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Disequilibrium, complexity, the Schottky effect, and q-entropies, in paramagnetism

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HIGHLIGHTS

- The concepts of disequilibrium and statistical complexity are employed to understand some paramagnetic phenomena.
- The Schottky effect receives special attention.
- q-entropies are found to best describe it when used to build up the statistical complexity.

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ABSTRACT

We investigate connections between statistical quantifiers and paramagnetism. More concretely, we apply the notions of (i) disequilibrium and (ii) statistical complexity, to a paramagnetic system of non-coupled dipoles. Interesting insights are thereby obtained. In particular, we encounter a kind of criticality, not associated to the temperature but to the disequilibrium.

1. Introduction

1.1. Disequilibrium and statistical complexity

Knowing about a system's unpredictability/randomness does not by itself means that one is adequately grasping the correlation structures that are reflected by the concomitant probability distribution (PD). One would wish to be able to capture the relations amongst the components of a given system in a way analogous to that in which entropy describes disorder. One has two extreme situations: (I) perfect order or (II) maximal randomness. These are not characterized endowed with strong correlations [1]. Between (I) and (II) variegated correlation-degrees may exist, represented by the characteristics of the pertinent PD. How are they represented? The answer is not an easily formulated one. We remind that Seth Lloyd encountered about 40 manners of defining a complexity, none of them satisfactory enough.

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A 1994-statement by Crutchfield is often mentioned [2,3] and repeated here again: *Physics does have the tools for detecting and measuring complete order equilibria and fixed point or periodic behavior and ideal randomness via temperature and thermodynamic entropy or, in dynamical contexts, via the Shannon entropy rate and Kolmogorov complexity. What is still needed, though, is a definition of structure and a way to detect and to measure it* .

López-Ruiz, Mancini, and Calvet (LMC) [1] advanced an intriguing functional of the probability distribution that indeed optimized Seth Lloyd's requirements. LMC use a product between Boltzmann's entropy (or information S, representing disorder) and the so called disequilibrium D, that reflects on the richness of structural details, and augments with it. Mathematically, D measures (in probability space) the distance from (a) the prevailing probability distribution to (b) the uniform probability, thus revealing the amount of structural details [1,4,5]. Thus, D is related to order. In the case of N-particles we have

$$D = \sum_{i=1}^{N} \left(p_i - \frac{1}{N} \right)^2 . \tag{1}$$

Here $p_1, p_2, \ldots, p_N$ are the individual probabilities normalized to unity ($\sum_{i=1}^{N} p_i = 1$) [1]. Our two ingredients S and D are joined by LMC to produce the complexity C_{LMC} [1,6–11]: $C_{LMC} = DS$. This quantity vanishes in the two above extremal instances (I) and (II).

Complexity can emerge as a property of large systems, which are too big to be understood in terms of the individual behavior of elementary constituents, but not so large that the effect of the individual contributions is completely washed out in statistical terms [12]. The most widespread notion of complex system refers to entities (made of many elementary constituents) that interact in an elementary fashion. Here the collective behavior is much richer than what the simplicity of the elementary behaviors would lead one to expect [12].

Paramagnetism is a collective phenomena much studied in statistical physics. It can, in the canonical ensemble, illustrate magnetism in simple terms. It makes it possible to relate macroscopic magnetic properties to the collective behavior of the microscopic magnetic moments. When the external magnetic field is created, the system experiences a state-change from complete randomization to complete orientation of the dipoles (with the magnetic field). In this sense, the system exhibits a behavior of the type order–disorder that would be amenable to study via the statistical complexity concept.

An interesting effect studied in the physics of solids is the so called Schottky anomaly: at low temperatures, a solid's specific heat capacity displays a peak. One speaks of an anomaly because, usually, either the heat capacity grows with the temperature T, or instead remains constant. We find it in systems with a discrete (usually few) number of energy levels, such that the energy grows in ladder-fashion, one step per available energy level. Given that the heat capacity is the energy derivative with respect to T, it exhibits a large peak whenever a level to level jump takes place. Schottky's anomaly is commonly detected, at low temperatures, in paramagnetic materials [13].

1.2. Our goal

We aim here to show that statistical complexity and disequilibrium can shed some light into structural details of paramagnetic phenomena, the Schottky anomaly in particular, in the case of an M-level system.

First, we will focus on the paramagnetism system of non-coupled magnetic moments of spin J, and then we will study with more detail the system with total spin $J = 1/2$, which constitutes an important example of a two-level system.

The structure of this paper is the following. In Section 2 we recapitulate the relevant background, i.e., the pertinent formalism in the canonical ensemble. The main results of the paper are in Section 3, in which we apply our ideas to paramagnetic systems of order J. In Section 4 we focus attention on a paramagnetic system with spin total $J = 1/2$. In Section 5 we concentrate our effort on the q-statistical complexities constructed with Rényi's and Tsallis' entropies, and we discuss their main properties (for the model in question with $J = 1/2$). Finally, we draw some conclusions in Section 6.

2. Disequilibrium in the canonical ensemble

In this section, we begin reviewing some notions for the canonical ensemble developed by López-Ruiz in Ref. [4,14], in which the system considered is a classical ideal gas in thermal equilibrium, i.e., N identical particles in a volume V at temperature T. However, for our present purposes, instead of a classical system we deal with a discrete system of identical levels of energy E_i, labeled with $i = 1, 2, \ldots, N$. The pertinent Boltzmann probability distribution then reads [15]

$$p_i = \frac{e^{-\beta E_i}}{Q_N(V,T)}, \tag{2}$$

where, as usual, $\beta = 1/k_B T$ and k_B is Boltzmann's constant. The canonical partition function Q_N is

$$Q_N(V,T) = \sum_i e^{-\beta E_i}, \tag{3}$$

and the Helmholtz' free energy A is related to Q_N as [15]

$$A(N,V,T) = -k_B T \ln Q_N(V,T). \tag{4}$$

R. López-Ruiz shows in Ref. [14] that, in this context, the disequilibrium $D(N, V, T)$ becomes

$$D(N, V, T) = e^{2\beta\,[A(N,V,T)-A(N,V,T/2)]}. \tag{5}$$

LR replaces now T by $T/2$ in Eq. (4) and inserts this into Eq. (5), finding

$$D(N, V, T) = \frac{Q_N(V, T/2)}{[Q_N(V, T)]^2}, \tag{6}$$

an important expression as we will see below.

3. Paramagnetic systems

3.1. The paramagnetic model

We provide here a brief description of a non-interacting magnetic system which consists of N identical magnetic dipoles of moments $\boldsymbol{\mu}$ and total spin J in the presence of the external magnetic field $\mathbf{H} = H\widehat{z}$, oriented along z-axis. The magnetic dipole moments in the direction of the external field have arbitrary values. The potential energy of the dipoles is $E = -N\boldsymbol{\mu}\cdot\mathbf{H}$, where $\mu = g\mu_B\sqrt{J(J+1)}$, g being the Landé factor and μ_B the Bohr magneton [15,16]. In such scenario, the corresponding partition function becomes [15]

$$Q_N(J, \eta) = \left(\frac{\sinh(\eta(J+1/2))}{\sinh(\eta/2)}\right)^N, \tag{7}$$

with a parameter η defined by

$$\eta = \frac{g\mu_B H}{k_B T}, \tag{8}$$

where T is the temperature. The relevant thermodynamic quantities that we will consider in the present proposal are [15,16]

$$A = -Nk_BT \ln\left(\frac{\sinh(\eta(J+1/2))}{\sinh(\eta/2)}\right), \tag{9}$$

$$S = Nk_B\left[\ln\left(\frac{\sinh(\eta(J+1/2))}{\sinh(\eta/2)}\right) - \eta J B_J(\eta)\right], \tag{10}$$

and

$$M = g\mu_B N J B_J(\eta), \tag{11}$$

for the Helmholtz free energy, entropy, and mean magnetization in the direction of the field, respectively. The Brillouin function B_J of order J is defined as [15,16]

$$B_J(\eta) = \frac{1}{J}\left((J+1/2)\coth(\eta(J+1/2)) - \frac{1}{2}\coth(\eta/2)\right), \tag{12}$$

and plays an important role in these considerations. Illuminating references are [2,17]. Here we focus on what we can learn from the concept of disequilibrium, not considered in the two references just cited.

3.2. Disequilibrium

Replacing Eq. (7) into Eq. (6) that defines to the disequilibrium in the canonical ensemble, we arrive at D for the paramagnetic system. Its analytical form is given by

$$D_N(J, \eta) = \left(\frac{\tanh(\eta/2)}{\tanh(\eta(J+1/2))}\right)^N. \tag{13}$$

Remember that the disequilibrium is a quantifier of a system's structural details' richness. We draw in Fig. 1 the shape of the disequilibrium per dipole that we call $d_J(\eta) = (D_N(J, \eta))^{1/N}$. Note that $0 \leq d_J(\eta) \leq 1$. We see that $d_J(\eta)$ grows with η until it saturates for medium η-values. This saturation is an artifact of the discrete level structure of the system. It does not occur in the case of a gas, for instance. The saturation entails that there exist a maximum degree of structure that the system can attain. This degree is minimal at very high temperatures, as expected.

Note the following asymptotic limiting cases: for $\eta \to 0$, we get $d_J(0) \approx 1/(2J+1)$, and for $\eta \to \infty$ we obtain $d_J(\infty) = 1$ for all J. For $J \to \infty$ the disequilibrium $d_\infty(\eta) \to 0$ for $\eta = 0$.

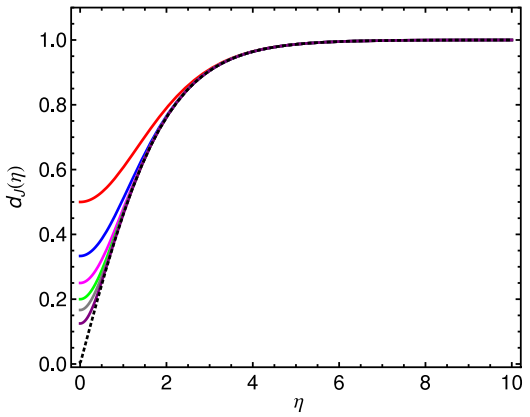

Fig. 1. Disequilibrium per dipole $d_J(\eta)$ as a function of $\eta = g\mu_B H/k_B T$ for $J = 1/2$, 1, 3/2, 2, 5/2, and 7/2. $J = 1/2$ is the red curve and the dotted curve represents the case $J = \infty$ (classical case). (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.)

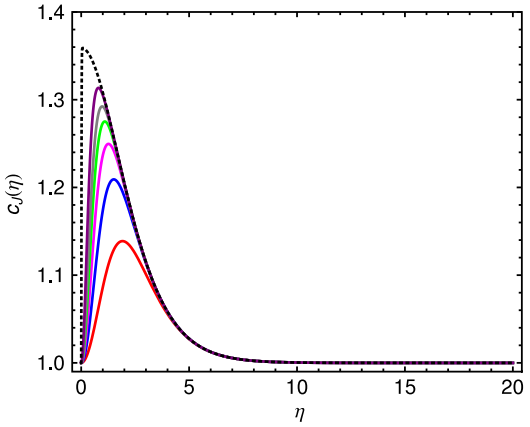

Fig. 2. Behavior of the statistical complexity per dipole $c_J(\eta)$ as a function of $\eta = g\mu_B H/k_B T$ for $J = 1/2$, 1, 3/2, 2, 5/2, and 7/2. $J = 1/2$ is the red curve and the dotted curve represents the limit at $J = \infty$. (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.)

3.3. Statistical complexity

We use here a slightly modified complexity (per dipole) definition introduced by Catalan et al. in Ref. [18], to avoid possible negative values. For the LMC-statistical complexity per dipole, this version is given by

$$c_J(\eta) = d_J(\eta)\, e^{S/Nk_B}, \tag{14}$$

with $d_J(\eta)$ defined in Eq. (13) and the entropy given by Eq. (10). In view of this, thus c_J becomes

$$c_J(\eta) = \frac{\cosh(\eta(J+1/2))}{\cosh(\eta/2)}\, e^{-\eta J B_J(\eta)}. \tag{15}$$

It is clear, from Eq. (15), that $c_J(\eta)$ vanishes for total disorder ($\eta = 0, c_J(0) = 1$, for all J) but remains finite (although minimal) for perfect order. $\eta \to \infty$ corresponds to $c_j(\infty) \to 0$ (maximal order). For $J = \infty$, the statistical complexity is given by the dotted curve, attaining there its maximum value. Here all conceivable orientation are possible. The situation here described is observed in Figs. 2 and 3.

4. Two-level model

4.1. The model

An important case, much studied in the literature, is that of the spin-1/2 system, in which $J = 1/2$ and $g = 2$. Each dipole has two orientations: ϵ and $-\epsilon$, with $\epsilon = \mu_B H$ [15]. Thus, setting $\eta = 2\beta\epsilon$ in Eq. (7) and using hyperbolic identities, the

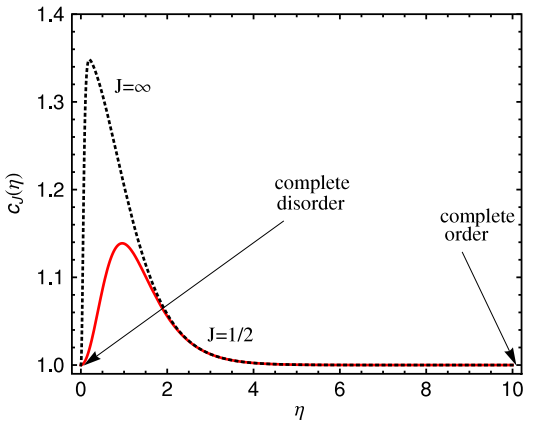

Fig. 3. Behavior of the statistical complexity per dipole $c_J(\eta)$ as a function of $\eta = g\mu_B H/k_B T$ for $J = 1/2$ and ∞. We indicate the regions of order and disorder, respectively.

partition function now becomes

$$Q_N(\beta, \epsilon) = (2\cosh(\beta\epsilon))^N. \tag{16}$$

Let us here introduce the main thermodynamic quantities that we will use later. These are [15]

$$A = -Nk_B T \ln(2\cosh(\beta\epsilon)), \tag{17}$$

$$S = -\left(\frac{\partial A}{\partial T}\right)_H = Nk_B \ln(2\cosh(\beta\epsilon)) - \beta\epsilon\tanh(\beta\epsilon), \tag{18}$$

$$M = -\left(\frac{\partial A}{\partial H}\right)_T = N\mu_B \tanh(\beta\epsilon), \tag{19}$$

and

$$C_H = Nk_B(\beta\epsilon)^2 \mathrm{sech}^2(\beta\epsilon), \tag{20}$$

for the Helmholtz free energy, entropy, magnetization and specific heat, respectively.

Writing $\Delta = 2\epsilon$ for the energy difference between the two allowed states of the dipole (gap of energy), the specific heat is re-expressed as [13,15]

$$C_H = Nk_B(\beta\Delta)^2 \frac{e^{\beta\Delta}}{(1+e^{\beta\Delta})^2}. \tag{21}$$

This form is known as the Schottky specific heat and is characterized by a broad peak with an excitation Δ. The maximum of C_H/Nk_B occurs at $\beta_m \approx 2.4/\Delta$, or approximately for $k_B T_m/\epsilon \approx 0.8333$, i.e., for the temperature $T_m \approx 0.42\Delta/k_B$. Thus for a two-level system the temperature of the peak is directly proportional to the splitting between the energy levels [13]. This important result will be relevant for the developments of the next sections.

4.2. Disequilibrium and energy gap

Setting $J = 1/2$ in Eq. (13), the disequilibrium per dipole turns out to be

$$d_{1/2}(\beta, \epsilon) = \frac{\tanh(\beta\epsilon)}{\tanh(2\beta\epsilon)}, \tag{22}$$

that, after a some manipulation of the hyperbolic functions, in terms of the gap of energy Δ it can be rewritten as

$$d_{1/2}(\beta, \Delta) = \frac{1+e^{-2\beta\Delta}}{(1+e^{-\beta\Delta})^2}. \tag{23}$$

We illustrate things in Fig. 4. We see that the disequilibrium attain its minimum value equal to 1/2 in $\beta\Delta = 0$ and tends to 1 for $\beta\Delta \to \infty$.

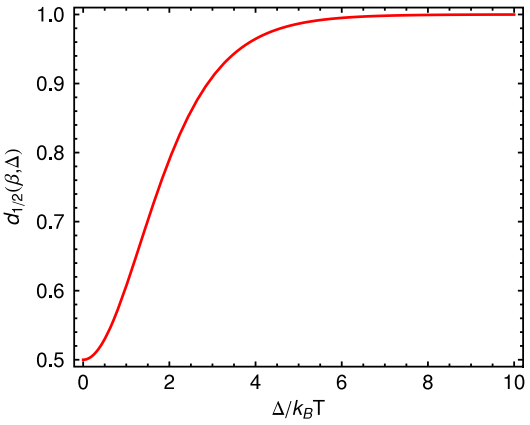

Fig. 4. Disequilibrium $d_{1/2}(\beta, \Delta)$ as a function of Δ/k_BT.

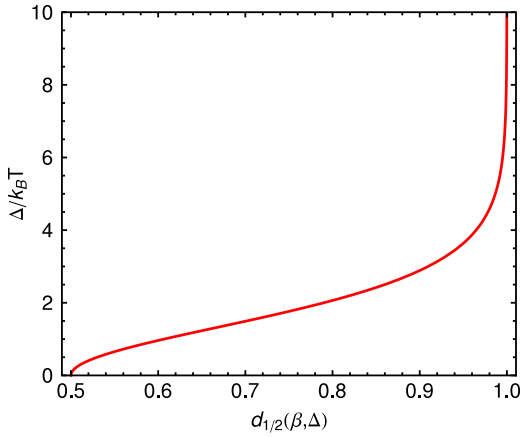

Fig. 5. Gap Δ/k_BT versus disequilibrium $d_{1/2}(\beta, \Delta)$.

Furthermore, we can determine the gap as a function of the disequilibrium by setting $u = \exp(-\beta\Delta)$ into Eq. (23), which gives

$$d_{1/2} = \frac{1+u^2}{(1+u)^2}. \tag{24}$$

Solving above equation we get

$$\beta\Delta = -\ln\left(\frac{-d_{1/2}+\sqrt{2d_{1/2}-1}}{d_{1/2}-1}\right), \tag{25}$$

that expresses the gap energy as a function of disequilibrium (see Fig. 5). One appreciates the fact that for the maximum disequilibrium $d = 1$, $\beta\Delta$ grows in unbounded fashion.

4.3. Disequilibrium and magnetic properties

Considering the definition of the magnetization (19) together with the hyperbolic identities, we find a relation between the disequilibrium with the magnetization, which looks like

$$d_{1/2}(\beta,\epsilon) = \frac{m(\beta,\epsilon)}{m(2\beta,\epsilon)}, \tag{26}$$

where we have defined $m(\beta, \epsilon) = M(\beta, \epsilon)/N\mu_B$ as the magnetization for dipole. In Fig. 6 we illustrate the shape of the disequilibrium curve and of the magnetization-one, for all temperatures.

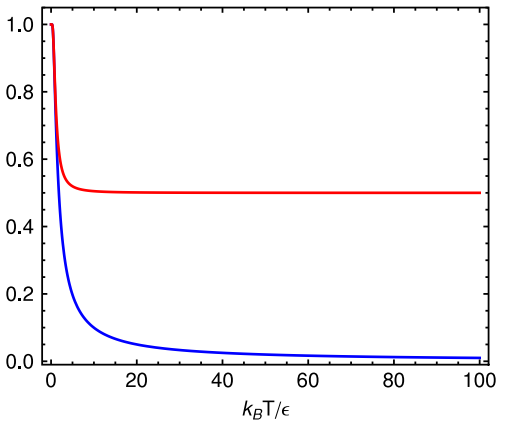

Fig. 6. Magnetization per dipole $m(\beta, \epsilon)$ (blue curve) and disequilibrium $d_{1/2}(\beta, \epsilon)$ (red curve) as a function of $k_B T/\epsilon$. (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.)

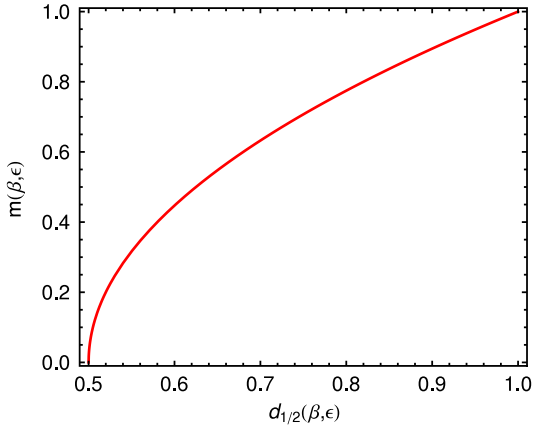

Fig. 7. Dependence of the magnetization per dipole $m(\beta, \epsilon)$ with the disequilibrium $d_{1/2}(\beta, \epsilon)$.

For high temperatures, $k_B T \gg \mu_B H$ or $\beta\epsilon \ll 1$ ($k_B T/\epsilon \gg 1$), $\tanh(\beta\epsilon) \approx \beta\epsilon$, and the ensuing result is $d(\beta, \epsilon) \to 1/2$, whereas $m(\beta, \epsilon) \to 0$. On the other hand, for low temperatures, $k_B T \ll \mu_B H$ or $\beta\epsilon \gg 1$ ($k_B T/\epsilon \ll 1$), since $\tanh(\beta\epsilon) \to 1$. Now we have $d(\beta, \epsilon) \to 1$ and $m(\beta, \epsilon) \to 1$.

Moreover, after a bit of algebraic manipulation, and using the identity $\tanh(2\beta\epsilon) = 2\tanh(\beta\epsilon)/(1 + \tanh^2(\beta\epsilon))$, we can cast the disequilibrium as

$$d_{1/2}(\beta, \epsilon) = \frac{1}{2} + \frac{1}{2} m^2(\beta, \epsilon). \tag{27}$$

At $H = 0$ and $\beta = 0$ we have $d_{1/2}(0, 0) = 1/2$ because $m(0, 0) = 0$. Thus, from the above equation we can recast the magnetization in terms of $d_{1/2}$ as follows

$$m(\beta, \epsilon) = \left(\frac{d_{1/2}(\beta, \epsilon) - d_{1/2}(0, 0)}{d_{1/2}(0, 0)} \right)^{1/2}. \tag{28}$$

Its behavior is represented in Fig. 7. Of course, if m grows, $d_{1/2}$ must increase, as the degree of order augments.

As just stated, when the disequilibrium increases, the magnetization grows as well. The ensuing degree of order augments until we reach a state of magnetic saturation (complete alignment of the dipoles). In the other extreme, zero magnetization implies complete randomization of the dipoles (complete disorder). So as to investigate the behavior of the magnetization near this "zero magnetization-point", lets us introduce the expansion parameter [19]

$$\delta = \frac{d_{1/2}(\beta, \epsilon) - d_{1/2}(0, 0)}{d_{1/2}(0, 0)}, \tag{29}$$

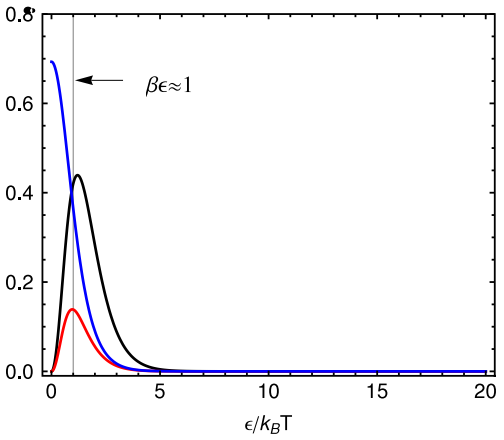

Fig. 8. Specific heat C_H/Nk_B (black curve), statistical complexity $c_{1/2}(\beta, \epsilon)$ (red curve) and entropy S/Nk_B defined in Eq. (18) (blue curve) as a function of ϵ/k_BT. The peak value of C_H/Nk_B occurs at $\beta\epsilon \approx 1.2$ and for $c_{1/2}(\epsilon, \beta)$ is at $\beta\epsilon \approx 1$. (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.)

entailing, in terms of the new variable δ, that

$$m(\delta) = \delta^{1/2}, \tag{30}$$

so that δ constitutes a kind of "order" parameter, with 1/2 being the critical-point exponent, and $d_{1/2}(0, 0)$ a critical point in the $m\, d_{1/2}$-plane. When the magnetization vanishes ($H = 0$, $\beta \to 0$). We see that δ is a measure of distance to the critical point $d_{1/2}(0, 0)$. In fact, the critical exponent of the function $m(\delta)$, according to Ref. [19], must satisfy

$$\lambda = \lim_{\delta \to 0} \frac{\ln m(\delta)}{\ln \delta} = \lim_{\delta \to 0} \frac{\ln \delta^{1/2}}{\ln \delta} = \frac{1}{2}, \tag{31}$$

showing that $\lambda = 1/2$ is indeed the critical exponent of the magnetization $m(\delta)$. Moreover, a λ positive entails that $m(\delta)$ tends to zero at the critical point [19]. Since $1/2 \leq d_{1/2} \leq 1$, then the range of δ is $0 \leq \delta \leq 1$. Our curve $m(\delta) = \delta^{1/2}$ versus δ looks exactly like that reported in Ref. [19], Fig. 3.25(b), page 137. From Eqs. (27) and (30) we also get

$$d_{1/2} = \frac{1}{2}\,(1 + \delta)\,, \tag{32}$$

which illuminates the behavior of the disequilibrium vs. the order parameter.

Note that we have obtained an exponent for the critical point that is not related to the temperature, but *to the disequilibrium*. Of course, here no phase transition is involved.

In addition, given that $m = M/N\mu_B$, we can recast δ as

$$\delta = \left(\frac{M}{N\mu_B}\right)^2, \tag{33}$$

an expression that quantifies the degree of ordering of the dipoles. When the magnetization is zero ($M = 0$) it is clear that $\delta = 0$ (perfect disorder). When the system reaches magnetic saturation ($M = \mu_B H$), we have $\delta = 1$ (perfect order). The case $\delta = 1/2$ entails that $M = \sqrt{2}N\mu_B/2$. Thus, half of the system's dipoles are ordered and the other half are not.

4.4. Statistical complexity and specific heat

In view of Eqs. (18) and (22), the LMC-statistical complexity per dipole becomes

$$c_{1/2}(\beta, \epsilon) = 2\frac{\sinh(\beta\epsilon)}{\tanh(2\beta\epsilon)}\, e^{-\beta\epsilon\, \tanh(\beta\epsilon)}. \tag{34}$$

The maximum of $c_{1/2}(\beta, \epsilon)$ occurs for $\beta\epsilon \approx 1$, that is $\beta\Delta \approx 2$.

In Fig. 8 we compare significant thermodynamic quantities like specific heat and entropy with the LMC-statistical complexity $c_{1/2}(\epsilon, \beta)$ for dipole. We note that, although the statistical complexity experiences an anomalous behavior similar to that of the specific heat, the peak values for C_H/Nk_B and $c_{1/2}(\epsilon, \beta)$ do not exactly coincide. The entropy does not display this type of anomaly. Now, the definition of statistical complexity is not unique. It depends on the information quantifier considered. We can improve the complexity performance by replacing Shannon's quantifier by another one. This is the subject of next Section.

5. Statistical complexity with q-entropies

In order to get more insight into the structure of the system, we will now appeal to q-entropies, that will replace Shannon's in the statistical complexity. We center our effort on Rényi's and Tsallis' entropies.

5.1. Rényi's entropy

Rényi's entropy R_q is an entropic functional of great relevance, because its manifold applications. Rényi's information measure is a generalization of the Shannon one, quantifying a system's diversity, uncertainty, or randomness. The degree of generalization is parameterized by a real parameter q. It is used in variegated areas of scientific research. One can mention, for instance, ecology, quantum information, the Heisenberg XY spin chain model, theoretical computer science, diffusion processes, several biological processes (a small sample is that of Refs. [20–31]). R_q is defined as [32]

$$R_q = \frac{k_B}{1-q} \ln \sum_i p_i^q, \tag{35}$$

where q is a real parameter, with $0 < q < \infty$, and $i = 1, 2, \ldots, M$ labels the energy-levels. For $q = 1$ we get the usual, Shannon's, thermodynamic entropy $R_1 \equiv S$. We have added, for convenience, the Boltzmann constant to the definition of R_q.

For the two-level system addressed in Section 4, it is clear that

$$\sum_{i=1}^{2} p_i^q = 2Q_1^{-q} \cosh(q\beta\epsilon), \tag{36}$$

where the sum runs over the energy levels and we have used the partition function (16) with $N = 1$. Thus, R_q per dipole becomes

$$\frac{R_q}{k_B} = \ln \left(\frac{2\cosh(q\beta\epsilon)}{(2\cosh(\beta\epsilon))^q} \right)^{1/(1-q)}. \tag{37}$$

Motivated by the above discussion, we propose here to adopt a Rényi-version, or q-statistical complexity (also studied by Sánchez-Moreno et al. in Ref. [33]), defined as

$$c_q^R(\beta, \epsilon) = d(\beta, \epsilon)\, e^{R_q(\beta,\epsilon)/k_B}, \tag{38}$$

with the disequilibrium $d(\beta, \epsilon)$ being that of Eq. (5). Of course, we have replaced the ordinary Shannon entropy by Rényi's one (for some properties see Ref. [4]).

Considering the above spin 1/2-system, and making use of Eqs. (22) and (37), after some algebraic manipulation we obtain

$$c_q^R(\beta, \epsilon) = \cosh(2\beta\epsilon) \cosh(q\beta\epsilon)^{1/(1-q)} (\cosh(\beta\epsilon))^{(q-2)/(1-q)}. \tag{39}$$

In Fig. 9 we display the behavior of c_q^R (given by (39)) for several values of q. In this graph, we also plot the specific heat for the 1/2-system. Clearly, the peak-value of the q-statistical complexity diminishes as q decreases. Given that we select q at will, we can find that optimum curve so that the positions of the complexity-peak and the specific heat-one coincide. The resulting q-value turns out to be $q = 0.51$. Thus, our present scenario is best described not by Shannon's entropy but by this specific Rényi one.

5.2. Tsallis' entropy

Tsallis' entropy is a generalization of the standard Shannon entropy S which is defined as [34–36]

$$S_q = k_B \frac{1 - \sum_i p_i^q}{q-1}, \tag{40}$$

with q any real number. In the limit $q \to 1$ one recovers $S_1 = S$. Note we have again added the Boltzmann constant. S_q constitutes a great advance in statistical mechanics and has been applied in variegated scientific disciplines with great success [34–36].

For our two-level system, taking into account Eq. (36), we immediately obtain S_q per dipole

$$\frac{S_q}{k_B} = \frac{1 - 2^{1-q} \cosh(\beta\epsilon)^{-q} \cosh(q\beta\epsilon)}{q-1}. \tag{41}$$

The Tsallis-version of the statistical complexity is

$$c_q^T(\beta, \epsilon) = d(\beta, \epsilon)\, e^{S_q(\beta,\epsilon)/k_B}, \tag{42}$$

whose ingredients are the disequilibrium (22) and the entropy S_q (41). The behavior of c_q^T is displayed in Fig. 10.

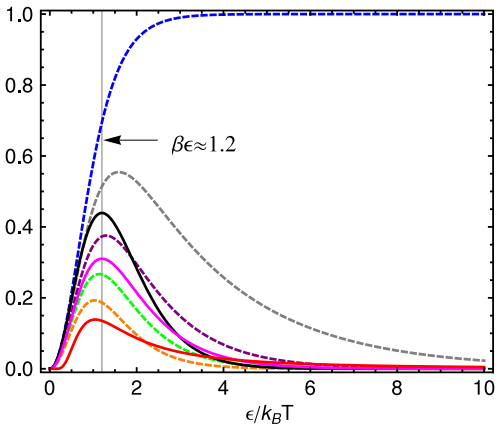

Fig. 9. Specific heat C_H/Nk_B (black curve) and statistical complexity $c_q^R(\beta,\epsilon)-1$ as a function of ϵ/k_BT for $q=0$, 0.2, 0.4, 0.51, 0.6, 0.8, and 1. The solid red curve corresponds to the $q=1$ case. Dotted curves represent c_q^R for other values of q. The dotted blue curve corresponds to $q=0$. The magenta (solid) curve is the optimum one with $q=0.51$. (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.)

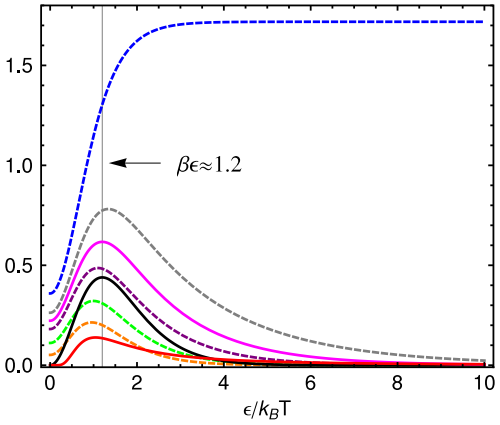

Fig. 10. Specific heat C_H/Nk_B (black curve) and statistical complexity $c_q^T(\beta,\epsilon)-1$ as a function of ϵ/k_BT for $q=0$, 0.2, 0.29, 0.4, 0.6, 0.8, and 1. The solid red curve corresponds to the $q=1$ case. Dotted curves represent c_q^T for other values of q. Th dotted blue curve corresponds to $q=0$. The magenta (solid) curve is the optimum one, with $q=0.294$. (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.)

6. Conclusions

Complementing studies made in Refs. [2,3], we have analyzed in this work the behavior of the disequilibrium D and the statistical complexity C_{LMC} for a paramagnetic system of non-coupled dipoles.

We have seen that the D-notion yields interesting insights. One appreciates that C_{LMC} matches exactly the peaks of the heat capacity in a Rényi's entropy-scenario with $q=0.294$ and in a Tsallis entropy-environment with $q=0.51$.

This makes the q-entropies a primordial tool to obtain fine details of the structure of our systems, together with the statistical complexity. The Schottky effect is explained by the fact that the associated peak takes place at the temperatures for which the system exhibits its maximum degree of q-complexity. Finally, we have seen that a kind of criticality-like effect emerges, that can be associated to D.

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