Microcanonical scaling in small systems

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Abstract

A microcanonical finite-size scaling ansatz is discussed. It exploits the existence of a well-defined transition point for systems of finite size in the microcanonical ensemble. The best data collapse obtained for small systems yields values for the critical exponents in good agreement with other approaches. The exact location of the infinite system critical point is not needed when extracting critical exponents from the microcanonical finite-size scaling theory.

Key words: critical phenomena, microcanonical finite-size scaling, Ising and Potts models

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In the canonical ensemble phase transitions appear exclusively in infinite systems. At the critical point of a continuous phase transition denoted by $T_c$ and $h_c$ the Gibbs free energy as a function of the temperature $T$ and of the field $h$ conjugate to the order parameter develops a non-analytic behaviour. As a consequence some thermodynamic functions as e.g. the specific heat and the susceptibility exhibit power law singularities $|T - T_c|^{-\alpha}$ and $|T - T_c|^{-\gamma}$ in the vicinity of $T_c$ and $h = h_c$ fixed, commonly with non-classical critical exponents $\alpha$ and $\gamma$. In finite systems all these singularities are rounded in the canonical ensemble. The appearance of this rounding is taken into account by finite-size scaling theory originally proposed on phenomenological grounds [1,2,3]. In the asymptotic limit $L \to \infty$ and $T \to T_c$ the behaviour of finite-size quantities is governed by scaling functions. The scaling functions are basically determined by the ratio $L/\xi(T)$ with $\xi(T)$ being the correlation length and $L$ the linear extension of the system. Note that the validity of finite-size scaling relations has been proven in renormalization group theory [1]. Over the years finite-size scaling theory has been shown to be a valuable tool for extracting critical exponents from finite-size data, as obtained for example from numerical simulations.

In the microcanonical analysis of finite systems one considers the entropy $S_N(E, M) = \ln \Omega_N(E, M)$ as a function of the energy $E$ and of the magnetization $M$ [4]. The density of states of a system with $N$ spins is denoted by $\Omega_N(E, M)$ and natural units with $k_B = 1$ are chosen. The entropy surface exhibits a well-defined transition point at an energy $E_c$ and magnetization $M_c$ although in finite systems $S_N(E, M)$ is everywhere perfectly analytic. The microcanonical analysis also shows that typical features of symmetry breaking, as for example the abrupt onset of several order parameter branches when the transition point is crossed from above, are already encountered in small systems [5,6,7]. With regard to these intriguing effects, it is tempting to ask whether a direct analysis of the microcanonical entropy also allows the determination of critical quantities from finite-size data.

In this Letter we provide numerical evidence that it is in principle possible to extract critical exponents from the behaviour of finite microcanonical systems. Considering different classical spin models belonging to different universality classes we show that the critical exponents can be obtained from systems which are moderately small. The scaling ansatz to be discussed in the following does not need any a priori knowledge of the infinite system. Especially, the knowledge of the exact location of the critical point of the infinite system is not needed.

In the following we discuss the nearest neighbour ferromagnetic Ising (I) model in three dimensions with the Hamiltonian

$$\mathcal{H}_I = -J \sum_{\langle i,j \rangle} S_i S_j$$

(1)
as well as a generalized Ising (GI) model with equivalent nearest and next-nearest neighbour interactions defined by the Hamiltonian

$$H_{GI} = -J \sum_{\langle i,j \rangle} S_i S_j - J \sum_{\langle i,k \rangle} S_i S_k.$$  \hspace{1cm} (2)

Here, $J > 0$ is the coupling constant and the spins $S_i$ can take on the values $\pm 1$. The first sum in equation (2) extends over nearest neighbour bonds whereas the second sum is over bonds connecting next-nearest neighbours. On the simple cubic lattice, a spin has 6 nearest neighbours and 12 next-nearest neighbours which yields the ground state energy per spin $\varepsilon_{GI} = -9J$ for the GI model. On the same lattice the simple Ising model has the ground state energy $\varepsilon_I = -3J$. The continuous phase transitions observed in both models belong to the same universality class. In addition, we investigate the three state Potts model in two dimensions whose Hamiltonian reads

$$H_P = -J \sum_{\langle i,j \rangle} \delta_{S_i, S_j},$$

with the spins taking on the values $S_i = 1, 2, 3$.

In a microcanonical analysis of finite systems with $N = L^d$ spins ($d$ being the number of space dimensions), the object of interest is the density of states $\Omega_N(E, M)$ as a function of the energy $E$ and the magnetization $M$. The spontaneous magnetization $M_{sp,N}(E)$ is defined to be the value of $M$ where the entropy $S_N(E, M)$ at a fixed value of the energy $E$ has its maximum with respect to $M$:

$$M_{sp,N}(E) : \iff S_N(E, M_{sp,N}(E)) = \max_M S_N(E, M).$$

(4)

This definition of the microcanonical spontaneous magnetization assures the equivalence of the canonical and microcanonical ensemble in the thermodynamic limit. At energies lower than a transition energy $E_{c,N}$ the entropy of the Ising universality class exhibits two maxima at $M = \pm M_{sp,N}$. When approaching the finite-size transition point $E_{c,N}$ from below the order parameter $M_{sp,N}$ vanishes with a square root behaviour in the finite system [5,7]. Thus the transition energy $E_{c,N}$ can be localized with high precision. This vanishing is also reflected in the divergence of the microcanonically defined finite-size zero-field susceptibility [5]. In Figure 1 the variation of the spontaneous magnetization per spin, $m_{sp,N} = M_{sp,N}/N$, as a function of the specific energy, $\varepsilon = E/N$, is shown for the two-dimensional nearest neighbour Ising model on an infinite and on a finite square lattice with $32^2$ spins. Both curves coincide at low energies. At higher energies, the square root behaviour close to the finite-size transition point can be observed. A similar behaviour is found for
the entropy surface of finite two-dimensional three state Potts models [8]. Note that the discreteness of the physical quantities of discrete spin systems such as the Ising model has to be considered with some care. There the language used here refers to continuous functions that describe the discrete data most suitably. In the microcanonical analysis of continuous spin systems as e.g. the XY [9] or the Heisenberg model this concern does not exist.

Fig. 1. Microcanonically defined order parameter vs specific energy for two-dimensional Ising models defined on an infinite square lattice (full line) and on a finite square lattice containing $32 \times 32$ spins (symbols). The finite-size spontaneous magnetization vanishes at a well-defined finite-size transition point.

In the canonical ensemble it is impossible to define an order parameter which exhibits the typical features of spontaneous symmetry breaking already in finite systems. Usually, a pseudo critical temperature is defined via the position of the maximum of some thermal quantity. However, this definition introduces an ambiguity as different quantities, e.g. the specific heat or the susceptibility, normally have their maxima located at different temperatures.

In order to determine relevant microcanonical quantities with high precision, very accurate estimations of the density of states are needed. The data presented here have been obtained with a very efficient algorithm [6] based on the concept of transition observables [10]. From these observables derivatives of the entropy with respect to the energy and/or magnetization are easily computed. This is a point of utmost importance as it is not the entropy itself which enters into the microcanonical analysis, but its derivatives with respect to $E$ and $M$.

The microcanonical finite-size scaling theory proposed and discussed in the following is formulated in such a way as to take advantage of the existence of
a well-defined transition point in finite microcanonical systems. This leads to the following scaling ansatz

\[ L^{\beta_{\varepsilon}/\nu_{\varepsilon}} m_{sp,N} (\varepsilon_{c,N} - \varepsilon) \sim W \left( C (\varepsilon_{c,N} - \varepsilon) L^{1/\nu_{\varepsilon}} \right) \]  

(5)

for the microcanonically defined order parameter in the limit of small scaling variables \( x = (\varepsilon_{c,N} - \varepsilon) L^{1/\nu_{\varepsilon}} \). \( C \) is a non-universal, model-dependent metric constant and \( W \) is a universal scaling function for a given universality class. Note that the microcanonical critical exponents in equation (5), which describe the behaviour of various quantities with respect to the specific energy, are not identical to the usual canonical exponents. For the order parameter one has \( \beta_{\varepsilon} = \beta/(1 - \alpha) \), whereas the microcanonical correlation length critical exponent is given by \( \nu_{\varepsilon} = \nu/(1 - \alpha) \) [11,5]. Here \( \beta, \alpha, \) and \( \nu \) are the canonical critical exponents. As the microcanonical order parameter varies like a square root in the vicinity of \( \varepsilon_{c,N} \) for all finite system sizes \( N [5,7] \) the scaling function \( W \) is asymptotically given as a square root \( W(x) \sim \sqrt{x} \) for small scaling variables \( x \). One remarkable feature of equation (5) is the absence of any non-universal quantity related to the infinite system. Especially, the location of the infinite system critical point \( \varepsilon_{c,\infty} \) does not enter in the definition of the scaling variable \( x \).

![Fig. 2. Microcanonical finite-size scaling plot for the three-dimensional Ising model.](image-url)

The values \( \beta_{\varepsilon}/\nu_{\varepsilon} = 0.54 \pm 0.03 \) and \( 1/\nu_{\varepsilon} = 1.43 \pm 0.04 \) result from the best data collapse.

In Figure 2 we test the ansatz (5) by plotting \( L^{\beta_{\varepsilon}/\nu_{\varepsilon}} m_{sp,N} \) as a function of \( x = (\varepsilon_{c,N} - \varepsilon) L^{1/\nu_{\varepsilon}} \) for several, altogether rather small, three-dimensional Ising models. Here, \( L \) ranges from 4 to 16. Using a recently proposed method for quantifying the nature of a data collapse [12], the optimal exponents and
their error bars can be obtained. For the 3d Ising model our small system data yield the values \( \beta_{\varepsilon}/\nu_{\varepsilon} = 0.54 \pm 0.03 \) and \( 1/\nu_{\varepsilon} = 1.43 \pm 0.04 \), in remarkable agreement with the expected values \( \beta_{\varepsilon}/\nu_{\varepsilon} = 0.52 \) and \( 1/\nu_{\varepsilon} = 1.43 \). For the GI model, a similar study for system sizes ranging from \( L = 4 \) to \( L = 12 \) yields the values \( \beta_{\varepsilon}/\nu_{\varepsilon} = 0.51 \pm 0.03 \) and \( 1/\nu_{\varepsilon} = 1.43 \pm 0.04 \), which again agrees with the literature values. For the 2d three state Potts models system sizes ranging from \( L = 6 \) to 18 have been investigated. The best data collapse results in the estimates \( 1/\nu_{\varepsilon} = 0.79 \pm 0.03 \) and \( \beta_{\varepsilon}/\nu_{\varepsilon} = 0.13 \pm 0.03 \) for the critical exponents. The agreement with the exactly known values \( 1/\nu_{\varepsilon} = 4/5 \) and \( \beta_{\varepsilon}/\nu_{\varepsilon} = 2/15 \) is again very good considering the smallness of the systems.

Fig. 3. Microcanonical finite-size scaling plot both for the Ising (I) and for the GI model. Adjusting the non-universal metric constants, see equation (5), with \( C_{GI}/C_I = 0.219 \), the data points of both models fall on a unique master curve, thus demonstrating the universality of the finite-size scaling function \( W \). The inset shows the scaling functions for the Ising model (solid curve) and the 2d Potts model (dashed). The scaling variable \( x \) of the Potts model is rescaled so that the amplitude of the square root function in the limit \( x \to 0 \) are identical (compare relation (5)). The curves are only displayed for the range of the scaling variable for which data for the Potts model have been obtained.

In Figure 3 we investigate whether the scaling function \( W \) is indeed universal. Adjusting the values of the non-universal constants \( C_I \) and \( C_{GI} \), the data of both models should fall on a common master curve for models within the same universality class. With \( C_{GI}/C_I = 0.219 \) a unique curve is observed, thus demonstrating the universality of the finite-size scaling function \( W \). In the inset of Figure 3 the scaling functions of the Ising model and of the Potts model are compared. As the two model systems belong to different universality classes different scaling functions are expected, which is indeed confirmed by the data.
Our approach differs from earlier attempts at a microcanonical finite-size scaling theory [5,13,14,15,16] in various regards. In Ref. [5,14] it was supposed that the entropy of finite systems was a homogeneous function in the vicinity of the transition point $\varepsilon_{c,\infty}$ of the infinite system. The resulting scaling relations involve $\varepsilon_{c,\infty}$ in the scaling variable and lead to rather poor results for the range of system sizes considered in the present work. However, the scaling relations deduced in [5] are expected to be valid in the asymptotic regime $L \to \infty$.

The authors of Ref. [16] studied the enthalpy instead of the entropy and developed a finite-size scaling theory in complete analogy to the canonical case. In the same way as in the canonical ensemble they defined a finite-size order parameter which differs from zero for all energies. No noticeable differences with canonical results were found in that approach.

In conclusion, we have presented numerical evidence that a suitable microcanonical finite-size scaling ansatz with the correct values of the critical exponents leads to good data collapse of microcanonical finite-size quantities of moderately small systems. It follows from this microcanonical ansatz that critical exponents can easily be obtained from finite microcanonical systems without any a priori knowledge of infinite system quantities. The expected universality of the scaling function for a given universality class has been demonstrated. The microcanonical finite-size scaling theory, presented for the order parameter in the present work, can also be formulated more generally in terms of scaling relations of the entropy of finite systems considered as a function of the energy, the magnetization and the inverse system size [17].

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