

Phase Transitions in the Two-Dimensional Ising Model from the Microcanonical Perspective

Kedkanok Sitarachu and Michael Bachmann

Soft Matter Systems Research Group, Center for Simulational Physics, Department of Physics and Astronomy, University of Georgia, Athens, GA 30602, USA

E-mail: Kedkanok.Sitarachu@uga.edu, bachmann@smsyslab.org

Homepage: <http://www.smsyslab.org>

Abstract. The continuous ferromagnetic-paramagnetic phase transition in the two-dimensional Ising model has already been excessively studied by conventional canonical statistical analysis in the past. We use the recently developed generalized microcanonical inflection-point analysis method to investigate the least-sensitive inflection points of the microcanonical entropy and its derivatives to identify transition signals. Surprisingly, this method reveals that there are potentially two additional transitions for the Ising system besides the critical transition.

1. Introduction

The Lenz-Ising model [1, 2] for spin systems provides an excellent foundation for the study of long-range correlations in a system with short-range interactions only. In the two-dimensional (2D) case, this cooperative behavior of local spins leads to a thermodynamic phase transition between the disordered paramagnetic and the ordered ferromagnetic phase [3]. However, the one-dimensional (1D) model does not show significant signs of cooperativity [2]. Although the 1D and 2D models were solved exactly many decades ago, the Ising model has inspired a multitude of studies thereafter and is probably the best-studied system exhibiting complex behavior in statistical physics.

Almost all of these studies have focused on canonical statistical properties of the critical behavior of the 2D system in the thermodynamic limit. Here, we follow a different conceptual approach and use recently expanded ideas of microcanonical thermodynamics [4, 5] for the analysis. The generalized microcanonical inflection-point analysis method [6] was developed to incorporate systems of finite size in the theory of phase transitions and to introduce a robust classification system for phase transitions that does not require the extrapolation toward the thermodynamic limit. This is particularly important for systems that are naturally finite, such as biological macromolecules, but the method can be used for the study of phase behavior in any system of interest, independently of system size.

As we will show in the following, microcanonical inflection-point analysis does not only correctly signal the expected second-order phase transition between the ferromagnetic and the paramagnetic phase. It also reveals two additional transitions of higher order, which do not seem to disappear in the thermodynamic limit.



2. Microcanonical analysis of least-sensitive inflection points

The typical classification of phase transitions is based on Ehrenfest's scheme, in which the order of a transition is determined by the order of the derivative of the appropriate thermodynamic potential (typically the Gibbs free enthalpy) with respect to its natural variables that exhibits a discontinuity at the transition point in the thermodynamic limit [7]. It thus makes use of the macroscopic state variables of the system, which are represented by averages over microscopic degrees of freedom in the canonical statistical ensemble. Since virtually all thermodynamic phase transitions that fit into this scheme are first- or second-order phase transitions, it is nowadays more common to distinguish only discontinuous and continuous transitions, respectively.

A significant drawback of the conventional canonical statistical analysis is that a unique identification of a phase transition relies on the necessity to study the system in the thermodynamic limit or to extrapolate to it in order to create a non-analyticity that signals a phase transition. This is not a problem for very large systems, for which the scaling to infinite size is possible and reasonable. However, for finite systems, there are no discontinuities. Therefore, in studies of systems like proteins, whose sizes cannot be extrapolated toward the thermodynamic limit, it has become popular to locate "peaks" and "shoulders" in canonical response quantities such as the specific heat, susceptibility, and fluctuations of order parameters. One problem with this approach is that these signals are not unique; the location of a transition point typically depends on the quantity used for its identification (see, e.g., Fig. 5 in Ref. [8]).

Another issue is that a peak in a fluctuating quantity does not necessarily signal a transition at all. The most prominent example is the 1D Ising model. There is no phase transition, but the specific heat curve possesses a pronounced peak, which remains finite even in the thermodynamic limit. Thus, if a system does not allow for the extrapolation toward the thermodynamic limit, a peak may or may not signal a transition. Yet, cooperative processes like the folding of a protein have many features in common with phase transitions. Therefore, it would be useful to have an analysis method that can provide unique transition signals even for systems of finite size. Microcanonical inflection-point analysis has been developed for this purpose and, in addition, allows for a systematic, hierarchical classification of the transitions [6].

The microcanonical entropy

$$S(E) = k_B \ln g(E), \quad (1)$$

where $g(E)$ is the density (or number) of states with energy E , and its derivatives $\beta(E) = dS(E)/dE$, $\gamma(E) = d^2S(E)/dE^2$, $\delta(E) = d^3S(E)/dE^3$, ... have a well-defined monotony in energy regions that do not include transition points. Thus, changes in monotony can be considered signals of peculiar behavior. Since entropy and energy drive thermodynamic phase transitions, these monotonic changes – represented by inflection points in the curves of $S(E)$ or its derivatives – are indicative signals of transitions in the system. More specifically, since transitions are typically associated with large fluctuations in energy, least-sensitive inflection points in these curves can serve as signals for transitions. The order of the transition is in correspondence with the order of the derivative of S that exhibits a least-sensitive inflection point [6]. For example, a least-sensitive inflection point in the first derivative, $\beta(E)$, indicates a second-order transition.

It is important to note that a least-sensitive inflection point can (but does not necessarily have to) occur together with a satellite signal at higher energy, which, if it is present, is always of higher order. This makes it necessary to distinguish *independent* and *dependent* transitions [6]. In the generalized inflection-point analysis method, an *independent transition* of odd order $(2k - 1)$ (k positive integer) is characterized by

$$\left. \frac{d^{(2k-1)}S(E)}{dE^{(2k-1)}} \right|_{E=E_{tr}} > 0, \quad (2)$$

whereas for even order $2k$

$$\left. \frac{d^{2k} S(E)}{dE^{2k}} \right|_{E=E_{\text{tr}}} < 0. \quad (3)$$

Since the dependent transitions are always of higher order than the transition they correspond to, their minimal order is 2. *Dependent transitions* of even order $2k$ satisfy

$$\left. \frac{d^{2k} S(E)}{dE^{2k}} \right|_{E=E_{\text{tr}}^{\text{dep}}} > 0, \quad (4)$$

and for odd-order transitions

$$\left. \frac{d^{(2k+1)} S(E)}{dE^{(2k+1)}} \right|_{E=E_{\text{tr}}^{\text{dep}}} < 0. \quad (5)$$

In the following, we apply this method to the 2D Ising model.

3. Results

The energy of a configuration $\mathbf{S} = (s_1, s_2, \dots, s_{L^2})$ of L^2 locally interacting spins with possible states $s_i = \pm 1$ on the $L \times L$ square lattice with periodic boundary conditions (i.e., a torus) is expressed in the Lenz-Ising model [1, 2] by

$$E(\mathbf{S}) = -J \sum_{\langle i, j \rangle} s_i s_j, \quad (6)$$

where $\langle i, j \rangle$ symbolizes that the sum only runs over pairs of spins that are nearest neighbors on the lattice. If $J > 0$, neighboring spins energetically prefer a parallel orientation, which can cause spontaneous ordering under appropriate thermodynamic conditions. Hence, the model allows to describe the phase transition between the paramagnetic phase of disordered spin configurations and the ferromagnetic phase with nonzero spontaneous magnetization. For antiferromagnetic coupling, $J < 0$, the ordered phase is dominated by configurations with an alternating spin pattern. In the following, for simplicity, we only discuss cases with even numbers of spins L in each row and column. This renders the density of states symmetric in energy space. In this case, the choice of the J sign does not actually matter and the results are identical for ferromagnetic and antiferromagnetic systems under the symmetry $E \rightarrow -E$. For convenience, we choose $J \equiv 1$ (and also set $k_B \equiv 1$) in the following. The microcanonical inverse temperature β is negative for the non-equilibrium states with $E > 0$ in the Ising model. Since we here intend to focus on the equilibrium phases, any signals in the positive-valued E space will be ignored.

For the analysis of the properties of the microcanonical entropy and its derivatives, we employ Beale's algorithmic method [9] for the exact evaluation of the density of states. The derivatives are calculated numerically using symmetric difference expressions. The thus obtained exact microcanonical results for systems with up to 192^2 spins are shown in Figs. 1 and 2.

We immediately recognize that, to leading order, the entropy S scales with system size [$\sim \mathcal{O}(L^2)$] in the space of the re-scaled energy $e = E/L^2$ [Fig. 1(a)]. The microcanonical inverse temperature β is virtually scale independent in the same space [Fig. 1(b)]. Since the entropy curves do not exhibit any least-sensitive inflection point (and, consequently, there is no extremum in β), a first-order transition does not exist.

The higher-order derivatives γ and δ , shown in Figs. 1(c) and (d), respectively, exhibit a nontrivial dependence on the system size within a narrow energy region. Outside this region, $\gamma \sim \mathcal{O}(1/L^2)$ and $\delta \sim \mathcal{O}(1/L^4)$ in the reduced energy space. The dependence and direction of change of these quantities with system size in the energy interval $e \in [-1.6, -1.0]$ is important. It determines if transitions in this energy region survive in the thermodynamic limit.

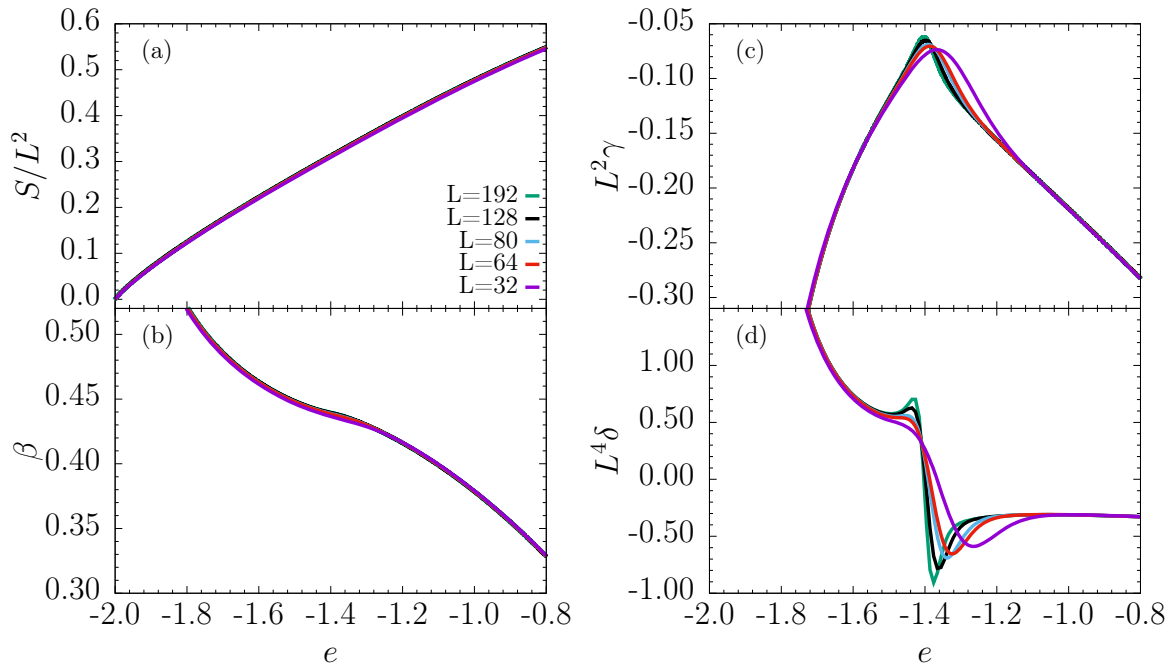


Figure 1. Microcanonical entropy per spin S/L^2 , β , $L^2\gamma$, and $L^4\delta$ plotted as functions of the energy per spin, $e = E/L^2$ for various system sizes.

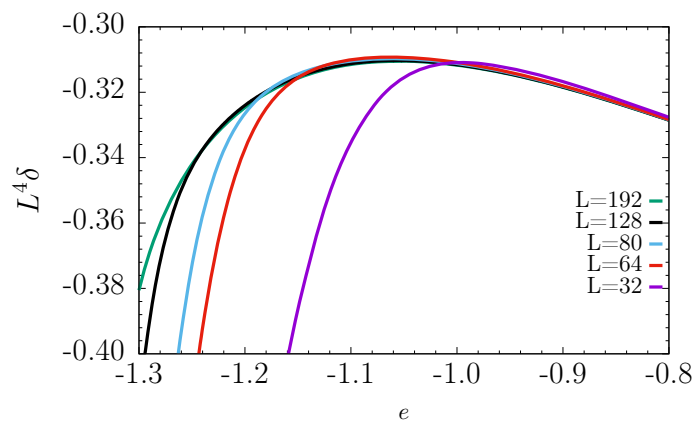


Figure 2. Enlarging the section of $L^4\delta$ above the critical transition in Fig. 1(d) makes the peaks associated with an additional third-order dependent transition clearly visible.

First of all, we clearly notice the peaks in the γ curves, associated with the respective least-sensitive inflection points in the β curves. According to our classification scheme, this signal indicates a second-order transition. For the system sizes studied, we also observe that the peak in γ becomes higher and sharper with increasing system size. It eventually will converge to $\gamma = 0$ in the thermodynamic limit $L \rightarrow \infty$ as this is the familiar second-order phase transition between the ferromagnetic and paramagnetic phase. The position of the γ peaks in e space and the corresponding β values at the inflection point of the individual systems enable the estimation of the transition temperature $T_{\text{tr}}(L)$ for each of the finite systems. In Fig. 3, we plot the dependence of the transition temperature on L . The points associated with the second-order

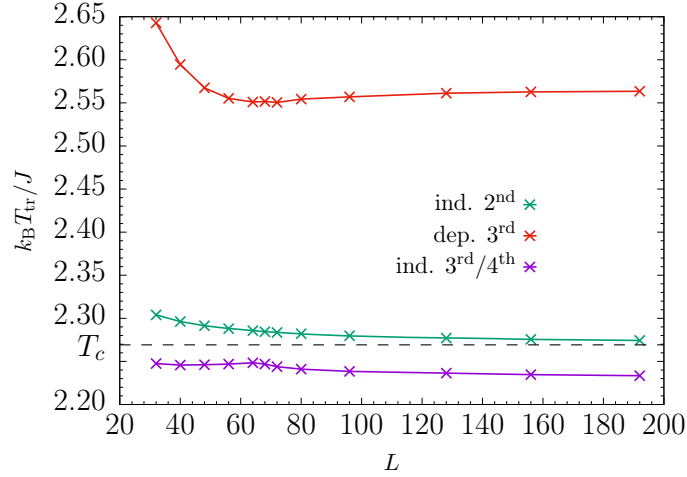


Figure 3. Transition temperatures T_{tr} as obtained by microcanonical analysis plotted as a function of L . Symbols indicate the system sizes, for which the actual calculations were performed. Lines connecting these points are guides to the eye. The curves do not suggest the merging of the three transition lines. We thus conclude that the additional higher-order transitions above and below the second-order ferromagnetic-paramagnetic transition line (which converges to $k_{\text{B}}T_c/J = 2/\ln(1 + \sqrt{2})$ as expected; dashed line) could survive even in the thermodynamic limit. Note the change in curvature of the upper-critical transition line near $L \approx 64$, where the transition characteristics changes from fourth to third order.

transition clearly converge toward the exact critical transition temperature $T_c = 2/\ln(1 + \sqrt{2})$. This confirms that microcanonical inflection-point analysis identifies the known second-order phase transition qualitatively and quantitatively correctly, as expected.

What is surprising, however, is the fact that the minimum that develops in δ with increasing system size at energies (and temperatures) below the critical point indicates an independent third-order transition (for $L \leq 64$ it is of fourth order) according to our classification scheme. Likewise, above the critical point, there is another signal in δ . The peak near $e \approx -1.1$ is interpreted as a dependent third-order transition, though, which is associated with the critical transition. Although the relative peak height on these scales does not increase with system size [Fig. 2], there is no clear sign of its extinction either (in fact the nearby minimum becomes deeper and deeper) and from the data available we conclude this transition might also exist in the thermodynamic limit.

The dependence of the corresponding transition temperatures on the system size is also shown in Fig. 3. For the system sizes studied, the exact results do not suggest a merger of these additional transitions with the critical transition in the thermodynamic limit. Microcanonical analysis cannot hint at the nature of these transitions; therefore an in-depth structural analysis of the results obtained in stochastic computer simulations for larger systems is necessary in future work.

4. Summary

We have employed the generalized microcanonical inflection-point analysis method [6] for the study of the transition behavior of the 2D Ising model on a square lattice with periodic boundary conditions. The analysis was based on the exact densities of states obtained by using Beale's evaluation method [9] for various system sizes with up to 192^2 spins. The method correctly identifies the known second-order phase transition and the transition points obtained for the

finite systems converge to the exactly known critical temperature in the thermodynamic limit. In addition, inflection-point analysis reveals two additional transitions, which are of higher-than-second order. One is located in the subcritical regime and it exists independently of the critical transition. For systems with $L > 64$, it is of third order. For smaller systems it shows the characteristics of a fourth-order transition. The other transition, which is of third order and found above the critical point, would not exist without the critical transition and thus depends on it. The origin and microscopic features of these additional transitions are not known yet. Based on the available results, no indication of a convergence of the transition points toward the critical temperature in the thermodynamic limit was found, which leads to the conclusion that they might also exist in the thermodynamic limit.

Acknowledgments

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