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Duality-based approximation for the critical point of the square lattice Ising ferromagnet within Tsallis statistics

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Abstract

Within the generalized thermostatistics of Tsallis, we propose for the spin-$\frac{1}{2}$ Ising ferromagnet a transmissivity variable which extends that defined by Tsallis and Levy for thermal magnetic systems. By using this generalized transmissivity as well as duality arguments, we calculate the q-dependence of the critical temperature corresponding to the square lattice, where q is the entropic index ($q = 1$ reproduces standard thermostatistics). Our approximate results are compared with those previously obtained using renormalization group and mean-field approximation.

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1. Introduction

The *thermal transmissivity* [1] (see also [2] and references therein) is a convenient variable introduced to treat classical discrete spin magnetic systems. One of the advantages of this variable arises from the fact that, in various standard situations, it maps the $[0, \infty]$ temperature interval into the $[0, 1]$ interval. Its key strength is that it provides a geometrical interpretation [3] for the flow of thermal information (we shall illustrate this below for the spin-$\frac{1}{2}$ Ising ferromagnet). Finally, it enables a simple approach for arbitrary finite clusters, the bonds of which are associated with arbitrary coupling constants (this is particularly convenient within real-space renormalization group).

For the λ-state *Potts Hamiltonian* defined by

$$\mathcal{H} = -\lambda J \sum_{\langle i,j \rangle} \delta_{\sigma_i,\sigma_j} \quad (\sigma_i = 1, 2, \dots, \lambda) \tag{1}$$

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($\langle i,j \rangle$ denotes the first neighbors; $\delta_{\sigma_i,\sigma_j}$ refers to Kroenecker delta function) the transmissivity is defined by (see [1, 2] and references therein)

$$t \equiv \frac{1 - e^{-\lambda J/k_B T}}{1 + (\lambda - 1)e^{-\lambda J/k_B T}}, \tag{2}$$

where k_B is the Boltzmann constant and T is the temperature.

In the case we shall focus on here (Ising model), $\lambda = 2$. Hence

$$t = \frac{1 - e^{-2J/k_B T}}{1 + e^{-2J/k_B T}} = \tanh\left(\frac{J}{k_B T}\right). \tag{3}$$

Recently, Tsallis [4] proposed a generalized entropy which leads to nonextensive statistical mechanics and thermodynamics. This generalized entropy is defined as follows:

$$S_q \equiv k_B \frac{1 - \sum_{i=1}^{W} p_i^q}{q - 1} \quad (q \in \mathscr{R}), \tag{4}$$

where $\{p_i\}$ are the occurrence probabilities of the W microstates of the system. The $q \to 1$ limit recovers the usual Shannon expression, i.e.,

$$S_1 = -k_B \sum_{i=1}^{W} p_i \ln p_i . \tag{5}$$

Several results of the literature have been extended using the Tsallis generalized statistics. Among them, we have Lévy-like [5] and correlated [6] anomalous diffusion, self-gravitating systems [7, 8], $d = 2$ turbulence [8], ferrofluid-like systems [9], hydrogen atom [10] and background cosmic radiation [11]. Also, it has been successfully used in the context of simulated-annealing optimization techniques [12], and a number of related aspects have been studied [13–26].

The influence of the nonextensitivity on phase transitions is certainly a field which should be explored. In particular, questions like the q dependence of critical points and critical exponents are wide open. The present work provides some clues along this line.

In the present work we focus on a simple magnetic system. Following the previous works [1, 2], we extend the transmissivity (denoted $t(q)$), from $q = 1$ to all q, within the framework of Tsallis statistics, thus generalizing the concept originally introduced within Boltzmann–Gibbs statistics.

In Section 2 we recall the relevant transmissivity concepts within the Boltzmann–Gibbs statistics ($q = 1$); in Section 3 we present the Tsallis statistics (for all q). Finally, we conclude in Section 4.

2. Boltzmann–Gibbs statistics ($q = 1$)

Let us briefly review the known transmissivity procedure for calculating the critical temperature within Boltzmann–Gibbs statistics (see Ref. [4]).

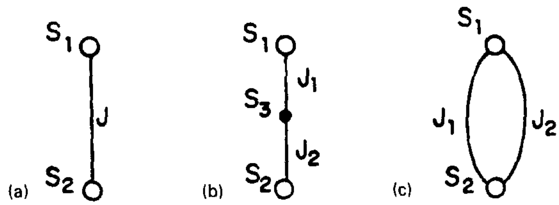

Fig. 1. Ising clusters for the (a) single bond, (b) two-series array, and (c) two-parallel array.

Consider the graphs in Fig. 1. The Boltzmann factor associated with Fig. 1(a) is given by

$$e^{-\beta\mathscr{H}_{12}} = e^{\beta J S_1 S_2} = \cosh(\beta J)[1 + \tanh(\beta J) S_1 S_2] \equiv A\left(1 + \frac{B}{A} S_1 S_2\right), \tag{6}$$

and the transmissivity is

$$t = \tanh(\beta J) \equiv \frac{B}{A}. \tag{7}$$

For Fig. 1(b) (*series* array) we have

$$e^{-\beta\mathscr{H}_{12}^{(s)}} = \sum_{S_3} e^{-\beta\mathscr{H}_{123}} = \sum_{S_3} e^{-\beta[J_1 S_1 S_3 + J_2 S_3 S_2]} \tag{8}$$

$$= \cosh(\beta J_1)\cosh(\beta J_2)[1 + S_1 S_2 \tanh(\beta J_1)\tanh(\beta J_2)], \tag{9}$$

which exemplifies the *series* composition algorithm

$$t_s = t_1 t_2 . \tag{10}$$

Consider now the *parallel* array (Fig. 1(c)). The Boltzmann factor is given by

$$e^{-\beta\mathscr{H}_{12}^{(p)}} = e^{\beta[J_1 S_1 S_2 + J_2 S_1 S_2]} = e^{\beta J_p S_1 S_2},$$

where $J_p = J_1 + J_2$. The associated transmissivity t_p is given by

$$t_p = \tanh(\beta J_p) = \tanh[\beta J_1 + \beta J_2] = \frac{\tanh(\beta J_1) + \tanh(\beta J_2)}{1 + \tanh(\beta J_1)\tanh(\beta J_2)};$$

hence

$$t_p = \frac{t_1 + t_2}{1 + t_1 t_2}, \tag{11}$$

which is the *parallel* composition algorithm. Eq. (11) can be rewritten as follows:

$$\frac{1 - t_p}{1 + t_p} = \frac{1 - t_1}{1 + t_1}\frac{1 - t_2}{1 + t_2}. \tag{12}$$

The *dual* transmissivity t^D [1, 27] is

$$t^D \equiv \frac{1-t}{1+t}, \tag{13}$$

so

$$t_p^D = t_1^D t_2^D, \tag{14}$$

which presents the parallel composition algorithm *in the form of the series one.*

The square lattice is self-dual. Using this fact, Kramers and Wannier [28] showed that the exact critical temperature for the Ising ferromagnet is given by $t_c = \sqrt{2} - 1$ (so, $k_B T_c / J = 2.269\ldots$). The graph dual of that of Fig. 1a is indicated in Fig. 2(a). Consequently, the critical point satisfies

$$t_c^D = t_c, \tag{15}$$

which implies

$$\frac{1-t_c}{1+t_c} = t_c; \tag{16}$$

hence $t_c = \sqrt{2} - 1$.

We repeat the procedure for the series array (see Fig. 2(b)). We obtain

$$t_c^2 = \frac{2t_c^D}{1 + [t_c^D]^2}, \tag{17}$$

which, once again, recovers the exact result $t_c = \sqrt{2} - 1$. If we used here the same procedure for increasingly larger clusters, we would *always* recover the exact answer $t_c = \sqrt{2} - 1$. We then see that the duality is a fundamental property, and that the transmissivity variable simplifies the calculation.

In the next section, we shall follow these two different paths (*single bond* and *series array of bonds*) just illustrated to extend this simple duality argument to arbitrary values of q; by simple we mean that it has not been necessary to consider the *entire* square lattice as in the original paper by Kramers and Wannier [28], who used duality arguments to derive $t_c = \sqrt{2} - 1$.

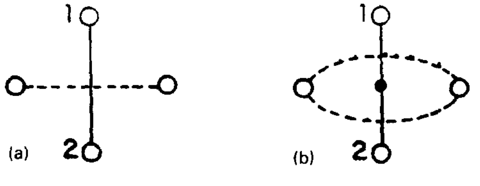

Fig. 2. Single (a) and two-series (b) bond arrays (solid lines), and their respective dual clusters (dashed lines).

3. General-q Tsallis statistics

We follow here the above procedure, replacing in the proper place the Boltzmann–Gibbs statistics ($q = 1$) by the general q result. For the Hamiltonian associated with Fig. 1(a)

$$-\beta\mathscr{H} = K_0 + KS_1S_2, \tag{18}$$

where $K \equiv BJ$ and K_0 is an additive constant. Eq. (6) yields

$$[1 + (1-q)(K_0 + KS_1S_2)]^{1/(1-q)} = A + BS_1S_2 = A\left(1 + \frac{B}{A}S_1S_2\right), \tag{19}$$

which yields the general transmissivity given by Eq. (7), $t \equiv B/A$, as before, where

$$A \equiv \tfrac{1}{2}\{a^+ + a^-\}, \tag{20}$$

$$B \equiv \tfrac{1}{2}\{a^+ - a^-\}, \tag{21}$$

with

$$a^+ \equiv [1 + (1-q)(K_0 + K)]^{1/(1-q)}, \tag{22}$$

$$a^- \equiv [1 + (1-q)(K_0 - K)]^{1/(1-q)}. \tag{23}$$

We recover the transmissivity $t = \tanh K$ when $q \to 1$. When the argument is negative the probability is to be taken zero [4].

We assume that Eq. (12) continues to be valid (at least as an approximation) for the generalized transmissivity $t(q)$. The self-duality of the square lattice implies $t_c^D(q) = t_c(q)$ for the critical point, or

$$\frac{1 - t_c(q)}{1 + t_c(q)} = t_c(q). \tag{24}$$

Consequently, the critical point is $t_c(q) = \sqrt{2} - 1$, which implies

$$\frac{a^+ - a^-}{a^+ + a^-} = \sqrt{2} - 1. \tag{25}$$

We present now the critical point for three cases, namely, $K_0 = 0$, $K_0 = K$ and $K_0 = -K$. For $K_0 = 0$ the critical point is given by

$$K_c^{-1} = (1-q)\frac{1 + (\sqrt{2}-1)^{1-q}}{1 - (\sqrt{2}-1)^{1-q}}. \tag{26}$$

In Fig. 3 we represent K_c^{-1} as a function of q.

For $K_0 = K$ we obtain, for the critical point,

$$K_c^{-1} = \frac{2(1-q)}{(\sqrt{2}+1)^{1-q} - 1}. \tag{27}$$

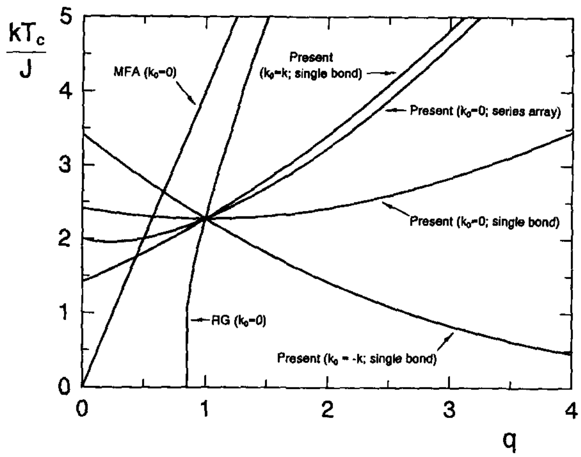

Fig. 3. Dimensionless critical temperature kT_c/J versus q for six different cases/approximations (we indicate the corresponding $q \to \infty$ asymptotic behavior): present single bond for $K_0 = 0$ ($kT_c/J \sim q$); present single bond for $K_0 = K$ ($kT_c/J \sim 2q$); present single bond for $K_0 = -K$.

In Fig. 3 we plot the corresponding function K_c^{-1} versus q. The third case, $K_0 = -K$, yields, for the critical point,

$$K_c^{-1} = \frac{2(1-q)}{1-(\sqrt{2}-1)^{1-q}}, \tag{28}$$

which is also shown in Fig. 3.

We see that all these cases reduce to the exact result for $q = 1$. For $q \neq 1$ they differ among them. For the $K_0 = 0$ case, we can compare the present results with other kinds of solution such as mean field approximations (MFA) [20] and renormalization group (RG) [29].

Let us now consider the $K_0 = 0$ case associated with the series array given by Fig. 1(b). The equivalent single bond graph is obtained as follows:

$$\begin{aligned}
&[1+(1-q)(K_0^s + K_s)S_1S_2]^{1/(1-q)} \\
&\quad = \sum_{S_3} [1+(1-q)K(S_1S_3 + S_3S_2)]^{1/(1-q)} \\
&\quad = [1+(1-q)K(S_1+S_2)]^{1/(1-q)} + [1-(1-q)K(S_1+S_2)]^{1/(1-q)} \\
&\quad \equiv C + DS_1S_2 = C\left[1 + \frac{D}{C}S_1S_2\right].
\end{aligned} \tag{29}$$

For $S_1 = S_2 = 1$ we obtain

$$[1+2(1-q)K]^{1/(1-q)} + [1-2(1-q)K]^{1/(1-q)} = C + D\,. \tag{30}$$

For $S_1 = -S_2 = 1$ we obtain

$$2 = C - D\,. \tag{31}$$

From (30) and (31) we determine C and D, and find

$$t_s(q) \equiv \frac{D}{C} = \frac{[1 + 2(1-q)K]^{1/(1-q)} + [1 - 2(1-q)K]^{1/(1-q)} - 2}{[1 + 2(1-q)K]^{1/(1-q)} + [1 - 2(1-q)K]^{1/(1-q)} + 2}\,. \tag{32}$$

For the parallel array given in Fig. 1(c) we have, for the equivalent single bond cluster (by using Eq. (19) for $K_0 = 0$),

$$\begin{aligned} 1 + (1-q)K_p S_1 S_2]^{1/(1-q)} &= [1 + 2(1-q)K S_1 S_2]^{1/(1-q)} \\ &= A(2K)[1 + t_p(q) S_1 S_2]\,, \end{aligned}$$

with

$$t_p(q) \equiv \frac{[1 + 2(1-q)K]^{1/(1-q)} - [1 - 2(1-q)K]^{1/(1-q)}}{[1 + 2(1-q)K]^{1/(1-q)} + [1 - 2(1-q)K]^{1/(1-q)}}\,. \tag{33}$$

The duality relation we are now considering is given by

$$t_s(q) = \frac{1 - t_p(q)}{1 + t_p(q)}\,, \tag{34}$$

which yields, for the critical point,

$$[1 + 2(1-q)K_c]^{1/(1-q)} - [1 - 2(1-q)K_c]^{1/(1-q)} = 2\,. \tag{35}$$

In Fig. 3 we present K_c^{-1} versus q.

We verify in the $K_0 = 0$ case that while the $q = 1$ discussion provides the exact answer *independently of the size of the clusters*, this is not for $q \neq 1$. Consequently, larger clusters should be investigated in order to improve the present approximations.

4. Discussion

Following the previous lines [1, 2] we generalize, within the Tsallis statistics, the transmissivity variable associated with the spin $\frac{1}{2}$ Ising ferromagnet. Then we use duality arguments in order to approach the critical temperature of this model for arbitrary q. Our main conclusions are:

(i) The critical temperature generically depends, as expected, on the value of the additive constant introduced in the Hamiltonian (this effect is suppressed only for $q = 1$). This result reinforces the same conclusion obtained within renormalization group techniques [29].

(ii) The discussion of the $K_0 = 0$ case illustrates the care that must be taken when doing approximations for $q \neq 1$. For example, all the approximations presently available yield, in the $q \to \infty$ limit, $k_B T_c / J \sim bq$, but great uncertainty is observed concerning the prefactor b; $b = 1$ within the present single bond approximation and $b = \frac{1}{2}$ within the series array approximation, to be compared with $b = 4$ for the mean field approximation [20] and $b = 5.5$ for a renormalization group approximation [29]. The sensitivity of the results on the size of the clusters involved in the approximation is reminiscent of the situation observed in quantum systems [30].

The present results could be useful in the discussion of magnetism in fractal structures where standard (extensive) thermodynamics are expected to fail. Further studies (like the present approach but using *larger* clusters, Monte Carlo techniques, and others) are welcome in order to better understand the influence of q on critical points.

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