\mu)} \mp 1}A(\vec{p};\omega). \quad (12)$$

So far we have discussed the one-particle properties. 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. We now relate the scattering function defined, for example, in Lovesey [14] in the q formalism as $S^{(q)}(\omega,\beta) = \int_{-\infty}^{\infty}(dt/2\pi)e^{-i\omega t}\langle\hat{A}^{\dagger}(0)\hat{A}(t)\rangle_q^{(c)}$, 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 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

$$S^{(q)}(\vec{k},\omega;\beta) = \int_C du\, K_q^{(2)}(u) Z_1(-\beta u(1-q)) \times S^{(1)}(\vec{k},\omega;-\beta u(1-q)) \,. \quad (13)$$

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

$$\mathrm{Im}\,\chi^{(q)}_{\hat{A}^{\dagger}\hat{A}}(\vec{k},\omega;\beta) = \pi\int_C du\, K_2^{(q)}(u) Z_1(-\beta u(1-q)) \times (1 - e^{-\beta u(1-q)\omega}) \times S^{(1)}(\vec{k},\omega;-\beta u(1-q)) \,. \quad (14)$$

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 three suggestions for possible experimental investigation of the validity of the q framework for nonextensive systems based on the results obtained here.

(A) Electron system.—The momentum distribution for electrons is given by Eq. (10) with the lower sign. This function is directly observable in positron annihilation experiments [12]. We use free electron spectral weight function, $A(\vec{p};\omega) = 2\pi\delta(\omega - \vec{p}^{\,2}/2m)$, in this calculation for simplicity of presentation. Details of the actual calculation will be given elsewhere. 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. Thus, $\langle\hat{N}(k_z)\rangle_q = V^{2/3}\int\int\frac{dk_x}{2\pi}\frac{dk_y}{2\pi}\langle\hat{N}(\vec{k})\rangle_q$. 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 $\langle\hat{N}(k_z)\rangle_q \propto (k_F^2 - k_z^2)[1 + \frac{(1-q)^2}{2-q}\frac{\pi^2}{5}\langle\hat{N}\rangle_1^2]$. In Fig. 1 we display a plot of the q dependence of the ratio $\langle\hat{N}(k_z)\rangle_q/\langle\hat{N}(k_z)\rangle_1$ 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 experiment [12] for small systems with $\langle\hat{N}\rangle_1 = 50$ and 100.

(B) Boson system.—The recent work on Bose condensation of atoms [13] involves condensation of a small number of atoms of the order of 100 to 170 confined to a small region of space by magnetic trapping. We here 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. (12) 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,

$$\frac{\langle\hat{N}\rangle_q}{\langle\hat{N}\rangle_1} \simeq \left(\frac{T_c^{(q)}}{T_c^{(1)}}\right)^{3/2}\frac{\Gamma(\frac{2-q}{1-q})}{(1-q)^{(1/2)}\Gamma(\frac{2-q}{1-q}+\frac{1}{2})} \times\left\{1 + \frac{\langle\hat{N}\rangle_1}{(1-q)^{(3/2)}}\frac{\zeta(5/2)}{\zeta(3/2)}\left(\frac{T_c^{(q)}}{T_c^{(1)}}\right)^{3/2} \times\left[\frac{\Gamma(\frac{2-q}{1-q}+\frac{1}{2})}{\Gamma(\frac{2-q}{1-q}+2)} - q\frac{\Gamma(\frac{2-q}{1-q})}{\Gamma(\frac{2-q}{1-q}+\frac{3}{2})}\right]\right\}. \quad (15)$$

In Fig. 2 we display a plot of $\langle\hat{N}\rangle_q/\langle\hat{N}\rangle_1$ versus $T_c^{(q)}/T_c^{(1)}$ for two representative values of $\langle\hat{N}\rangle_1$ for $q = 0.4$ and 0.8. Curilef [19] calculated $T_c^{(q)}/T_c^{(1)}$ for $q \approx 1$ and found it increasing for $\langle\hat{N}\rangle_q/\langle\hat{N}\rangle_1$ equal to unity; from our Fig. 2, we see a similar increasing trend as we go from $q = 0.4$ to 0.8 as $\langle\hat{N}\rangle_1$ goes from 75 to 150.

(C) Scattering experiments.—The fabrication of quasiperiodic superlattices was successfully realized as

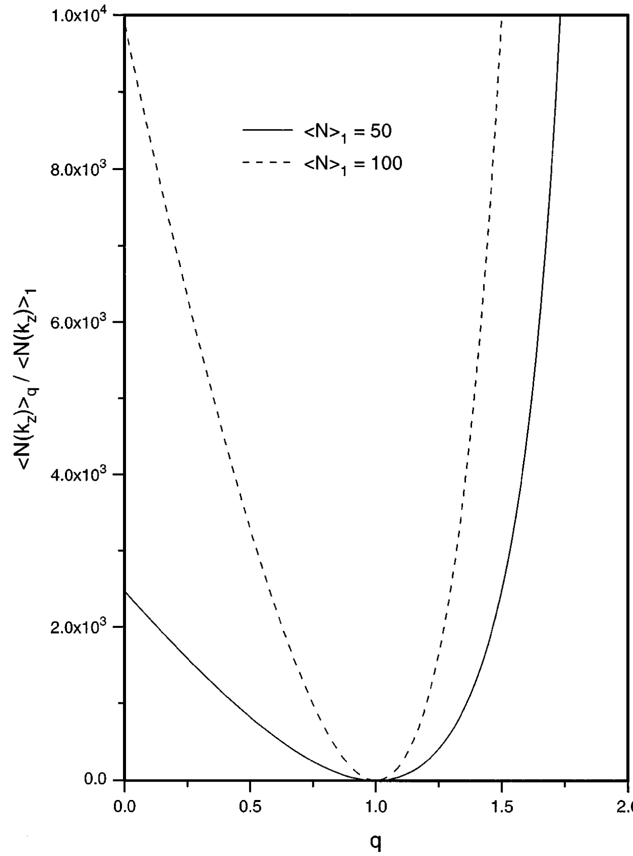

FIG. 1. Plot of $\frac{\langle\hat{N}(k_z)\rangle_q}{\langle\hat{N}(k_z)\rangle_1}$ as a function of q for $\langle\hat{N}\rangle_1 = 50$ and 100. Note that the value at $q = 1$ is unity.

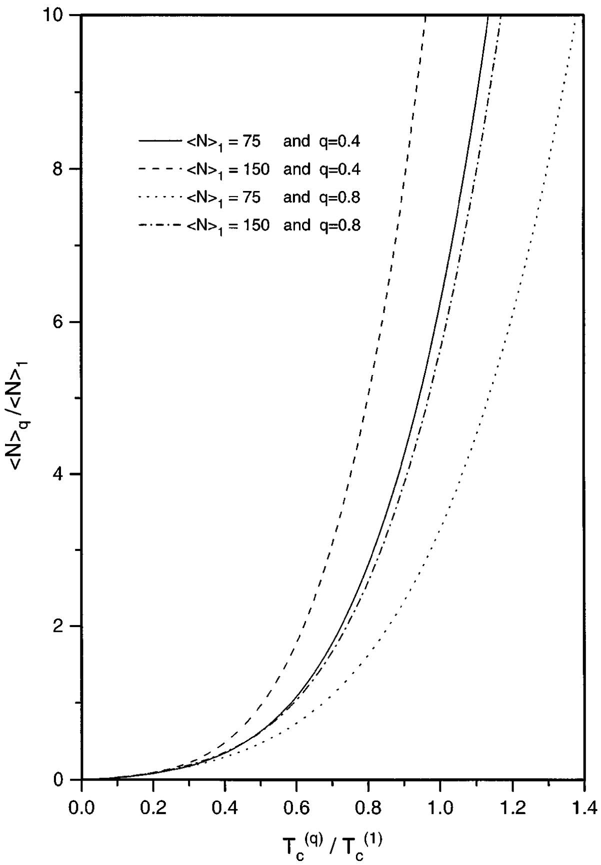

FIG. 2. Plot of $\langle \hat{N} \rangle_q$ as a function of $\frac{T_c^{(q)}}{T_c^{(1)}}$ for $\langle \hat{N} \rangle_1 = 75$ and 150, and for $q = 0.4$ and 0.8.

early as 1985 [20] and experimentally investigated by x-ray and neutron diffraction, etc. See Ref. [21]. These systems afford another class of possible experimental avenue to test the q framework when we consider *finite size effects* they might display. By using some known forms for the structure factor $S^{(1)}$ in Eq. (13) we can calculate that for $q < 1$, etc., as was done in the other two calculations. We propose to use our framework for such scattering cross section calculation to investigate these in some model structures in a separate communication.

In conclusion, we have here developed the q formalism of Tsallis 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 propose three possible experimental tests of this framework.

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