

Thermodynamics at negative temperatures in interacting systems: One-dimensional Ising model

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An exact microcanonical analysis of the one-dimensional Ising model is presented with emphasis on the emergence of negative temperatures. The number of states of the system is obtained as a function of the energy, the magnetization, and the number of spins. The Boltzmann and Gibbs entropy is computed, and the results are compared in the thermodynamic limit and for finite systems as well. According to the Boltzmann scenario, negative temperatures naturally appear as a consequence of the energy bounded spectrum. In this case, the Boltzmann entropy is not symmetric with the energy as soon as the magnetization is different from zero and does not vanish at the maximum allowed value of the energy. Along with entropy, the specific heat and magnetic susceptibility are analyzed as functions of the temperature. Although the specific heat is always positive, the symmetry is also broken in both branches of positive and negative temperatures for finite values of the magnetization. The susceptibility, in its turn, changes sign in the negative sector. In addition, the phase transition, which is present when the temperature goes to zero from the right, is totally suppressed when the temperature tends to zero from the left. Finite-size effects are also studied to understand the equivalence of the microcanonical and canonical formulations for this interacting model. Negative temperatures are not allowed according to the Gibbs formulation.

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I. INTRODUCTION

The microcanonical description of lattice spin systems has long occupied a central place in statistical mechanics, both as a conceptual framework and as a direct route to entropy-based thermodynamics (see, for instance, textbooks [1–5]). For low-dimensional systems with short-range interactions, the microcanonical ensemble is especially useful because it gives direct access to the entropy as a function of the relevant conserved or constrained macroscopic variables. This makes it possible to discuss temperature, response functions, and the relationship between different ensembles directly at the state counting level [6–8]. A particular issue brought about in the microcanonical ensemble is related to the case of negative absolute temperatures, which has attracted renewed attention in recent years, especially in systems whose energy spectrum is bounded from above. A central point in this debate concerns the appropriate definition of entropy. The Boltzmann *surface*

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entropy, for a particular magnetic system, is defined by

$$S_B(E, M, N) = k_B \ln \Omega(E, M, N), \quad (1)$$

where k_B is the Boltzmann constant and $\Omega(E, M, N)$ is the number of states with fixed energy E , magnetization M , and the number of particles N . In its turn, the Gibbs *volume* entropy is given by

$$S_G(E, M, N) = k_B \ln \Gamma(E, M, N), \quad (2)$$

where $\Gamma(E, M, N)$ is now the total number of states of a system with an energy less than or equal to E . $\Gamma(E, M, N)$ and $\Omega(E, M, N)$ are related by

$$\Gamma(E, M, N) = \sum_{E' \leq E} \Omega(E', M, N). \quad (3)$$

Swendsen and Wang argued that the Gibbs *volume* entropy (see, e.g., Refs. [9–12]) leads to incorrect thermodynamic predictions for systems with nonmonotonic densities of states, thereby supporting the consistency of negative temperatures within a Boltzmann-type *surface* framework [13]. Similar conclusions were reached by Frenkel and Warren [14] and by Poulter [15], who have emphasized that negative temperatures are physically meaningful equilibrium states in bounded-spectrum systems. An extensive comparison between canonical and microcanonical entropy definitions has been carried out by Matty *et al.* [7], while a later review by Swendsen [16] further clarified the conceptual status of entropy in situations involving negative temperatures, phase coexistence, and long-range interactions. More recently, related aspects of the Boltzmann-Gibbs debate have continued to be discussed from different perspectives [17]. In most of the above works, and even in statistical mechanics textbooks, noninteracting systems, such as ideal gas, harmonic oscillators, paramagnets, and independent particles with two (or more)-level energy have been used to exemplify the principal characteristics of the proposed entropy definitions. However, some interacting systems such as vortices in hydrodynamic flows [18] and studies treating nonlinear rotors [19] do have already been considered with negative temperatures (see also a review by Baldovin *et al.* [20]). Within this framework, the one-dimensional Ising model provides another ideal testing ground. Although simple, it is already an interacting system with a bounded spectrum, and its exact solvability makes it particularly suitable for clarifying the origin and meaning of negative temperatures in the Boltzmann microcanonical view together with a quantitative comparison to the Gibbs entropy definition. Although the microcanonical number of states has previously been studied in Ref. [21] for the one-dimensional model in chains and strips, only the symmetric case that does not depend on magnetization has been analyzed. We therefore investigate here the one-dimensional Ising model by exactly computing its complete relevant thermodynamic quantities within the microcanonical ensemble using the Boltzmann and Gibbs definition of entropy. We analyze the thermodynamics of the model in the entropy-energy plane for several values of the magnetization. Particular attention has been given to the structure of the inverse temperature and to the emergence of the negative-temperature regime in the Boltzmann case. This paper is organized as follows: Section II introduces the one-dimensional Ising model with open boundary conditions, the relevant extensive variables, and the microcanonical formulation to obtain the corresponding number of states. In Sec. III, the results of the Boltzmann entropy are presented with discussion of negative temperatures. A comparison between Boltzmann versus Gibbs entropy is discussed in Sec. IV. The effects of finite size and the route to the thermodynamic limit are presented in Sec. V. Some final remarks are discussed in the last section.

II. ONE-DIMENSIONAL ISING MODEL IN THE MICROCANONICAL ENSEMBLE

The Hamiltonian with only nearest-neighbor interactions of the one-dimensional Ising model can be written as

$$\mathcal{H} = -J \sum_{i=1}^{N-1} \sigma_i \sigma_{i+1}, \quad (4)$$

where $J > 0$ is the ferromagnetic exchange interaction, $\sigma_i = \pm 1$, and open boundary conditions are considered in the one-dimensional lattice consisting of N spins. Here, and in what follows, we will consider, without loss of generality, $J = 1$ and $k_B = 1$. This means that all energies are measured in units of J and temperatures in units of J/k_B . In the microcanonical ensemble, the internal energy E obtained from Hamiltonian (4), the magnetization $M = \sum_{i=1}^N \sigma_i$, and the number of spins N are kept fixed. In order to specify the spin configuration of the one-dimensional lattice, we closely follow, and summarize here for completeness, the procedure already done in Refs. [22,23] to compute the total number of microstates $\Omega(E, M, N)$. The same notation adopted in Ref. [23] is also used herein. The quantity $\Gamma(E, M, N)$ is then obtained directly from Eq. (3). First, it is noticed that the introduction of the number of up spins Q , the number of up spin domains B , and the number of up-down and down-up spin pairs K is enough to completely and uniquely specify E and M for a given total number of spins N . Thus, the energy obtained with the Hamiltonian (4) and the corresponding magnetization can be given, respectively, by

$$E = -(N - 1 - K) + K = -(N - 1) + 2K, \quad (5)$$

$$M = Q - (N - Q) = 2Q - N. \quad (6)$$

Inserting *walls* between spins of different signs, the one-dimensional lattice is viewed as boxes containing either up or down spins (for more details, see Ref. [23]). Since we have in total $K + 1$ boxes and the up spin domains comprise B boxes, the number of boxes containing down spins is simply $K + 1 - B$. It means that the computation of the total number of states is just replaced by the equivalent problem of counting the number of ways of distributing balls in boxes, in this particular case Q up spins in B boxes and $N - Q$ down spins in $K + 1 - B$ boxes. All possible configurations obtained after this counting process are given by (details can be found in Ref. [23])

$$\Omega(E, M, N) = (1 + \delta_{2B-\alpha, 2Q-1}) \frac{(Q-1)!}{(Q-B)!(B-1)!} \frac{(N-Q-1)!}{(N-Q-B+\alpha-1)!(B-\alpha)!}, \quad (7)$$

where $\delta_{2B-\alpha, 2Q-1}$ is the Kronecker delta symbol, and

$$Q = \frac{M + N}{2}, \quad (8)$$

$$B = \frac{E + N - 1}{4} + \frac{\alpha}{2}, \quad (9)$$

with $\alpha = 0, 1, 2$. In the thermodynamic limit, where one has $N \rightarrow \infty$ with $u = E/N$ and $m = M/N$ finite, the microcanonical entropy

$$S(E, M, N) = Ns(u, m) = \ln \Omega(E, M, N) \quad (10)$$

can, after some algebra and using the Stirling approximation, be written as

$$\begin{aligned} s(u, m) = & q \ln q + (1 - q) \ln(1 - q) - (q - b) \ln(q - b) \\ & - (1 - q - b) \ln(1 - q - b) - 2b \ln b, \end{aligned} \quad (11)$$

where

$$q = \frac{Q}{N} = \frac{m + 1}{2} \quad \text{and} \quad b = \frac{B}{N} = \frac{u + 1}{4}. \quad (12)$$

The above procedure then furnishes the desired entropy as a function of the corresponding extensive variables for finite systems as well as in the thermodynamic limit.

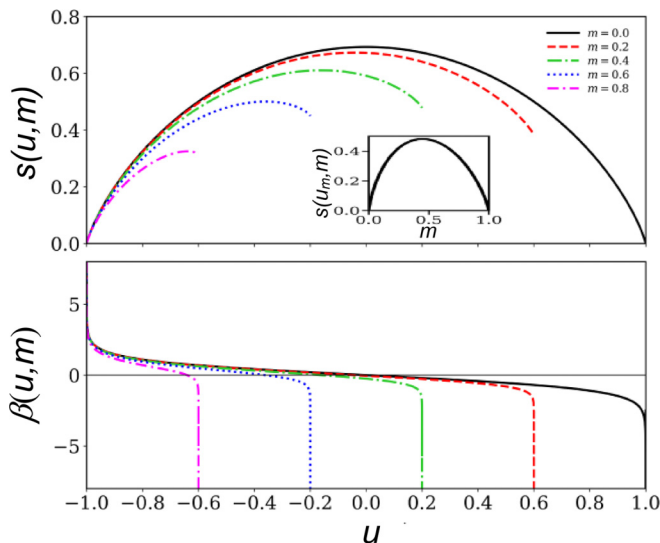


FIG. 1. Reduced entropy per spin $s(u, m)$ (upper panel) and the corresponding microcanonical inverse temperature $\beta(u, m)$ (lower panel), for the one-dimensional Ising chain in the thermodynamic limit, shown for several fixed values of the magnetization m . The legends in the upper panel also hold for the lower panel. For each m , the energy and the temperature are restricted to the finite interval $-1 \leq u \leq u_m$. The inset in the upper panel shows the entropy $s(u_m, m)$.

III. BOLTZMANN ENTROPY IN THE THERMODYNAMIC LIMIT

Having established the exact microcanonical relation $s(u, m)$, we are now in a position to analyze the thermodynamic consequences of negative temperatures. Because the one-dimensional Ising model has a bounded energy spectrum at fixed magnetization, the entropy is not a monotonic function of the energy over the entire physically allowed interval. As a result, the inverse temperature changes sign at the entropy maximum, naturally separating the thermodynamic description into positive- and negative-temperature sectors. In this section, we examine how this structure is reflected in the main thermodynamic observables. In particular, we discuss the behavior of the entropy, the inverse temperature, the specific heat at fixed magnetization, and the isothermal susceptibility, emphasizing how the bounded spectrum and the fixed magnetization constraint shape the response of the system in both thermal branches.

A. Entropy and negative temperature

Equations (11) and (12) provide a transparent framework to analyze the thermodynamic behavior of the model. For each fixed value of magnetization m , the energy is confined to the finite interval

$$-1 \leq u \leq u_m, \quad \text{with} \quad u_m = 1 - 2|m|, \quad (13)$$

which is the essential condition for the existence of negative temperatures. Figure 1 summarizes the thermodynamic behavior of the energy and temperature of the one-dimensional Ising chain in the thermodynamic limit at fixed magnetization. Starting from the lowest-energy state, $u = -1$, the entropy increases with u , reaches a maximum at

$$u^* = -m^2, \quad (14)$$

and then decreases as the energy approaches the upper boundary of the allowed interval. This behavior is a direct consequence of the bounded energy spectrum. As the energy increases from its minimum value, the number of accessible microstates has a fast initial increase, but beyond a certain

point it begins to decrease. As a result, the derivative $\partial s/\partial u = 1/T$, where T is the temperature, changes sign. This behavior is shown in the upper panel of Fig. 1 for several values of magnetization m . It is clearly seen that the symmetry of the entropy as a function of the energy, with respect to its maximum value u^* , breaks as soon as the magnetization is different from zero, with a steeper slope (as we shall see below) after the maximum. This sign change is clearly reflected in the inverse of the temperature $\beta(u, m)$, with $\beta = 1/T$, shown in the lower panel of Fig. 1. At low energies, $\beta(u, m) > 0$, corresponding to the usual positive-temperature regime. At the point where $s(u, m)$ reaches its maximum, one has $\beta(u^*, m) = 0$, which corresponds to the infinite-temperature limit. For higher energies, the entropy decreases with increasing u , so that $\beta(u, m) < 0$ in the energy interval

$$u^* < u \leq u_m, \quad (15)$$

characterizing the negative-temperature sector. Thus, within the microcanonical ensemble, negative temperatures arise naturally whenever the entropy ceases to be an increasing function of the energy. Figure 1 also shows that increasing m reduces both the accessible energy interval and the maximum entropy. Physically, this reflects the fact that the magnetization constraint restricts the number of spin configurations compatible with the system. However, for all nonzero values of m considered here, there remains a finite energy window in which $\beta < 0$. The negative temperature is therefore not a peculiarity of the unmagnetized chain but a robust feature of the model in its microcanonical description. Another important feature is that the entropy does not vanish at the maximum allowed energy value. At the bottom edge, $u \rightarrow -1$, the system approaches the most ordered low-energy configurations, and the number of compatible microstates becomes exponentially small with just one possible ordered state for $u = -1$ and $s(-1, m) = 0$ for any value of m . On the other hand, at the top edge, $u \rightarrow u_m$, the magnetization being nonzero implies an unbalanced number of up-down spins that can be arranged in so many different ways that an entropic effect is also present in the system. The entropy in this limit is given by

$$s(u_m, m) = \frac{(1+m)}{2} F[(1-m)/(1+m)], \quad (16)$$

where

$$F(x) = -x \ln x - (1-x) \ln(1-x). \quad (17)$$

However, between these two limits, $s(u, m)$ exhibits a single broad maximum, which identifies the most probable macrostate at fixed m and coincides with the point where the inverse temperature changes sign. Such a structure has, in fact, a simple physical interpretation. On the positive-temperature branch, adding energy increases disorder and drives the system away from the ordered low-energy sector. On the negative-temperature branch, in contrast, the system lies in the upper part of a bounded spectrum, where further energy input reduces the number of accessible microstates. In this sense, the negative-temperature sector is not anomalous, but rather a natural continuation of the microcanonical equation of state beyond the entropy maximum. It should also be stressed here that the temperature indeed goes to zero as the energy approaches its maximum value u_m . This can be clearly seen in the bottom panel of Fig. 1, where $\beta \rightarrow -\infty$ when $u \rightarrow u_m$. In fact, one has

$$\lim_{u \rightarrow u_m} \frac{\partial s}{\partial u} \rightarrow -\infty. \quad (18)$$

The above limit is not apparent on the vertical axis scale of the upper panel in Fig. 1.

B. Specific heat behavior

Figure 2 shows the specific heat at fixed magnetization $c_m(T)$ as a function of temperature T for several values of m . The curve naturally splits into two branches, corresponding to the positive- and negative-temperature sectors identified in the microcanonical equation of state. An important result

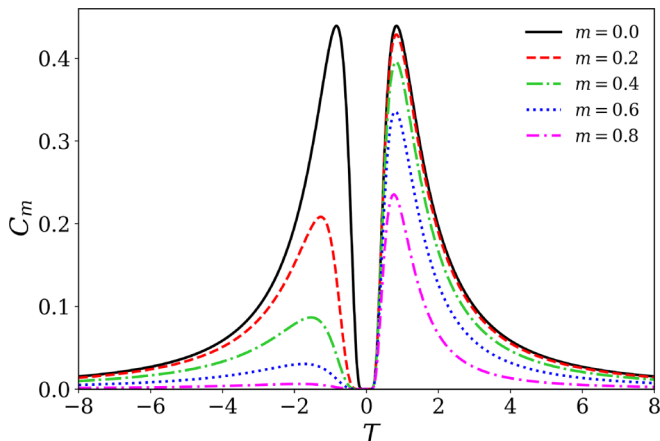


FIG. 2. Specific heat at fixed magnetization c_m as a function of the temperature T in the thermodynamic limit for several values of the magnetization m (indicated in the legend). The figure displays both the positive- and negative-temperature branches allowed by the bounded energy spectrum of the model.

is that $c_m(T)$ remains positive in both branches. This follows from the concavity of the entropy $s(u, m)$, since

$$c_m = \left(\frac{\partial u}{\partial T} \right)_m = -\frac{1}{T^2} \left[\left(\frac{\partial^2 s}{\partial u^2} \right)_m \right]^{-1}, \quad (19)$$

and $s(u, m)$ is concave in the allowed energy interval; one has $(\partial^2 s / \partial u^2)_m < 0$, which ensures $c_m > 0$ for both $T > 0$ and $T < 0$. Thus, although the sign of the temperature changes across the entropy maximum, the thermal response remains well defined and positive throughout the physically accessible region. The specific heat vanishes in three limiting regimes, namely, as $T \rightarrow 0^+$, as $T \rightarrow 0^-$, and as $|T| \rightarrow \infty$. The suppression of specific heat as $T \rightarrow 0^+$ reflects the freezing of thermal fluctuations near the edge of the ground-state $u = -1$, where only a very small number of low-energy configurations remain accessible. A similar effect occurs as $T \rightarrow 0^-$, but now at the upper spectral boundary $u \rightarrow u_m$, where the number of accessible microstates decreases. In the opposite limits, $|T| \rightarrow \infty$, the specific heat also tends to zero because the entropy becomes locally flat around its maximum, in a way that the system responds only weakly to further thermal changes. Between these limiting regimes, $c_m(T)$ exhibits a broad maximum in each branch, signaling the crossover between edge-dominated configurations and the highly degenerate intermediate-energy sector. For $m = 0$, the specific heat is symmetric with respect to $T = 0$. As the magnetization increases, the asymmetry also increases, with the two maxima presenting different peak heights. However, both peaks are progressively lower and have shifted in their position. This is a reflection of the reduction of the accessible energy window and the corresponding depletion of configurational entropy. In this sense, the general evolution of $c_m(T)$ with m is fully consistent with the narrowing of the entropy curves discussed above.

C. Isothermal susceptibility behavior and zero temperature transition

The isothermal susceptibility can be computed using Eqs. (11) and (12) to obtain first the equation of state

$$\left(\frac{\partial s}{\partial m} \right)_u = -\frac{h}{T}, \quad (20)$$

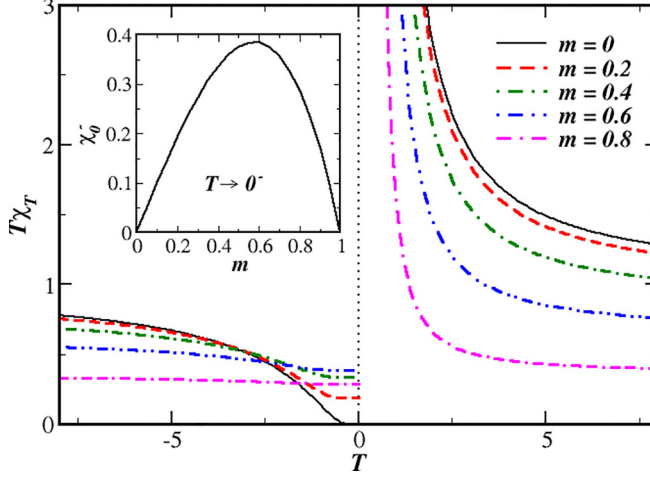


FIG. 3. Temperature times the isothermal susceptibility $T\chi_T$ as a function of temperature T (shown in the main graph) for several fixed values of the magnetization m (given in the legend) in the thermodynamic limit. For $T \rightarrow 0^+$, $T\chi_T \rightarrow \infty$ for all values of $m < 1$. For $T \rightarrow 0^-$, $T\chi_T \rightarrow \chi_0^-$, with χ_0^- given in Eq. (26) as a function of m shown in the inset.

which can be written as

$$\frac{h}{T} = \operatorname{arsinh} \left[\frac{me^{-2/T}}{\sqrt{1-m^2}} \right], \quad (21)$$

where h is here the external field in units of J .

The isothermal magnetic susceptibility, defined as

$$\chi_T = \left(\frac{\partial m}{\partial h} \right)_T, \quad (22)$$

can be obtained by taking the derivative of Eq. (21):

$$\frac{\partial}{\partial m} \left(\frac{h}{T} \right)_T = \frac{Te^{-2/T}}{(1-m^2)\sqrt{1-m^2+m^2e^{-4/T}}}. \quad (23)$$

From the above equation, we finally have

$$\chi_T(T, m) = \frac{e^{2/T}(1-m^2)\sqrt{1-m^2+m^2e^{-4/T}}}{T}. \quad (24)$$

This expression immediately reveals the strong asymmetry between the positive- and negative-temperature sectors, as can be clearly seen in Fig. 3, which shows the temperature times the isothermal susceptibility $T\chi_T$ as a function of T for several fixed values of m . Even at zero magnetization, the susceptibility is not antisymmetric at all, as would be suggested at first sight. For $T > 0$, one has $\chi_T > 0$, as expected for the usual paramagnetic response, whereas for $T < 0$ the susceptibility becomes negative. The sign change is entirely controlled by the factor T in front of Eq. (24), while the remaining factors are positive throughout the physically allowed region. On the positive-temperature branch, χ_T grows rapidly as $T \rightarrow 0^+$ and goes to infinity for any value of $m < 1$, indicating that the low-energy sector becomes increasingly sensitive to an external magnetic disturbance. Physically, this reflects the proximity to the lower spectral edge, where a weak field can efficiently reorganize the domain structure compatible with the magnetization constraint. In other words, in this limit one has a phase transition at zero temperature [24]. The corresponding scaling

form of $T\chi_T$ close to the right-handed limit to zero temperature is given by

$$T\chi_T \simeq \chi_0^+ t^{-\gamma}, \quad (25)$$

where $t = e^{-2/T}$, the critical exponent of susceptibility $\gamma = 1$, and χ_0^+ is a constant that depends on m . In contrast, on the negative-temperature branch, χ_T is negative as well and approaches a constant value as $T \rightarrow 0^-$, namely,

$$T\chi_T \simeq \chi_0^- = m(1 - m^2), \quad (26)$$

where χ_0^- (which is shown in the inset of Fig. 3) is a constant that also depends on m . In this case, the phase transition, as predicted by the scaling relation given in Eq. (25), is suppressed for negative temperatures. This behavior is a direct consequence of the bounded spectrum: Near the upper spectral edge, the system occupies a population-inverted sector, so that the magnetic response is reversed relative to the conventional positive-temperature regime. Figure 3 also shows that the magnitude of susceptibility decreases as magnetization increases. This suppression is consistent with the prefactor $(1 - m^2)$ in the exact expression above and reflects the progressive reduction of magnetic fluctuations under stronger magnetization constraints. In other words, as the system is forced in the direction of larger fixed values of m , the number of accessible spin rearrangements decreases and the response to an external field becomes correspondingly weaker.

D. General comments

The susceptibility provides a particularly clear signature of the distinction between the two thermal sectors. While the specific heat remains positive on both branches, the susceptibility changes sign across the infinite-temperature point, sharply distinguishing the ordinary positive-temperature regime from the negative-temperature sector associated with the upper part of the bounded energy spectrum. In addition, the phase transition seen as one approaches $T \rightarrow 0^+$ is suppressed in the negative sector $T \rightarrow 0^-$. Together, these results reveal a coherent thermodynamic picture. The entropy curve determines a monotonic inverse-temperature branch that connects positive and negative temperatures through the maximum-entropy point. The specific heat remains positive and displays finite-temperature maxima on both sides of the spectrum, while the susceptibility sharply distinguishes the conventional positive-temperature regime from the anomalous negative-temperature sector. The progressive suppression of all these responses with increasing m reflects the same fundamental mechanism: Fixing a larger magnetization m reduces the number of accessible microstates, which in turn narrows the allowed energy interval, and weakens the thermal and magnetic fluctuations of the system.

IV. BOLTZMANN VERSUS GIBBS ENTROPY

For comparison with the Boltzmann entropy, it is useful to analyze the Gibbs entropy defined by Eqs. (2) and (3). The corresponding Gibbs entropy per spin is then

$$s_G(u, m) = \frac{1}{N} S_G(E, M, N) = \frac{1}{N} \ln \Gamma(E, M, N). \quad (27)$$

The thermodynamic-limit form of $s_G(u, m)$ follows directly from the large- N behavior of the Boltzmann multiplicity. Indeed, with Eq. (10) one has

$$\Omega(E, M, N) = \exp[Ns_B(u, m)], \quad (28)$$

which means that the cumulative sum $\Gamma(E, M, N)$ in Eq. (3) is asymptotically dominated by the largest value of $s_B(v, m)$ among all energies $v \leq u$. Therefore,

$$s_G(u, m) = \lim_{N \rightarrow \infty} \left[\frac{1}{N} \ln \Gamma(E, M, N) \right] = \sup_{v \leq u} (s_B(v, m)), \quad (29)$$

where $\sup(x)$ is the least upper bound (supremum) of the variable x . This relation provides a particularly simple interpretation of the Gibbs construction in the thermodynamic limit: Instead of assigning to each energy shell its own entropy, as in the Boltzmann prescription, the Gibbs entropy is determined by the most entropically favorable shell among all states with energy below u . For the present model, the Boltzmann entropy $s_B(u, m)$ is defined in the bounded interval $-1 \leq u \leq u_m$ and exhibits a single maximum at $u^* = -m^2$. As a consequence, the supremum in Eq. (29) can be evaluated explicitly. For energies below the maximum, $s_B(u, m)$ is still increasing, and therefore the largest value below u is simply $s_B(u, m)$ itself. However, for energies above u^* , the Boltzmann entropy decreases, so that the cumulative counting is dominated by the shell at $u = u^*$. Thus, one obtains the following piecewise result:

$$s_G(u, m) = \begin{cases} s_B(u, m), & -1 \leq u \leq u^*, \\ s_B(u^*, m), & u^* \leq u \leq u_m. \end{cases} \quad (30)$$

Equation (30) shows that the Gibbs entropy coincides with the Boltzmann entropy only on the increasing branch of $s_B(u, m)$. Beyond the entropy maximum, the Gibbs entropy no longer follows the decreasing part of the Boltzmann curve, but instead remains constant. In other words, the upper portion of the spectrum is replaced by a plateau,

$$s_G(u, m) = \text{const}, \quad u^* \leq u \leq u_m. \quad (31)$$

The height of this plateau can be obtained explicitly. Writing

$$q = \frac{1+m}{2}, \quad b = \frac{1+u}{4},$$

the maximum occurs at

$$u = u^*, \quad b^* = \frac{1+u^*}{4} = \frac{1-m^2}{4} = q(1-q). \quad (32)$$

Substituting $b = b^*$ into the Boltzmann entropy, one has

$$s_B(u^*, m) = -q \ln q - (1-q) \ln(1-q). \quad (33)$$

Thus, in the thermodynamic limit, the Gibbs entropy takes the explicit form

$$s_G(u, m) = q \ln q + (1-q) \ln(1-q) - (q-b) \ln(q-b) - (1-q-b) \ln(1-q-b) - 2b \ln b, \quad (34)$$

for $-1 \leq u \leq u^*$ [which is exactly Eq. (11) reproduced here for completeness], and

$$s_G(u, m) = -q \ln q - (1-q) \ln(1-q), \quad (35)$$

for $u^* \leq u \leq u_m$. This result has an immediate thermodynamic consequence. Since $s_G(u, m)$ is nondecreasing by construction, its derivative never becomes negative. The corresponding inverse temperature,

$$\beta_G(u, m) = \left(\frac{\partial s_G}{\partial u} \right)_m, \quad (36)$$

is therefore given by

$$\beta_G(u, m) = \begin{cases} \beta_B(u, m), & -1 \leq u < u^*, \\ 0, & u^* < u \leq u_m. \end{cases} \quad (37)$$

In particular, the negative-temperature branch present in the Boltzmann description is completely suppressed in the Gibbs construction and replaced by a zero-slope entropy plateau. This contrast between the two entropy definitions is particularly transparent in the present model. The Boltzmann

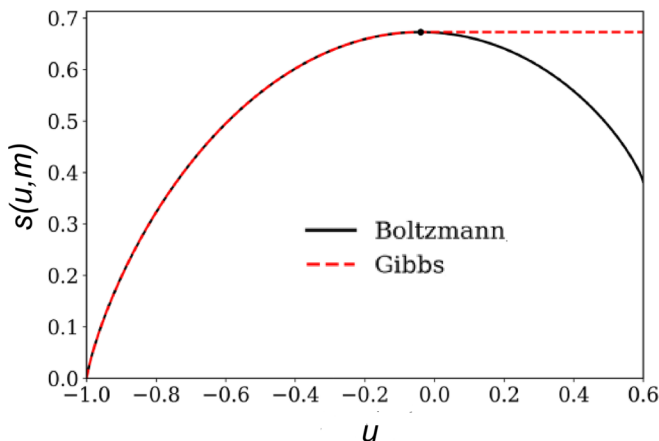


FIG. 4. Comparison between the Boltzmann and Gibbs entropies per spin, $s(u, m)$, as functions of the energy $u = E/N$ for fixed magnetization $m = 0.2$ in the thermodynamic limit. The solid curve corresponds to the Boltzmann entropy, while the dashed curve represents the Gibbs entropy. The two definitions coincide on the increasing branch of the entropy, but differ in the high-energy sector, where the Gibbs entropy saturates at a constant value whereas the Boltzmann entropy decreases.

entropy resolves the shell structure of the spectrum and therefore becomes nonmonotonic, giving rise to a negative-temperature branch once the number of accessible states begins to decrease with increasing energy. The Gibbs entropy, in contrast, counts all states with energy below a given value and is therefore dominated, in the high-energy region, by the shell of maximal entropy. As a result, it becomes insensitive to the decreasing branch of $s_B(u, m)$ and does not support a negative-temperature regime. This behavior is illustrated in Fig. 4, where we compare $s_G(u, m)$ and $s_B(u, m)$ as functions of energy u for the specific case of magnetization $m = 0.2$. Similar curves are obtained for other values of m . It should be worthwhile to stress here that the overall scenario depicted in Fig. 4 is not particular of the details of the present model, but has already been obtained in previous studies on different systems, as is discussed in Fig. 4 of Ref. [20]. Moreover, similar conclusions have been also achieved from rather general arguments [25].

V. FINITE-SIZE ANALYSIS

Since for the present model one has all quantities as a function of the size of the one-dimensional lattice, it will be illustrative to analyze the thermodynamic behavior of the system as N increases. This can be done following two distinct situations: First, how the two entropies compare for finite systems, and second, perhaps more interesting, how the microcanonical- and canonical-like ensembles compare with the length of the one-dimensional lattice. In the first case, at finite lattices N , the Gibbs entropy plateau is not perfectly sharp because the cumulative sum in Eq. (3) still reflects the discreteness of the spectrum. Nevertheless, as the number of spins N increases, the Gibbs entropy rapidly approaches the piecewise form (30), and the flattening of the upper branch becomes increasingly evident. The thermodynamic-limit behavior is therefore already anticipated at large but finite sizes, even though the exact cancellation of the slope is only achieved asymptotically. It is also interesting to examine, as a subproduct of this model, how the microcanonical description at fixed energy and magnetization approaches the corresponding canonical behavior when the system size remains finite. For the one-dimensional Ising chain, no genuine ensemble inequivalence is expected in the thermodynamic limit, since the model is short ranged. The physically relevant question is therefore not whether the two ensembles are fundamentally different, but rather how the discrete shell structure of the finite system is smoothed out by canonical energy fluctuations

and how the thermodynamic-limit equivalence is progressively recovered as the number of spins N increases. In the microcanonical description, the starting point is the finite- N entropy $S(E, M, N)$. Since both E and M are sharply fixed, the entropy is defined only on a discrete set of energy shells. Consequently, the caloric curve is also discrete, and the inverse temperature must be extracted from finite differences of the entropy between neighboring shells rather than from a smooth function derivative. For a direct comparison with the microcanonical results at fixed magnetization, it is convenient to introduce the restricted canonical partition function

$$Z_M(\beta, N) = \sum_E \Omega(E, M, N) e^{-\beta E}. \quad (38)$$

This formulation describes a canonical ensemble in which the magnetization is fixed, while the energy is allowed to fluctuate. The corresponding mean energy is then obtained from

$$U_M(T, N) = - \frac{\partial \ln Z_M(\beta, N)}{\partial \beta} \quad (39)$$

and provides a smooth caloric curve $u(T) = U_M/N$.

The difference between the two descriptions is therefore immediate. In the microcanonical ensemble, each energy shell is treated individually, and the temperature reflects the detailed shell-by-shell variation of the multiplicity. In the restricted canonical ensemble, in contrast, the temperature is associated with a weighted average over many shells, so that the resulting caloric curve is continuous even for finite N . Thus, the discrepancy between the two ensembles at finite size is not a sign of true inequivalence, but a consequence of spectral discreteness in the microcanonical description and of thermal averaging in the canonical one.

A particularly important point in the present problem is the fate of the negative-temperature branch. Because the Ising chain has a bounded spectrum, the microcanonical entropy may already become nonmonotonic at finite N , and negative temperatures appear as soon as the multiplicity starts to decrease with increasing energy. In the finite system, however, this branch is represented only by a finite set of discrete points. The canonical description, on the other hand, replaces this shell structure by a smooth interpolation between the low-energy positive-temperature sector and the high-energy negative-temperature sector. The comparison therefore makes it possible to see, in a very direct way, how the negative-temperature regime is already present in finite chains, while its thermodynamic-limit structure emerges only after the discrete shell spacing becomes sufficiently small.

Figure 5 compares the microcanonical and restricted canonical caloric curves for finite one-dimensional Ising chains. The upper panels correspond to the sector $m = 0$, while the lower panels correspond to $m = 0.2$. In all cases, the microcanonical temperature, obtained from finite differences of the entropy, appears as a discrete set of points, reflecting the shell structure of the finite spectrum. In contrast, the restricted canonical temperature is a continuous function of the mean energy, since it results from thermal averaging over all states compatible with a fixed magnetization.

Figure 5 shows that both descriptions already capture the same global thermodynamic structure: a positive-temperature branch at low energies, a crossover through the infinite-temperature region, and a negative-temperature branch in the upper part of the spectrum. Their difference is therefore not qualitative, but finite size in origin. The microcanonical caloric curve retains the discreteness of the underlying energy shells, whereas the canonical curve smooths this structure through energy fluctuations. As the system size increases from $N = 10$ to $N = 20$, the microcanonical points become denser and progressively approach the canonical curves, illustrating the expected recovery of ensemble equivalence in the thermodynamic limit.

A central result of this comparison is that the negative-temperature branch is not an artifact of the thermodynamic-limit treatment. It is already present in finite chains and follows directly from the bounded spectrum and the exact shell-by-shell counting of states. What changes with increasing N is not the existence of this branch, but only its representation: For small systems, it appears as a discrete sequence of temperature values controlled by the entropy differences between neighboring shells,

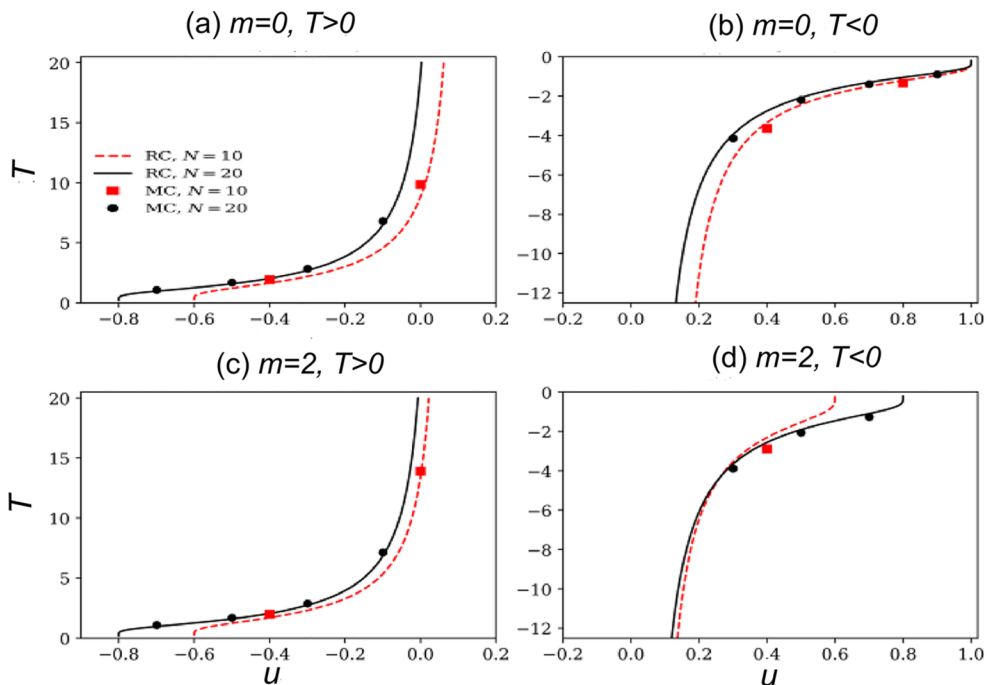


FIG. 5. Comparison between the microcanonical (MC) and restricted canonical (RC) caloric curves for finite one-dimensional Ising chains. The upper panels correspond to the sector $m = 0$, while the lower panels correspond to $m = 0.2$. Panels (a) and (c) show the positive-temperature branches, whereas panels (b) and (d) display the negative-temperature branches. In each case, the microcanonical results are represented by discrete points, reflecting the shell structure of the finite spectrum, while the restricted canonical results are shown as continuous curves obtained by thermal averaging at fixed magnetization. Results are displayed for $N = 10$ and $N = 20$.

while for larger systems it tends toward the smooth behavior predicted by the thermodynamic-limit microcanonical theory.

VI. CONCLUSION

In this work, an exact microcanonical treatment of the one-dimensional Ising model at fixed energy, magnetization, and number of spins has been developed. The resulting entropy in the thermodynamic limit makes the thermodynamic structure of the model particularly transparent. For fixed magnetization, the bounded energy interval naturally leads to an entropy that increases from the lower spectral edge, reaches a single maximum, and then decreases as the upper boundary is approached. As a consequence, the inverse temperature changes sign, separating the physical domain into positive- and negative-temperature sectors. In this sense, the one-dimensional Ising chain provides a fully analytic example of how negative temperatures arise in an interacting system having a bounded spectrum.

For comparison, we also examined the Gibbs entropy at fixed magnetization. As a result, the Gibbs construction suppresses the decreasing branch of the entropy and yields no negative-temperature regime. This provides a particularly simple and explicit illustration of the conceptual difference between the two entropy definitions in a bounded-spectrum interacting model.

Finally, our finite-size analysis shows that the negative-temperature branch is not an artifact of the thermodynamic-limit treatment. It is already encoded in the exact shell structure of finite chains, where the microcanonical caloric curve appears as a discrete sequence of temperature values, while

the restricted canonical description smooths this structure through thermal averaging. As the system size increases, the microcanonical points become denser and progressively approach the canonical curves, recovering the expected ensemble equivalence in the thermodynamic limit.

Overall, the one-dimensional Ising model provides an especially clear setting in which to analyze the interplay between refined microcanonical counting, bounded spectra, and negative temperatures. From a physical point of view, it provides a fully analytic example of negative-temperature thermodynamics in an interacting spin system. These results suggest that the same strategy may be profitably extended to other short-range lattice models with additional local variables or constraints, where refined microcanonical structures remain of both conceptual and practical interest.

DATA AVAILABILITY

There are no publicly available research data or software supporting this manuscript. Requests for further information or data should be sent to the authors.

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