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Transmuted finite-size scaling at first-order phase transitions

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Abstract

It is known that fixed boundary conditions modify the leading finite-size corrections for an L^3 lattice in $3d$ at a first-order phase transition from $1/L^3$ to $1/L$. We note that an exponential low-temperature phase degeneracy of the form 2^{3L} will lead to a different leading correction of order $1/L^2$. A $3d$ gonihedric Ising model with a four-spin interaction, plaquette Hamiltonian displays such a degeneracy and we confirm the modified scaling behaviour using high-precision multicanonical simulations.

We remark that other models such as the Ising antiferromagnet on the FCC lattice, in which the number of "true" low-temperature phases is not macroscopically large but which possess an exponentially degenerate number of low lying states may display an effective version of the modified scaling law for the range of lattice sizes accessible in simulations.

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Keywords: First-order phase transitions, finite-size scaling, extensive degeneracy

To some extent first-order phase transitions have been the poor cousins of continuous transitions when it comes to numerical investigations, in spite of their prevalence in nature, see, e.g., the articles in Herrmann et al. (1992). Initial studies of finite-size scaling for first-order transitions were carried out by Imry (1980); Binder (1981); Fisher and Berker (1982) and further pursued by Privman and Fisher (1983); Binder and Landau (1984); Challa et al. (1986); Peczak and Landau (1989); Privman and Rudnik (1990). Later, rigorous results for periodic boundary conditions were derived using Pirogov-Sinai theory and similar techniques applied to the case of non-periodic boundary conditions, for a review see Janke (2003a).

It is possible to derive the finite-size scaling behaviour at first-order phase transitions using straightforward heuristic arguments discussed in Janke (1993), rather than the more sophisticated approach of Borgs and Kotecký (1990, 1992). To do this, we introduce a simple two-phase model in which the system spends a fraction W_{o} of its total time in one of q ordered phases (as in a q-state Potts model) and a fraction $W_{\mathrm{d}} = 1 - W_{\mathrm{o}}$ in the disordered phase. The corresponding energies are $\hat{e}_{\mathrm{o}}$ and $\hat{e}_{\mathrm{d}}$, respectively, where the hat is introduced for quantities evaluated at the inverse phase transition temperature of the infinite system, β^{∞}. Physically, the model neglects fluctuations within the phases and also treats the flips between the phases as instantaneous jumps. With these assumptions the energy moments are just the weighted

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average over the phases, $\langle e^n \rangle = W_o \hat{e}_o^n + (1 - W_o)\hat{e}_d^n$, and from this we can calculate various other derived observables. The specific heat $C_V(\beta, L) = -\beta^2 \partial e(\beta, L)/\partial\beta$ is given by

$$C_V(\beta, L) = L^d \beta^2 \left(\left\langle e^2 \right\rangle - \langle e \rangle^2 \right) = L^d \beta^2 W_o (1 - W_o) \Delta\hat{e}^2 \tag{1}$$

with $\Delta\hat{e} = \hat{e}_d - \hat{e}_o$. Differentiating with respect to W_o then gives a maximum $C_V^{\max} = L^d(\beta^\infty \Delta\hat{e}/2)^2$ at $\beta^{C_V^{\max}}(L)$ for $W_o = W_d = 0.5$, where the disordered and ordered peaks of the energy probability density have equal *weight*. We can see that this immediately recovers the L^d scaling of the peak in $C_V^{\max}$.

The leading corrections can also be obtained by Taylor expanding the ratio of weights around β^∞. The probability of being in any one of the ordered states or the disordered state is related to the free-energy densities $\hat{f}_o, \hat{f}_d$ of the states by

$$p_o \propto e^{-\beta L^d \hat{f}_o} \text{ and } p_d \propto e^{-\beta L^d \hat{f}_d} \tag{2}$$

and the fraction of time spent in the ordered states is proportional to qp_o. The ratio of weights is thus $W_o/W_d \simeq qe^{-L^d \beta \hat{f}_o}/e^{-\beta L^d \hat{f}_d}$ (up to exponentially small corrections in L, see Borgs and Janke (1992); Janke (1993)). Taking the logarithm of this ratio gives $\ln(W_o/W_d) \simeq \ln q + L^d \beta(\hat{f}_d - \hat{f}_o)$ and expanding around β^∞ at the finite-size specific-heat maximum where $W_o = W_d$ gives $0 = \ln q + L^d \Delta\hat{e}(\beta - \beta^\infty) + \ldots$, which can be solved for the finite-size peak loation of the specific heat:

$$\beta^{C_V^{\max}}(L) = \beta^\infty - \frac{\ln q}{L^d \Delta\hat{e}} + \ldots \, . \tag{3}$$

The $1/L^d$ leading correction to scaling is immediately apparent. Similar calculations of Janke (1993) for the location $\beta^{B^{\min}}(L)$ of the minimum of the energetic Binder parameter

$$B(\beta, L) = 1 - \frac{\langle e^4 \rangle}{3\langle e^2 \rangle^2} \tag{4}$$

give

$$\beta^{B^{\min}}(L) = \beta^\infty - \frac{\ln(q\hat{e}_o^2/\hat{e}_d^2)}{L^d \Delta\hat{e}} + \ldots \tag{5}$$

which again displays the $1/L^d$ correction.

The key observation is now that an exponential degeneracy in q, the number of low-temperature phases, will alter the scaling behaviour because of the presence of the various $\ln(q)$ factors in the leading scaling terms in Eqs. (3), (5). One model with precisely this feature is a $3d$ plaquette (4-spin) interaction Ising model on a cubic lattice,

$$\mathcal{H} = -\frac{1}{2} \sum_{[i,j,k,l]} \sigma_i \sigma_j \sigma_k \sigma_l \, , \tag{6}$$

where the ground-state degeneracy of $q = 2^{3L}$ on an L^3 lattice (cf. Fig. 1) was shown by Pietig and Wegner (1996) to be unbroken throughout the low-temperature phase. This is a member of a family of so-called gonihedric Ising models which were originally formulated as a lattice discretization of string-theory actions in high-energy physics which depend solely on the extrinsic curvature of the string worldsheet, for a review see Johnston et al. (2008). This

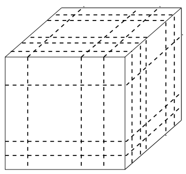

Fig. 1. A typical ground state of the $3d$ plaquette Hamiltonian showing planes of spins flipped with respect to a purely ferromagnetic ground state dotted. Since *any* plane of spins may be flipped, the degeneracy is $q = 2^{3L}$.

plaquette Hamiltonian has attracted attention because it displays a strong first-order transition observed first by Espriu et al. (1997) and evidence of glass-like behaviour at low temperatures discovered by Lipowski (1997); Johnston et al. (2008).

In the plaquette gonihedric model with $q = 2^{3L}$, Eqs. (3), (5) become

$$\beta^{C_V^{\max}}(L) = \beta^{\infty} - \frac{\ln 2^{3L}}{L^3 \Delta\hat{e}} + O\left((\ln 2^{3L})^2 L^{-6}\right) = \beta^{\infty} - \frac{3\ln 2}{L^2 \Delta\hat{e}} + O\left(L^{-4}\right) \tag{7}$$

and

$$\beta^{B^{\min}}(L) = \beta^{\infty} - \frac{\ln(2^{3L}\hat{e}_o^2/\hat{e}_d^2)}{L^3 \Delta\hat{e}} + O\left((\ln(2^{3L}\hat{e}_o^2/\hat{e}_d^2))^2 L^{-6}\right) = \beta^{\infty} - \frac{3\ln 2}{L^2 \Delta\hat{e}} - \frac{\ln(\hat{e}_o^2/\hat{e}_d^2)}{L^3 \Delta\hat{e}} + O\left(L^{-4}\right) \tag{8}$$

so the leading contribution to the finite-size corrections is now, as expected with the exponential degeneracy, $\propto L^{-2}$. For the extremal values one also finds non-standard scaling corrections

$$C_V^{\max}(L) = L^3 \left(\frac{\beta^{\infty}\Delta\hat{e}}{2}\right)^2 + O(L) \tag{9}$$

and

$$B^{\min}(L) = 1 - \frac{1}{12}\left(\frac{\hat{e}_o}{\hat{e}_d} + \frac{\hat{e}_d}{\hat{e}_o}\right)^2 + O(L^{-2})\,, \tag{10}$$

where the leading correction terms are also modified by a factor of L due to the exponential degeneracy compared with the standard case.

To verify the modified scaling we used in Mueller et al. (2014) the multicanonical Monte Carlo algorithm of Berg and Neuhaus (1991, 1992); Janke (1992, 1998) where rare states lying between the ordered and disordered phases are promoted artificially, decreasing the autocorrelation time and allowing the system to oscillate more rapidly between phases. We systematically improve guesses of the energy probability distribution using recursive estimates of Janke (2003b) before the actual production run with of the order of $(100-1000)\times 10^6$ sweeps. Canonical estimators can then be retrieved by weighting the multicanonical data to yield Boltzmann-distributed energies. Reweighting techniques are very powerful when combined with multicanonical simulations, and allow the calculation of observables over a broad range of temperatures. Errors on the measured quantities have been extracted by jackknife analysis using 20 blocks for each lattice size. The observables such as the specific heat (1) and Binder's energy parameter (4) have been calculated from the data as function of temperature by reweighting. This enables us to determine the positions of their peaks, $\beta^{C_V^{\max}}(L)$ and $\beta^{B^{\min}}(L)$, with high precision.

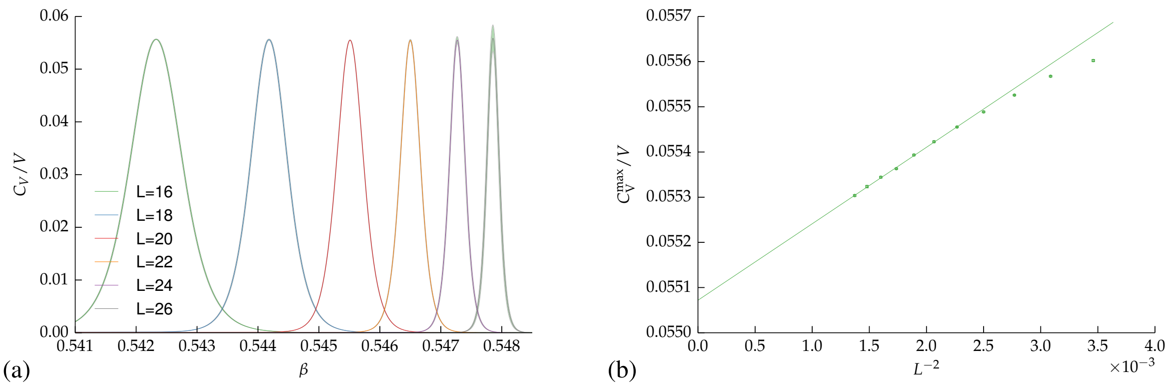

Fig. 2. (a) Specific-heat curves as function of β and (b) their maxima, $C_V^{\max}(L)/V$, vs $1/L^2$ showing clearly the (non-standard) $O(L^{-2})$ behaviour of the leading correction. The best fit line of 0.055072(4) + 0.1693(21)L^{-2} through the measured values is drawn.

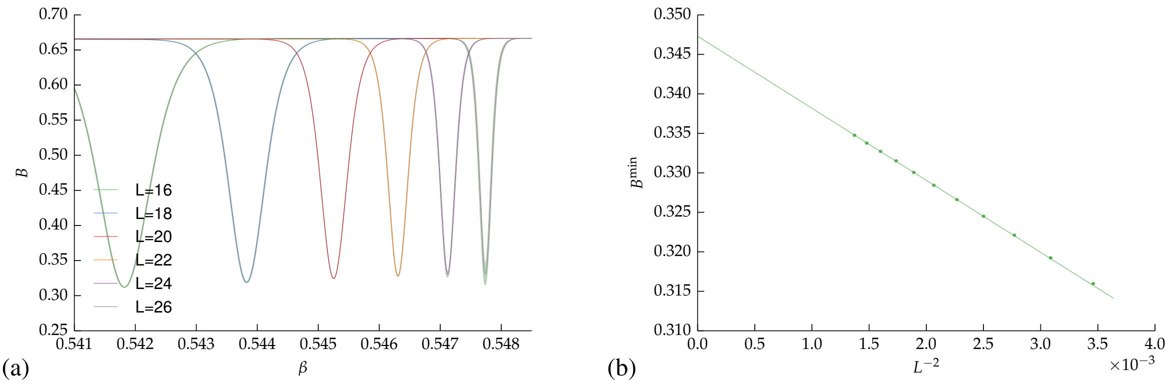

Fig. 3. (a) Curves of the Binder parameter as function of β and (b) their minima, $B^{\min}(L)$, vs $1/L^2$ also showing the (non-standard) $O(L^{-2})$ behaviour of the leading correction. The best fit line of $0.34729(7) - 9.12(4)L^{-2}$ through the measured values is drawn.

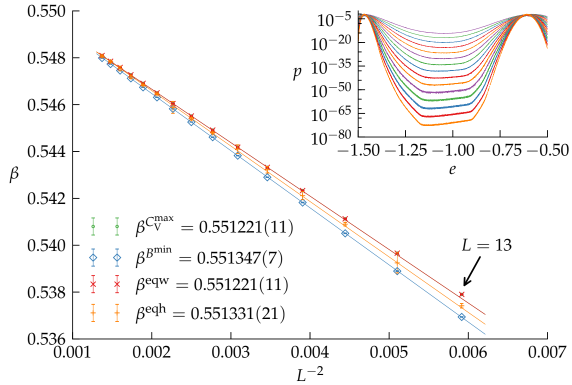

Fig. 4. Best fits using the leading $1/L^2$ scaling for the (finite lattice) peak locations of the specific heat $C_V^{\max}$, Binder's energy parameter $B^{\min}$; or inverse temperatures β^{eqw} and β^{eqh}, where the two peaks of the energy probability density are of same weight or have equal height, respectively. The values for β^{eqw} and $\beta^{C_V^{\max}}$ are indistinguishable in the plot. The omitted corrections which we discuss in detail in Mueller et al. (2014) give the slightly different effective slopes. The inset shows the energy probability density $p(e)$ over $e = E/L^d$ at β^{eqh} for lattice sizes $L \in \{13, 14, \ldots, 26, 27\}$.

We first verify the modified scaling for $C_V^{\max}(L)$ and $B^{\min}(L)$ given in Eqs. (9), (10). From Figs. 2 and 3 it is apparent that the $1/L^2$ scaling of the leading correction term engendered by the degeneracy $q = 2^{3L}$ is clearly displayed by both quantities. The data and fits in Fig. 4 for the two estimates for the inverse transition temperatures using Eqs. (7), (8) also clearly display the transmuted scaling laws with $1/L^2$ corrections. In obtaining the best fit lines we have left out the smaller lattices systematically, until a goodness-of-fit value of at least $Q = 0.5$ was found for each observable individually. We have also included estimates of the transition temperatures using the additional estimators $\beta^{\mathrm{eqw}}(L)$ and $\beta^{\mathrm{eqh}}(L)$, chosen systematically to minimize

$$D^{\mathrm{eqw}}(\beta) = \left(\sum_{e<e_{\min}} p(e,\beta) - \sum_{e\geq e_{\min}} p(e,\beta)\right)^2 \quad \text{and} \quad D^{\mathrm{eqh}}(\beta) = \left(\max_{e<e_{\min}}\{p(e,\beta)\} - \max_{e\geq e_{\min}}\{p(e,\beta)\}\right)^2 , \tag{11}$$

respectively, where the energy of the minimum between the two peaks, $e_{\min}$, is determined beforehand to distinguish between the different phases. From error weighted averages (refraining from a full cross-correlation analysis as discussed by Weigel and Janke (2010)) of the inverse transition temperatures $\beta^{C_V^{\max}}$, $\beta^{B^{\min}}$, β^{eqw}, and β^{eqh} given in Fig. 4 we find $\beta^{\infty} = 0.551\,291(7)$ for the infinite lattice inverse transition temperature, where the final error estimate is taken as the smallest error bar of the contributing β estimates. The precision of the simulation results and the broad range of lattice sizes clearly excludes fits in all cases to the standard finite-size scaling ansatz, where the first correction is proportional to the inverse volume.

Any model with an exponentially degenerate low-temperature phase will display the modified scaling at a first-order phase transition described for the $3d$ gonihedric model here. Apart from higher-dimensional variants of the gonihedric model or its dual, there are numerous other fields where the scenario could be realized. Examples range from ANNNI models discussed by Selke (1988) to topological "orbital" models in the context of quantum computing reviewed by Nussinov and van den Brink (2013) which all share an extensive ground-state degeneracy. Among the orbital models for transition metal compounds, a particularly promising candidate is the $3d$ classical compass or t_{2g} orbital model where a highly degenerate ground state is well known and signatures of a first-order transition into the disordered phase have recently been found numerically by Gerlach and Janke (2014).

Numerous other systems, such as the Ising antiferromagnet on a $3d$ FCC lattice, have an exponentially degenerate number of ground states but a small number of true low-temperature phases. Nonetheless, they do possess an exponentially degenerate number of low-energy excitations so, depending on the nature of the growth of energy barriers with system size, an *effective* modified scaling could still be seen at a first-order transition for the lattice sizes accessible in typical simulations. The crossover to the true asymptotic standard scaling would then only appear for very large lattices. Indeed, previous simulations of Beath and Ryan (2006) appear to have found non-standard scaling for the first-order transition in the Ising antiferromagnet on a $3d$ FCC lattice.

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