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Dynamic Linear Response Theory for a Nonextensive System Based on the Tsallis Prescription

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We develop here a dynamic linear response theory of many-body nonextensive systems based on the maximization of the Tsallis entropy associated with the density matrix and the concomitant suitably defined mean total energy, number, etc., where the averaging is over the qth power of the density matrix, q being a parameter characterizing the nonextensivity. This formulation is shown to preserve causality (Kramers-Kronig), time reversal, and Onsager reciprocity, while a different form of fluctuation-dissipation theorem is obtained. The traditional theory for extensive systems is obtained in the special case where $q = 1$. [S0031-9007(96)00087-7]

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There are many physical systems where spatial and/or temporal *long-range* interactions are present which make their behavior nonextensive. This may occur (a) in large systems such as those in astrophysics with long-range (gravitational) interactions, (b) in small nanometric systems in condensed matter, for example, where the range of interactions is comparable to system size, (c) in situations where *long-time memory* persists, and (d) in systems with fractally structured space-time. These situations demand an enlargement of the standard statistical mechanics and thermodynamics [1]. Tsallis [2] has proposed a generalization which retains [3] much of the formal structure of the standard theory and has successfully been applied in recent years to explain many of the above types of situations. We cite here a few of these among the many: stellar polytropes [4,5], Ising chain [6,7] and ferrofluids [8], fractal random walks [9] and anomalous diffusion [10], two-dimensional Euler turbulence [5], cosmic microwave background radiation [11], quantum uncertainty principle [12], exotic quantum statistics [13,14], Lévy-type anomalous superdiffusion [15], and an overview [16]. There are novel applications of this framework in other contexts which we do not mention here.

The purpose of the present work is to develop the corresponding generalization of the statistical-mechanical theory of irreversible processes based on the Tsallis prescription which, in the special case of $q = 1$ recovers the well-known formulation of Kubo [1,17]. Just as the Kubo theory proved to be an extremely valuable tool in its ability to give quick estimates of many types of transport properties for extensive systems, the corresponding formulas derived here are expected to be similarly useful in examining nonextensive system properties. While the static fluctuation-dissipation theorem in this framework exists [18] in the literature, the dynamic theory does not. With this development we hope to provide here the dynamic linear response and hence also a Green function formulation of many-body nonextensive systems within the Tsallis prescription. We explore all the ramifications of this prescription in much the same way as in the work of Kubo [1,17]. Such a theory is expected to be of immense value in understanding the anomalous frequency dependence in amorphous systems, in glasses, and in fractal systems, for example.

In developing the traditional linear-response formalism one deals with a Hermitian operator $\hat{B}$, whose average is driven away from its equilibrium average value $\langle \hat{B} \rangle_0$ by means of a time-dependent external field $X(t)$. In the standard quantum-mechanical formulation, the average of $\hat{B} - \langle \hat{B} \rangle_0 \equiv \Delta \hat{B}$ is given by

$$\langle \Delta \hat{B}(t) \rangle = \mathrm{Tr}[\hat{\rho}(t)\hat{B}] - \mathrm{Tr}(\hat{\rho}_0 \hat{B}) = \mathrm{Tr}[\hat{\rho}(t)\Delta \hat{B}],$$
$$\text{with } \mathrm{Tr}\hat{\rho}(t) = 1 = \mathrm{Tr}\hat{\rho}_0 . \tag{1}$$

Here $\hat{\rho}_0$ is the equilibrium density matrix determined from the maximum von Neumann entropy of the system for given constraints and $\hat{\rho}(t)$ is the time-dependent density matrix obeying a quantum Liouville–von Neumann equation determined by a Hamiltonian that incorporates the effect of $X(t)$:

$$\hat{H} - \hat{A}X(t)\,. \tag{2}$$

The operator conjugate to $X(t)$ is here denoted by $\hat{A}$.

We now depart from this traditional approach here by employing the Tsallis prescription [2,3] as follows. The equilibrium density matrix $\hat{\rho}_0$ is determined by maximizing the Tsallis entropy defined by

$$S_q = k_B(1 - \mathrm{Tr}\hat{\rho}^q)/(q-1), \quad \text{with } \mathrm{Tr}\hat{\rho} = 1\,, \tag{3}$$

where q is a parameter which characterizes the nonextensive nature of the system, and thus depends on the long-range nature of interactions present in the system. We take k_B to be the usual Boltzmann constant, for simplicity of presentation here, and may in principle depend on q (C. Tsallis, the last reference in [3]). The equilibrium canonical ensemble prescription requires the constraint of fixed q mean energy defined by

$$U_q = \mathrm{Tr}(\hat{H}\hat{\rho}^q)\,. \tag{4}$$

Henceforth we shall use the notation $\hat{P}(\hat{H};q) = \hat{\rho}^q(\hat{H})$, in order to keep in focus the Tsallis prescription and not to confuse it with the traditional method. Note that $\mathrm{Tr}\hat{P} = \mathrm{Tr}\hat{\rho}^q \neq 1$ for $q \neq 1$. Thus the equilibrium density matrix with a temperature (Lagrange) parameter β is found to be

$$\begin{aligned} \hat{P}(\hat{H};q,\beta) &= \hat{Q}(\hat{H};q,\beta)/[Z(\hat{H};q,\beta)]^q, \\ \text{where } \hat{Q}(\hat{H};q,\beta) &= [1-\beta(1-q)\hat{H}]^{q/(1-q)}, \\ Z(\hat{H};q,\beta) &= \mathrm{Tr}[1-\beta(1-q)\hat{H}]^{1/(1-q)}. \end{aligned} \tag{5}$$

The corresponding entropy is given by calculating it using Eq. (5). We also modify the definition of the linear response to conform to the Tsallis prescription by employing the q averages:

$$\langle \Delta\hat{B}(t)\rangle_q \equiv \mathrm{Tr}[\hat{P}(t)\hat{B}] - \mathrm{Tr}[\hat{P}(\hat{H};q,\beta)\hat{B}]\,. \tag{6}$$

Note that this differs from the traditional definition in Eq. (1) because $\mathrm{Tr}\hat{P} = \mathrm{Tr}\hat{\rho} \neq 1$ for $q \neq 1$.

The traditional quantum principles allow us to write the Liouville–von Neumann equation for the P operator introduced above as

$$i\hbar\frac{\partial\hat{P}(t)}{\partial t} = [\hat{H},\hat{P}(t)] - [\hat{A},\hat{P}(t)]X(t)\,, \tag{7}$$

with the initial condition $\hat{P}(t=-\infty) = \hat{P}(\hat{H};q,\beta)$ given by Eq. (5). The solution of this to linear order in $X(t)$ is then found by standard procedures:

$$\begin{aligned} \hat{P}(t) \cong \hat{P}(\hat{H};q,\beta) - \frac{1}{i\hbar}\int_{-\infty}^{t} dt'\, e^{-i(t-t')\hat{H}/\hbar} \\ \times [\hat{A},\hat{P}(\hat{H};q,\beta)]X(t')e^{i(t-t')\hat{H}/\hbar}. \end{aligned} \tag{8}$$

Thus we obtain

$$\begin{aligned} \langle\Delta\hat{B}(t)\rangle_q &= \int_{-\infty}^{t} dt'\,\phi_{\mathrm{BA}}(t-t')X(t')\,, \\ \phi_{\mathrm{BA}}(t) &= -\frac{1}{i\hbar}\mathrm{Tr}\{[\hat{A},\hat{P}(\hat{H};q,\beta)]\hat{B}(t)\} \\ &= \frac{1}{i\hbar}\mathrm{Tr}\{[\hat{A},\hat{B}(t)]\hat{P}(\hat{H};q,\beta)\}\,. \end{aligned} \tag{9}$$

If $X(t) = X_0\cos\omega t$, we may define

$$\begin{aligned} \langle\Delta\hat{B}(t)\rangle_q &= \mathrm{Re}\{\chi_{\mathrm{BA}}(\omega)X_0e^{i\omega t}\}, \\ \text{where } \chi_{\mathrm{BA}}(\omega) &= \lim_{\varepsilon\to 0}\int_0^{\infty} dt\,\phi_{\mathrm{BA}}(t)e^{-i\omega t-\varepsilon t}\,. \end{aligned} \tag{10}$$

We can prove the following identity for the commutator occurring in Eq. (8) which is a generalization of the corresponding one due to Kubo [17].

Identity A:

$$\begin{aligned} [\hat{A},\hat{P}(\hat{H};q,\beta)] = q\hat{P}(\hat{H};q,\beta)\int_0^{\beta} d\lambda[\hat{P}(\hat{H};q,\lambda)]^{-1} \\ \times [\hat{H},\tilde{A}_\lambda]\hat{P}(\hat{H};q,\lambda)\,, \end{aligned} \tag{11}$$

$$\tilde{A}_\lambda = \frac{1}{1-\lambda(1-q)\hat{H}}\,\hat{A}\,\frac{1}{1-\lambda(1-q)\hat{H}}\,.$$

From this we obtain another expression for the response function

$$\begin{aligned} \phi_{\mathrm{BA}}(t) = -q\mathrm{Tr}\hat{P}(\hat{H};q,\beta)\int_0^{\beta} d\lambda[\hat{P}(\hat{H};q,\lambda)]^{-1} \\ \times \tilde{A}_\lambda\hat{P}(\hat{H};q,\lambda)\dot{\hat{B}}(t)\,. \end{aligned} \tag{12}$$

The overdot on operator B represents its time derivative. Similarly the isothermal admittance is obtained by considering static applied force and calculating the expression

$$\langle\Delta\hat{B}\rangle_q^T = \mathrm{Tr}\hat{P}(\hat{H}-X\hat{A};q,\beta)\hat{B} - \mathrm{Tr}\hat{P}(\hat{H};q,\beta)\hat{B}\,, \tag{13}$$

to leading order in X. To calculate this we need another identity, which is a generalization of that due to Karplus and Schwinger [19] for the exponential operators. This is proved in a straightforward way and it is as follows.

Identity B:

$$\hat{Q}(\hat{H}-\hat{A}X;q,\beta)=\hat{Q}(\hat{H};q,\beta)+qX\hat{Q}(\hat{H};q,\beta)\int_0^\beta d\lambda[\hat{Q}(\hat{H};q,\lambda)]^{-1}\tilde{A}'_\lambda\hat{Q}(\hat{H}-\hat{A}X;q,\lambda),$$
$$\text{where } \tilde{A}'_\lambda=[1-\lambda(1-q)(\hat{H}-X\hat{A})]^{-1}[1-\lambda(1-q)\hat{H}]\tilde{A}_\lambda, \tag{14}$$

with $\tilde{A}_\lambda$ defined in Eq. (11) . Here $\hat{Q}$ is the operator defined in Eq. (5). Working to linear order in X, in Eq. (14), we obtain the isothermal response function, corresponding to the dynamical one obtained in Eq. (10):

$$\chi^T_{\mathrm{BA}}=q\left\{\mathrm{Tr}\int_0^\beta d\lambda\,\hat{P}(\hat{H};q,\beta)[\hat{P}(\hat{H};q,\lambda)]^{-1}\tilde{A}_\lambda\hat{P}(\hat{H};q,\lambda)\hat{B}\right\}-q\left(\mathrm{Tr}\int_0^\beta d\lambda\,\hat{R}(\hat{H};q,\beta)\tilde{A}_\lambda\right)[\mathrm{Tr}\hat{P}(\hat{H};q,\beta)\hat{B}],$$
$$\text{Here } \hat{R}(\hat{H};q,\beta)=[1-\beta(1-q)\hat{H}]^{1/(1-q)}/Z(\hat{H};q,\beta). \tag{15}$$

A discussion of the equality between the zero frequency limit and this expression involves the same subtleties as in the extensive case given in detail in [1,17]. In general $\chi_{\mathrm{BA}}(\omega=0)\neq\chi^T_{\mathrm{BA}}$, unless one makes ergodicity assumption, etc. We would also like to remark here that, for $q=1$, these results go over to their counterparts in the theory for extensive systems given originally by Kubo [17]. In this way we have placed the Tsallis prescription on par with the traditional approach to linear response theory. Some of the finer aspects of the linear response theory discussed recently in [20], namely, that one is using near-equilibrium density matrices and that the source of irreversibility is the introduction of a nonunitary component in the undriven dynamics, carry over here as well.

We can also define the "relaxation function" as the relaxation of $\langle\hat{B}\rangle_q$ after removal of the external disturbance and is given as in [17]:

$$\Phi_{\mathrm{BA}}(t)=\lim_{\varepsilon\to0^+}\int_t^\infty dt'\,\phi_{\mathrm{BA}}(t')e^{-\varepsilon t'}=\sum_{i,j}\left(\frac{P(i)-P(j)}{E_i-E_j}\right)\langle i|\hat{A}|j\rangle\langle j|\hat{B}|i\rangle e^{it(E_j-E_i)/\hbar}, \tag{16}$$
$$\text{where } P(i)=[1-\beta(1-q)E_i]^{q/(1-q)}/(Z)^q.$$

We have used the complete set of eigenfunctions of the Hamiltonian operator $\hat{H}|i\rangle=E_i|i\rangle$, in deriving the second expression in Eq. (16). From this expression, we deduce three important relations, all of which are proved quite easily: (1) $\Phi_{\mathrm{BA}}(t)$ is real; (2) $\Phi_{\mathrm{BA}}(-t)=\Phi_{\mathrm{AB}}(t)$ (time-reversal symmetry); and by defining

$$\sigma_{\mathrm{BA}}(\omega)=\int_0^\infty dt\,\Phi_{\mathrm{BA}}(t)e^{-i\omega t},$$

we obtain (3) the Onsager relationships

$$\mathrm{Re}\sigma_{\mathrm{AB}}(\omega)=\mathrm{Re}\sigma_{\mathrm{BA}}(-\omega),$$
$$\mathrm{Im}\sigma_{\mathrm{AB}}(\omega)=-\mathrm{Im}\sigma_{\mathrm{BA}}(-\omega).$$

One may also define a correlation function involving the q average over the anticommutator combination of the operators

$$\Psi_{\mathrm{BA}}(t)=\frac{1}{2}\mathrm{Tr}\hat{P}(\hat{H};q,\beta)\{\hat{A}\hat{B}(t)+\hat{B}(t)\hat{A}\}$$
$$=\sum_{i,j}\left(\frac{P(i)+P(j)}{2}\right)\langle i|\hat{A}|j\rangle\langle j|\hat{B}|i\rangle e^{it(E_j-E_i)/\hbar}. \tag{17}$$

Now we derive in a formal way the dynamical fluctuation-dissipation theorem by formally writing

$$e^{i(t/\hbar)(E_j-E_i)}=e^{i(t/\hbar)E_j}e^{-i(t'/\hbar)E_i},$$

and setting $t=t'$ at the end of the calculation. Then we obtain the interesting relation between these two functions:

$$\Psi_{\mathrm{BA}}(t,t')=\frac{a(-\partial_{t'})+a(\partial_t)}{2[a(-\partial_{t'})-a(\partial_t)]}i\hbar(\partial_{t'}+\partial_t)\Phi_{\mathrm{BA}}(t,t'), \tag{18}$$
$$\text{where } a(\partial_t)=[1+\beta(1-q)i\hbar\partial_t]^{q/(1-q)}.$$

Thus the general fluctuation-dissipation theorem for finite frequencies for the nonextensive system is found to be a little more involved, even though we recover the well-known result for $q=1$. This generalizes a result due to Kubo [17] for extensive systems, with the same notations,

$$\Psi_{\mathrm{BA}}(t)=E_\beta(-i\partial_t)\Phi_{\mathrm{BA}}(t),$$
$$E_\beta(\omega)=\frac{\hbar\omega}{2}\coth\frac{\beta\hbar\omega}{2}. \tag{18'}$$

Equation (18) reduces to this simple form for extensive systems where $q=1$.

A fluctuation-dissipation theorem for zero frequency was obtained in [18]; the same result is obtained from the isothermal result in Eq. (15), as can be proved by considering the q-free energy of the system, as follows. We consider a time independent constant force Y corresponding to the operator $\hat{B}$ and consider a new Hamiltonian $\hat{H}-X\hat{A}-Y\hat{B}$. Following Eq. (5), we find the q-free energy associated with the system in the Tsallis prescription is [3] given by

$$F(\hat{H}-X\hat{A}-Y\hat{B};q,\beta)=\frac{1}{\beta(q-1)}\times\{[Z(\hat{H}-X\hat{A}-Y\hat{B};q,\beta)]^{1-q}-1\}. \tag{19}$$

From this we find by differentiating with respect to Y that the q mean value of $\hat{B}$ is given by

$$-\frac{\partial F(\hat{H} - X\hat{A} - Y\hat{B}; q, \beta)}{\partial Y} = \mathrm{Tr}\hat{P}(\hat{H} - X\hat{A} - Y\hat{B}; q, \beta)\hat{B} = \langle \hat{B} \rangle_q . \quad (20)$$

Another derivative of this with respect to X and evaluating the result for $X = Y = 0$, we obtain a different but equivalent form of the result for the isothermal response function, Eq. (15), which may now be expressed in the familiar form $-\partial^2 F/\partial X \partial Y|_{X=Y=0} = \chi^T_{\mathrm{BA}}$. This is the result of Chame and de Mello [18]. This is also the result obtained by Tsallis [16] for isothermal static spin susceptibility where the operators refer to spin. In the static case, the Onsager relations have been proved in [21].

Another point of interest is to note that the real and imaginary parts of the susceptibility defined in Eq. (10) obeys the Kramers-Kronig relation because

$$\chi_{\mathrm{BA}}(\omega) = \chi^R_{\mathrm{BA}}(\omega) + i\chi^1_{\mathrm{BA}}(\omega), \quad \chi^R_{\mathrm{BA}}(\omega) = P\sum_{ij} \frac{\langle i|\hat{A}|j\rangle\langle j|\hat{B}|i\rangle[P(i) - P(j)]}{\hbar\omega + E_i - E_j}$$
$$\chi^1_{\mathrm{BA}}(\omega) = \pi \sum_{ij} \langle i|\hat{A}|j\rangle\langle j|\hat{B}|i\rangle[P(i) - P(j)]\delta(\hbar\omega + E_i - E_j). \quad (21)$$

Thus we see that the Kramers-Kronig relation holds for any q. This points out that the Tsallis prescription preserves the causality condition, which is understood when we recall that it is only a way of prescribing the initial condition in solving the Liouville–von Neumann equation, Eq. (7).

It is also worth noting that a Green function theory for many-body systems which are nonextensive may be constructed by the Tsallis prescription as was done above for response functions. For example, a one particle Green function in this framework is defined by

$$G_q(1,2) = \frac{1}{i\hbar}\,\mathrm{Tr}[\hat{P}(\hat{H}; q, \beta)T(\hat{\psi}(1)\hat{\psi}^\dagger(2))], \quad (22)$$

where T is the usual time ordering operator, and the other operators are the one particle destruction and creation operators, and 1 here refers to space-time, $(\vec{r}_1, t_1)$, etc. Further development of this proceeds along the same lines as in the theory of thermal Green functions.

In conclusion, we have employed the Tsallis prescription for nonextensive systems to deduce dynamic linear response function and its various properties. We may also observe that the von Neumann and Tsallis prescriptions are just two different ways of prescribing the initial thermodynamic equilibrium condition in solving the quantum Liouville–von Neumann equation. All those properties which do not depend on the actual form of the initial density matrix, such as time-reversal symmetry, causality, Onsager reciprocity relations are satisfied while a different form of the dynamical fluctuation-dissipation theorem is obtained exhibiting the dependence on the initial density matrix. The development given here should be a valuable tool in analyzing dynamical properties of systems exhibiting anomalous time and/or frequency dependences; see, for example, papers in [22].

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