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Finite-size scaling corrections in two-dimensional Ising and Potts ferromagnets

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Abstract. Finite-size corrections to scaling of critical correlation lengths and free energies of Ising and three-state Potts ferromagnets are analysed by numerical methods, on strips of width N sites of square, triangular and honeycomb lattices. Strong evidence is given that the amplitudes of the 'analytical' correction terms, N^{-2}, are identically zero for triangular and honeycomb Ising systems. For Potts spins, our results are broadly consistent with this lattice-dependent pattern of cancellations, though for correlation lengths non-vanishing (albeit rather small) amplitudes cannot be entirely ruled out.

1. Introduction

The systematic study of subdominant terms in scaling provides researchers with guidelines on how to extrapolate, e.g. finite-size results to the thermodynamic limit [1–5]. Also, it may in itself bring out connections to underlying physical properties. These latter may be universal, such as the relationship between critical free-energy finite-width correction and conformal anomaly of the corresponding universality class [6], or otherwise relate to details of the system under consideration [7]. In this work we investigate the possible existence of a link between lattice structure and presence (or absence) of specific subdominant terms in finite-size scaling. A numerical analysis is made of correlation-length and free energy data at criticality, as given by the largest eigenvalues of the transfer matrix (TM) [8], for Ising and three-state Potts ferromagnets on strips of square, triangular and honeycomb lattices with homogeneous, isotropic nearest-neighbour couplings, and periodic boundary conditions (PBC) across.

We recall the following results from conformal invariance [9] for the critical spin–spin correlation length, ξ_N, and (dimensionless) negative free energy per site, f_N, on strips of width N sites with PBC [6, 7, 10, 11]:

$$N/\pi\xi_N = \eta + a_\xi N^{-\omega} + b_\xi N^{-\omega_1} + \cdots \tag{1}$$

$$N^2(f_N - f_\infty) = c\pi/6 + a_f N^{-\omega} + b_f N^{-\omega_1} + \cdots \tag{2}$$

where η is the decay-of-correlations exponent and c the conformal anomaly number, with respective exact values $\eta = \frac{1}{4}$, $c = \frac{1}{2}$ (Ising); $\eta = \frac{4}{15}$, $c = \frac{4}{5}$ (three-state Potts) [6, 9, 10]. In terms of the two largest eigenvalues Λ_N^0 and Λ_N^1 of the column-to-column TM, $\xi_N^{-1} = \zeta \ln(\Lambda_N^0/\Lambda_N^1)$; $Nf_N = \zeta \ln \Lambda_N^0$; the factor ζ is unity for the square lattice and, in triangular or honeycomb geometries, corrects for the fact that the physical length added upon each application of the TM differs from one lattice spacing [11–13].

Studies of the operator content of conformally invariant theories, and the perturbation theory (for finite-size systems, with N^{-1} as the perturbation variable) for the corresponding operator product expansion [14] have shown how, in two dimensions, the allowed values of the exponents ω, ω_1 etc are related to the scaling dimensions of the respective set of (model-specific) irrelevant operators. These exponents are therefore universal, as the set of their allowed values is fixed for a given model. It must be noted that terms with $\omega = 2$, the so-called 'analytical' corrections, are expected in any theory, as they are related to the conformal block of the identity operator [14]. It has also been shown [15, 16] that no first-order corrections are expected for ground-state energies, the dominant terms being second-order; this will be particularly relevant for the three-state Potts model, as seen below.

Many numerical studies of corrections to scaling pertaining to two-dimensional classical (i.e. Ising, Potts etc) systems have actually been carried out in their *one*-dimensional *quantum* counterparts [16–19], by taking advantage of well known correspondences [20, 21]. While this is expected to have no effect on the determination of the universal correction exponents, the amplitudes a_ξ, a_f, b_ξ, b_f etc are generally believed to be non-universal, although, for example in certain quantum chain systems, they display similar dependences (Privman–Fisher universality) [11] on the anisotropy parameter [17]. On the other hand, the relationship between $(1+1)$-dimensional chains and two-dimensional spin systems is such that the latter are necessarily located on a square lattice. Thus, much less is known about corrections to scaling for spins on, say, triangular or honeycomb symmetries than on their square counterpart. So far, the only explicit (published) reference to the connection between lattice symmetry and corrections to scaling seems to be a remark on the fact that, on a square lattice operators of spin ± 4 will appear, giving rise to N^{-2} corrections [14].

Our main purpose here is to estimate, through numerical work, the first few amplitudes and exponents (i.e. lowest-order) as given in equations (1) and (2), for Ising and three-state Potts spins on square, triangular and honeycomb geometries. We shall usually assume, for each model, definite values for the two or three exponents used in our fits, taking our hints from conformal invariance theory [14–16].

In particular, we shall seek instances in which, for a given spin model and exponent, the corresponding amplitude appears to vanish for one or more lattices and is non-zero otherwise. The idea of linking accidentally (or otherwise) vanishing amplitudes to underlying physical properties has been exploited fruitfully in the past [7]: the absence of vacancy corrections (with an exponent $\frac{4}{3}$) has been demonstrated for some Ising-like models, implying completeness of the corresponding set of irrelevant operators; investigation also showed that this is particular to Ising systems, and that for $q = 2 + \epsilon$ Potts spins such corrections are of order ϵ. In the present case, we expect to probe the interplay between lattice symmetries and the set of irrelevant operators for the respective spin systems. To our knowledge, no attempt to draw such a connection has been made, despite the wealth of data available for two-dimensional conformally invariant systems.

2. Ising ferromagnets

We start by considering the Ising model. Exact expressions for the eigenvalues of the TM are available for all lattices concerned: square [1, 22, 23], triangular [24] and honeycomb [11, 25]. From their inspection, one readily sees that the finite-size estimates ξ_N and f_N of equations (1) and (2) must have well-defined parity as functions of N^{-1}. Therefore, we assume consistently with: (i) analytical evidence derived for ξ_N on square [1] and honeycomb [11] lattices (ii) numerical analysis of f_N on the square lattice [2]; (iii) the universal result connecting f_N and conformal anomaly [6], and (iv) results for quantum Ising chains [17, 19], that for all

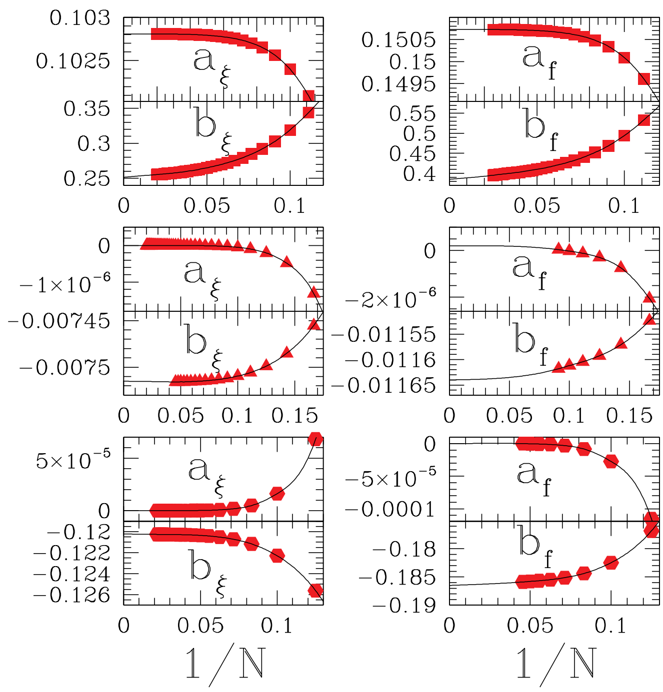

Figure 1. Two-point fits of coefficients in equations (3) and (4). Splines are guides to the eye. Lattices and N-ranges displayed are (top to bottom) square: a_ξ, b_ξ: 9–50; a_f, b_f: 9–40; triangular: a_ξ: 6–27; b_ξ: 6–22; a_f, b_f: 6–11; honeycomb: a_ξ, b_ξ: 8–46; a_f, b_f: 8–22.

cases one has

$$N/\pi\xi_N = \tfrac{1}{4} + a_\xi N^{-2} + b_\xi N^{-4} + \cdots \tag{3}$$

$$N^2(f_N - f_\infty) = \frac{\pi}{12} + a_f N^{-2} + b_f N^{-4} + \cdots. \tag{4}$$

The bulk-free energies f_∞ can be calculated in closed form [26], again for all three lattices. Truncating the series above at N^{-4}, one gets finite-size approximants (also referred to as two-point fits) to the amplitudes $a_{\xi,f}$, $b_{\xi,f}$ from pairs of ξ_N and f_N for consecutive widths $N-1$ and N ($N-2$ and N for the honeycomb). The approximants themselves still exhibit a weak N-dependence, on account of the truncation just mentioned. In fact they usually converge rather smoothly as N increases, allowing reliable extrapolations to be produced; for example, a_ξ for the square lattice agrees with the exact result [1] to two parts in 10^5. We have found the sequences of two-point fits for a_ξ, b_ξ to behave better than those for a_f, b_f. For these latter on triangular and honeycomb geometries, as well as b_ξ on the triangular lattice, numerical instabilities or sudden trend reversals arose for large N; the worst such cases were a_f, b_f on the triangular lattice where behaviour changed abruptly for $N > 11$. We did not pursue the analysis of such deviations, since by then we already had a fairly large sample of well-behaved data from which to extrapolate (albeit with less accuracy than in other instances, where monotonic trends seem to extend all the way as $N \to \infty$; for instance, from a logarithmic plot one finds for the honeycomb $a_\xi(N) \propto N^{-6.4}$ for $6 \leqslant N \leqslant 46$). Graphical illustrations and extrapolated numerical estimates are shown respectively in figure 1 (where use of $1/N$ on the horizontal axis is for ease of representation, not implying assumption of a specific scaling form), and table 1.

Table 1. Extrapolated ($N \to \infty$) amplitudes for Ising model (see equations (3) and (4)). Uncertainties in last quoted digits shown in parentheses.

Lattice	a_ξ	b_ξ	a_f	b_f
Square	0.102 810(2)[a]	0.251 5(5)	0.150 730(2)	0.385(1)
Triangular	$<10^{-8}$	−0.007 515(5)	$<10^{-6}$	−0.011 65(5)
Honeycomb	$<10^{-10}$	−0.120 22(5)	$<10^{-6}$	−0.186 5(10)

[a] Exact: $\pi^2/96 = 0.102\,808\,379\ldots$ [1].

The above results strongly suggest that the coefficients of the N^{-2} corrections are exactly zero in both equations (3) and (4), for triangular and honeycomb geometries.

3. Three-state Potts ferromagnets

In order to check whether the (apparently exact) vanishing of the analytical corrections is a model-independent, purely lattice-related phenomenon, we proceeded to study the next simplest spin system, the three-state Potts ferromagnet. Exact critical temperatures and exponents, and closed forms for bulk-free energies, are again avaliable for all three lattices [26]. Compared with the Ising case, the main differences are: (i) no exact expressions are forthcoming for the eigenvalues of the TM, implying that one must rely on numerical diagonalization, and also that the simple argument for definite parity of eigenvalues as functions of N^{-1}, plausible in the Ising case, need not apply here; and (ii) (corroborating the point just made) a correction exponent $\omega_0 = \frac{4}{5}$ is expected to arise [27], overshadowing higher-order terms.

We tackled (i) by generating the data displayed in table 2, for strip widths 3–14 (square); 3–12 (triangular) and 4–14 (honeycomb; N even). The data in part (b) are displayed without the geometric factor ζ, in order to match the bulk-free energies as given in closed form in [26]. Thus they must be multiplied respectively by $2/\sqrt{3}$ (triangular) and $\sqrt{3}$ (honeycomb) to fit equation (2) with $c = \frac{4}{5}$.

As regards (ii), we took recourse to predictions from conformal invariance, namely: (a) analytical (N^{-2}) corrections are always expected [14]; (b) first-order corrections to the ground-state free energy must be absent [15, 16]. Therefore we assumed:

$$N/\pi\xi_N = \tfrac{4}{15} + a_\xi^{\omega_0} N^{-4/5} + a_\xi^{2\omega_0} N^{-8/5} + a_\xi N^{-2} + a_\xi^{3\omega_0} N^{-12/5} + \cdots \tag{5}$$

$$N^2(f_N - f_\infty) = 2\pi/15 + a_f^{2\omega_0} N^{-8/5} + a_f N^{-2} + a_f^{3\omega_0} N^{-12/5} + \cdots. \tag{6}$$

Because of the small value of ω_0, second-, and even third-order perturbation terms may give rise to corrections of comparable magnitude to the analytical ones. Obviously, one cannot simultaneously and reliably fit all coefficients displayed in equations (5) and (6) from the data of table 2. We thus resorted to selective truncations. Recall that our main goal is to check whether the presence or absence of analytical corrections follows the same lattice-dependent pattern found above.

For correlation-length data we started by trying (a1) two-point fits for $a_\xi^{\omega_0}$ and $a_\xi^{2\omega_0}$, assuming $a_\xi \equiv 0$; (a2) same for $a_\xi^{\omega_0}$ and a_ξ, assuming $a_\xi^{2\omega_0} \equiv 0$; (b1) three-point fits for $a_\xi^{\omega_0}$, $a_\xi^{2\omega_0}$ and a_ξ; (b2) three-point fits for $a_\xi^{\omega_0}$, $a_\xi^{2\omega_0}$ and $a_\xi^{3\omega_0}$, assuming $a_\xi = 0$. Least-squares fits for varying ranges of N were also performed to the forms used in (a1)–(b2), always giving similar values of $\chi^2 \sim 10^{-5}$–10^{-6} per degree of freedom.

For each lattice, all procedures gave reasonably consistent trends for $a_\xi^{\omega_0}$, no doubt because of the small value of ω_0, and the wide gap separating it from all other assumed secondary

Table 2. Finite-width data for three-state Potts ferromagnet.

	(a) $\eta_N = N/\pi\xi_N$		
N	Square	Triangular	Honeycomb
3	0.292 265 133 729	0.274 124 359 026	
4	0.282 270 742 335	0.272 011 393 185	0.271 730 743 990
5	0.277 362 861 763	0.270 966 103 989	
6	0.274 717 716 167	0.270 319 649 167	0.270 584 629 588
7	0.273 119 422 538	0.269 867 269 140	
8	0.272 058 600 969	0.269 527 830 301	0.269 822 520 229
9	0.271 304 554 006	0.269 261 539 672	
10	0.270 741 340 874	0.269 045 974 456	0.269 315 733 294
11	0.270 304 823 980	0.268 867 303 915	
12	0.269 956 670 152	0.268 716 440 914	0.268 957 780 730
13	0.269 672 553 348		
14	0.269 436 295 211		0.268 691 595 289
∞[a]	$\frac{4}{15}$	$\frac{4}{15}$	$\frac{4}{15}$

	(b) $(1/N)\ln\Lambda_N^0$		
N	Square[b]	Triangular	Honeycomb
3	2.121 091 261 980	2.002 959 900 939	
4	2.097 704 520 030	1.985 008 921 770	2.287 656 371 786
5	2.087 460 663 806	1.976 777 367 483	
6	2.082 063 689 903	1.972 321 291 068	2.279 250 879 301
7	2.078 863 356 335	1.969 638 661 220	
8	2.076 806 333 203	1.967 899 052 250	2.276 305 887 939
9	2.075 404 683 690	1.966 707 034 799	
10	2.074 406 246 134	1.965 854 709 111	2.274 943 228 054
11	2.073 669 695 186	1.965 224 253 551	
12	2.073 110 712 019	1.964 744 836 946	2.274 203 278 951
13	2.072 676 417 341		
14	2.072 332 267 371		2.273 757 232 635
∞[c]	2.070 187 162 576	1.962 224 155 163	2.272 522 658 739

[a] Conformal invariance [9].
[b] Data for $N = 3$–11 available in [2].
[c] Evaluated in closed form [26].

exponents; on the other hand, since these latter are so close to one another, we could generally extract no clear-cut information from their respective fitted coefficients: in all cases, any pair of terms (or single term) among $a_\xi^{2\omega_0}$, a_ξ, $a_\xi^{3\omega_0}$ could do a reasonable job of standing in for effective corrections when the other(s) was (were) assumed absent. Furthermore, we noticed that sequences of finite-N estimates were much more stable than any of the above if we used an *ad hoc* form inspired in the Ising case, namely

$$N/\pi\xi_N = \frac{4}{15} + a_\xi^{\omega_0} N^{-4/5} + a_\xi N^{-2} + b_\xi N^{-4}. \tag{7}$$

Indeed, in figure 2 one sees that, although for each lattice all forms (a1)–(b2) yield estimates of $a_\xi^{\omega_0}$ whose extrapolated values might conceivably coincide (as illustrated by the splines), data from equation (7) exhibit the smallest residual N-dependence of all, leading to the least uncertainties upon extrapolation. Such stability shows up also in the estimates of a_ξ of equation (7) and, to a more limited extent, in those of b_ξ. This contrasts with the corresponding sequences of $a_\xi^{2\omega_0}$ etc in procedures (a1)–(b2), which generally display a much broader variation. See table 3 for the respective extrapolations against $1/N$.

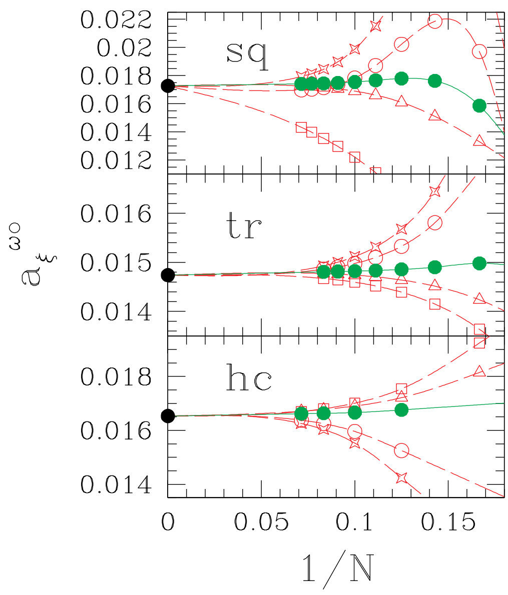

Figure 2. Finite-N estimates of $a_\xi^{\omega_0}$ in equation (5) from different truncation procedures (see text). Squares: (a1); triangles: (a2); stars: (b1); empty circles: (b2); full circles: equation (7). Splines are guides to the eye, joining the vertical axis at central estimates from equation (7); see table 3. Top to bottom: square, triangular, honeycomb.

The small absolute values of a_ξ for triangular and honeycomb lattices remind one of the corresponding case for Ising spins. For (a2) on the triangular lattice, and (b1) on the honeycomb, error bars actually include the origin. However, turning now to the most regular series given by equation (7), we recall that the respective estimates are reached by crossing the horizontal axis, on extrapolation of rather monotonic sequences; so it seems improbable that by going to larger widths, for example, a change of trend would occur, causing error bars to be consistent with $a_\xi = 0$ in this case. A different possibility, connected with the *ad hoc* character of equation (7), is that there may be a *systematic* error implicit in assuming this particular set of scaling corrections. One might ask what combination, if any, of power-law corrections would be consistent with the absence of analytical terms. However, having already examined all reasonable forms suggested by theory (namely procedures (a1)–(b2) and associated least-squares fits), and having found none among them associated with clearly superior results, as regards smooth convergence and/or quality of fit, we decided not to proceed along these lines.

We now turn to free energies. Attempts to include a first-order term, $a_f^{\omega_0} N^{-\omega_0}$, in equation (6) consistently produced very small, and steadily decreasing with increasing N, values of $a_f^{\omega_0}$ ($<10^{-5}$, on extrapolation) for all three lattices. Thus, our numerical data are in entire accord with the prediction from conformal invariance [15, 16] that $a_f^{\omega_0} \equiv 0$.

Going to higher-order terms, we first recall earlier results, all for the square lattice or, equivalently, quantum chains. A single-correction estimate gave $\omega = 2$ [2]. Assuming terms proportional to $N^{2\omega_0}$ to be negligible, contradictory results were obtained upon comparing numerical estimates and conformal-invariance predictions for gap amplitudes related to N^{-2} [18]. This was later explained [19] by showing that, though the amplitude of the $N^{2\omega_0}$ terms was indeed small, it could not be neglected. Specifically as regards free energies, the following values were calculated, using the notation of our equation (6): $a_f^{2\omega_0} = 0.001\,721(3)$, $a_f = 0.0280(5)$ [19].

Again, we tried selective truncations of equation (6), namely (a1) two-point fits for $a_f^{2\omega_0}$ and a_f, assuming $a_f^{3\omega_0} \equiv 0$; (a2) same for $a_f^{2\omega_0}$ and $a_f^{3\omega_0}$, assuming $a_f \equiv 0$; (b) three-point fits for $a_f^{2\omega_0}$, a_f and $a_f^{3\omega_0}$. Least-squares fits for varying ranges of N were also performed to

Table 3. Extrapolated ($N \to \infty$) amplitudes for Potts correlation lengths. See text for definitions of procedures (a1)–(b2), and equation (7). Uncertainties in last quoted digits shown in parentheses.

Procedure	$a_\xi^{\omega_0}$	$a_\xi^{2\omega_0}$	a_ξ	$a_\xi^{3\omega_0}$	b_ξ
			Square		
(a1)	0.018 9(7)	0.0352(6)	—	—	—
(a2)	0.018 0(5)	—	0.119(6)	—	—
(b1)	0.015(2)	0.04(3)	0.05(5)	—	—
(b2)	0.016(1)	0.038(15)	—	0.13(5)	—
Equation (7)	0.017 27(4)	—	0.133(1)	—	0.10(2)
			Triangular		
(a1)	0.015 0(2)	0.000(1)	—	—	—
(a2)	0.014 9(1)	—	0.001(1)	—	—
(b1)	0.014 1(6)	0.012(7)	−0.017(10)	—	—
(b2)	0.014 4(3)	0.006(3)	—	0.012(6)	—
Equation (7)	0.014 74(1)	—	0.0046(1)	—	−0.026(10)
			Honeycomb		
(a1)	0.016 1(7)	0.0045(30)	—	—	—
(a2)	0.016 3(4)	—	0.008(3)	—	—
(b1)	0.017 6(20)	−0.016(25)	0.028(31)	—	—
(b2)	0.017(1)	−0.005(9)	—	0.016(14)	—
Equation (7)	0.016 53(2)	—	0.0061(1)	—	−0.31(2)

the forms used in (a1)–(b). The results were generally undistinguished, much as was the case for η above. The only exception was (a2) for the square lattice where, contrary to all other cases, we found a steadily growing $a_f^{3\omega_0}$ with increasing N. This clearly signals, consistently with earlier results [2, 19], that for the square lattice analytical terms are present with a large coefficient.

In order to make contact with conformal invariance work, we investigated the convergence of $a_f^{2\omega_0}$ and a_f in procedure (a1), for the square lattice. We found these estimates to vary significantly with N; in fact, Bulirsch–Stoer [28, 29] extrapolations pointed to effective corrections $\sim N^{-x}$, $x \simeq 2.5$, with respective final estimates $a_f^{2\omega_0} \simeq 0.02$, $a_f \simeq 0.25$. This gives a value $\sim$12.5 for the ratio $a_f/a_f^{2\omega_0}$, to be compared with Reinicke's estimate, 16.3(3) [19]. Given the number and severity of approximations involved in our calculations, this result may be regarded as broadly consistent with universality of the ratio $a_f/a_f^{2\omega_0}$, as expected from conformal invariance.

Since, for all procedures and lattices, the overall picture was very similar to that described in the preceding paragraph, we decided to try the simpler scheme of [2], namely assuming effective one-power corrections $N^2(f_N - f_\infty) = 2\pi/15 + a_f^{\rm eff} N^{-\omega_0}$, and allowing ω_0 to vary, searching for good fits. We determined the following optimum values for ω_0: 1.9–2.0, (square lattice, again in accordance with the early estimate $\omega = 2$ [2]); 1.6–1.7 (triangular); $\sim$1.5 (honeycomb). Similarly scattered results arose recently from Monte Carlo calculations of magnetization, susceptibility and specific heat for three-state Potts spins on square $N \times N$ systems [30], where widely differing values of ω_0 were obtained for the corrections of each quantity. As regards the possible connection between lattice symmetry and presence, or absence, of analytical corrections, the above one-power corrections are broadly consistent with a similar picture to that found for Ising systems. In such a scenario, the triangular-and honeycomb-effective exponents would reflect a non-zero coefficient for $N^{-2\omega_0} = N^{-1.6}$, and a null one for the analytical term, while for the square lattice the explanation would be as discussed above: both terms are present, with N^{-2} having an amplitude one order of magnitude larger than $N^{-1.6}$.

4. Conclusions

We have analysed corrections to scaling in critical Ising and three-state Potts ferromagnets on the three main two-dimensional lattices. By studying the simplest non-trivial systems available and well-defined lattice symmetries we have left aside, for example, anisotropy-induced crossover phenomena and dealt with power-law finite-size corrections alone, avoiding marginal operators (which arise in four-state Potts systems, for instance) with their associated logarithmic terms. We have given strong evidence that the amplitudes of the N^{-2} corrections of inverse correlation length and free energy of Ising systems vanish both on triangular and honeycomb geometries, but not on the square lattice.

For the inverse correlation length of the Potts model, the main correction is well fitted by an $N^{-4/5}$ term, in accord with theory and earlier numerical work [16, 18, 19]. We have found the values of the N^{-2} coefficients for the triangular and honeycomb lattices to be certainly much smaller than for a square geometry, though we have not been able to ascertain that they vanish.

For Potts free energies, the $N^{-4/5}$ term is always absent, as predicted by conformal invariance [15, 16]; we have estimated the power arising in an effective single-term correction to be an apparently lattice-dependent exponent in the range 1.5–2.0. Our results for the square lattice are consistent with earlier work, in predicting $N^{-1.6}$ and N^{-2} corrections whose amplitude ratio is $\sim$12.5, to be compared with the previously obtained estimate 16.3(3) [19]. As regards triangular and honeycomb geometries, the respective exponents for the effective single-term corrections are much closer to $2\omega_0 = \frac{8}{5}$ (the second-order perturbation value predicted by conformal invariance) than to 2. This may, or may not, mean that the N^{-2} term is absent in these cases.

Several questions arise: (i) can one prove, e.g. on the basis of conformal invariance properties, that the amplitudes of the N^{-2} corrections are exactly zero for triangular and honeycomb Ising systems? If so, (ii) how do such amplitudes behave, for example, in an anisotropic triangular lattice as one crosses over towards a square symmetry, by reducing the strength of the bonds along one of its main directions? And (iii) how does the $2+\epsilon$–state Potts model behave in triangular or honeycomb geometries, as regards the N^{-2} correction? (iv) Do the amplitudes of the N^{-2} corrections really vanish for the three-state Potts model on the same lattices as it appears to be the case for Ising systems? If so, can it be established by conformal invariance theory? We plan to investigate numerical aspects of these and related matters in future work.

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