Generalization of the Mean-Field Ising Model
Within Tsallis Thermostatistics

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Abstract

In this study, the mean-field Ising model, using the Bogolyubov inequality which has been obtained in the framework of the generalized statistical thermodynamics (GST), and is suitable for nonextensive systems, has been investigated. Generalized expressions for the mean-field magnetization and free energy have been established. These new results have been verified by the fact that they transform to the well-known Boltzmann-Gibbs results in the $q \to 1$ limiting case. For the index $q$ which characterizes the fractal structure of the magnetic system, an interval has been established where the generalized mean-field free energy has a minimum and mean-field magnetization has a corresponding finite value. The interval of $q$ is consistent with paramagnetic free spin systems [14].

1 Introduction

Boltzmann-Gibbs statistics is used in Physics to study the systems having the conditions (i) the spatial range of the microscopic interactions are short-ranged (ii) the time range of the microscopic memory is short-ranged (iii) the system evolves in a Euclidean-like space-time. These kind of systems are said

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to be extensive. Whenever a system does not obey these restrictions (non-extensive systems), Boltzmann-Gibbs statistics fails and a non-extensive formalism of statistics must be needed.

In the recent years, a trend towards the non-extensive physics is rapidly increasing. In this context, the endeavour of the generalization of some of the conventional concepts such as entropy, free energy, etc. have been under investigation. These generalizations could roughly be classified under two subject titles: namely the generalized statistical thermodynamics (GST) and quantum groups. In a recent paper [1], the author called attention to a possible relation between these two subjects which appear to be very distinct.

In 1988, C. Tsallis proposed a generalized entropy [2]

$$S_q = k \frac{1 - \sum_{i=1}^{W} p_i^q}{q - 1} \quad (1)$$

where $k$ is a positive constant, $p_i$ is the probability of the system to be in a microstate, $W$ is the total number of the configurations of the system and $q$ is a parameter relevant to the measure. Tsallis entropy has the usual standard entropy properties such as positivity, equiprobability, concavity and irreversibility but in general lacks the property of additivity. This entropy transforms to the well-known additive Shannon entropy in $q \to 1$ limit.

From the year 1988 up to the present days, numerous concepts of the statistical mechanics and thermodynamics have been tackled in the frame of this generalization. Amongst them, the specific heat of the harmonic oscillator [3], one-dimensional Ising model [4], the Boltzmann H-theorem [5], the Ehrenfest theorem [6], the von Neumann equation [7], quantum statistics [8,9], the fluctuation-dissipation theorem [10], Langevin and Focker-Planck equations [11], paramagnetic systems [14], Callen identity [15], infinite-range spin-1/2 Ising ferromagnet [16], generalization of Planck radiation law [17,18], Kolmogorov entropy and fractals [19], quantum uncertainty [20], anisotropic rigid rotator [21], Haldane exclusion statistics [22,23] and Bose-Einstein condensation [24] could be enumerated.

The generalization which has been successfully applied to the preceding concepts has also been prosperous in some of the physical applications where the Boltzmann-Gibbs statistics was inadequate. The establishment of finite mass for the astrophysical systems in the frame of polytropic structures [25], the calculation of the specific heat of the unionized hydrogen atom [26], the derivation of Levy-type anomalous diffusion [27-30], the construction of a
comprehensive thermodynamic description of $d = 2$ Euler turbulence [31] and solar neutrino problem [32] are the examples that could be mentioned herewith. For a review of the subject see [33] and the mathematical investigations of the $q$-entropies are now available in [34-36].

In this study, starting from the generalized Bogolyubov inequality [12], the generalized free energy is found for the mean-field Ising model. In addition to this, within GST, the generalized magnetization of the mean-field Ising model is obtained and the critical temperature is found to be the same as the expression given by Sarmento in ref.[15]. The graphical solutions of the generalized magnetization are examined and it is observed that the finite solutions relevant to the corresponding generalized free energy exist only for a range of $q$ values.

2 Ising Model and the Bogolyubov Inequality

One of the successful models of the interacting spin systems is the Ising model. A spin variable $s_i$, which is allowed to take the values $\mp 1$, is placed on each lattice site. The spins interact according to the Hamiltonian

$$\mathcal{H} = -J \sum_{<ij>} s_i s_j - \lambda \sum_i s_i$$

(2)

where $J$ is the exchange energy and the first term is responsible for the ferromagnetism, i.e. the cooperative phenomenon and the possibility of a phase transition. $<ij>$ denotes a sum over nearest neighbour spins. Here the most important interaction is the exchange interaction $J$ and is very dependent on interparticle distance. Therefore the nearest neighbours interactions have been taken into account and distant interactions ignored. If $J = 0$ the eq.(2) is the Hamiltonian of paramagnet. $\lambda$ is termed as the mean-field having the dimension of the magnetic field and could be considered as a variation parameter. Unfortunately, very few statistical models have been exactly solved. In three dimensions not even the nearest neighbour spin model is tractable. Therefore it is necessary to resort to approximation methods. One of the most widely used amongst them is P.R.Weiss’ mean-field theory approach [37].

For a given Hamiltonian one way of deriving the mean-field is to start from the Bogolyubov inequality
\[ F \leq \Phi = F_0 + \langle \mathcal{H} - \mathcal{H}_0 \rangle_0 \]  

(3)

where \( \mathcal{H} \) is the actual Hamiltonian under consideration but not easily handled for the solution and \( \mathcal{H}_0 \) is a trial Hamiltonian possessing a solution which depends on the parameter \( \lambda \). \( F \) and \( F_0 \) are respectively the free energies associated with the Hamiltonians \( \mathcal{H} \) and \( \mathcal{H}_0 \). \( \langle \cdots \rangle_0 \) denotes an average taken in the ensemble defined by \( \mathcal{H}_0 \).

In order to calculate the right hand side of eq.(3) the trial Hamiltonian \( \mathcal{H}_0 \) has been chosen such that; each variable in the system interact not with the other variable but with an effective field. This interaction could be defined in terms of a parameter \( \lambda \). On the other hand, the mean-field is described as the minimum value of eq.(3) with respect to \( \lambda \):

\[ F_{mf} = \min_{\lambda} \{ \Phi \} \]  

(4)

We consider the nearest neighbour Ising model in a zero field, defined by the Hamiltonian given in eq.(2) with \( \lambda = 0 \), on a lattice of \( N \) sites with each site having \( z \) nearest neighbours (coordination number, e.g. for the simple cubic lattice \( z = 0 \)). Thus it follows that

\[ \mathcal{H} = -J \sum_{<ij>} s_i s_j . \]  

(5)

The trial Hamiltonian which decomposes into a sum of functions of individual spins and satisfies the requirement of translational invariance could be expressed in terms of a single parameter \( \lambda \)

\[ \mathcal{H}_0 = -\lambda \sum_i s_i . \]  

(6)

\( \mathcal{H}_0 \) is the Hamiltonian of a paramagnet. In this case the difference of the Hamiltonians is expressed by

\[ \mathcal{H} - \mathcal{H}_0 = -J \sum_{<ij>} s_i s_j + \lambda \sum_i s_i . \]  

(7)
3 Bogolyubov Inequality in the Generalized Statistical Thermodynamics (GST)

A. Plastino and C. Tsallis have obtained the Bogolyubov inequality in GST with the variational methods as a result of the concavity (not necessarily extensivity) property of the Tsallis entropy [12]:

\[ F \leq \frac{F_0}{H} + \left(1 - \frac{1}{H}\right) \frac{1}{\beta(1-q)} \quad \text{for } q < 2 \tag{8} \]

\[ = \frac{F_0}{H} - \left(1 - \frac{1}{H}\right) \frac{1}{\beta} \quad \text{for } q = 2 \tag{9} \]

\[ \geq \frac{F_0}{H} + \left(1 - \frac{1}{H}\right) \frac{1}{\beta(1-q)} \quad \text{for } q > 2 \tag{10} \]

where

\[ H \equiv \left\langle \frac{1 - \beta(1-q)\mathcal{H}_0}{1 - \beta(1-q)\mathcal{H}} \rightangle_0 , \tag{11} \]

\[ \beta = 1/k_B T, \quad k_B \text{ is the Boltzmann constant and } T \text{ is the temperature of the system.} \]

In the \( q \to 1 \) limit one gets

\[ H \approx 1 + \beta(1-q) \left\langle \mathcal{H} - \mathcal{H}_0 \right\rangle_0 \tag{12} \]

and in this manner eqs.(8),(9),(10) transform to the original Bogolyubov inequality given by eq.(3).

The partition function belonging to the Ising model corresponding to the Hamiltonian \( \mathcal{H}_0 \), for an individual spin, could be written in GST with the expression

\[ (Z_0)_q = \sum_i \left[ 1 - \beta(1-q) (\mathcal{H}_0)_i \right]^{\frac{1}{1-q}} \tag{13} \]

namely
\[ (Z_0)_q = \left[ 1 + \beta \lambda (1 - q) \right]^{\frac{1}{1-q}} + \left[ 1 - \beta \lambda (1 - q) \right]^{\frac{1}{1-q}} . \]  

(14)

A major difficulty arises from the nonextensivity (nonadditivity) of GST when we’re dealing with the system which is composed of \( N \) non-interacting single-spins. The difficulty is that the partition function of the system with \( N \) independent spin cannot be factorized into the product of \( N \) partition functions for system with single spin as it can be done in standard formalism \((q = 1)\). More explicitly this unusual property arises from the following inequality :

\[ [1 + (1 - q)(A + B)]^{\frac{1}{1-q}} \neq [1 + (1 - q)A]^{\frac{1}{1-q}} [1 + (1 - q)B]^{\frac{1}{1-q}} . \]  

(15)

A closed analytical expression for the \( N \) independent many-body system can only be obtained by following an approximation scheme like in ref.[8], namely by taking eq.(15) as an equality. This problem has also been pointed out by Pennini et al. [38] for the generalized distribution functions and they made a numerical application for a simple system without an approximation (see also [39]). In addition to this, eq.(15) has widely analyzed in ref.[18] and it is realized that this factorization scheme provides a bound to the exact answer. In fact, it can be seen that this procedure is analogous to the standard mean-field approach, which, through Bogolyubov inequality, also is a bound of the exact result.

Therefore, by using this approximation scheme, in GST the free energy of a system which is composed of \( N \) non-interacting single-spins becomes

\[ (F_0)_q = \frac{\left\{ [1 + (1 - q)\beta \lambda]^{\frac{1}{1-q}} + [1 - (1 - q)\beta \lambda]^{\frac{1}{1-q}} \right\}^{N(1-q)}}{\beta (1 - q)} - 1 . \]  

(16)

On the other hand, in the \( q \to 1 \) limit eq.(16) transforms to the standard expression

\[ (F_0)_1 = -\frac{N}{\beta} \log \cosh(\beta \lambda) \]  

(17)

Within our factorization scheme, generalized average value of a single spin within a system of \( N \) independent spins is assumed to be equal to the mean
value corresponding to a system consisting of just one spin. Since the average individual spin is \( \langle s \rangle_0 = \sum_i s^i \), in GST one gets

\[
\langle s \rangle_q = \frac{[1 + \beta \lambda(1-q)]^{\frac{q^2}{2}} - [1 - \beta \lambda(1-q)]^{\frac{q^2}{2}}}{[1 + \beta \lambda(1-q)]^{\frac{q^2}{2}} + [1 - \beta \lambda(1-q)]^{\frac{q^2}{2}}}. \quad (18)
\]

Similarly, in the \( q \to 1 \) limit eq.(18) transforms to the well-known expression

\[
\langle s \rangle_1 = \tanh(\beta \lambda). \quad (19)
\]

Taking into consideration eqn.(5) and (6), performing the sums one obtains

\[
H = \frac{1 + \beta(1-q)\lambda N \langle s \rangle_q}{1 + \beta(1-q)\lambda N \langle s \rangle_q} \quad (20)
\]

where the factorization of the interaction term is possible since \( H_0 \) includes only the single-site terms. In eq.(20), for a translationally invariant system \( \langle s_i \rangle_q = \left( \langle s_j \rangle_q = \langle s \rangle_q \right) \), and \( zN/2 \) is the number of bonds on the lattice.

Substitution of eqs.(16) and (20) in the right-hand side of the Bogolyubov inequality given by eq.(8), leads to the following relation

\[
\Phi_q = \frac{(F_0)_q \left[ 1 + \beta(1-q)\frac{1}{2}JzN \langle s \rangle^2_q \right] + \lambda N \langle s \rangle_q - \frac{1}{2}JzN \langle s \rangle^2_q}{1 + \beta(1-q)\lambda N \langle s \rangle_q}. \quad (21)
\]

In the \( q \to 1 \) limit, by taking into consideration eqs.(17) and (19), one gets from eq.(21):

\[
\Phi_1 = (F_0)_1 + \lambda N \langle s \rangle_1 - \frac{1}{2}JzN \langle s \rangle^2_1 \quad (22)
\]

which is identical with the result obtained from eq.(3) with the same approximation using the Boltzmann distribution [40]. \( \Phi_q \) could be minimized by choosing

\[
\lambda = Jz \langle s \rangle_q. \quad (23)
\]

This minimum of the mean-field magnetization is substituted in eq.(18) giving a new expression for the magnetization which could be named as \textit{generalized mean-field magnetization}.
\[(\langle s \rangle_0)_q = f \left( \langle (s)_0 \rangle_q \right) = \frac{1 + \beta J_z (1 - q) \langle (s)_0 \rangle_q}{1 + \beta J_z (1 - q) \langle (s)_0 \rangle_q} \]

which in the \( q \to 1 \) transforms to the expected result

\[
\langle (s)_0 \rangle_1 = \tanh \beta J_z \langle (s)_0 \rangle_1
\]

i.e. identical with the original mean-field magnetization [40].

In order to determine the critical temperature, the gradients of the curves \( y = \langle (s)_0 \rangle_q \) and \( y = f \left( \langle (s)_0 \rangle_q \right) \) should be equated at the origin which leads to the result

\[
T_c = qJ_z k
\]

which is identical with the result given in ref.[15]. Standard value of critical temperature \( T_c = Jz / k_B \) is recovered in the \( q \to 1 \) limit. It is important to note that \( T_c \) depends on \( z \) (the number of nearest neighbours) as well as \( q \), but not on the other parameters of the lattice structure such as dimensionality.

**Generalized mean-field free energy** corresponding to the minimum \( \lambda \) is obtained by the substitution of eq.(23) into eq.(21):

\[
(F_{mf})_q = \frac{(F_0)_q \left[ 1 + \beta (1 - q) \frac{1}{2} JzN \left( \langle s \rangle_0^2 \right)_q \right] + \frac{1}{2} JzN \left( \langle s \rangle_0^2 \right)_q}{1 + \beta (1 - q) JzN \left( \langle s \rangle_0^2 \right)_q} .
\]

As usual, in the \( q \to 1 \) limiting case eq.(27) transforms to be the conventional result [40]

\[
(F_{mf})_1 = (F_0)_1 + \frac{1}{2} JzN \left( \langle s \rangle_0^2 \right)_1 .
\]

By means of the Bogolyubov inequality given by eqs.(8)-(10) in GST and the choice of an easily solvable expression for \( \mathcal{H}_0 \) in a paramagnetic system, the right-hand side of the inequality could be solved exactly and an upperbound for the free energy of the actual Hamiltonian could be established. The most
probable free energy \((F_{mf})_q\) of the system in terms of the free energy \((F_0)_q\) of the individual spins are in the form of eq.(27) which has been obtained from the mean-field theory. Corresponding to eqs.(8),(9) and (10), the Bogolyubov inequality takes the following forms in GST:

\[
F \leq (F_{mf})_q \quad \text{for } q < 2 \quad (29)
\]

\[
F = (F_{mf})_q \quad \text{for } q = 2 \quad (30)
\]

\[
F \geq (F_{mf})_q \quad \text{for } q > 2 \quad (31)
\]

4 Graphical Solutions of Generalized Mean-Field Magnetization Consistent with the Generalized Mean-Field Free Energy

In the standard mean-field Ising model, the unique solution of the magnetization for temperatures greater than \(T_c\), is \(\langle (s)_0 \rangle_1 = 0\) which corresponds to the paramagnetic phase. On the other hand, for temperatures less than \(T_c\), there exist two solutions corresponding to the values \(\langle (s)_0 \rangle_1 = 0\) and finite \(\langle (s)_0 \rangle_1\). The mean-field free energy corresponding the finite \(\langle (s)_0 \rangle_1\) value is a minimum and the system under consideration is in stable ferromagnetic phase. The minima of the generalized mean-field free energy for various \(q\) values are presented in Fig.1 whereas the finite values of the corresponding generalized mean-field magnetization is demonstrated in Fig.2 (standard values appear in the case of \(q = 1\)).

As it is recognized from Fig.1, the mean-field free energy exhibits a minimum for \(q\) values in the interval \(1 < q < 3\). In this case, it is expected that, the generalized mean-field magnetization possesses a finite solution. From the curve plotted in Fig.2, it is noticed that, \(y = f \left[\langle (s)_0 \rangle_q\right]\) has a solution only if \(q\) takes values in the interval \(1 < q < 3\). This result coincides with the \(q\) values calculated by another method which is completely different from
the approximation method used in this study where the distributions of the total magnetic moments of the magnetic systems in the thermodynamical equilibrium have been taken into account [14].

5 Conclusions

In this study, a step has been taken towards the enlargement of the areas of applications in the generalized statistical thermodynamica (GST). In this manner, our effort in the aspect of the investigation of the phase transitions with GST has been strengthened. In this framework, by the approximate scheme which we have used here, closed and analytical expressions for the generalized mean-field magnetization and the generalized mean-field free energy have been derived for the \( N \) independent single-spin systems. From the graphical representations it is seen that, the stable solutions consistent with each other are obtained if and only if \( q \) lies in the interval \( 1 < q < 3 \). This interval is the same as the one obtained in ref.[14]. In the \( q \to 1 \) case, it is observed that, both of the two expressions transforms to the results obtained in the standard Boltzmann-Gibbs statistics. In addition to this, \( q \)-dependent mean-field critical temperature \( T_c(q) \) is deduced. It is observed that our result which is obtained for the square lattice within a renormalization group calculation [39]. The consistency of these results can be taken as a validification of our approximation.

Acknowledgments

It is a great pleasure for the authors to express their sincere thanks to Professor C. Tsallis (CBPF, Brazil) and Professor T. Altanhan (Ankara University, Turkey) for their kind interest and bringing to their attention the present status of the subject. We are indebted to TUBITAK for providing our communication with Professor C. Tsallis.
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Figure Captions

Fig. 1. Generalized mean-field free energy versus generalized mean-field magnetization for various $q$ values. Standard result is depicted for $q = 1$ case.

Fig. 2. Graphical solution of the generalized mean-field magnetization. The solid line is the curve $y = (\langle s \rangle_0)_q$, while the others represent $y = f \left[ (\langle s \rangle_0)_q \right]$ (eq.(24)) plots for various $q$ values. Standard result is depicted for $q = 1$ case.