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Research Article

Microcanonical Entropy of the Infinite-State Potts Model

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In this investigation we show that the entropy of the two-dimensional infinite-state Potts model is linear in configurational energy in the thermodynamic limit. This is a direct consequence of the local convexity of the microcanonical entropy, associated with a finite system undergoing a first-order transition. For a sufficiently large number of states q, this convexity spans the entire energy range of the model. In the thermodynamic limit, the convexity becomes insignificant, and the microcanonical entropy (the logarithm of the density of states) tends to a straight line. In order to demonstrate the behaviour of the convexity, we use the Wang-Landau Monte-Carlo technique to numerically calculate the density of states for a few finite but high values of q. Finally, we calculate the free energy and discuss the generality of our results.

1. Introduction

A thermodynamic system can be considered small when the characteristic length scale for the interaction between the subunits is comparable to the system size itself. In such systems, properties that are extensive in the thermodynamic limit, such as entropy and free energy, do not scale linearly with system size [1]. In addition, a traditional viewpoint concerning small systems has been that phase transitions cannot be defined for them since their partition functions are finite and, thus, analytic. According to such a viewpoint, only systems in the thermodynamic limit can undergo phase transitions since they exhibit the necessary discontinuities in temperature derivatives of thermodynamic potentials. This classification is unsatisfactory for two reasons. First, the thermodynamic limit is a theoretical construct that does not exist in nature. Second, several investigations have been performed to understand phase transitions in macroscopic systems based on transitions in downscaled, finite systems. A modern, proposed classification scheme for phase transitions in finite systems is based on canonical partition function zeros [2]. It has also been noted that finite systems undergoing a first-order phase transition exhibit an inverted curvature of a thermodynamic potential [3, 4].

A specific case of inverted curvature is the occurrence of negative specific heat in the microcanonical ensemble. This is a peculiar effect associated with small systems undergoing a first-order phase transition [4, 5]. Mathematically, this is equivalent to a region of local convexity in an otherwise concave microcanonical entropy [6]. The significance of this *convex intruder* [6] vanishes in the thermodynamic limit where the thermodynamics becomes extensive and there is no difference between microcanonic and canonic properties. This has been very nicely discussed by the late Gross in a series of papers, advocating the utilization of microcanonical thermostatistics as a foundation of thermodynamics, see, for instance, [6–8].

The purpose of the current investigation is to use this finite-size property of the microcanonical entropy to express the analytical solution to a well-known lattice spin model, the infinite-state Potts model in the thermodynamic limit [9, 10].

The standard, q-state, Potts model [11] is a lattice model with nearest neighbor interaction. Each lattice site, i, is assigned a spin state, $s_i = 1, \ldots, q$, and the spins interact according to the Hamiltonian:

$$H = -J\sum_{i>j}\delta\left(s_i, s_j\right), \tag{1}$$

where J is the interaction strength and δ is the Kronecker delta, which has the property that $\delta(x, y) = 1$ if $x = y$ and 0 otherwise. The summation is over the nearest neighbors, and each interaction is only counted once. The partition function is given by $Z = \sum_{\{s\}} \exp(-\beta H)$ where $\{s\}$ indicates summation over all spin configurations and β has its usual meaning of $1/k_B T$, where k_B is Boltzmann's constant and T is temperature. Since a vast majority of the microstates are highly degenerate, it is convenient to rewrite the partition function in the form:

$$Z = \sum_{E} \Omega(E) e^{-\beta E}, \tag{2}$$

where the microcanonical partition function, $\Omega(E)$, also known as the density of states, represents the degeneracy factor for the energy E in the canonical partition function (2). It is easy to verify that, for a two-dimensional (2D) square lattice with N points, the energy can take all integer multiples of J from $-2NJ$ to 0.

The Potts model provides an excellent model framework for the study of phase transitions (see, e.g., [6, 12, 13]) and has a lot of applications in diverse fields, for an overview, see [11]. In 2D, the Potts model undergoes a first-order phase transition for $q > 4$ and a continuous one for $q \leq 4$ [11]. In the limit of large q, the model is also known as the infinite-state Potts model, and interesting applications can be found in foam coarsening [14] and number theory [15, 16]. Wu et al. [16] has shown that the infinite-state Potts model is equivalent to the problem of restricted partitioning of integers. Based on this analogy, Wu [15] has solved the infinite-state Potts model in two and three dimensions. Although ingenious, it is not straightforward to extract thermodynamic information, such as the density of states, $\Omega(E)$, from Wu's partition function.

In this investigation we show that the microcanonical entropy of the 2D Potts model is linear in configurational energy in the limit of large q and in the thermodynamic limit. By simulations, we demonstrate the behaviour of the microcanonical entropy as q and N are varied. We base our proof on the asymptotic properties of the convex intruder.

2. Simulation Method

We use the Wang-Landau algorithm [17] to calculate the density of states, $\Omega(E)$. This is a Monte Carlo histogram technique, which yields the density of states with arbitrary precision while it is ergodic, meaning that every point in phase space is visited an (approximately) equal amount of times.

A major advantage with this method compared to conventional Monte Carlo techniques is that repeated simulations at multiple temperatures are avoided. Instead, the entire density of states is calculated in one single simulation run per system. Knowing the density of states admits calculation of both microcanonical and canonical thermodynamic properties.

The Wang-Landau algorithm is an iterative procedure based on a random walk in energy space with the purpose of modifying the density of states and updating a histogram. When the histogram is (sufficiently) flat, the modification factor is refined, the histogram is reset, and a new iteration starts. Ultimately, the density of states converges to its true value. The algorithm is outlined in detail in [17]. In that paper, a comparison with an analytically solved system, the 2D Ising model, is made. Here it was found that the relative errors in internal energy and canonical entropy calculated from the Wang-Landau density of states as compared to the exact analytical expressions were smaller than 0.09% and 1.2%, respectively. Since the q-state Potts model has not been exactly solved, the same kind of error analysis cannot be made for that case. However, we have no reason to believe that the simulation error for the q-state Potts model should be significantly different than that for the Ising model.

In the current investigation, the microcanonical entropy, S_μ, which is given by the logarithm of the density of states,

$$S_\mu(E) = k_B \ln \Omega(E), \tag{3}$$

is calculated for 2D Potts models on square lattices with varying lattice size, $N = L \times L$, and varying q. All simulations are performed with periodic boundary conditions. We define the energy in unit J and the temperature in J/k_B. The units are chosen so that $J = 1$ and $k_B = 1$, which enables a dimensionless notation.

3. Results and Discussion

We will demonstrate that the entropy of the 2D square lattice Potts model becomes linear in energy for large q in the thermodynamic limit and is given by the asymptotic expression for the entropy per site,

$$s(\varepsilon) \sim \left(1 + \frac{\varepsilon}{2}\right) \ln q, \quad -2 \leq \varepsilon \leq 0, \; q \longrightarrow \infty, \tag{4}$$

where ε is the configurational energy per site, $\varepsilon = E/N$. To demonstrate this, we will consider the degeneracy factors for the ground state and the most excited state, the latent heat as $q \to \infty$, and the vanishing of the convex intruder in the thermodynamic limit.

We start our line of investigation by writing the microcanonical entropy in the general form,

$$S_\mu(E) = \sigma(E) - \psi(E), \tag{5}$$

where σ is linear in energy and ψ is a correction function [18]. This expression is valid also for finite lattices.

An explicit expression for σ can be written down if at least two degeneracy factors are known. For the ferromagnetic ($J > 0$) Potts model, the ground state, where every spin is the same, is q-fold degenerate,

$$\Omega(-2N) = q. \tag{6}$$

At the highest excited state, $\Omega(0)$, every neighboring lattice site has different spin. In fact, $\Omega(0)$ is equal to the chromatic polynomial, $P(G, q)$, over the graph, G [11]. In our case, G is the 2D square lattice with N sites (vertices) and periodic boundary conditions. $P(G, q)$ is a polynomial in q with degree N and leading order coefficient 1. The signs of the coefficients, which depend on N and G, alternate, and the coefficient of the q^{N-1} term is equal to the negative of the number of edges [19], that is, $-2N$ in our case. Since $P(G,q)$ is a polynomial in q with degree N, we have that $P(G,q) \sim q^N$ as $q \to \infty$, for any positive N.

Let us now investigate the large N limit. It has been shown that the limit $W = \lim_{N\to\infty} P(G,q)^{1/N}$ exists and that $\lim_{q\to\infty} q^{-1}W = 1$ [20]. This means that $P(G,q) \sim q^N$ also when we take the limit $N \to \infty$ before the limit $q \to \infty$. More formally, it has been shown that the two limits in the expression $\lim_{q\to q_s}\lim_{N\to\infty} P(G,q)^{1/N}$ commute if $q_s > \chi(G)$ [21], where $\chi(G)$ is the chromatic number of G [22]. The 2D square lattice is a planar graph, and, since all planar graphs are four colorable, meaning that $\chi(G) \le 4$, the limits clearly commute for $q_s \to \infty$.

This means that $\Omega(0)$ approaches q^N asymptotically,

$$\Omega(0) \sim q^N, \quad q \longrightarrow \infty, \tag{7}$$

for any positive N. Our specific approach is based on taking the large q limit before the thermodynamic limit. However, since the limits commute, the final expression, (4), is independent on the order of the limits.

Now we can write the expression for σ, the straight line between $\ln\Omega(-2N)$ and $\ln\Omega(0)$,

$$\sigma(E) = \left(N + \frac{N-1}{2N}E\right)\ln q, \quad -2N \le E \le 0. \tag{8}$$

For the correction function, ψ, we cannot give an explicit expression. That would correspond to solving the q-state Potts model analytically, which clearly is beyond the scope of the current investigation. We will instead be satisfied by demonstrating that ψ in (5) becomes insignificant in the thermodynamic limit of the infinite-state Potts model. We start by describing how the microcanonical entropy changes as q is increasing. For small values of q, there is a local maximum in S_μ. For $q = 2$, the Ising model, this maximum is at the midpoint of the energy scale. As q is increased, this local maximum shifts to higher energies and finally turns into a global maximum at $E = 0$, tending to $N\ln q$, in agreement with (7).

These aspects are illustrated in Figure 1, where we show S_μ as a function of E for $q = 10$, 100, and 1000 for an $N = 100$ lattice. For finite thermodynamic systems undergoing a first-order phase transition, a certain part of the entropy becomes convex [23]. This *convex intruder* can indeed be seen as a signature of a first-order phase transition in a finite system [6]. The local convexity is located between the energies, E_- and E_+, where $E_+ - E_-$ is equal to the latent heat. In Figure 1, the convexity is clearly visible in the $q = 100$ and 1000 curves but not directly visible in the $q = 10$ curve. We also see that the width of the convex region increases with increasing q. For combinatorial reasons, a few configurations with energies close to the ground state will never be accounted for. Specifically, for periodic boundary conditions, we have $\Omega(1-2N) = \Omega(2-2N) = \Omega(3-2N) = \Omega(5-2N) = 0$, which explains the irregular appearance of $S_\mu(E)$ at low E.

Due to computer time limitations, S_μ for arbitrarily large q and N cannot be calculated, but, in Figure 2, we show the

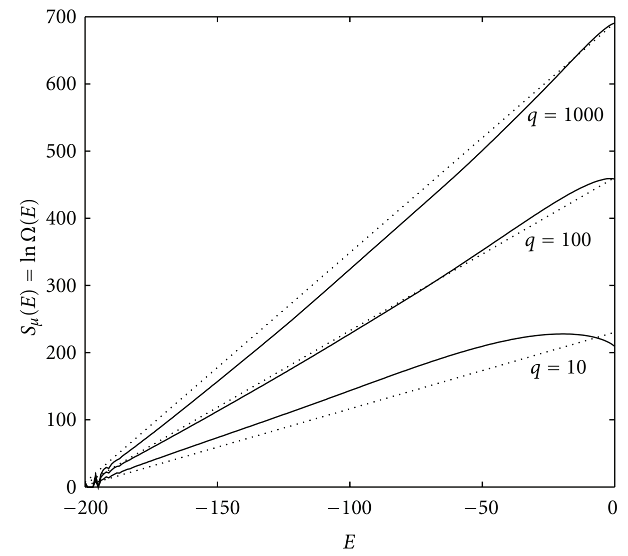

Figure 1: The solid curves represent the microcanonical entropy, $S_\mu(E)$, plotted as a function of energy, E, for three different values of q: 10, 100, and 1000. The lattice size is $N = 100$. The dotted lines represent σ and are straight lines from $\ln q$ to $N\ln q$. The local convexity of $S_\mu(E)$ is clearly visible in the $q = 100$ and $q = 1000$ cases.

convex intruder $\delta S/N = (S_{\text{lin}} - S_\mu)/N$, where S_{lin} is the line between E_- and E_+ (not to be confused with σ, which is the line between $-2N$ and 0), for $q = 10$ and 100 for various lattice sizes. Here we see that the convex intruder flattens out as N increases, illustrating how the microcanonical entropy responds to variations in q and N.

Baxter has derived an expression for the latent heat per site, Q, of the 2D Potts model [24], and from this we extract that $Q \to 2$ as $q \to \infty$. Thus, in the limit of large q, the convex intruder spans the entire energy interval. This leads us to the following large-q properties of ψ,

$$\psi(0) \longrightarrow 0, \qquad q \longrightarrow \infty, \tag{9}$$

at the high energy endpoint and

$$\psi(E) > 0, \qquad -2N < E < 0, \qquad q \longrightarrow \infty \tag{10}$$

at the interior. We also note that $\psi(-2N) = 0$ for all values of q. In other words, as $q \to \infty$, ψ becomes identical to the convex intruder.

In the thermodynamic limit, this intruder becomes insignificant by necessity. That is, $\lim_{N\to\infty}\psi(E)/N = 0$, which is in agreement with our simulations shown in Figure 2, since as $q \to \infty$, $S_{\text{lin}} \to \sigma$ and $\delta S \to \psi$ with the properties of (9) and (10). As discussed by Gross et al. [6], any convexity of the microcanonical entropy, $s(\varepsilon)$, for an infinite system with short-range interaction is forbidden [6]. A concave $s(\varepsilon)$ is required for an extensive thermodynamics.

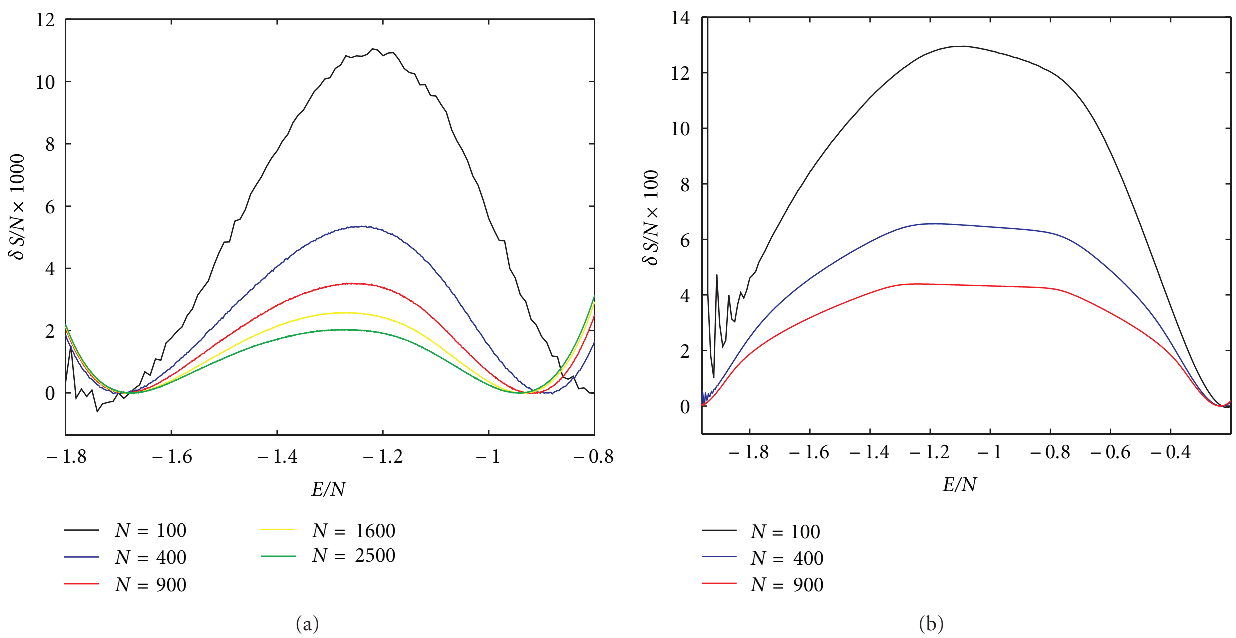

FIGURE 2: The convex intruder, $\delta S/N$, is shown as a function of E for (a) $q = 10$ and for (b) $q = 100$ for various lattice sizes. Only the central branches of the curves, that is, the parts between the local minima at E_- and E_+, are of significance here.

With these facts established, we can calculate the entropy per site in the thermodynamic limit of the infinite-state Potts model as

$$s(\varepsilon) = \lim_{N\to\infty} \frac{S_\mu(E)}{N} = \lim_{N\to\infty}\left[\left(1+\frac{E}{2N}\right)\ln q - \frac{\psi(E)}{N}\right] = \left(1+\frac{\varepsilon}{2}\right)\ln q, \tag{11}$$

which proves (4).

We have now shown that the microcanonical entropy of the infinite-state Potts model in the thermodynamic limit is given by (8). Combining this with (3) and (2), we can write down an explicit expression for the canonical partition function, Z. From this we calculate the free energy per site, f, which is given by

$$-\beta f = \lim_{N\to\infty}\frac{1}{N}\ln Z. \tag{12}$$

Using the elementary rule for summation of a geometrical series, we find that

$$f \sim \begin{cases} -\beta^{-1}\ln q, & \beta < \ln\sqrt{q}, \\ -2, & \beta \geq \ln\sqrt{q}. \end{cases} \tag{13}$$

The reader should be aware that this is an asymptotic relation, valid for $q \to \infty$. For any finite (but large) value of q, (13) can be regarded as an approximation. This result agrees with the mean field calculations by Mittag and Stephen [9], which are known to be exact in the $q \to \infty$ limit [10].

Finally, it is straightforward to generalize our reasoning to any dimension, $d > 1$. The Potts model on a d-dimensional hypercubic lattice takes energies from $-dN$ to 0. For large enough q, the phase transition is of first order, and the latent heat per site in the thermodynamic limit and the large q limit is given by $Q \to d$, for a d-dimensional square lattice [9]. In other words, for any $d > 1$ there is a convex intruder spanning the entire configurational energy interval. In the thermodynamic limit, the effect of this intruder vanishes, and the microcanonical entropy tends to its concave hull.

4. Conclusion

In summary, we have shown that the microcanonical entropy of the 2D standard Potts model approaches a straight line in the limit of large q and in the thermodynamic limit. This leads directly to an asymptotic form for the partition function, from which we calculate the free energy. We have also shown that it is straightforward to generalize this result to higher dimension since the phase transition is of first order and since the associated convex intruder takes up the entire energy range.

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