Tsallis non-extensive statistical mechanics of the self-gravitating gas

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Outline I

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Statistical mechanics is one of the most important branches of physics, born to provide theoretical foundation to the phenomenologically constructed thermodynamics.


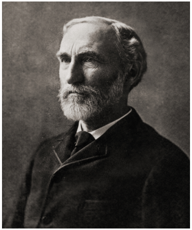

Figure: Ludwig Boltzmann and Josiah W. Gibbs

Introduction

Boltzmann-Gibbs (BG) Statistical Mechanics

The most important quantity in BG Statistics is the entropy, using the Shannon's formula:

$$S_{BG} = -k_B \sum_{i=1}^{\Omega} p_i \ln p_i; \tag{1}$$

with the sum of the probabilities of each state is normalized,

$$\sum_{i=1}^{\Omega} p_i = 1. \tag{2}$$

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For the particular case where each microstate has the same probability, $p_i = 1/\Omega \;\forall\; i$, the very familiar expression for the microcanonical entropy is found,

$$S_{BG} = k_B \ln \Omega. \tag{3}$$

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Introduction

Boltzmann-Gibbs (BG) Statistical Mechanics

- Microcanonical ensemble just requires that the system under study is closed and isolated.
- The probability density of microstates for this ensemble is constant.

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- The probability density of microstates for this ensemble is constant.

Additional ensembles can be constructed adding constrictions, e.g., the **canonical ensemble**, for which all possible energies ϵ_i are assumed to have a probability p_i

$$\sum_i \epsilon_i p_i = \langle E \rangle = U. \tag{4}$$

- The system is in thermal equilibrium with its sorroundings.

We could ask:

Why the need of a different and more general formalism for Statistical Mechanics?

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Before to answer this question, we review some of the features of BG statistics.

[1] A. Campa, T. Dauxois, S. Ruffo, *Phys. Rep.* **480** (2009) 57–159.

Features of Boltzmann-Gibbs Statistics

Features: Extensivity and Additivity

Before to answer this question, we review some of the features of BG statistics.

- Entropy and other thermodynamic potentials are **extensive and additive functions.**

1. Additivity: for the entropies of two independent systems A and B,
$$S_{BG}(A+B) = S_{BG}(A) + S_{BG}(B).$$
2. Extensivity: entropy is proportional to the size of the system, $S_{BG} \propto N$.

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Additivity implies extensivity and non-extensivity implies non-additivity, but not the reverse [1].

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Another feature required for systems is the **concavity** of entropy S_{BG}.

- Entropy must be a **concave function of its parameters** in order to be thermodynamically stable.

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Another feature required for systems is the **concavity** of entropy S_{BG}.

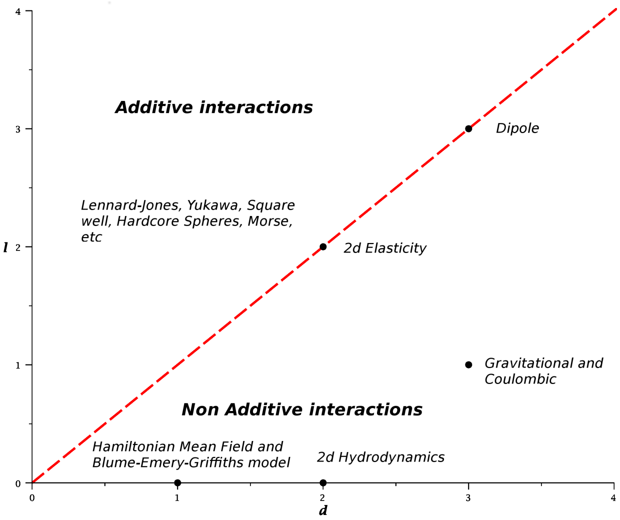
- Entropy must be a **concave function of its parameters** in order to be thermodynamically stable.

A very important feature of BG statistics is the **ensemble equivalence**:

- Thermodynamic information obtained from different statistical ensembles is the same, up to small fluctuations.
- This allows to study systems using the most suitable ensemble, depending on their physical conditions, e.g., controlled pressure, fixed temperature, etc.

These features of BG Statistical Mechanics, are limited to a very particular set of interaction potentials: Additive interactions.

A classification for interactions



Long-range (Non-additive) interactions (LRI)

Definition

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- Considering an interaction potential which decays with distance as r^{-l}.

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In the pairwise approximation, LRI can be defined as follows:

- Considering an interaction potential which decays with distance as r^{-l}.
- For a system in a d-dimensional space, energy per each particle pair is,

$$e = \int_{\delta}^{R} \frac{\rho C}{r^l} d^d r = \rho C \Omega_d \int_{\delta}^{R} r^{(d-1)-l} dr$$
$$= \frac{\rho C \Omega_d}{d-l} [R^{d-l} - \delta^{d-l}]; \qquad \text{if} \quad l \neq d; \tag{5}$$

- The above integral diverges when $l \leq d$.

Types of Long-range interactions

Long range interactions

Interaction	l l/d	Comments
Large systems		
Gravity	1 $1/3$	Long Range
Coulomb	1 $1/3$	Long Range with Debye screening
Dipole	3 1	Limit case
2D Hidrodynamics	0 0	Logaritmic Interactions
Small systems		
Atomic and molecular Clusters Bose–Einstein condensates		Range of the interaction is of the order of the size of the system

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The gravitational interaction is an interesting case, even for LRI.

- Gravitational systems have the following features:

[2] W. Thirring, *Z. Phys.* **235** (1970) 339
[3] M. D'Agostino et al., *Phys. Lett. B* **473** (2000) 219–225.
[4] A. Campa, T. Dauxois, S. Ruffo, *Phys. Rep.* **480** (2009) 57–159.

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Long-range Interactions and the BG Statistics

The Gravitational Case

The gravitational interaction is an interesting case, even for LRI.

- Gravitational systems have the following features:
  1. Thermodynamic instability, due to the purely attractive nature of gravity [2].
  2. Ensemble inequivalence: Microcanonical specific heat can be negative for these systems [3].
  3. Non-additivity and no-extensivity: interaction quantities between subsystems are not negligible $E_{int} \nrightarrow 0$.
  4. Thermodynamic limit is not well defined: The traditional $N \to \infty, V \to \infty, N/V = constant$, does not holds up.
  5. Non-concavity of entropy.
  6. Ergodicity break: Not all accessible thermodynamic states are connected by intermediate ones [4].

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[3] M. D'Agostino et al., *Phys. Lett. B* **473** (2000) 219–225.

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Tsallis Non-extensive (non-additive) Statistics

- Several generalizations for entropy were proposed, to deal (and to try solve the several issues related) with:

$$S(A,B) \neq S(A) + S(B);$$

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- The most well known of these generalizations is the **q-Entropy** or Tsallis entropy, proposed by C. Tsallis [5], which establish that:

$$S_q(A+B) = S_q(A) + S_q(B) + (1-q)S_q(A)S_q(B)\,. \qquad (6)$$

where q is a free parameter which measures the non-extensivity.

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where q is a free parameter which measures the non-extensivity.

- Non-extensivity is achieved by modifying (or generalizing) the definition of entropy:

$$S_q = -k_B \sum_{i=1}^{\Omega} p_i^q \ln_q p_i = \frac{1 - \sum_{i=1}^{\Omega} p_i^q}{1-q}\,. \tag{7}$$

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- The function $\ln_q$ is defined as:

$$\ln_q x = \frac{x^{1-q} - 1}{1 - q} \, . \tag{8}$$

Recovers the usual natural logarithm in the limit $q \to 1$.

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- Microcanonical q-Entropy satisfies the normalization condition,

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- Canonical q-entropy requires the following constriction for energy:

$$\langle E \rangle_q = \frac{\sum_{i=1}^{\Omega} p_i^q \epsilon_i}{\sum_{j=1}^{\Omega} p_j^q} = U_q. \tag{10}$$

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Tsallis Non-extensive (non-additive) Statistics

Modified themodynamic limit

Non-extensive statistics also requires a modification in the thermodynamic limit!!

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Modified themodynamic limit

Non-extensive statistics also requires a modification in the thermodynamic limit!!

- Instead of the well known limit,

$$N \to \infty\,, V \to \infty\,,\ \text{and}\ N/V = const. \tag{11}$$

  This new limit should be considered to take into account the non-additivity, adding a weight factor N^* to some variables as:

$$N^* \propto N^{1-l/d}. \tag{12}$$

- In the gravitational case $d = 3$ and $l = 1$, $N^* \propto N^{2/3}$.

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With the modified limit variables can be classified in:

Tsallis Non-extensive (non-additive) Statistics

Modified themodynamic limit

With the modified limit variables can be classified in:

- Extensives as,

$$\lim_{N,V\to\infty} \frac{S}{N}, \frac{V}{N} = const\,, \tag{13}$$

- Pseudo-extensives (energy type) as,

$$\lim_{N\to\infty} \frac{F^*}{N\,N^*} = const\,, \tag{14}$$

- Pseudo-intensives as

$$\lim_{N\to\infty} \frac{T^*}{N^*}, \frac{P^*}{N^*} = const\,. \tag{15}$$

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Other notions have to be generalized as well. Depending on the ensemble, different quantities are obtained for Tsallis statistics and its respective distribution functions.

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- The Tsallis temperature is defined as

$$T_q \equiv \frac{1}{k_B \beta} = \left(\frac{\partial S_q}{\partial E} \right)^{-1}_{V,N} . \tag{16}$$

- And the Tsallis pressure as

$$P_q = T_q \left(\frac{\partial S_q}{\partial V} \right)_{E,N} . \tag{17}$$

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Tsallis Non-extensive (non-additive) Statistics

However, based on a generalized notion of equilibrium[6][7], instead of the intensive variables above, the true physical intensive quantities for q-statistics are:

[6] S. Abe, et al, Physics Letters A 281, 126 (2001).
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- Tempeature

$$T^* = \left(1 + \frac{1-q}{k_B} S_q\right) \left(\frac{\partial S_q}{\partial E}\right)^{-1}_{V,N} =: \frac{1}{k_B \beta_q}\,, \tag{18}$$

- Pressure

$$P^* = \frac{T^*}{1 + \left[(1-q)/k_B\right] S_q} \left(\frac{\partial S_q}{\partial V}\right)_{E,N} \,. \tag{19}$$

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T he inverse physical temperature is defined as β_q, and proportionality between β and β_q is commonly referred to as c, i.e.,

$$c = 1 + \frac{1-q}{k_B} S_q\,, \qquad (20)$$

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The Newtonian Self-gravitating gas

Considering a non relativistic and isolated system of N point particles interacting via a Newtonian gravitational potential

$$-\frac{1}{|\mathbf{q_i}-\mathbf{q_j}|_A} = \begin{cases} -\frac{1}{|\mathbf{q_i}-\mathbf{q_j}|} & |\mathbf{q_i}-\mathbf{q_j}| \geq A \\ \\ +1/A & |\mathbf{q_i}-\mathbf{q_j}| \leq A. \end{cases} \tag{21}$$

Where A is a short distance cut-off, which satisfies $A \ll L$, with L is the size of the system.

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Where A is a short distance cut-off, which satisfies $A \ll L$, with L is the size of the system. The Hamiltonian of such a system is

$$\mathcal{H} = \mathcal{T} + \mathcal{U} = \sum_{i=1}^{N} \frac{p_i^2}{2m} - Gm^2 u\left(|\mathbf{q_i}-\mathbf{q_j}|\right); \tag{22}$$

The potential $u(|\mathbf{q_i}-\mathbf{q_j}|)$ has been defined as

$$u(|\mathbf{q_i}-\mathbf{q_j}|) = \sum_{1\leq i<j\leq N} \frac{1}{|\mathbf{q_i}-\mathbf{q_j}|_A}. \tag{23}$$

Starting with the canonical ensemble, the partition function is:

$$Z_q = \frac{1}{N! h^{3N}} \int d^{3N}q \, d^{3N}p \, \exp_q\left(-\beta_q \mathcal{H}(\mathbf{p}, \mathbf{q})\right), \tag{24}$$

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- After performing some calculations, Z_q can be written as,

$$\begin{aligned} Z_q &= \frac{V^N \Gamma\left(\frac{2-q}{1-q}\right)}{N! \, h^{3N}} \left(\frac{2\pi m}{(1-q)\beta_q}\right)^{3N/2} \frac{i}{2\pi} \\ &\oint_C dt(-t)^{-\frac{2-q}{1-q} - \frac{3N}{2}} e^{-t} \int d^{3N}r \, e^{\eta_q u(|\mathbf{r_i} - \mathbf{r_j}|)}; \end{aligned} \qquad (25)$$

introducing a dimensionless variable η, and an effective dimensionless potential $u(\cdot)$, which are:

$$\eta = \frac{G m^2 N \beta_q}{L}, \quad u\left(|\mathbf{r_i} - \mathbf{r_j}|\right), \text{ for } 0 < \mathbf{r_k} < 1. \qquad (26)$$

To obtain an explicit expression for the self-gravitating gas, a dilute regime, which assumes low density is considered.

- Taylor expansion of the interaction potential can be carried out, i.e., up to second order,

$$e^{\eta_q u(|\mathbf{r_i}-\mathbf{r_j}|)} \approx 1 + \eta_q u + \frac{1}{2!}\eta_q^2 u^2 \,. \qquad (27)$$

where $\eta_q = \frac{(-t)(1-q)}{N}\eta$.

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  where $\eta_q = \frac{(-t)(1-q)}{N}\eta$.
- In this low density limit the interaction potential can be written as a sum of identical two-body interactions,

$$\begin{aligned} u(|\mathbf{r_i}-\mathbf{r_j}|) &= \frac{1}{|\mathbf{r_1}-\mathbf{r_2}|}\left[(N-1)+(N-2)+\ldots+1\right] \\ &= \frac{1}{|\mathbf{r_1}-\mathbf{r_2}|}\sum_{k=1}^{N}(N-k)\,. \end{aligned} \tag{28}$$

- In the limit $N \to \infty$,

$$u(|\mathbf{r_i} - \mathbf{r_j}|) = \frac{N(N-1)}{2\,|\mathbf{r_1} - \mathbf{r_2}|}\,. \tag{29}$$

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- The quadratic term in (27) can be simplified in a similar manner,

$$\begin{aligned} u(|\mathbf{r_i} - \mathbf{r_j}|))^2 = \quad & \frac{N(N-1)}{2\,|\mathbf{r_1} - \mathbf{r_2}|^2} + \frac{N(N-1)(N-2)}{|\mathbf{r_1} - \mathbf{r_2}|\,|\mathbf{r_1} - \mathbf{r_3}|} \\ & + \frac{N(N-1)(N-2)(N-3)}{4\,|\mathbf{r_1} - \mathbf{r_2}|\,|\mathbf{r_3} - \mathbf{r_4}|}\,. \end{aligned} \tag{30}$$

- In the limit $N \to \infty$,

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- Plugging all of these things into the coordinate integral,

$$e^{\eta_q u(|\mathbf{r_i} - \mathbf{r_j}|))} \approx 1 - tN^2A + t^2N^2B\,. \tag{31}$$

- where,

$$A = \frac{\eta(1-q)b_0}{2N}\left(1-\frac{1}{N}\right), \tag{32}$$

$$B = \frac{\eta^2(1-q)^2}{2N^2}\left[\frac{b_0^2}{4}\left(1-\frac{1}{N}\right)\left(1-\frac{2}{N}\right)\left(1-\frac{3}{N}\right) + \frac{b_2}{2N^2}\left(1-\frac{1}{N}\right) + \frac{b_1}{N}\left(1-\frac{1}{N}\right)\left(1-\frac{2}{N}\right)\right], \tag{33}$$

- Further we have defined the gravitational virial coefficients as

$$
\begin{aligned}
b_0 &= \int_0^1 d^3r_1 d^3r_2 \, \frac{1}{|\mathbf{r_1} - \mathbf{r_2}|} \,, && (34) \\
b_0^2 &= \int_0^1 d^3r_1 d^3r_2 d^3r_3 d^3r_4 \, \frac{1}{|\mathbf{r_1} - \mathbf{r_2}|} \frac{1}{|\mathbf{r_3} - \mathbf{r_4}|} \,, && (35) \\
b_1 &= \int_0^1 d^3r_1 d^3r_2 d^3r_3 \, \frac{1}{|\mathbf{r_1} - \mathbf{r_2}|} \frac{1}{|\mathbf{r_1} - \mathbf{r_3}|} \,, && (36) \\
b_2 &= \int_0^1 d^{3N}r_1 d^{3N}r_2 \, \frac{1}{|\mathbf{r_1} - \mathbf{r_2}|^2} \,. && (37)
\end{aligned}
$$

- These coefficients are just numbers which change depending on the symmetry of the box where the box is contained.

With those approximations, the integral [8] over the auxiliary variable t be can computed,

$$Z_q \approx \left[\frac{2\pi m}{(1-q)\beta_q}\right]^{3N/2} \frac{V^N}{N!\,h^{3N}} \frac{\Gamma\left(\frac{2-q}{1-q}\right)}{\Gamma\left(\frac{2-q}{1-q}+\frac{3N}{2}\right)}$$

$$\times\left[1 + AN^2 \frac{\Gamma\left(\frac{2-q}{1-q}+\frac{3N}{2}\right)}{\Gamma\left(\frac{1}{1-q}+\frac{3N}{2}\right)} + BN^2 \frac{\Gamma\left(\frac{2-q}{1-q}+\frac{3N}{2}\right)}{\Gamma\left(\frac{q}{1-q}+\frac{3N}{2}\right)}\right]$$

$$= Z_q^{(IG)} \cdot Z_q^{(grav)}$$

In the absence of gravitational interaction, $\eta = 0$ (and $A = B = 0$), the result os the same than for the Tsallis canonical ideal gas.

[8] D. Prato, Physics Letters A 203, 165 (1995).

The next step is to calculate the modified thermodynamic limit. Considering $N \to \infty$,

$$\lim_{N\to\infty} \frac{1}{N} \ln Z_q^{(grav)} \simeq \frac{\eta(1-q)b_0}{2} + \eta^2(1-q)^2\left(\frac{b_1}{2} - \frac{b_0^2}{2}\right) \quad (38)$$

This expression allow to calculate relevant thermodynamic quantities.

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- The equation of state for pressure can be calculated with,

$$\frac{P^*}{k_B T^*} = \left(\frac{\partial \ln Z_q}{\partial V}\right)_{T^*}, \quad (39)$$

  which is,

$$\frac{P^* V}{N k_B T^*} = 1 - \frac{\eta}{3N} \frac{\partial}{\partial \eta} \ln Z_q^{(grav)} . \quad (40)$$

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- Substituting (38) into (40), allows us to compute the thermodynamic limit of the equation of state.

$$\frac{P^* V}{N k_B T^*} \simeq 1 - \frac{\eta(1-q)b_0}{6} - \frac{\eta^2(1-q)^2}{3}\left(b_1 - b_0^2\right) . \qquad (41)$$

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  Which exhibits a explicit dependence on the parameter q.

- It is also instructive to consider the specific heat capacity at constant volume, defined in the Tsallis statistics as

$$(c_V)_q = -\frac{T^*}{N} \left(\frac{\partial^2 F^*}{\partial T^*}\right)_V . \tag{42}$$

  Which in the diluted regime is,

$$\frac{(c_V)_q}{k_B} \simeq \frac{3}{2} + \eta^2 (1-q)^2 \left(b_1 - b_0^2\right) . \tag{43}$$

  This result is always positive also in the presence of gravitational forces.

Conclusions

The non-extensive Tsallis formalism has been applied to a Newtonian self-gravitating gas.

- Reasonable and physically sound results were obtained from the application of Tsallis statistics, achieving convergence of important thermodynamic functions and state equations.

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- Tsallis statistics has proved to be a viable tool for the description of systems with long-range forces, but that its application has to be carried out with care.
- In the hopes to find ensemble equivalence in this formalism, the microcanonical ensemble was explored (not shown here); however, it was only partially achieved, up to a factor of $(1-q)$ in the state equation.

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- Another possible way to investigate the equivalence of ensembles is to check whether the probability distribution functions of microcanonical and canonical ensembles are related via a Laplace transformation.

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- The question of ensemble equivalence need more detailed investigations, especially on the exact and correct formulation of the microcanonical ensemble in Tsallis statistics.

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