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1994 J. Phys. A: Math. Gen. 27 5707

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The classical N -body problem within a generalized statistical mechanics

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Received 22 February 1994, in final form 27 May 1994

Abstract. The modifications that must be introduced within the framework of standard, classical N -body statistical mechanics techniques, in order to deal with the recently proposed generalized scenario of non-extensive statistical mechanics are discussed. A generalized version of the equipartition theorem is shown to hold. The ideal gas is revisited as a simple application.

Non-extensivity (or non-additivity) is a term much in vogue nowadays in some areas of physics, by way of reference to some interesting generalizations of traditional concepts. These generalizations exhibit a somewhat holistic (context dependent) nature and flow mainly along two separate streams: generalized statistical mechanics, on one hand [1–19], and quantum groups [20–33] on the other. A tentative connection between these two fields has recently been advanced [34].

The extension of statistical mechanics we are referring to here was proposed in [1], inspired by multifractals, on the basis of a generalized entropy S_q that possesses the usual properties of positivity, equiprobability, concavity and irreversibility, and suitably generalizes the standard additivity (it is non-extensive if $q \neq 1$) as well as the Shannon theorem [3]. It reads

$$S = k(q - 1)^{-1} \sum_m p_m (1 - p_m^{q-1}) \quad (1)$$

where k is a conventional positive constant, q is any real number (characterizing a particular statistics) and the sum runs over all the microscopic configurations (whose probabilities are $\{p_m\}$). By introducing the generalized internal energy

$$\langle E \rangle_q = \sum_m p_m^q \epsilon_m \quad (2)$$

Curado and Tsallis show [3] that the entire (Legendre-transform) mechanical structure of thermodynamics is preserved. By recourse to information theory (IT) concepts [35] it has been shown that the corresponding generalization for non-diagonal quantum density

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operators is easily achieved [7]. The conventional theory (Boltzmann–Gibbs statistics) is that particular instance in which one chooses $q = 1$.

Most concomitant applications refer to quantal instances [1–19], while relatively scarce attention has been paid to classical ones. The classical N -body gravitational problem constitutes one of the possible interesting applications of the generalized statistical mechanics [6]. (Levy flights [8] and self-organization in biological systems [9] constitute other interesting applications, recently established.) As is well known [36,37], the canonical ensemble for such a problem poses (thus far) insurmountable difficulties within the conventional Boltzmann–Gibbs scenario.

A D -dimensional N -body gravitational-like system consist of N classical particles *attractively* interacting through two-body interactions characterized by a potential $U(r) = A/r^\alpha$ ($A < 0$ if $\alpha > 0$, and $A > 0$ if $\alpha < 0$). The one body internal energy is characterized, *within Boltzmann–Gibbs statistics*, by the integral

$$I(D, \alpha) = \int_{\text{cut-off}}^{\infty} dr r^{D-1} r^{-\alpha} \exp(-\beta A/r^\alpha) \quad (3)$$

(the cut-off, which avoids possible $r = 0$ divergences, is physically very natural due to unavoidable quantum effects). We straightforwardly verify that, for any finite temperature, $I(D, \alpha)$ *diverges* if $0 < \alpha < D$ and *converges* if $\alpha < 0$ or if $\alpha > D$ ($\alpha = 0$ and $\alpha = D$ are marginal cases to be discussed on their own). Newtonian gravitation ($\alpha = D - 2$) belongs to the forbidden region for $D = 3$ (this fact is, of course, well known [36]). In other words, *the Boltzmann–Gibbs statistical description of canonical thermal equilibrium fails if $\alpha \in (0, D)$* . Consequently, something has to be done! Naturally, our present suggestion is to replace standard thermo-statistics by the generalized one, where q is a function of (D, α) to be determined (of course, one expects to recover $q = 1$ if $\alpha \notin (0, D)$). This task should probably be accomplished by carefully discussing the dynamics of the system. For collisionless systems, the standard formalism [35] yields maximum entropy (phase space) distributions that imply a non-physical infinite mass for the associated system [6,38]. It has been shown in [6] that for q sufficiently different from 1 this divergence disappears. In order to treat more general situations than the collisionless one it would be of interest to discuss some particular aspects of the generalized statistical mechanics in connection with the classical many-body problem, as some difficulties arise in connection with the concomitant partition function. *These seem so acute that not even the classical ideal gas has yet been adequately discussed within this generalized scenario* [39]. The discussion of the ideal gas (essentially corresponding to $\alpha = D = 0$, constituting therefore a marginal example with respect to the considerations expounded in the preceding paragraph) can further provide useful insight concerning these matters. Additionally, the study we shall here undertake could be of some utility in connection with stellar systems with polytropic phase distributions, which have been shown to be of the generalized maximum entropy form [6].

In the Boltzmann–Gibbs statistics the exponential form of the canonical ensemble probability distribution [40] allows for the explicit integration, in evaluating the partition function Z , of the momentum-dependent part (kinetic energy) of $\exp(-\beta H)$ (β is the inverse temperature and H refers to the Hamiltonian of the system). This fact, reduces the work involved in computing Z to the evaluation of integrals over just the configuration variables r_i , $i = 1, \dots, DN$, where N refers to the number of particles and D is the dimension of the one-body configuration space. The corresponding multiple integral is conventionally called

the configurational partition function. For

$$H = \sum_{i=1}^{DN} (p_i^2/2m) + U(r_1, \dots, r_{DN}) \tag{4}$$

we have

$$\begin{aligned} Z_{q=1} &= \frac{1}{N!h^{DN}} \left(\frac{2\pi m}{\beta h^2}\right)^{DN/2} \int \dots \int \exp\{-\beta U\} dr_1 \dots dr_{DN} \\ &= \frac{1}{N!h^{DN}} \left(\frac{2\pi m}{\beta h^2}\right)^{DN/2} Z_{q=1}^{\text{conf.}} \end{aligned} \tag{5}$$

Of course, this nice property is lost for $q \neq 1$, as, instead of (5) we have to deal with [1, 3]

$$Z_q = \frac{1}{N!h^{DN}} \int \dots \int \{1 - \beta(1 - q)H\}^{1/(1-q)} dr_1 \dots dr_{DN} \tag{6}$$

which does not lend itself to an obvious factorization process.

In the present paper we wish to address that this problem in an adequate fashion, which will, as a bonus, yield the general treatment of the classical ideal gas.

We set

$$\mathbf{R} = (r_1, \dots, r_{DN}) \quad \mathbf{P} = (p_1, \dots, p_{DN}) \tag{7}$$

and write the generalized (canonical) phase space distribution function [1-19]

$$f(\mathbf{R}, \mathbf{P}) = Z_q^{-1} [1 - \beta(1 - q)H(\mathbf{R}, \mathbf{P})]^{1/(1-q)} \tag{8}$$

where, as usual, we include in (6) division by the factor $\eta = N!h^{DN}$ so as to have a dimensionless partition function and probably account for the fact of having to deal with N undistinguishable particles (h is the size of a typical 'cell' in phase space). It must be stressed that, by definition [1, 3], the distribution function (8) vanishes, for $q < 1$, whenever the bracket in this equation is ≤ 0 (cut-off condition of generalized probability distribution). A similar condition exists for $q > 1$ [9].

Going over now to 'polar' coordinates in our DN -dimensional momentum space we set

$$(p_1, \dots, p_{DN}) \rightarrow (P, \phi_1, \dots, \phi_{(DN-1)}) \tag{9}$$

(P is the radial coordinate and $\phi_1, \dots, \phi_{DN-1}$ are the angular ones). The integrand in (6) depends only upon P . The integral over the angular variables ϕ_i is immediately performed [41] and contributes a factor $\delta = 2\pi^{DN/2}/\Gamma(DN/2)$ to the generalized partition function Z_q .

We shall herefrom concentrate our efforts on the interesting physical range [38] of q -values for the present problem, namely, the region $q < 1$, assuming, of course, $\beta > 0$ (we recall that the energy spectrum is unbounded from above, hence $\beta < 0$ is physically inaccessible). Towards the end of this paper we shall discuss other q -values. With the transformation (9) we can recast Z_q , after introducing the definition

$$W(\mathbf{R}) = 2m\{\beta(1 - q)\}^{-1} [1 - \beta(1 - q)U(\mathbf{R})] \tag{10}$$

in the fashion

$$Z_q = \eta^{-1} \delta[\beta(1-q)/2m]^{1/(1-q)} \int \{W(\mathbf{R}) - P^2\}^{1/(1-q)} P^{DN-1} dP d^{DN}r. \quad (11)$$

The cut-off condition enters here (cf the discussion following equation (8)), which entails that the factor $\{W(\mathbf{R}) - P^2\}$ should be set equal to zero whenever it becomes negative [1, 3]. As a consequence, configurations \mathbf{R} for which $W(\mathbf{R}) < 0$ do not contribute in the integral (11). Moreover, in order to enforce the cut-off condition we can accept as valid 'P-contributions' to (11) those that obey the restriction

$$0 \leq P^2 \leq W(\mathbf{R}) \quad (12)$$

which tells us that the P -integral limits are zero and the square-root of $W(\mathbf{R})$. Additionally, we are entitled to change variables according to

$$[P^2/W(\mathbf{R})] = \cos^2 \theta \quad 0 \leq \theta \leq \pi/2 \quad (13)$$

so as to replace the P -integration process by a θ one, recasting Z_q in the fashion

$$Z_q = \eta^{-1} \delta[\beta(1-q)/2m]^{1/(1-q)} I_p I_c \quad (14)$$

with

$$I_p = \int_0^{\pi/2} \cos^{DN-1}(\theta) \sin^{(3-q)/(1-q)}(\theta) d\theta \quad (15)$$

and

$$I_c = \int W(\mathbf{R})^{(1/(1-q)+DN/2)} d^{DN}r. \quad (16)$$

The angular integral can be expressed in terms of beta functions (Euler's integrals of the first kind) which in turn can be rewritten with the help of gamma functions [41] so that, finally, we have

$$\begin{aligned} I_p &= \frac{1}{2} \Gamma(DN/2) \Gamma((2-q)/(1-q)) / \Gamma((2-q)/(1-q) + DN/2) \\ &\equiv \frac{1}{2} \Gamma(DN/2) \{\Gamma_1 / \Gamma_2\}. \end{aligned} \quad (17)$$

In writing down (14), together with the closed result (17), we have achieved our main aim, i.e. that of reducing the evaluation of Z_q to the computation of just one integral over the configuration variables (cf equation (16)). We shall now apply this result to the classical ideal gas.

For the ideal gas the potential energy $U(\mathbf{R})$ vanishes, so that the associated quantity $W(\mathbf{R})$ (cf equation (10)) verifies

$$W(\mathbf{R}) = 2m/[\beta(1-q)] = \text{constant} \quad (18)$$

and, as a consequence (cf equation (16)),

$$I_c = \{2m/\beta(1-q)\}^{[1/(1-q)+DN/2]} V^N \quad (19)$$

where V is the D -dimensional volume accessible to our gas. Consequently, equation (14) becomes

$$Z_q = (V^N/N!)[2\pi m/h^2(1-q)\beta]^{DN/2}(\Gamma_1/\Gamma_2) \tag{20}$$

which, by introduction of the two quantities

$$\Lambda = (1/N!)[2\pi m/h^2]^{DN/2} \tag{21}$$

$$d(q) = (1-q)^{-DN/2}\Gamma_1/\Gamma_2 \tag{22}$$

can be recast in the fashion

$$Z_q = \Lambda d(q)V^N(kT)^{DN/2} \tag{23}$$

where we have used $\beta = 1/kT$.

The generalized Helmholtz' free energy is [3]

$$F_q = -kT(Z_q^{1-q} - 1)/(1-q) \tag{24}$$

so that we find

$$F_q = -kT(1-q)^{-1}([\Lambda d(q)]^{1-q}V^{(1-q)N}(kT)^{(1-q)DN/2} - 1) \tag{25}$$

and the specific heat is

$$\begin{aligned} C_q &= T \left[\frac{\partial S_q}{\partial T} \right]_{N,V} = \left[\frac{\partial U_q}{\partial T} \right]_{N,V} = -T[\partial^2 F_q/\partial T^2]_{N,V} \\ &= \frac{kND}{2} [1 + (1-q)DN/2] \\ &\quad \times \left\{ \frac{\Gamma \left[\frac{2-q}{1-q} \right]}{\Gamma \left[\frac{2-q}{1-q} + \frac{1}{2}DN \right]} (1-q)^{-DN/2} (V^N/N!) \left[\frac{2\pi mkT}{h^2} \right]^{DN/2} \right\}^{1-q} \end{aligned} \tag{26}$$

This result holds for $q \leq 1$ and has been here derived for the first time. By recourse to the Hilhorst's transform, one of us [38] has discussed the ideal gas in the q -range

$$1 \leq q \leq 1 + (2/DN). \tag{27}$$

Unfortunately, Hilhorst's transform cannot be employed for $q < 1$ [39]. It is to be remarked that the treatment discussed in this paper can also be applied in the case of q -values belonging to the interval (27). Extra care must be taken in accommodating the (analogous to the $q < 1$ case) cut-off condition, but no essential differences arise with respect to what we have so far expanded. We obtain, via a quite different procedure, the same results obtained in [38].

Equation (26) exhibits the *loss of universality* that the present generalized statistics introduces. Indeed, if $(q-1) \neq 0$, the specific heat depends on m (analogously to what happens in the $q = 1$ quantum statistics). Also, for the $q < 1$ case, we verify that, in the $N \rightarrow \infty$ limit, an interesting *crossover* occurs in the *prefactor* of the specific heat. Indeed,

it increases as N if $q = 1$ and as N^2 if $q < 1$. This is to be mentioned in connection with a similar behaviour discussed by Saslaw [36] for $D = 3$ gravitation.

It is instructive to rederive equation (29) with reference to a generalized version of the equipartition theorem, that, as we now proceed to show, *also holds within the present generalized framework*.

Let $A(\mathbf{R}, \mathbf{P})$ denote a generic quantity. Its generalized mean value is given by (cf equation (2)) [3]

$$\begin{aligned} \langle A \rangle_q &= \frac{1}{N!h^{DN}} \int A(\mathbf{R}, \mathbf{P}) \{f(\mathbf{R}, \mathbf{P})\}^q d\Omega \\ &= \frac{1}{N!h^{DN}} Z_q^{-q} \int A(\mathbf{R}, \mathbf{P}) [1 - \beta(1 - q)H]^{q/(1-q)} d\Omega \end{aligned} \quad (28)$$

and we shall use this to *derive* a generalized equipartition theorem.

Let us now assume that our Hamiltonian H can be split into two pieces in the fashion

$$H = h + g \quad (29)$$

where g is a homogeneous quadratic function of L canonical variables of which say ν are generalized coordinates and the remaining ones are $\mu = L - \nu$ generalized momenta

$$g = g(r_1, \dots, r_\nu, p_1, \dots, p_\mu) \quad (30)$$

and h does not depend upon these L variables. By Euler's theorem [41] we have

$$2g = \sum_{i=1}^{\nu} r_i (\partial g / \partial r_i) + \sum_{i=1}^{\mu} p_i (\partial g / \partial p_i) \quad (31)$$

so that the generalized mean value of g reads

$$\langle g \rangle_q = \frac{1}{2} \left(\sum_{i=1}^{\nu} \langle r_i (\partial g / \partial r_i) \rangle_q + \sum_{i=1}^{\mu} \langle p_i (\partial g / \partial p_i) \rangle_q \right). \quad (32)$$

We shall now discuss in some detail one generic term of this equation. Consider

$$\langle r_k (\partial g / \partial r_k) \rangle_q = \frac{Z_q^{-q}}{N!h^{DN}} \int r_k (\partial g / \partial r_k) [1 - \beta(1 - q)H]^{q/(1-q)} d\Omega. \quad (33)$$

This is a multidimensional ($2DN$) integral. Let us evaluate the integral over r_k . This variable ranges between, say, r_a and r_b , these values being given by the cut-off condition mentioned in connection with the probability distribution (8). We have

$$J \equiv \int_{r_a}^{r_b} r_k (\partial g / \partial r_k) [1 - \beta(1 - q)H]^{q/(1-q)} dr_k \quad (34)$$

so that

$$\langle r_k (\partial g / \partial r_k) \rangle_q = \frac{Z_q^{-q}}{N!h^{DN}} \int \dots \int J dr_1 \dots dr_{k-1} dr_{k+1} \dots dp_{DN}. \quad (35)$$

In order to obtain J we integrate by parts. To do so we first notice that, on account of equations (29) and (30)

$$\frac{\partial}{\partial r_k} \{ [1 - \beta(1 - q)H]^{1/(1-q)} \} = -\beta(\partial g / \partial r_k) [1 - \beta(1 - q)H]^{q/(1-q)} \quad (36)$$

which, since the integrated part will vanish because of the cut-off condition, leads to

$$J = \beta^{-1} \int [1 - \beta(1 - q)H]^{1/(1-q)} dr_k. \quad (37)$$

Using the normalization condition for $f(\mathbf{R}, P)$, namely

$$\frac{1}{N! h^{DN}} Z_q^{-1} \int [1 - \beta(1 - q)H]^{1/(1-q)} d\Omega = 1 \quad (38)$$

this yields, upon insertion into (35)

$$\langle r_k (\partial g / \partial r_k) \rangle_q = \beta^{-1} (Z_q)^{1-q}. \quad (39)$$

It is apparent that each term in the sums appearing in (32) will yield a contribution of the type (39), so that

$$\langle g \rangle_q = (L/2) kT (Z_q)^{1-q} \quad (40)$$

which is the generalized version of the equipartition theorem. For the ideal gas discussed above, the total energy E is a homogeneous quadratic function of DN momenta, which allows one to write

$$\langle E \rangle_q = \frac{1}{2} DN kT (Z_q)^{1-q} \quad (41)$$

which, after differentiation with respect to the temperature, leads once more to the specific heat (26).

Now, in order to ascertain the thermal behaviour as q moves away from 1 (at fixed values of N, V, β) we present the first-order expansion of the equation of state in terms of $(1 - q)$, namely,

$$PV/NkT \simeq 1 + (1 - q) [(DN/2) \ln(2\pi m V^{2/D} / h^2 \beta) - \ln(N!)]. \quad (42)$$

It is seen that the pressure ($P = -(\partial F_q / \partial V)_T$) tends to change as N^2 (non-extensivity!) with large N , which reminds one of the gravitational gas behaviour in two dimensions [36].

We conclude by restating that our present methodology allows for a straightforward application of statistical mechanics techniques to classical systems within the generalized scenario [1] under consideration. It can be also mentioned that the existence of a generalized equipartition theorem is another manifestation of the coherence of the generalized mean values [1, 3], which were earlier shown, within a quantum framework, to obey the constraints posed by Ehrenfest's theorem [7]. The appearance of the N -body partition function in (40) is a clear manifestation of the holistic character (i.e. context dependent even in the absence of interactions at the Hamiltonian level) of the present generalization of statistical mechanics. As evidenced by equation (41), a particular degree of freedom, although contributing with the same amount to the total energy, is coupled to all the remaining degrees of freedom through Z_q , which carries with it information concerning the structure of the whole system. This is a patent manifestation of the non-extensive entropy we have used herein.

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