**Generalized Fluctuation Theory based on the reparametrization invariance of the microcanonical ensemble**

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**Abstract**

The main interest of the present work is the generalization of the Boltzmann-Gibbs distributions and the fluctuation theory based on the consideration of the reparametrization invariance of the microcanonical ensemble. This approach allows a novel interpretation of some anomalous phenomena observed in the non extensive systems like the existence of the negative specific heats as well as possibilities the enhancing of some Monte Carlo methods based on the Statistical Mechanics.

I. INTRODUCTION

We have been witness in the last years of an important reconsideration of the Foundations of the Thermodynamics and the Statistical Mechanics originated from the interest to use this kind of description in systems which are outside the context of their traditional applications. An important area of the nowadays developments is found in the Thermo-statistical description of the called non extensive systems.

The non extensive systems are those non necessarily composed by a huge number of constituents, they could be mesoscopic or even small systems, where the characteristic radio of some underlaying interaction is comparable or larger than the characteristic linear dimension of the system, particularity leading to non existence of statistical independence due to the presence of long-range correlations. In the last years a significant volume of evidences of thermodynamic anomalous behaviors are been found in the study of the non screened plasmas and the turbulent diffusion, astrophysical systems, nuclear, molecular and the atomic clusters, granular matter and complex systems \[^1\] \[^2\] \[^3\] \[^4\] \[^5\] \[^6\] \[^7\] \[^8\] \[^9\] \[^10\] \[^11\].

It is usual to find in this context equilibrium thermodynamic states characterized by exhibiting a negative heat capacity, that is, thermodynamic states where an increment of the total energy leads to a decreasing of the temperature. This behavior is associated to the convexity of the entropy and the corresponding ensemble inequivalence and can appear as a consequence of the small character of the systems (during the first-order phase transitions in molecular and atomic or nuclear clusters \[^12\] \[^13\] \[^14\]) or because of the long-range character of the interactions (see in the astrophysical systems \[^12\]).

The existence of such anomalous thermodynamical behaviors demands new developments within the Equilibrium Statistical Mechanics and the Thermodynamics. An important contribution to the understanding of such phenomena is found in the formulation of the Microcanonical Thermo-statistics by D. H. E. Gross \[^7\]. a theory which returns to the original basis of the Statistical Mechanics with the reconsideration of the well-known Boltzmann epitaph:

\[
S = \log W, \tag{1}
\]

and allows the study of phase transitions in systems outside the thermodynamic limit. Since \(W\) is the number of microscopic states compatible with a given macroscopic state, the Boltzmann entropy \(W\) is a measure of the size of the microcanonical ensemble. Within Classical Statistical Mechanics \(W\) is just the microcanonical accessible phase space volume, that is, a geometric quantity. This explains why the entropy \(W\) does not satisfy the concavity and the extensivity properties, neither demands the imposition of the thermodynamic limit or a probabilistic interpretation like the Shannon-Boltzmann Gibbs extensive entropy:

\[
S_e = - \sum_k p_k \log p_k. \tag{2}
\]

Such geometric character of the Boltzmann entropy leads naturally to the development of geometric formulations of any statistical formulation derived from microcanonical basis.

Motived by the successes of the Gross’ formulation \[^7\], we have performed in the refs.\[^17\] \[^18\] an analysis about the geometric features of the microcanonical ensemble. Particularly, we have shown in the previous paper \[^17\] that the microcanonical description is characterized by the presence of an internal symmetry whose existence is related to the dynamical origin of this ensemble, which has been coined by us as the reparametrization invariance. Such symmetry leads naturally to the development of a non Riemannian geometric formulation within the microcanonical description, which leads to an unexpected generalization of the Gibbs canonical ensemble and the classical fluctuation theory for the open systems, the improvement of Monte Carlo simulations based on the canonical ensemble, as well as a reconsideration of any classification scheme of the phase transitions based on the concavity of the microcanonical entropy.

I shall continuous in the present paper the study of the geometric aspects related to the existence of the reparametrization invariance. The present work addresses the study of those equilibrium situations char-
acterized by the consideration of several control parameters. The main interest will be focussed in the generalization of the well-known Boltzmann-Gibbs distributions and the fluctuation theory related with the consideration of the reparametrization invariance ideas. I realize while writing this work that some of the present ideas have been also rediscovered by Toral in ref. [19] by starting from the Information Theory.

II. ISOLATED SYSTEM

Let us consider an isolated dynamical system whose macroscopic description could be carried out by starting from microcanonical basis. Let \( \hat{I} \equiv \{ \hat{I}_1, \hat{I}_2, \ldots, \hat{I}_n \} \) be the set of all those fundamental physical quantities determining the microcanonical distribution function \( \hat{\omega}_m \):

\[
\hat{\omega}_m(I) = \frac{1}{\Omega(I)} \delta[I - \hat{I}],
\]

which are simultaneously measurable, that is \( [\hat{I}_i, \hat{I}_j] = 0 \), being \( \Omega(I) = \text{Sp} \{ \delta(I - \hat{I}) \} \) the microcanonical partition function. Let us suppose that the eigenvalues of the set \( \hat{I} \) belong to certain subset \( \mathcal{R}_I \) of the Euclidean n-dimensional space \( \mathbb{R}^n \).

Let us consider another subset \( \mathcal{R}_\Theta \subset \mathbb{R}^n \) which is diffeomorphic equivalent to the subset \( \mathcal{R}_I \), that is, there exists a diffeomorphic bijective map \( \Theta : \mathcal{R}_I \rightarrow \mathcal{R}_\Theta \) with a non vanishing Jacobian:

\[
\left| \frac{\partial \Theta}{\partial I} \right| = \text{det} \left[ \frac{\partial \Theta^k(I)}{\partial I^i} \right] \neq 0,
\]

for every point \( I \in \mathcal{R}_I \). It is said that the map \( \varphi \) defines a reparametrization change of the Euclidean subset \( \mathcal{R}_I \). The set of functionals derived from the above map \( \Theta, \hat{\Theta} = \{ \hat{\Theta}^1, \hat{\Theta}^2, \ldots, \hat{\Theta}^n \} = \Theta [\hat{I}] \), determines the same microscopic Physics of the set \( \hat{I} \): every eigenstate \( |\Psi_r\rangle \) of \( \hat{I}, \hat{\Theta} |\Psi_r\rangle = I_n |\Psi_r\rangle \), is also an eigenstate of the set \( \Theta, \hat{\Theta} |\Psi_r\rangle = \Theta [\hat{I}] |\Psi_r\rangle = \Theta (\hat{I} |\Psi_r\rangle) = \Theta (|\Psi_r\rangle \Theta |\Psi_r\rangle) = \Theta_n |\Psi_r\rangle \), and the physical quantities \( \hat{k}^\Theta, \hat{m} \hat{\Theta} \) are also simultaneously measurable, \( [\hat{k}^\Theta, \hat{m} \hat{\Theta}] = 0 \). There is nothing strange that the set \( \hat{\Theta} \) determines also the same macroscopic Physics of the set \( \hat{I} \). Taking into account the well-known property of the Dirac delta function:

\[
\delta(\Theta - \hat{\Theta}) = \left[ \frac{\partial \Theta}{\partial I} \right]^{-1} \delta[I - \hat{I}] \Rightarrow \Omega(\Theta) = \left[ \frac{\partial \Theta}{\partial I} \right]^{-1} \Omega(I),
\]

and therefore:

\[
\frac{1}{\Omega(\Theta)} \delta(\Theta - \hat{\Theta}) = \frac{1}{\Omega(I)} \delta[I - \hat{I}],
\]

The above identity \( \text{[6]} \) expresses an internal symmetry which will be referred as a reparametrization invariance of the microcanonical ensemble. The reparametrization invariance of the microcanonical distribution function \( \hat{\omega}_m \) leads to the reparametrization invariance of the expectation value of any microscopic quantity \( \hat{A} \), \( \hat{A} = \text{Sp} \{ \hat{A} \hat{\omega}_m \} \Rightarrow \hat{A}(I) \equiv \hat{A}(\Theta) \), that is, the expectation values of the microscopic observables behaves as scalar functions under any reparametrization change \( \Theta \).

Mathematically speaking, it is said that the Euclidean subsets \( \mathcal{R}_I \) and \( \mathcal{R}_\Theta \) are identical representations of certain abstract space \( \mathfrak{3} \). The totality of the reparametrization changes among the admissible representations of the space \( \mathfrak{3} \) constitutes a group, the Group of Diffeomorphisms of the space \( \mathfrak{3} \). The reparametrization invariance of the microcanonical ensemble means that such description provides the same macroscopic Physics for all admissible representations of the abstract space \( \mathfrak{3} \).

The microcanonical partition function \( \Omega \) defines an invariant measure \( d\mu = \Omega(\Theta) d\Theta \equiv \Omega(I) d\hat{I} \) which provides the number of microstates \( W_n = \int_{\pi_\sigma} d\mu \) belonging to a small subset \( \pi_\sigma \) of certain coarse grained partition

\[
\mathcal{P} = \{ \pi_\sigma \subset \mathfrak{3} | \bigcup_\pi_\sigma = \mathfrak{3} \}
\]

of the abstract space \( \mathfrak{3} \), and allows us to introduce the Boltzmann entropy \( S_B [\pi_\sigma] = \ln W_\sigma \). Hereafter, I will consider that the number of macrostates \( W_n \) grows exponentially with the increasing of the number \( n \) of the degrees of freedom of the interest system, so that the thermodynamic limit:

\[
s = \lim_{n \rightarrow \infty} \frac{S_B [\pi_\sigma]}{n},
\]

exists and it is independent of the nature of the coarse grained partition \( \pi_\sigma \) of the space \( \mathfrak{3} \) whenever every subset \( \pi_\sigma \) be small. This hypothesis allows us to take the reduced entropy \( s \) as a continuous scalar function defined on the space \( \mathfrak{3} \). When the interest system is large enough, the number of microstates \( W_n \) can be estimated in the practice by \( W_1 \simeq \Omega(I) \delta I_0 \), where \( \delta I_0 \) is a small constant volume. The estimate \( W_1 \) differs from the one obtained in other representation \( W_2 \simeq \Omega(\Theta) \delta \Theta_0 \). However these estimations should lead to the same reduced entropy in the thermodynamic limit \( n \rightarrow \infty \):

\[
s = \lim_{n \rightarrow \infty} \frac{\ln W_2}{n} = \lim_{n \rightarrow \infty} \frac{\ln W_1}{n} \equiv \lim_{n \rightarrow \infty} \frac{1}{n} \ln \left[ \frac{\partial \Theta(\hat{I})}{\partial \hat{I}} \right] \delta I_0 \delta \Theta_0 = 0,
\]

which imposes the restriction that the Jacobian of the reparametrization cannot grow exponentially with \( n \). I shall assume for practical purposes the validity of the approximation \( S \equiv S_1 = \ln W_1 \simeq S_2 = \ln W_2 \) when the interest system is large enough.
III. OPEN SYSTEM

Let us now consider an experimental setup where the interest system is put in contact with certain external apparatus \( \phi_s \), which controls its macroscopic behavior in a way that the expectation values of the physical quantities \( \Theta \equiv \Theta (\hat{I}) \) are kept fixed:

\[
\langle \hat{\Theta} \rangle = S_p \left\{ \Theta^k (\hat{I}; \hat{\omega}) \right\}.
\]  

(10)

The equilibrium distribution function \( \hat{\omega} \) of the interest system under these conditions can be derived from the standard procedure of maximization of the entropy:

\[
S[\hat{\omega}] = -S_p (\hat{\omega} \ln \hat{\omega}),
\]

(11)

which leads directly to the following generalized Boltzmann-Gibbs distribution:

\[
\hat{\omega}_{BG} (\beta) = \frac{1}{Z(\beta)} \exp \left\{ -\beta \hat{I} \right\},
\]

(13)

which is just a special case of the generalized distribution \( \hat{\omega}_{BG} \) with \( \Theta (\hat{I}) \equiv \hat{I} \). The convention \( \lambda_k \cdot \varphi^k \equiv \lambda \cdot \varphi \) will be hereafter adopted in order to simplify our notation. Since the operator:

\[
\exp \left[ -\eta \cdot \Theta (\hat{I}) \right] = \int \exp \left[ -\eta \cdot \Theta (I) \right] \delta \left[ I - \hat{I} \right] dI,
\]

(14)

the canonical partition function \( Z(\eta) \) can expressed as follows:

\[
Z(\eta) = \int \exp \left[ -\eta \cdot \Theta (I) \right] \Omega (I) dI,
\]

(15)

where \( \Omega (I) = S_p \left\{ \delta [I - \hat{I}] \right\} \) is the microcanonical partition function in the representation \( \mathcal{R}_I \) of the space \( \mathfrak{Z} \).

The integral \( \mathcal{R}_I \) when \( \Theta (I) \equiv I \) is just the Laplace transformation:

\[
Z(\beta) = \int \exp [-\beta \cdot I] \Omega (I) dI,
\]

(16)

which supports in the thermodynamic limit \( n \to \infty \) the validity of the well-known Legendre transformation:

\[
P(\beta) = \inf_{I^*} \{ \beta \cdot I - S (I) \},
\]

(17)

between the Planck thermodynamic potential \( P(\beta) = -\ln Z(\beta) \) of the Boltzmann-Gibbs distribution \( \text{(13)} \) and the coarse grained entropy \( S(I) = \ln \Omega (I) \delta I_0 \) of the microcanonical ensemble \( \text{(3)} \). The identity \( \text{(17)} \) represents that a macrostate of the Boltzmann-Gibbs ensemble \( \text{(13)} \) with canonical parameter \( \beta \) is equivalent in the thermodynamic limit \( n \to \infty \) to a macrostate of the microcanonical ensemble \( \text{(3)} \), whose set \( I^* \) represents the point of global minimum of the functional:

\[
P(I; \beta) = \beta \cdot I - S (I),
\]

(18)

within the representation \( \mathcal{R}_I \) of the abstract space \( \mathfrak{Z} \), which satisfies the conditions:

\[
\beta_i = \frac{\partial S(I^*)}{\partial I^i}, \quad \kappa_{ij} = \frac{\partial^2 S(I^*)}{\partial I^i \partial I^j},
\]

(19)

where the entropy Hessian \( \kappa_{ij} \) must be a negative defined matrix, that is, the entropy must be locally concave in the point \( I^* \in \mathcal{R}_I \). Such exigency implies that all those regions of the Euclidean subset \( \mathcal{R}_I \) where the entropy \( S \) is not locally concave will never be equivalent to a macrostate of the Boltzmann-Gibbs ensemble \( \text{(13)} \). This situation is usually referred as an ensemble inequivalence.

Let \( \mathcal{B}_I \) be the Euclidean n-dimensional subset composed by all admissible values of the canonical parameters \( \beta \) of the external apparatus leading to a thermodynamic equilibrium of the interest system characterized by the Boltzmann-Gibbs distribution \( \text{(13)} \). According to the condition \( \text{(19)} \), such thermodynamic equilibrium is characterized by the identification \( \beta = \hat{\beta} \) of the canonical parameters \( \beta \) of the external apparatus with the components \( \hat{\beta} \) of the gradient of the microcanonical entropy, the map \( \psi_I \):

\[
\psi_I : \mathcal{R}_I \to \mathcal{B}_I \equiv \left\{ \hat{\beta} \in \mathcal{B}_I \left| \beta_i = \frac{\partial S(I)}{\partial I^i} \right. \right\},
\]

(20)

in the representation \( \mathcal{R}_I \) of the space \( \mathfrak{Z} \). When the entropy is locally concave in certain subset \( \pi_\alpha \subset \mathcal{R}_I \), the map \( \psi_I \) establishes a bijective correspondence between the subset \( \pi_\alpha \) and certain subset \( \Lambda_\alpha \subset \mathcal{B}_I \). During the ensemble inequivalence the bijective character of the map \( \psi \) is lost. The set \( \hat{\beta} \in \mathcal{B}_I \) of canonical parameters of the external apparatus leads to a macrostate with ensemble inequivalence when there exist at least two distinct points \( I_1 \) and \( I_2 \in \mathcal{R}_I \), where \( \hat{\beta} = \psi_I (I_1) = \psi_I (I_2) \). Thus, the ensemble inequivalence can be seen as a thermodynamic equilibrium where exist a competition among all those microcanonical states \( I_k \in \mathcal{R}_I \) where \( \psi_I (I_k) = \hat{\beta} \).

Let us return to the case of the generalized Boltzmann-Gibbs ensemble \( \text{(12)} \). Taking into account the reparametrization invariance of the measure \( d\mu = \Omega (I) dI = \Omega (\Theta) d\Theta \), the integral \( \text{(15)} \) can be rephrased as follows:

\[
Z(\eta) = \int \exp [-\eta \cdot \Theta] \Omega (\Theta) d\Theta,
\]

(21)

which allows a natural extension of the conventional Statistical Mechanics and Thermodynamics with a simple
reparametrization change $I \to \Theta$ and $\beta \to \eta$: The Legendre transformation between the thermodynamic potentials $P(\eta) = -\ln Z(\eta)$ and $S(\Theta) = \ln \Omega(\Theta) \delta \Theta_0$:

$$P(\eta) = \inf_{\Theta} \{ \eta \cdot \Theta - S(\Theta) \}, \quad (22)$$

and the conditions of the ensemble equivalence:

$$\eta_k = \frac{\partial S(\Theta^*)}{\partial \Theta^k}, \quad \kappa_{km} = \frac{\partial^2 S(\Theta^*)}{\partial \Theta^k \partial \Theta^m}, \quad (23)$$

where the entropy Hessian $\kappa_{km}$ in the representation $R_\Theta$ must be a negative definite matrix, that is, the entropy $S(\Theta)$ must be locally concave in the point $\Theta^* \in R_\Theta$. The above results deserve some remarks.

**Remark 1** While a reparametrization change does not alter the microcanonical description of an isolated system, for an open system such transformation implies a substitution of the external apparatus $\varphi_3 \to \varphi_\eta$ which controls its thermodynamic equilibrium, and consequently, generalized Boltzmann-Gibbs ensembles with different representation $R_\Theta$ and $R_\phi$ provide in general different thermodynamical descriptions.

**Remark 2** The validity of the Legendre transformation (22) implies the local equivalence of the macrostates of different generalized Boltzmann-Gibbs ensembles in the thermodynamic limit $n \to \infty$ whenever they are equivalent to the same macrostate of the microcanonical ensemble. Such equivalence implies a relation among the canonical parameters of the generalized thermostat and an ordinary thermostat: Since $S(I) \equiv S(\Theta)$ when $n \to \infty$, the conditions (12) and (23) lead the following transformation rule during a reparametrization change $\Theta \to I$:

$$\beta_i = \frac{\partial S}{\partial I^i}, \quad \eta_k = \frac{\partial S}{\partial \Theta^k} \Rightarrow \beta_i = \frac{\partial \Theta^k}{\partial I^i} \eta_k, \quad (24)$$

while the entropy Hessian obeys:

$$\kappa_{ij} = \frac{\partial \Theta^k}{\partial I^i} \frac{\partial \Theta^m}{\partial I^j} \kappa_{km} + \frac{\partial^2 \Theta^k}{\partial I^i \partial I^j} \eta_k. \quad (25)$$

Since $R_I$ and $R_\Theta$ are just two admissible representations of the abstract space $3$, the above transformation rules are also applicable to any two admissible representations of $3$. Equation (24) is just the transformation rule of the components of a covariant vector within a differential geometry. However, the entropy Hessian does not represent a second rank covariant tensor, since the transformation rule should be given by:

$$\tau_{ij} = \frac{\partial \Theta^k}{\partial I^i} \frac{\partial \Theta^m}{\partial I^j} \tau_{km} \quad (26)$$

instead of the rule (25). This result leads to an important third remark.

**Remark 3** Since the entropy Hessian is not a second rank covariant tensor, the concavity properties of the entropy may change during the reparametrization changes. Consequently, the regions of ensemble inequivalence between the Boltzmann-Gibbs ensemble and the microcanonical ensemble in the representation $R_I$ does not coincide to the regions of ensemble inequivalence in the representation $R_\Theta$.

Let us consider a trivial example taken from our previous work [17]. Let $s$ be a positive real map defined on a seminfinite Euclidean line $L$, $s : L \to R^+$, which is given by the concave function $s(x) = \sqrt{x}$ in the representation $R_x$ of $L$ (where $x > 0$). Let $\varphi$ be a reparametrization change $\varphi : R_x \to R_y$ given by $y = \varphi(x) = x^t$. The map $s$ in the new representation $R_y$ of the seminfinite Euclidean line $L$ is now given by the function $s(y) = y^2$ (with $y > 0$), which is clearly a convex function.

The third remark implies a revision of our conceptions about the classification of the phase transitions based on the concavity of the entropy and the generalization of some Monte Carlo methods with distribution functions inspired on the Statistical Mechanics.

The first-order phase transitions are closely related with the phenomenon of ensemble inequivalence. Since the ensemble inequivalence depends on the nature of the external apparatus controlling the thermodynamic equilibrium of the interest system, the existence of this anomaly reflects the inability of the external apparatus to control all microcanonically admissible equilibrium states of the interest system, and consequently, this kind of phenomenon can not be relevant within the microcanonical description. The interested reader can see a long discussion about this subject in the ref. [17].

The phenomenon of ensemble inequivalence also implies an important lost of information about the thermodynamical properties of a given system during the phase coexistence in regard to the thermodynamical information which can be derived from the microcanonical description. Such lost of information also leads to the failure of ordinary Monte Carlo methods based on the Boltzmann-Gibbs ensemble in the neighborhood of the first-order phase transitions [20].

The ensemble inequivalence can be successfully avoided by using an appropriate representation $R_\Theta$ within the generalized Boltzmann-Gibbs distribution (12). Therefore, the simple consideration of the reparametrization changes allows a suitable extension of some Monte Carlo methods. This question was discussed in the ref. [18] for the particular case of the Gibbs canonical ensemble. I shall consider below a formal extension of the methodology developed in that reference for enhancing the well-known Metropolis importance sample algorithm [21] by focussing only the most important features. The reader could see the ref. [18] for more details.

The probability of acceptance of a Metropolis move based on the generalized Boltzmann-Gibbs distribution...
where $\Delta \Theta^k = \Theta^k (I + \Delta I) - \Theta^k (I)$. When $n$ is large enough $\Delta I \ll I \Rightarrow \Delta \Theta^k \simeq \{ \partial \Theta^k (I) / \partial I \} \Delta I$, and consequently:

$$
p (I | I + \Delta I) \equiv \min \{ 1, \exp \left[ -\tilde{\beta} \cdot \Delta I \right] \}
$$

(28)

where the effective canonical parameter $\tilde{\beta}_i = \beta_i (I; \eta)$ is given by:

$$
\tilde{\beta}_i = \beta_i (I; \eta) = \frac{\partial \Theta^k (I)}{\partial I} \cdot \eta_i.
$$

(29)

Reader can notice that the above definition is very similar to the transformation rule (24). The difference resides now in the fact that the set $I$ does not take the equilibrium value $I^*$, but it changes during the Monte Carlo dynamics. Thus, the present generalized Metropolis algorithm looks-like an ordinary Metropolis algorithm and the transformation rule (24), the matrix $\Pi$ connects the ensemble equivalence within the generalized Boltzmann-Gibbs description [12] and the transformation rule (24). As already shown in ref. [18], this feature of the present Metropolis algorithm allows the Monte Carlo dynamics to explore the anomalous regions of the subset $R_I$ where the ensemble inequivalence within the Boltzmann-Gibbs description (13) takes place. The reader can see an example of application of this method in the section V. The above observations lead directly to a fourth remark which clarifies us the nature of the generalized thermostat $\varphi_\eta$.

**Remark 4** When the interest system is large enough, the generalized thermostat or reservoir $\varphi_\eta$ leading to the generalized Boltzmann-Gibbs distribution (12) is almost equivalent to an ordinary thermostat $\varphi_\beta$ whose canonical parameters $\tilde{\beta}$ fluctuates with the fluctuations of the physical quantities $I$ of the interest system according to the rule (24).

The fourth remark is particularly interesting. Conventional Thermodynamics usually deals with equilibrium situations where the fundamental physical quantities $I$ are kept fixed when the interest system is isolated (a microcanonical description) or the physical quantities $I$ fluctuate and corresponding canonical parameters $\beta$ are kept fixed by the thermostat (“within canonical description”). The generalized Boltzmann-Gibbs ensemble (12) is just a natural framework for consider all those equilibrium situations where both the fundamental physical quantities $I$ of the interest system and the corresponding effective canonical parameters $\tilde{\beta}$ of the external thermostat fluctuate as a consequence of their mutual interaction. Thus, the ordinary condition for the thermodynamic equilibrium between the canonical parameters of the interest system $\tilde{\beta}$ and the external apparatus $\tilde{\beta}$ only takes place for their corresponding average values:

$$
\langle \tilde{\beta} \rangle = \langle \beta \rangle.
$$

(30)

The last observation leads directly to the main objective of the present study: the implementation of a generalized fluctuation theory based on the reparametrization invariance of the microcanonical ensemble.

**IV. GENERALIZED FLUCTUATION THEORY**

**A. Fundamental results**

Let $\delta I = I - I^*$ and $\delta \beta = \tilde{\beta} - \beta$ be dispersions of the fundamental physical quantities $I$ of the interest system and the effective canonical parameters $\beta$ of the generalized thermostat respectively. Our aim is to obtain the correlations $\langle \delta I^i \delta I^j \rangle$, $\langle \delta \beta_i \delta \beta_j \rangle$ within the generalized Boltzmann-Gibbs description (12) and identify their mutual relationships. It is very important to remark that such correlations depends crucially on the interaction between the interest system and the generalized thermostat, and consequently, the values of these quantities are modified with the change of the external control apparatus.

Let us began from the correlation $\langle \delta I^i \delta I^j \rangle$:

$$
\langle \delta I^i \delta I^j \rangle = \frac{1}{Z(\eta)} \int \delta I^i \delta I^j \exp \left[ -\eta \cdot \Theta (I) \right] \Omega (I) dI,
$$

(31)

where the Gaussian approximations leads directly to the result:

$$
\langle \delta I^i \delta I^j \rangle = \left( \Pi_{ij}^{(I)} \right)^{-1}.
$$

(32)

where the matrix $\Pi_{ij}^{(I)}$ is given by:

$$
\Pi_{ij}^{(I)} = \eta_k \frac{\partial^2 \Theta (I^*)}{\partial I^i \partial I^j} - \frac{\partial^2 S (I^*)}{\partial I^i \partial I^j}.
$$

(33)

The above result generalizes the classical relation among the correlations $\langle \delta I^i \delta I^j \rangle$ and the entropy Hessian $\kappa_{ij}$ [10], $\langle \delta I^i \delta I^j \rangle = -\kappa_{ij}^{-1}$ derived from the Boltzmann-Gibbs distribution (13). Taking into consideration the transformation rule (25), the matrix $\Pi_{ij}^{(I)}$ can be rewritten as follows:

$$
\Pi_{ij}^{(I)} \equiv -\frac{\partial \Theta^k}{\partial I^i} \frac{\partial \Theta^m}{\partial I^j} \kappa_{km}.
$$

(34)

where $\kappa_{km}$ is the entropy Hessian [23] in the representation $R_\Theta$ of the abstract space $\mathcal{Z}$.

The expectation values $\Theta^* = \langle \Theta^k \rangle$ and $\langle \delta \Theta^k \delta \Theta^m \rangle$ with $\delta \Theta = \Theta - \Theta^*$ within the generalized Boltzmann-Gibbs description (12) can be obtained from the Planck thermodynamic potential $P (\eta)$ in the representation $R_\Theta$
The Gaussian estimation of $\langle \delta \Theta^k \delta \Theta^m \rangle$ is given now by the inverse of the entropy Hessian (23):

$$
\langle \delta \Theta^k \delta \Theta^m \rangle = -\kappa^{-1}_{km} = \left( \Pi^{(e)}_{km} \right)^{-1}.
$$

(36)

Taking into account the result (34):

$$
\Pi^{(I)}_{ij} = \frac{\partial \Theta^k}{\partial I^j} \frac{\partial \Theta^m}{\partial I^i} \Pi^{(e)}_{km},
$$

(37)

and therefore, the correlations $\langle \delta I^i \delta I^j \rangle$ and $\langle \delta \Theta^k \delta \Theta^m \rangle$ are related by a transformation rule of second rank contravariant tensors:

$$
\langle \delta I^i \delta I^j \rangle = \frac{\partial I^i}{\partial \Theta^k} \frac{\partial I^j}{\partial \Theta^m} \langle \delta \Theta^k \delta \Theta^m \rangle,
$$

(38)

where the correlations $\langle \delta I^i \delta I^j \rangle$ can be expresses in terms of the Planck thermodynamic potential $P(\eta)$ as follows:

$$
\langle \delta I^i \delta I^j \rangle = -\frac{\partial I^i}{\partial \Theta^k} \frac{\partial I^j}{\partial \Theta^m} \frac{\partial^2 P(\eta)}{\partial \Theta^m \partial \Theta^k \partial \eta_{lm}}.
$$

(39)

The correlations $\langle \delta \beta_i \delta I^j \rangle$ and $\langle \delta \beta_i \delta \beta_j \rangle$ can be derived easily from the correlations $\langle \delta I^i \delta I^j \rangle$. Since $\delta I \ll I^*$ when the interest system is large enough, the dispersion $\delta \beta$ of the effective canonical parameters $\beta = \beta(I; \eta)$ defined in the equation (29) can be estimated in terms of the dispersions $\delta I$ as follows:

$$
\delta \beta_i \equiv \eta_k \frac{\partial^2 \Theta^k \left( I^* \right)}{\partial I^i \partial I^j} \delta I^j,
$$

(40)

and therefore:

$$
\langle \delta \beta_i \delta I^j \rangle = \eta_k \frac{\partial^2 \Theta^k \left( I^* \right)}{\partial I^i \partial I^j} \langle \delta I^n \delta I^j \rangle = F_{in} \langle \delta I^n \delta I^j \rangle.
$$

(41)

Since the definition (33) of the matrix $\Pi^{(I)}_{ij}$ allows us to express the matrix $F_{ij}$ derived from the second derivatives of the map $\Theta$ as follows:

$$
F_{ij} \equiv \eta_k \frac{\partial^2 \Theta^k \left( I^* \right)}{\partial I^i \partial I^j} = \Pi^{(I)}_{ij} + \frac{\partial^2 S \left( I^* \right)}{\partial I^i \partial I^j},
$$

(42)

the correlations $\langle \delta \beta_i \delta I^j \rangle$ can be given by:

$$
\langle \delta \beta_i \delta I^j \rangle = \delta_i^j + \frac{\partial^2 S \left( I^* \right)}{\partial I^i \partial I^j} \langle \delta I^n \delta I^j \rangle,
$$

(43)

where the delta Kronecker $\delta_i^j$ appears as consequence of the presence of the terms $\Pi^{(I)}_{ij} \langle \delta I^n \delta I^j \rangle \equiv \delta_i^j$ which is straightforwardly followed from the equation (32).

Finally, the approximation (40) and the identity (41) allows us to express the correlations $\langle \delta \beta_i \delta \beta_j \rangle$ as follows:

$$
\langle \delta \beta_i \delta \beta_j \rangle = F_{in} F_{jm} \langle \delta I^n \delta I^m \rangle = F_{jm} \langle \delta \beta_i \delta I^m \rangle,
$$

(44)

and considering the relation:

$$
F_{jm} = \langle \delta \beta_i \delta I^m \rangle \Pi^{(I)}_{nm},
$$

(45)

I arrive to the following result:

$$
\langle \delta \beta_i \delta \beta_j \rangle = \langle \delta \beta_i \delta I^m \rangle \Pi^{(I)}_{nm} = \Pi^{(I)}_{nm} \langle \delta \beta_i \delta I^m \rangle.
$$

(46)

The relations (43) and (46) are the fundamental results of the present subsection. Introducing the nomenclature for the correlations tensors $G^{ij} = \langle \delta I^i \delta I^j \rangle$, $M^{ij} = \langle \delta \beta_i \delta I^j \rangle$ and $T_{ij} = \langle \delta \beta_i \delta \beta_j \rangle$, the fundamentals relations can be rewritten as follows:

$$
M^{ij} = M^{ij} \Pi^{(I)}_{nm} M^{nm},
$$

(47)

$$
T_{ij} = M^{ij} G_{nm} M^{nm},
$$

(48)

where $G_{nm} = \left( G^{-1} \right)_{nm} \Pi^{(I)}_{nm}$.

I can substitute (47) in (49) in order to express the correlation matrix $M^{ij}$ in terms of the entropy Hessian $\kappa_{ij}$ and the correlation matrix $G^{ij}$:

$$
T_{ij} = M^{ij} G_{nm} \left( \delta^{i \mu} + \kappa_{i\mu} G^{\mu \nu} \right),
$$

(49)

which can be rewritten as follows:

$$
G^{\mu \nu} T_{ij} = \delta^j_{\mu} + 2G^{\mu \eta} \kappa_{ij} + G^{\mu \nu} \kappa_{i\mu} G^{\nu \kappa} \kappa_{j\kappa} = \left( \delta^j_{\mu} + G^{\mu \eta} \kappa_{ij} \right),
$$

(50)

Therefore, the identity (48) can be expressed as follows:

$$
\langle \delta I^i \delta I^j \rangle \langle \delta \beta_n \delta \beta_j \rangle = \langle \delta I^i \delta \beta_n \rangle \langle \delta I^n \delta \beta_j \rangle.
$$

(51)

The reader may notice that no one of the above identities makes any explicit reference to the representation $R_\alpha$ used in the generalized Boltzmann-Gibbs ensemble $\alpha$, and consequently, such thermodynamical identities possesses a general validity for the case of an external apparatus controlling the average values of the fundamental quantities $I$ of the interest system throughout the identification of the average values of the effective canonical parameters $\beta$ of the external apparatus with the corresponding average values of the parameters $\beta = \partial S/\partial I$ derived from the gradient of the microcanonical entropy $S$ of the interest system.

Since the thermodynamical variables $I$ and $\beta$ are just an admissible representation from the parametrization
invariance viewpoint, the reparametrization change \( I \rightarrow \Theta \) and \( \beta \rightarrow \eta \) leads also to the validity of the relations:

\[
\langle \delta \eta_i \delta \Theta^m \rangle = \delta_k^m + \frac{\partial^2 S (\Theta)}{\partial \Theta^k \partial \Theta^n} \langle \delta \Theta^n \delta \Theta^m \rangle,
\]

(52)

\[
\langle \delta \Theta^i \delta \Theta^m \rangle \langle \delta \eta_i \delta \eta_k \rangle = \langle \delta \eta_i \delta \Theta^m \rangle \langle \delta \eta_i \delta \Theta^r \rangle,
\]

(53)

which means that the fundamental results also exhibit reparametrization invariance.

**B. Some anomalous behaviors revised**

As elsewhere shown \([22]\), the entropy Hessian provides important information about the fluctuations of thermodynamic quantities during the thermodynamic equilibrium of an open system. Such connection is usually derived from the Boltzmann-Gibbs distribution \([13]\) which leads directly within the Gaussian approximation to the following result:

\[
\kappa_{ij} = \frac{\partial^2 S}{\partial I^i \partial I^j} \rightarrow -\kappa_{im} \langle \delta I^m \delta I^j \rangle = \delta^i_j.
\]

(54)

The correlation matrix \( G^{ij} = \langle \delta I^i \delta I^j \rangle \) is always nonnegative, which is easily verified from the following reasonings:

\[
\left( \xi_i \delta I^i \right)^2 = \xi_i \xi_i \langle \delta I^i \delta I^j \rangle = \xi_i G^{ij} \xi_j \geq 0,
\]

(55)

where the equality only takes place when \( \xi \equiv 0 \). Consequently, the applicability of the relation (54) is limited to those regions of the subset \( \mathcal{R} \) where the entropy Hessian be a negative definite matrix, that is, the regions in which is ensured the equivalence between the Boltzmann-Gibbs ensemble \([12]\) and the microcanonical ensemble. Thus, the extrapolation of the formula (54) towards regions of ensemble inequivalence has no sense within the conventional Thermodynamics. Let us consider a very simple example.

Let be a system whose thermodynamical state is determined only by the total energy \( E \). The corresponding canonical parameter is the inverse temperature \( \beta \) of the Gibbs thermostat. The relation (54) is given now by:

\[
-\frac{\partial^2 S (E)}{\partial E^2} \langle \delta E^2 \rangle = 1,
\]

(56)

which can be conveniently rewritten by using the microcanonical inverse temperature \( \beta (E) = 1/T (E) = \partial S (E) / \partial E \) as follows:

\[
\langle \delta E^2 \rangle = - \left( \frac{\partial^2 S (E)}{\partial E^2} \right)^{-1} = - \left( \frac{\partial \beta (E)}{\partial E} \right)^{-1}
\]

\[
= T^2 \frac{dT}{dE} = T^2 C,
\]

(57)

where \( C \) is the heat capacity. Since the average square dispersion of the total energy energy \( \langle \delta E^2 \rangle \geq 0 \), the heat capacity should be nonnegative \( C \geq 0 \). As already mentioned, such relation is only applicable during the ensemble inequivalence.

There is nothing wrong in assuming that all those energetic regions with a convex entropy \( \partial^2 S (E) / \partial E^2 > 0 \) are just thermodynamical states with a negative heat capacity \( C < 0 \). Such anomalous behaviors are well-known since the famous Lyndel-Bell work \([10]\) and them have been also observed recently in experiments involving nuclear or molecular clusters \([12, 13, 14]\). However, the relation between the heat capacity \( C \) with the average energy fluctuations \([57]\) has to be generalized in order to attribute some reasonable physical meaning to these anomalous thermodinamical states in terms of a suitable fluctuation theory. Such generalization is provided precisely by the formula:

\[
\langle \delta \beta \delta E \rangle = 1 + \frac{\partial^2 S (E)}{\partial E^2} \langle \delta E^2 \rangle,
\]

(58)

which is a particular expression of the fundamental result \([13]\) to the unidimensional case (only one control parameter). While the inverse temperature can be kept fixed \( \delta \beta = 0 \) in order to control a microcanonical state with a positive heat capacity \( C > 0 \), such control parameter can not be kept fixed when we deal with microcanonical states with non positive heat capacities \( C \leq 0 \). There \( \langle \delta \beta \delta E \rangle \geq 1 \), which means that the fluctuations \( \beta \) and \( I \) should be correlated in order to ensure the control of such anomalous thermodynamical states, that is, in order to ensure the ensemble equivalence. As already commented in the subsection above, this feature is the key for the success of the Metropolis algorithm based on the generalized Boltzmann-Gibbs ensemble \([12]\).

The heat capacity \( C \) is a very simple example of a response function which characterizes how sensible is the system energy \( E \) (controlled quantity) during a small change of the temperature \( T \) of the thermostat (control parameter). Another example of response function is the magnetic susceptibility \( \chi_B = \partial M / \partial B \), which characterizes how sensible is the system magnetization \( M \) (controlled quantity) during a small change of the external magnetic field \( B \) (control parameter). Thus, the well-known thermodynamical identities:

\[
C = \frac{\partial E}{\partial T} = \beta^2 \langle \delta E^2 \rangle, \quad \chi_B = \frac{\partial M}{\partial B} = \beta \langle \delta M^2 \rangle,
\]

(59)

can be considered as response-fluctuation theorems. As already pointed out, such relations are non applicable during the ensemble equivalence where \( C \) or \( \chi_B \) can admits negative values, and therefore, such thermodynamic theorems should find a natural extension within the present framework.

**C. Microcanonical thermodynamic formalism**

The geometric framework developed in the present work constitutes a natural generalization of the thermo-
dynamic formalism of the conventional Thermodynamics. A key for the success is to perform a thermodynamical description whose essence be so close to the macroscopic picture provided by the microcanonical ensemble, which possesses a hierarchical supremacy in regard to any generalized Boltzmann-Gibbs description \[12\].

The total differentiation of the microcanonical entropy:

\[ dS = \beta_i dI^i \quad \text{with} \quad \beta_i = \frac{\partial S}{\partial I^i}, \quad (60) \]

provides the expectation values of the effective canonical parameters \( \beta \) of an external generalized thermostat and the physical quantities \( I \) in the representation \( \mathcal{R}_I \) of the abstract space \( \mathcal{I} \). The symmetry of the entropy Hessian \( \kappa_{ij} \) leads to what could be considered as the Maxwell identities within the microcanonical description:

\[ \kappa_{ij} = \frac{\partial^2 S}{\partial I^i \partial I^j} = \kappa_{ji} \Rightarrow \frac{\partial \beta_i}{\partial I^j} = \frac{\partial \beta_j}{\partial I^i}, \quad (61) \]

The reparametrization invariance imposes some restrictions to the admissible parameters used in the generalized Boltzmann-Gibbs canonical description within the present geometric framework. As already shown in the equation \[24\], the canonical parameters \( \beta_i \) are just the components of a covariant vector. Such status can not be attributed to the ordinary temperature \( T \) or the external magnetic field \( B \). For example, the Gibbs canonical ensemble written for a ferromagnetic system with Hamiltonian \( \hat{H} \) under an external magnetic field \( B \) directed along the z-axis:

\[ \dot{\omega}_G = \frac{1}{Z(\beta; B_z)} \exp \left[ -\beta \left( \hat{H} - B \hat{M}_z \right) \right], \quad (62) \]

can be considered as a Boltzmann-Gibbs distribution with canonical parameters \( \beta \) and \( \lambda = -\beta B \), whose microcanonical description is given by:

\[ \dot{\omega}_M = \frac{1}{\Omega(U, M_z)} \delta \left( U - \hat{H} \right) \delta \left( M_z - \hat{M}_z \right). \quad (63) \]

While the parametrization \( (\beta, \lambda) \) is just a covariant vector within a differential geometry, such character is not exhibited by the the pair \( (T, B) \), and therefore, this last is not a suitable parametrization of the generalized canonical description from the reparametrization invariance point of view. The above observation inspires a reasonable and necessary redefinition of the concept of response functions in order to preserve the geometric covariance of the thermodynamic formalism developed in this work.

The element of the generalized response matrix \( \chi^{ij} \):

\[ \chi^{ij} = -\frac{\partial \langle I^i \rangle}{\partial \beta_j}, \quad (64) \]

characterizes the rate of change of the average of the \( i \)-th physical quantity \( \langle I^i \rangle \) under a small variation of the \( j \)-th average effective control parameter \( \beta_j = \langle \tilde{\beta}_j \rangle \) of the generalized thermostat. Thus, \( \chi^{ij} \) is a measure of the sensibility of the interest system under the control of the external apparatus. Strictly speaking, the response matrix \( \chi^{ij} \) \[61\] is not a second-rank contravariant tensor. Such character is straightforwardly followed from the fact that the microcanonical counterpart \( \tilde{\chi}_{ij} \) of the inverse response matrix \( \chi^{ij} \):

\[ \chi_{ij} = -\frac{\partial \delta_{ij}}{\partial \langle I^i \rangle}, \]

is just the negative entropy Hessian \( \tilde{\chi}_{ij} = -\kappa_{ij} \) \[19\] which obviously is not a second-rank covariant tensor. The connection between the generalized response matrix \( \chi^{ij} \) and the entropy Hessian \( \kappa_{ij} \) leads directly to rephrased the microcanonical Maxwell identities \[61\] as the symmetric character of the generalized response matrix:

\[ \chi^{ij} = \chi^{ji}, \quad (65) \]

The ensemble equivalence within the generalized Boltzmann-Gibbs ensemble \[12\] in the representation \( \mathcal{R}_I \) demands the negative definition of the entropy Hessian \( \kappa_{ij} \), which is equivalent to demand the positive definition of the generalized response matrix \( \chi^{ij} \) \[61\]. Thus, regions of ensemble equivalence are just regions with anomalous behavior in the response functions \( \chi^0 \).

The correlations matrixes \( G^{ij} = \langle \delta I^i \delta I^j \rangle \), \( M^i = \langle \delta \beta_i \delta I^j \rangle \) and \( T_{ij} = \langle \delta \beta_i \delta \beta_j \rangle \) are related by a set of thermodynamical identities which could be referred as the generalized fluctuation relations:

\[ \langle \delta \beta_i \delta I^j \rangle = \delta_{ij} + \kappa_{ij} \langle \delta I^m \delta I^n \rangle, \quad (66) \]

\[ \langle \delta I^i \delta I^m \rangle \langle \delta \beta_n \delta \beta_j \rangle = \langle \delta \beta_j \delta I^n \rangle \langle \delta \beta_n \delta I^i \rangle, \quad (67) \]

within the representation \( \mathcal{R}_I \). The connection between the entropy Hessian \( \kappa_{ij} \) with the generalized response matrix \( \chi^{ij} \) allows us to rephrase the first-generalized relation \[66\] as follows:

\[ \chi^{ij} = \chi^{im} \langle \delta \beta_m \delta I^i \rangle + \langle \delta I^i \delta I^j \rangle, \quad (68) \]

which is the generalized response-fluctuation theorem. A fundamental difference of the above expressions in regard to the conventional result \[67\] is the presence of a non vanishing correlation matrix \( M^i_j = \langle \delta \beta_i \delta I^j \rangle \). Moreover, the identity \[67\] has no counterpart within the conventional Thermodynamics. Such correlations are not present within the ordinary Boltzmann-Gibbs distribution \[12\] since the canonical parameters of the thermostat are keep fixed, so that \( \delta \beta \equiv 0 \Rightarrow \langle \delta \beta_i \delta I^j \rangle = \langle \delta \beta_i \delta \beta_j \rangle \equiv 0 \). Such limitation does not allow to the Boltzmann-Gibbs description to access to all those regions with a anomalous behavior of the response functions, i.e. regions with a negative heat capacity. As already shown by us in the refs. \[17, 18\], the only way to access to such anomalous regions with ensemble inequivalence within a Boltzmann-Gibbs-like description is by using a generalized thermostat with a fluctuating effective
canonical parameters $\tilde{\eta} = \eta \cdot \partial \tilde{\Theta} / \partial I$ in order to control the thermodynamic equilibrium of the interest system by keeping fixed the averages of the ordinary equilibrium conditions $\langle \tilde{\beta}_i \rangle = \langle \beta_i \rangle$.

The generalized fluctuation relations \cite{16} admit another interpretation. Let us consider a representation $R_J$ where the entropy Hessian be a diagonal matrix in a given point $J$, $\kappa_{ij} = \kappa_i \delta_{ij}$, which can be obtained from the representation $R_J$ by using an appropriate orthogonal rotation. Whenever an Hessian eigenvalue $\kappa_i > 0$ (when the interest point belongs to a regions with ensemble inequivalence) the corresponding correlation $\langle \delta \beta_i \delta J^i \rangle = 1 + \kappa_i \langle (\delta J^i)^2 \rangle$, and consequently:
\begin{equation}
\langle \delta \beta_i \delta J^i \rangle \geq 1. \tag{69}
\end{equation}
Such inequality looks-like an uncertainty relation which talks about that the physical quantity $J^i$ and the corresponding canonical parameter $\beta_i$ of the generalized thermostat can not be kept fixed when the corresponding eigenvalue $\kappa_i$ of the entropy Hessian be nonnegative, that is, when the thermodynamical state of the interest system belongs to a region of ensemble inequivalence. Thus, the quantities $\beta_i$ and $J^i$ can be considered within the present framework as complementary thermodynamic quantities.

This interpretation allows us to refer the generalized fluctuation identities \cite{16} as uncertainty thermodynamic relations \cite{17}.

It is necessary before end this subsection to devote some comments about the phase transitions. The phase transitions within the conventional Thermodynamics are mathematically identified by the non analyticities of the thermodynamic potential which is relevant in a given application. Within the microcanonical description of an isolated system the only relevant thermodynamic potential is the microcanonical entropy $S$.

The microcanonical entropy $S$ is always a continuous function, and it is analytical whenever the number of degrees of freedom of the interest system $n$ be finite. Thus, as in the conventional Thermodynamics, the non analyticities of the entropy per particle $s = S/n$ can appear only in the thermodynamic limit $n \to \infty$. Since the microcanonical entropy is a scalar function from the viewpoint of the reparametrization invariance, its nonanalyticities will appears in any representation $R_\Theta$ of the abstract space $\mathcal{S}$, and therefore, these mathematical anomalies are reparametrization invariant. Thus, the lost of analyticity of the microcanonical entropy is identified in the present geometric framework as the mathematical signature of the microcanonical phase transitions. It is said microcanonical phase transitions in order to distinguish them from other macroscopic anomalies which are related with the occurrence of the phenomenon of ensemble inequivalence in an open system. Generally speaking, there exist two generic types of microcanonical phase transitions: the microcanonical discontinuous phase transitions (associated to a discontinuity in some of the first derivatives of the microcanonical entropy $S$) and the microcanonical continuous phase transitions (associated to lost of analyticity of the microcanonical entropy $S$ with continuous first derivatives).

The dynamical origin of the microcanonical ensemble leads to identify any microcanonical phase transition as the occurrence of some kind of dynamical anomaly in the microscopic picture of the system. The evidences analyzed in the previous work \cite{17} suggest strongly that the microcanonical phase transitions are directly related with the occurrence of the ergodicity breaking phenomenon, which takes place when the time averages and the ensemble averages of certain macroscopic observables can not be identified due to the microscopic dynamics is effectively trapped in different subsets of the configurational or phase space during the imposition of the thermodynamic limit $n \to \infty$ \cite{23}.

As elsewhere shown, the convexity of the microcanonical entropy leads to the existence of a lost of analyticity of the Planck thermodynamical potential $P(\beta)$ in the thermodynamic limit via the Legendre transformation \cite{17}. Such discontinuity in some of the first derivatives of $P(\beta)$ is the signature of the first-order phase transitions in the conventional Thermodynamics. It is necessary to remark at this point that this kind of anomalies can not be microcanonically relevant since they have only sense for the open systems instead of the isolated ones \cite{17}. The first-order phase transitions are untimely related with the phenomenon of ensemble inequivalence appearing as a consequence of the non negative definition of the entropy Hessian $\kappa_{ij}$ in a given representation $R_\Theta$ of the abstract space $\mathcal{S}$. Therefore, the existence of the ensemble inequivalence depends crucially on the nature of the external apparatus controlling the thermodynamic equilibrium of the interest system. Thus, the first-order phase transitions can be considered as avoidable thermodynamical anomalies of the open systems. This last feature can be used for enhancing the available Monte Carlo methods based on the Statistical Mechanics in order to avoid the ensemble inequivalence by considering the generalized Boltzmann-Gibbs distributions \cite{17}.

I recommend to the interested reader to read the long discussion exposed in the ref. \cite{17} for a better understanding about all these important questions. I shall consider in the section an example where the existence of a first-order phase transition in the canonical description hides the occurrence of two microcanonical phase transitions in the thermodynamical description of the $q = 10$ states Potts model system.

D. Conjugate variables and the Riemannian interpretation of the fluctuations

The introduction of the dispersion $\delta \omega_i$:
\begin{equation}
\delta \omega_i = \delta \beta_i - \kappa_i \delta I^i, \tag{70}
\end{equation}
allows to rewrite the fundamental relation \cite{18} as follows:
\begin{equation}
\langle \delta \omega_i \delta I^i \rangle = \delta_i^2. \tag{71}
\end{equation}
The correlations \( \langle \delta \omega_i \delta \omega_j \rangle \) can be derived as follows:

\[
\begin{align*}
= (\delta \beta_i \delta \omega_j) - \kappa_{in} (\delta I^n \delta \omega_j), \\
= (\delta \beta_i \delta \omega_j) - \kappa_{ij}, \\
= T_{ij} - \kappa_{ij},
\end{align*}
\]

where the substitution of equation (17) and (19) leads finally to the following result:

\[
\langle \delta \omega_i \delta \omega_j \rangle = G_{ij}.
\]  

(73)

It is very easy to notice that the quantity \( \omega_i \) is just the difference between the effective canonical parameter \( \tilde{\beta} = \eta \cdot \partial \Theta / \partial I \) of the external apparatus \( \varphi_\eta \) and the canonical parameter of the system \( \beta = \partial S / \partial I \), \( \omega_i \equiv \tilde{\beta}_i - \beta_i \), that is:

\[
\omega_i = \eta_k \frac{\partial \Theta_k}{\partial I^i} - \frac{\partial S}{\partial I^i} = \frac{\partial}{\partial I^i} P(\Theta; \eta),
\]

(74)

where \( P(\Theta; \eta) \) is the functional:

\[
P(\Theta; \eta) = \eta \cdot \Theta - S.
\]  

(75)

The quantities \( \omega = \{ \omega_i \} \) and \( I = \{ I^i \} \) can be classified as conjugated variables since they obey the relations:

\[
\langle I^{i'} I^j \rangle = G \delta_{ij}, \quad \langle \delta \omega_i I^{i'} \rangle = \delta \omega_i G^{i'}, \quad \langle \delta \omega_i \delta \omega_j \rangle = G_{ij}.
\]  

(76)

In fact, the approximation (40) leads directly to the following transformation rule between the fluctuations \( \delta \omega ' s \) and \( \delta I ' s \):

\[
\delta \beta_i = F_{ij} \delta I^j \Rightarrow \delta \omega_i = G_{ij} \delta I^j;
\]

(77)

which allows us to obtain the second and third identities from the definition of the correlation matrix \( G^{ij} \) in the equations (70).

The generalized Boltzmann-Gibbs distribution (12) can be rephrased as follows:

\[
d\omega_{GC} \{ I \} = \frac{1}{Z(\eta)} \exp \left[ -\eta \cdot \Theta(I) + S(I) \right] \frac{dI}{\delta I_0},
\]

\[
eq \frac{1}{Z(\eta)} \frac{dI}{\delta I_0} \exp \left[ -P(\Theta; \eta) \right] dI.
\]

(78)

The power expansion of the functional \( P(\Theta; \eta) \) in the neighborhood of its minimum is given by:

\[
P(\Theta; \eta) = P(\Theta^*; \eta) + \frac{\partial P(\Theta^*; \eta)}{\partial I^i} \delta I^i + \frac{1}{2} \frac{\partial^2 P(\Theta^*; \eta)}{\partial I^i \partial I^j} \delta I^i \delta I^j + \ldots
\]

\[
= P^* + \omega_i^* \delta I^i + \frac{1}{2} G_{ij} \delta I^i \delta I^j + \ldots
\]

(79)

where

\[
\omega_i^* = \frac{\partial P(\Theta^*; \eta)}{\partial I^i} = 0, \quad G_{ij} = \frac{\partial^2 P(\Theta^*; \eta)}{\partial I^i \partial I^j}.
\]

(80)

The Gaussian approximation allows us to estimate the canonical partition function as follows:

\[
Z(\eta) \cong \exp \left[ -P^* \right] \sqrt{\det (2 \pi G^{ij})} \delta I_0^{-1},
\]

(81)

which allows us to estimate finally the generalized Boltzmann-Gibbs distribution in terms of the variable \( I \) by:

\[
d\omega_{GC} \{ I \} = \frac{1}{\sqrt{\det (2 \pi G^{ij})}} \exp \left\{ -\frac{1}{2} G_{ij} \delta I^i \delta I^j \right\} dI.
\]

(82)

The transformation from \( I \) towards the conjugated variables \( \omega \) allows us to rewrite the above results as follows:

\[
d\omega_{GC} \{ \omega \} = d\omega \int \delta (\omega - \omega(I)) d\omega_{GC} \{ I \},
\]

(83)

which leads immediately within the Gaussian approximation to the result:

\[
d\omega_{GC} \{ \omega \} \equiv \frac{1}{\sqrt{\det (2 \pi G^{ij})}} \exp \left\{ -\frac{1}{2} G^{ij} \omega_i \omega_j \right\} d\omega.
\]

(84)

The correlation tensor \( G^{ij} \) or \( G^{ij} \) arises as a consequence of the interaction between the generalized thermostat \( F_{ij} \) and the interest system \( \{ \kappa_{ij} \} \) within the generalized Boltzmann-Gibbs description \( G_{ij} = F_{ij} - \kappa_{ij} \). Such tensor provides in this context a Riemannian interpretation of the fluctuations, where the norm:

\[
\delta s^2 = G_{ij} \delta I^i \delta I^j,
\]

(85)

is directly related to the probability of occurrence of a given fluctuation \( \delta I = I - I^* \) around the thermodynamic equilibrium of the system in accordance with the equation (82). I refer to a Riemannian metric since the correlation matrix \( G_{ij} \) behaves as a second-rank tensor under a given reparametrization \( \nu : R_I \rightarrow R_I \) within the same representation \( R_\eta \) of the generalized Boltzmann-Gibbs ensemble. Taking into account \( J = \nu(I) \Rightarrow \Theta(I) = \Theta[\nu^{-1}(J)] \), the expression of the correlation matrix in the representation \( R_J \) is:

\[
G_{\alpha \beta} = \frac{\partial^2 P(\Theta^*; \eta)}{\partial J^\alpha \partial J^\beta} = \frac{\partial I^i \partial I^j}{\partial J^\alpha \partial J^\beta} G_{ij} + \frac{\partial^2 I^i}{\partial J^\alpha \partial J^\beta} \omega_i^*.
\]

(86)

where the vanishing of the second terms takes place as a consequence of the stationary conditions (80). This result generalizes the other Riemannian interpretations of the Thermodynamics obtained in the past (22). While the covariant second-rank tensor \( G_{ij} \) characterizes the probabilities of the fluctuations of the physical quantities \( I = \{ I^i \} \) of the interest system, its corresponding contravariant tensor \( G^{ij} \) characterizes the probabilities of the fluctuations of the conjugated variables \( \omega = \{ \omega_i \} \) in the neighborhood of its expectation \( \omega^* = \langle \omega \rangle = \langle \tilde{\beta} \rangle - \langle \tilde{\beta} \rangle \equiv 0 \) in accordance with the equation (83),
which provides us information about the unusual thermodynamic equilibrium between the generalized thermostat and the interest system. Thus, the conjugated character of the variables $\omega$ and $I$ is closely related with the complementary character of the canonical parameters $\hat{\beta}$ or $\hat{\beta}$ and their corresponding physical quantities of the interest system $I$.

V. A FORMAL APPLICATION

Let us reconsider again the example about a ferromagnetic system under the influence of an external magnetic field $B$ directed along the $z$-axis. Let us introduce a distinction between the internal Hamiltonian $\hat{H}$ (related with the system internal energy $U$) and the total Hamiltonian $\hat{H}_B = \hat{H} - BM_z$ (related with the total energy $E = U - BM_z$). As already commented, the Boltzmann-Gibbs distribution of the system under these conditions:

$$\hat{\omega}_G = \frac{1}{Z(\beta; B)} \exp \left[ -\beta \hat{H}_B \right], \quad (87)$$

can be reinterpreted as a Boltzmann-Gibbs distribution (BGE) with canonical parameters $\beta$ and $\lambda = -\beta B$:

$$\hat{\omega}_G = \frac{1}{Z(\beta; \lambda)} \exp \left[ -\beta \hat{H} - \lambda \hat{M}_z \right]. \quad (88)$$

The above observation allows to distinguish the usual microcanonical description (IME):

$$\hat{\omega}_M = \frac{1}{\Omega(U; B)} \delta \left( U - \hat{H}_B \right), \quad (89)$$

from the detailed microcanonical description (DME):

$$\hat{\omega}_M = \frac{1}{\Omega(U, M_z)} \delta \left( U - \hat{H} \right) \delta \left( M_z - \hat{M}_z \right). \quad (90)$$

While the canonical ensembles (87) and (88) are identical, the microcanonical ensembles (89) and (90) are essentially inequivalent. The above interpretation allows us to consider the modulus of the external magnetic field $B$ or more exactly, the quantity $\lambda = -\beta B$ as the canonical control parameter which is thermodynamically complementary to the magnetization of the system $M_z$. Consequently, the macroscopic description provided by ensemble (89) can be considered as an intermediate description between the DME (90) and the BGE (88), which leads to the following hierarchy among these ensembles: DME $\Rightarrow$ IME $\Rightarrow$ BGE. This hierarchy presupposes that the description DME contains more information than the IME description, and at the same time this last one contains more information than the BGE description.

Let us consider the analysis of the above magnetic system in terms of the thermodynamic formalism. The total differential of the microcanonical entropy of the detailed ensemble $\hat{\omega}_M$ $S(U, M_z)$ is simply given by:

$$dS = \beta dU + \lambda dM, \quad (91)$$

where:

$$\beta = \frac{\partial S}{\partial U}, \quad \lambda = \frac{\partial S}{\partial M_z} \Rightarrow \left( \frac{\partial \lambda}{\partial U} \right)_{M_z} = \left( \frac{\partial \beta}{\partial M_z} \right)_{U}. \quad (92)$$

The introduction of the total energy $U = E + BM_z$ allows to rewrite the above expression as follows:

$$dS = \beta (dU - B dM) = \beta (dE + M_z dB), \quad (93)$$

from which are derived the relations:

$$\tilde{S}(E; B) = S(U, M_z), \quad (94)$$

$$\beta = \frac{\partial \tilde{S}}{\partial E}, \quad \beta M_z = \frac{\partial \tilde{S}}{\partial B} \Rightarrow \left( \frac{\partial (\beta M_z)}{\partial E} \right)_B = \left( \frac{\partial \beta}{\partial B} \right)_E. \quad (95)$$

Thus, the consideration of the total energy $E$ instead of the internal energy $U$ corresponds to a reparametrization where $(U, M_z) \Rightarrow (E, B)$. Reader can notice that such transformation does not correspond to the diffeomorphic transformation considered by the reparametrization invariance of the microcanonical ensemble discussed in the present work. Finally, the Planck potential $P(\beta, \lambda)$ of the BGE is derived from the DME microcanonical entropy $S(U, M_z)$ throughout the Legendre transformation as follows:

$$P(\beta, \lambda) = \beta U + \lambda M_z - S(U, M_z), \quad (96)$$

which is equivalent to the one obtained from the IME microcanonical entropy $\tilde{S}(E; B)$ by considering the relations $\lambda = -\beta B$ and $E = U - BM_z$:

$$P(\beta, \lambda) = \beta U - \beta BM - S(U, M_z) = \beta E - \tilde{S}(E; B) = P(\beta; B). \quad (97)$$

The microcanonical partition functions $\Omega(U, M_z)$ and $\Omega(E; B)$ are related as follows:

$$\Omega(E; B) = \int \Omega(U, M_z) \delta \left( U - E - BM_z \right) dU dM_z, \quad (98)$$

which leads to the following maximization problem in the thermodynamic limit:

$$\tilde{S}(E; B) = \sup_{M_z} \{ S(E + BM_z, M_z) \}, \quad (99)$$

whose stationary conditions are given by:

$$\frac{\partial S(U, M_z)}{\partial U} B + \frac{\partial S(U, M_z)}{\partial M_z} = 0, \quad (100)$$

$$B \frac{\partial^2 S}{\partial U^2} + 2B \frac{\partial^2 S}{\partial U \partial M_z} + \frac{\partial^2 S}{\partial M_z^2} < 0. \quad (101)$$
The relation \( \xi \) clarifies the precise meaning of the relation \( \xi \), which talks us that the reparametrization \((U, M) \rightarrow (E, B)\) in the thermodynamic limit is just a kind of projection where it could be involved an important lost of thermodynamic information.

Taking into consideration that \( \beta = \partial S/\partial U \) and \( \lambda = \partial S/\partial M \), the condition \( \xi \) is just the relation \( \lambda = -\beta B \). On the other hand, the general solution of this stationary condition leads to what could be called as the microcanonical magnetization curve at a given magnetic field \( B \), \( M = M(U; B) \). Generally speaking, such microcanonical magnetization curve could be a multivalued function of the internal energy, that is, there could be more than one admissible value of the magnetization \( M \) at a given value of the internal energy \( U \). However, only those points of the microcanonical magnetization curve satisfying the stability condition \( \xi \) will be observed within the IME description. Such condition is related with the negative definition of the entropy Hessian \( \kappa \), which can be rephrased by eliminating the magnetic field \( B \) as follows:

\[
\xi = \lambda^2 \kappa_{UU} + \lambda \beta (\kappa_{UM} + \kappa_{MU}) + \kappa_{MM} \beta^2 < 0, \quad (102)
\]

where the stationary condition \( \xi \) was taken into account. Thus, all those points where \( \xi > 0 \) can not be observed in the IME description, and consequently, such possibility involves a lost of thermodynamic information in regard to the one provided by DME description. Thus, some branches of the microcanonical magnetization curve can disappear within the IME description, leading in this way to the existence of discontinuities. Such discontinuities can be considered as the signature of microcanonical discontinuous phase transitions within the IME description because of them represent discontinuities in the first derivative

\[
\beta M = \frac{\partial \tilde{S}}{\partial B} \quad (103)
\]

of the IME microcanonical entropy \( \tilde{S}(E; B) \). The lost of information is more significant in the BGE description, which demands now the negative definition of the entropy Hessian:

\[
\kappa_{UU} < 0, \quad \kappa_{MM} \kappa_{UU} - \kappa_{UM} \kappa_{MU} > 0, \quad (104)
\]

which is more restrictive than the condition \( \xi \), that is, the attainability of the condition \( \xi \) leads to the attainability of \( \xi \), but the converse is not true.

The picture described above can be observed during the study of the thermodynamic properties of the \( q = 10 \) states Potts model [24]:

\[
\tilde{H} = \sum_{\langle ij \rangle} (1 - \delta_{\sigma_i \sigma_j}) \quad (105)
\]

where the sum involves only neighbor-neighbor interactions on a square lattice \( L \times L \) with periodic boundary conditions. The spin variable of the \( i \)-th site \( \sigma_i = 1, 2, ..., 10 \) are rephrased as bidimensional vector \( \mathbf{s}_i = [\cos(\omega \sigma_i), \sin(\omega \sigma_i)] \) with \( \omega = 2\pi/q \), which allows to introduce the microscopic magnetization as follows \( M = \sum_i s_i \).

The study of this model system with \( L = 25 \) by using the Gibbs canonical ensemble [57] is characterized by the existence of a discontinuous phase transition at \( \beta_c \simeq 1.42 \) with \( B = 0 \), which is recognized by the existence of a plateau in the caloric curve \( \beta \) versus \( \varepsilon \) \((\varepsilon = E/N \) is the energy per particle with \( N = L^2 \)) from \( \varepsilon_1 \simeq 0.319 \) to \( \varepsilon_2 \simeq 0.909 \) corresponding to a latent heat \( q_0 = \varepsilon_2 - \varepsilon_1 \simeq 0.78 \). As already commented, the first-order phase transition within the Gibbs canonical ensemble is a consequence of an ensemble inequivalence between this description and the IME description [89], which takes place as a consequence of the existence of thermodynamical states with a negative specific heat. These anomalous states manifest themselves as a backbending in the caloric curve within the IME microcanonical ensemble [89].

![Caloric curve](image)
ical phase transitions at

e shows a comparative study between two Monte Carlo

lines indicate the limit of the energetic region with a negative

heat capacity hidden by the ensemble inequivalence.

The study of the magnetic properties of this system

within the IME microcanonical ensemble [S9] at B = 0

is shown in the FIG[2]. This figure reveals the existence of
two microcanonical phase transitions which are hidden

by the ensemble inequivalence within the Gibbs canonical
description. It is easy to show that such anomalies

are directly related with the lost of analyticity of the

microcanonical entropy \( \hat{s}(\varepsilon; B) \) in the thermodynamic

limit as well as the occurrence of ergodicity breaking

in the microscopic picture of the system. The interested

reader can see more details about this study in the

refs.[17, 18]. In spite of the significant amount of ther-

odynamical information provided by the IME description

[S9] in regard to the BGE [S7], the discontinuous

character of the magnetization curve is a clear indica-

tion about the lost of information of the IME description

in regard to the DME one [M10] appearing as a conse-

quence of the unattainability of the condition (102) for

some macrostates. The Monte Carlo simulations shows

the existence of several metastable states with differ-

ent magnetizations in the energetic region \( (\varepsilon_A, \varepsilon_B) \)

with \( \varepsilon_A \simeq 0.7 \) and \( \varepsilon_B \simeq 0.93 \), which indicates clearly the mul-
tivariate character of the microcanonical magnetization

curve \( M = M(U; B = 0) \) in the DME description, which

should exhibit an anomalous branch characterized by an

increasing of the magnetization with the increasing of the

internal energy \( \partial M/\partial U > 0 \).

In complete analogy with the Gibbs canonical ensemble

case, the existence of metastable states provokes an

exponential divergence of the correlation times with the

increasing of the system size during the Monte Carlo sim-

ulations, a dynamical phenomenon referred in the litera-

ture as supercritical slowing down. The existence of this

phenomenon is untimely related with the lost of informa-
tion associated to the ensemble inequivalence. To avoid

this difficulty is necessary to perform a thermodynamic

description within the DME ensemble. This aim could be

carried out in an appropriated canonical-way within

a generalized Boltzmann-Gibbs description [M12] whose

generalized thermostat exhibits two fluctuating effective

control parameters \( \beta \) and \( \lambda \). This is just an unusual

equilibrium situation from the conventional Thermody-

namics viewpoint characterized by a fluctuating tempera-
ture \( \tilde{T} = 1/\beta \) and a fluctuating external magnetic field

\( B = -\lambda/\beta \).

The dependence of the canonical parameters \( \beta = \partial S/\partial U \)

and \( \lambda = \partial S/\partial M \), with the microcanonical vari-

ables \( (U, M_z) \) can be obtained by computing the averages

\( \beta = \langle \hat{\beta} \rangle, \lambda = \langle \hat{\lambda} \rangle, U = \langle \hat{U} \rangle \) and

\( M_z = \langle \hat{M}_z \rangle \). (107)

The components of the entropy Hessian \( \kappa_{ij} = \{\kappa_{UU}, \kappa_{UM}, \kappa_{MU}, \kappa_{MM}\} \)

can be derived from the gener-

alized fluctuations relations:

\[
\langle \delta \beta \delta U \rangle = 1 + \kappa_{UU} \langle \delta U^2 \rangle + \kappa_{UM} \langle \delta M_z \delta U \rangle, \tag{108}
\]

\[
\langle \delta \beta \delta M_z \rangle = \kappa_{UU} \langle \delta U \delta M_z \rangle + \kappa_{UM} \langle \delta M_z^2 \rangle, \tag{109}
\]

\[
\langle \delta \lambda \delta U \rangle = \kappa_{MU} \langle \delta U \delta M_z \rangle + \kappa_{MM} \langle \delta M_z \delta U \rangle, \tag{110}
\]

\[
\langle \delta \lambda \delta M_z \rangle = 1 + \kappa_{MU} \langle \delta U \delta M_z \rangle + \kappa_{MM} \langle \delta M_z^2 \rangle. \tag{111}
\]

Reader can see all these behaviors in the FIG[11] which

shows a comparative study between two Monte Carlo

simulations of this toy system at \( B = 0 \): the well-

known Swedsen-Wang clusters algorithm (SW) based on

the Gibbs canonical ensemble [K20] and the Metropolis

Monte Carlo algorithm (GMMC) based on the gen-

eralized Boltzmann-Gibbs ensemble [K12] explained in the

section III and the ref.[18]. The SW algorithm is unable

to describe all those states with a negative heat capacity,

a task successfully performed by using the GMMC al-

gorithm. The key for the success of this last Monte Carlo

method is precisely the using of a generalized Gibbs ther-

mostat with a fluctuating inverse temperature \( \beta \). The

caloric curve is obtained here by computing the average

values \( \beta = \partial \hat{s}(\varepsilon; B) / \partial \varepsilon = \langle \hat{\beta} \rangle \) and

\( \varepsilon = \langle \hat{\varepsilon} \rangle \), while the

curvature or entropy Hessian \( \kappa = \partial^2 \hat{s}(\varepsilon; B) / \partial \varepsilon^2 \) can be derived from the unidimensional generalized fluctuation relation:

\[
\langle \delta \beta \delta \varepsilon \rangle = 1 + \kappa \langle \delta \varepsilon^2 \rangle \tag{106}
\]

by computing the correlations \( \langle \delta \beta \delta \varepsilon \rangle \) and \( \langle \delta \varepsilon^2 \rangle \). Reader

can notice that no abrupt change of the energy appear

by using the GMMC algorithm, which illustrates us the

avoidable character of the first-order phase transitions,

and therefore, the irrelevance of such anomalies within a

microcanonical description.

FIG. 2: Magnetic properties of the \( q = 10 \) states Potts model

at zero magnetic field \( B \) within the IME microcanonical de-

scription in which is shown the existence of two microcan-

onical phase transitions at \( \varepsilon_{fp} \simeq 0.7 \) (ferro-ferro, discontinuous

PT) and \( \varepsilon_{fp} \simeq 0.8 \) (ferro-para, continuous PT). The dash-dot

lines indicate the limit of the energetic region with a nega-

tive heat capacity hidden by the ensemble inequivalence.

FIG.

II

III

ferromag.

phases

discontinuous

phase transition

paramag.

phase

derivative

edges of the region

with \( \kappa > 0 \)

paramag.

phases

discontinuous

phase transition

microcanonical description.
by computing the four components of the correlation matrix \( M^2 = \{ \delta \delta U, \delta \delta M, \delta \lambda \delta U, \delta \lambda \delta M \} \) and the four component of the correlation matrix \( G^2 = \{ \langle U^2 \rangle, \delta U \delta M, \delta M \delta U, \langle M^2 \rangle \} \). The microcanonical entropy \( S(U, M) \) can be derived from the direct numerical integration of the canonical parameters \((\beta, \lambda)\) and the entropy Hessian \( \kappa_{ij} \). The possibility of perform such study will be accounted in a forthcoming paper.

As already shown in the subsection IV C, the above generalized fluctuation relations can be rewritten by introducing the generalized response matrix \( \chi^2 \):

\[
\chi^{UU} = \frac{\partial U}{\partial \beta}, \quad \chi^{UM} = \frac{\partial U}{\partial \lambda},
\]

\[
\chi^{MU} = -\frac{\partial M}{\partial \beta}, \quad \chi^{MM} = -\frac{\partial M}{\partial \lambda},
\]

as follows:

\[
\chi^{UU} = \langle \delta U^2 \rangle + \chi^{UU} \langle \delta \delta U \rangle + \chi^{UM} \langle \delta \delta M \rangle, \quad \chi^{UM} = \langle \delta U \delta M \rangle + \chi^{UU} \langle \delta \delta U \rangle + \chi^{UM} \langle \delta \delta M \rangle, \quad \chi^{MU} = \langle \delta M \delta U \rangle + \chi^{MU} \langle \delta \delta U \rangle + \chi^{MM} \langle \delta \delta M \rangle, \quad \chi^{MM} = \langle \delta M^2 \rangle + \chi^{MU} \langle \delta \delta U \rangle + \chi^{MM} \langle \delta \delta M \rangle.
\]

The above expressions exhibit the intrinsic reparametrization invariance of the geometrical theory developed in the present work. However, conventional Thermodynamics usually deals with the total energy \( E = U - BM \) and the external magnetic field \( B \) instead of the internal energy \( U \) and the magnetization \( M \). This is the reason why it is very interesting to rephrased the above results in terms of \( E \) and \( B \).

Let us began with the components of the generalized response matrix, which can be rephrased as:

\[
\chi^{UU} = -\frac{\partial E}{\beta} + B \frac{\partial M}{\beta} + \frac{1}{\beta} \left( \frac{\partial E}{\partial B} + B \frac{\partial M}{\partial B} + M \right), \quad \chi^{UM} = \frac{\partial E}{\beta} \left( \frac{\partial E}{\partial B} + B \frac{\partial M}{\partial B} + M \right),
\]

\[
\chi^{MU} = -\frac{\partial M}{\beta} + \frac{1}{\beta} B \frac{\partial M}{\partial B}, \quad \chi^{MM} = \frac{1}{\beta} \frac{\partial M}{\partial B},
\]

where the symmetric property \( \chi^{UM} = \chi^{MU} \) leads to the well-known thermodynamical identity:

\[
\frac{\partial E}{\partial B} = -\beta \frac{\partial M}{\partial \beta} - M = T \frac{\partial M}{\partial T} - M.
\]

The fluctuations \( \delta U \) should be rewritten in terms of the fluctuations \( \delta E \), where \( \delta U = \delta E + B \delta M + M \delta B \). The ordinary response-fluctuation relations corresponding to \( \delta \beta = \delta B = 0 \) are given by:

\[
\frac{\partial E}{\partial \beta} = \frac{\delta E}{\delta \beta} = \chi_{EE}, \quad \frac{\partial M}{\partial \beta} = \frac{\delta M}{\delta \beta} = \chi_{EM} = 1 \frac{\partial M}{\partial B} = \chi_{MM}, \quad \frac{\partial E}{\partial B} = \frac{\delta E}{\delta B} = \chi_{EE} = \frac{1}{\beta} \frac{\partial M}{\partial B} = \chi_{EM}, \quad \frac{\partial M}{\partial B} = \frac{\delta M}{\delta B} = \chi_{MM} = -1 \frac{\partial M}{\partial \beta} = \chi_{EM}.
\]

where it was introduced what can be considered as the components of the response matrix \( \chi^2 = \{ \chi_{EE}, \chi_{EM}, \chi_{MM} \} \) in the representation \( (E, M) \). The reader can notice that \( \chi_{EE} = T^2 C \) and \( \chi_{MM} = T \chi_B \), where \( C \) and \( \chi_B \) are the heat capacity and the magnetic susceptibility respectively. These classical expressions lost their validity when the response functions present some anomalous behavior, like \( C < 0 \) or \( \chi_B < 0 \). As already commented, this problem could be solved within the fluctuation theory by considering the generalized response-fluctuation relations when \( \delta \beta \neq 0 \) and \( \delta B \neq 0 \), which can be expressed as follows:

\[
\frac{\partial E}{\partial \beta} = \frac{\delta E}{\delta \beta} = \chi_{EE} = \frac{1}{\beta} \frac{\partial M}{\partial B} = \chi_{EM}, \quad \frac{\partial M}{\partial \beta} = \frac{\delta M}{\delta \beta} = \chi_{MM} = -1 \frac{\partial M}{\partial \beta}.
\]

The equations (124) constitutes the generalized response-fluctuation relations in terms of the usual control parameters of the conventional Thermodynamics for a magnetic system, \((E, M; \beta, B)\). The corresponding generalized expressions for a fluid system is very easy to obtain by considering the correspondence \((E, M; \beta, B) \leftrightarrow (E, p; \beta, V)\) where \( p \) is the pressure and \( V \) the volume of the container:

\[
\frac{\partial E}{\partial \beta} = \frac{\delta E}{\delta \beta} = \chi_{EE} = \frac{1}{\beta} \frac{\partial p}{\partial V}, \quad \frac{\partial M}{\partial \beta} = \frac{\delta M}{\delta \beta} = \chi_{EM} = -1 \frac{\partial p}{\partial V},
\]

where the symmetric condition \( \chi_{EE} = \chi_{PP} \) leads to the well-known thermodynamic identity:

\[
\frac{\partial E}{\partial V} = -\beta \frac{\partial p}{\partial \beta} - p = T \frac{\partial p}{\partial T} - p.
\]

The generalized response-fluctuation relations are given
now by:

\[
\begin{align*}
\dot{\chi}^{EE} &= \langle \delta Q \rangle^2 + \chi^{EE} \langle \delta \beta \delta Q \rangle + \chi^{EP} \langle \delta k \delta Q \rangle, \\
\dot{\chi}^{EP} &= \langle \delta Q \delta p \rangle + \chi^{EE} \langle \delta \beta \delta p \rangle + \chi^{EP} \langle \delta k \delta p \rangle, \\
\chi^{PP} &= \langle \delta p \rangle^2 + \chi^{PE} \langle \delta \beta \delta p \rangle + \chi^{PP} \langle \delta k \delta p \rangle,
\end{align*}
\]

where \(\delta Q = \delta E + p \delta V\) and \(\delta k = -\delta \beta V\).

VI. SUMMARY

It has been considered a generalization of the Boltzmann-Gibbs distributions \([13]\) based on the reparametrization invariance of the microcanonical ensemble. The resulting distribution functions correspond to an equilibrium situation where an interest system is put in contact with a generalized thermostat in order to keep fixed the average values of the quantities \(\hat{\Theta} = \Theta (\hat{I})\): an external control apparatus becoming equivalent for the case of a large enough interest system to the ordinary thermostat with effective fluctuating canonical parameters \(\hat{\beta} = \beta + \delta \hat{\beta}\). It is shown that the ordinary equilibrium condition between the canonical parameters of the thermostat \(\hat{\beta}\) and the corresponding canonical parameters of interest system \(\beta \equiv \delta S/\delta I\) is only satisfied now in average \(\left\langle \hat{\beta} \right\rangle = \left\langle \beta \right\rangle\) and these ideas are used for enhance the possibilities of the well-known Metropolis importance sample algorithm in regions characterized by the ensemble inequivalence.

The generalized Boltzmann-Gibbs ensemble leads in a natural way towards a suitable extension of the classical fluctuation theory of the conventional Thermodynamics by using a non Riemannian geometric framework which accounts for the reparametrization changes within the microcanonical description. Surprisingly, the present approach leads to a novel interpretation of the thermodynamic states with negative specific heat and other anomalous behavior of the response functions as macrostates which can be only controlled by an external apparatus with fluctuating control parameters \(\hat{\beta}\). Thus, the generalized fluctuation relations \((66)\) act as certain kind of thermodynamic uncertainly relations where the physical observables of the interest system \(I\) and the corresponding effective canonical parameters of the external generalized thermostat \(\hat{\beta}\) behave as complementary thermodynamical quantities. The above results constitute the basis what could be considered a generalized thermodynamic formalism within the microcanonical description. A rephrasing the generalized fluctuation relations is carried out with the introduction of the concept of the conjugate canonical variables \((\omega, I)\) where \(\omega = \hat{\beta} - \beta\), a representation which possibilities a Riemannian interpretation of the fluctuations within the generalized Boltzmann-Gibbs description \([12]\), constituting in this way a natural extension of other geometric interpretations of the classical fluctuation theory developed in the past \([22]\). As example of application, it was obtained the generalized response-fluctuation relations for a magnetic system (and a fluid system) in terms of the natural control parameters of the geometric framework, as well as the usual control parameters of the conventional Thermodynamics.

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