Hyperscaling in the Ising model on the simple cubic lattice

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High-temperature series for the second spherical moment $M_2 = \sum_{\vec{x}} x^2 \langle \sigma_0 \sigma_{\vec{x}} \rangle$ are presented to 15 terms for the spin-$\frac{1}{2}$ Ising model, on both the simple cubic and body-centered-cubic lattices. These results are combined with previously known series to study hyperscaling to 15 terms on the simple cubic lattice. Some of the evidence suggests a violation of hyperscaling.

In the course of studying lattice field theories, I have computed the high-temperature series for the full two-spin correlation function for all graphs with up to 15 internal lines, on both the simple cubic and body-centered-cubic lattice. The results hold for any scalar theory with a spin density distribution which is even in *s*.

Details and some analysis of the results will be published elsewhere. Here I wish to concentrate on the implications for critical indices and hyperscaling in the Ising model.

High-temperature series for the susceptibility χ in the Ising model have already been computed[1] for sc and bcc lattices up to 17 and 15 lines, respectively. But the most complete results for

$$M_2 \equiv \sum_{\vec{x}} x^2 \langle \sigma_0 \sigma_{\vec{x}} \rangle$$

extended to 12 lines.[2] My results are[3] $(v = \tanh J/kT)$

$$M_2 = 6v + 72v^2 + 582v^3 + 4032v^4 + 25\,542v^5 + 153\,000v^6 + 880\,422v^7 + 4\,920\,576v^8 + 268\,796\,70v^9 + 144\,230\,088v^{10} + 762\,587\,910v^{11} + 3\,983\,525\,952v^{12} + 20\,595\,680\,694v^{13} + 105\,558\,845\,736v^{14} + 536\,926\,539\,990v^{15} \ , \quad (1)$$

$$M_2 = 8v + 128v^2 + 1416v^3 + 13\,568v^4 + 119\,240v^5 + 992\,768v^6 + 7\,948\,840v^7 + 61\,865\,216v^8 + 470\,875\,848v^9 + 3\,521\,954\,816v^{10} + 25\,965\,652\,936v^{11} + 189\,180\,221\,184v^{12} + 1\,364\,489\,291\,848v^{13} + 9\,757\,802\,417\,152v^{14} + 69\,262\,083\,278\,152v^{15} \ , \quad (2)$$

for the sc and bcc cases, respectively.

The results for M_2 and χ can be combined to compute ν, the exponent for the correlation length near the critical point

$$\xi^2 = \frac{M_2}{6\chi} \sim D_+^2 \tau^{-2\nu} \ , \quad (3)$$

where

$$\tau = (1 - T_c/T), \quad T > T_c, \text{ the critical temperature} \ . \quad (4)$$

First, following Baker[4] I computed ν using critical-point renormalization.[5] If

$$f(v) = \sum f_j v^j \sim (v - v_c)^{-\psi} \ , \quad (5)$$

$$g(v) = \sum g_j v^j \sim (v - v_c)^{-\phi} \ , \quad (6)$$

then

$$h(x) = \sum \frac{f_j}{g_j} x^j \sim (1 - x)^{-(\psi - \phi + 1)} \quad (7)$$

near $x = 1$. Using

$$f(v) = M_2(v) = \sum_{j=1}^{15} M_{2j} v^j \ , \quad (8)$$

$$g(v) = \chi(v) = 1 + \sum_{j=1}^{15} \chi_j v^j \ , \quad (9)$$

then

$$(1 - x) \frac{d}{dx} \ln h(x) |_{x=1} = 2\nu + 1 \ . \quad (10)$$

Because Nickel's results[3] on the bcc lattice are more extensive than mine, I will restrict my analysis

TABLE I. Padé estimates for 2ν for the function defined in Eq. (11). N and D are the degrees of the numerator and denominator polynomials. Asterisks denote defects (close poles and zeros, with residue ≤ 0.01).

$D \backslash N$	1	2	3	4	5	6	7	8	9	10	11	12
1	1.2314	1.2518	1.2696	1.2994	1.2889	1.2884	1.2846	1.2859	1.2840	1.2853	1.2834	1.2841
2	1.2524	1.5136	1.219*	1.2918	1.2884	1.289*	1.2856	1.285*	1.2848	1.285*	1.2839	
3	1.2704	1.220*	0.849*	1.2895	1.306*	1.2844	1.2845	1.2846	1.232*	1.285*		
4	1.3026	1.2925	1.2906	1.2869	1.2860	1.2845	1.2846	1.285*	1.285*			
5	1.2871	1.2900	1.295*	1.2861	1.288*	1.2846	1.285*	1.284*				
6	1.2908	1.288*	1.2833	1.2847	1.2848	1.2838	1.285*					
7	1.2807	1.2853	1.2845	1.2848	1.285*	1.287*						
8	1.2899	1.2848	1.2847	1.285*	1.284*							
9	1.2754	1.2847	1.285*	1.285*								
10	1.219*	1.2844	1.285*									
11	1.290*	1.2840										
12	1.281*											

to the simple cubic lattice. The standard technique[4] is to compute the Padé approximants to

$$p(x) = (1-x)\frac{d}{dx}\ln h(x) \qquad (11)$$

and evaluate these at $x=1$. The results for 2ν are shown in Table I. It is noteworthy that the Padé approximants obtained from using 14 or 15 terms are plagued with defects (nearby zeros and poles), so that the results are quite unreliable. By restricting attention only to the first 13 terms one deduces

$$\nu = 0.6423 \pm 0.0008 \qquad (12)$$

using the Hunter and Baker[6] estimate for the error. It is clear from the defect-free Padé approximants for 15 lines that $p(x)$ has a pole near $x=-1$ and another near $x=+2$. So we can make a linear fractional transformation.

$$z = \frac{x}{\alpha + (1-\alpha)x}\ , \qquad (13)$$

which leaves both the origin and $x=1$ invariant, and which maps the other singularities as far from the origin as possible. The mapping

$$z = \frac{x}{\frac{4}{5} + x/5} \qquad (14)$$

accomplishes this, and the results in Table II show the results of a Padé analysis of p in the variable z. All poles have moved well outside the unit circle in z but the problem of defects remains and Eq. (12) remains the most reliable estimate.

TABLE II. Padé estimates for 2ν after mapping Eq. (14).

$D \backslash N$	1	2	3	4	5	6	7	8	9	10	11	12
1	1.2314	1.2481	1.2619	1.2844	1.2896	1.2898	1.2881	1.2868	1.2858	1.2853	1.2849	1.2845
2	1.2487	1.5136	1.205*	1.2919	1.2898	1.290*	1.281*	1.2835	1.2845	1.2839	1.282*	
3	1.2621	1.206*	0.849*	1.2891	1.2791	1.2866	1.2836	1.288*	1.2842	1.290*		
4	1.2884	1.2913	1.2904	1.2869	1.2862	1.2853	1.2847	1.284*	1.2839			
5	1.2907	1.2906	1.292*	1.2863	1.288*	1.2845	1.283*	1.286*				
6	1.2906	1.291*	1.289*	1.2852	1.2847	1.2838	1.286*					
7	1.2838	1.2867	1.2805	1.2849	1.287*	1.289*						
8	1.2863	1.285*	1.2842	1.2844	1.290*							
9	1.286*	1.284*	1.2844	1.284*								
10	1.2850	1.2845	1.284*									
11	1.285*	1.299*										
12	1.2843											

TABLE III. Neville table for 2ν. $q_j^{(0)}$ is defined in Eq. (16), with h_i defined in Eqs. (7)–(9). Subsequent columns are defined by $q_j^{(r)}=[jq_j^{(r-1)}-(j-2r)q_{j-1}^{(r-1)}]/2r$.

	$q_j^{(0)}$	$q_j^{(1)}$	$q_j^{(2)}$	$q_j^{(3)}$	$q_j^{(4)}$	$q_j^{(5)}$
2	2.800 000					
4	1.725 484	0.650 967				
6	1.549 504	1.197 546	1.470 836			
8	1.473 635	1.246 028	1.294 509	1.235 733		
10	1.431 182	1.261 371	1.284 386	1.277 637	1.288 113	
12	1.404 266	1.269 687	1.286 319	1.288 251	1.293 559	1.294 648
14	1.385 590	1.273 531	1.283 142	1.278 908	1.271 900	1.263 236
3	1.850 000					
5	1.551 397	1.103 491				
7	1.467 196	1.256 693	1.371 595			
9	1.422 863	1.267 697	1.281 452	1.236 381		
11	1.395 796	1.273 995	1.285 017	1.287 988	1.307 340	
13	1.377 557	1.277 243	1.284 550	1.284 006	1.281 518	1.273 771
15	1.364 332	1.278 367	1.281 456	1.276 815	1.270 522	1.265 024

To extract meaningful numbers for 14 and 15 lines one can abandon the Padé approach and go back to the ratio test. If $h(x)$ behaves like $(1-x)^{-(1+2\nu)}$ near $x=1$ and

$$h(x)=\sum h_j x^j \; , \tag{15}$$

then the coefficients

$$q_j^{(0)}=n\left[\frac{h_j}{h_{j-1}}-1\right] \tag{16}$$

should tend to 2ν for large j. For the series defined by Eqs. (7)–(9), the sequence $q_j^{(0)}$ is smoother if the coefficients for even j and odd j are treated separately. The Neville table[7] for this series is shown in Table III. The sequence of first differences

$$q_j^{(1)}=[jq_j^{(0)}-(j-2)q_{j-2}^{(0)}]/2 \tag{17}$$

is better convergent than the original sequences $q_j^{(0)}$. The sequence

$$q_j^{(2)}=[jq_j^{(1)}-(j-4)q_{j-2}^{(1)}]/4 \tag{18}$$

has lost the monotonicity required for really believing the Neville table analysis.

Table IV shows the Neville tables for the series in

TABLE IV. Neville table for 2ν after the mapping (14).

	$q_j^{(0)}$	$q_j^{(1)}$	$q_j^{(2)}$	$q_j^{(3)}$	$q_j^{(4)}$	$q_j^{(5)}$
2	2.240 000					
4	1.556 422	0.872 844				
6	1.438 745	1.203 390	1.368 663			
8	1.395 101	1.264 169	1.324 948	1.310 377		
10	1.370 986	1.274 525	1.290 059	1.266 800	1.255 906	
12	1.355 482	1.277 965	1.284 846	1.279 632	1.286 048	1.292 077
14	1.344 677	1.279 847	1.284 551	1.284 159	1.287 554	1.288 156
3	1.657 358					
5	1.468 358	1.184 857				
7	1.410 669	1.266 448	1.327 641			
9	1.380 950	1.276 930	1.290 032	1.271 228		
11	1.362 300	1.278 379	1.280 914	1.273 315	1.274 098	
13	1.349 589	1.279 676	1.282 595	1.284 556	1.291 581	1.296 826
15	1.340 389	1.280 591	1.283 108	1.283 879	1.283 286	1.279 138

TABLE V. Padé estimates for $2\Delta-\gamma$.

D \ N	1	2	3	4	5	6	7	8	9	10	11	12	13
1	1.9821	1.9281	1.8998	1.9003	1.898*	1.8868	1.884*	1.8824	1.8828	1.884*	1.8848	1.886*	1.8860
2	1.9481	1.6501	1.9004	1.900*	1.926*	1.8784	1.882*	1.8827	1.882*	1.852*	1.8874	1.8870	
3	4.6712	1.916*	1.888*	1.875*	1.8825	1.883*	1.8856	1.8847	1.8875	1.8853	1.8869		
4	1.8935	1.884*	1.8795	1.8808	1.883*	1.882*	1.885*	1.885*	1.8859	1.886*			
5	1.887*	1.878*	1.8806	1.876*	1.8905	1.8853	1.886*	1.8865	1.8867				
6	1.8821	1.8813	1.8837	1.8891	1.882*	1.886*	1.888*	1.8867					
7	1.8814	1.882*	1.8931	1.885*	1.885*	1.8861	1.8867						
8	1.882*	1.880*	1.884*	1.885*	1.885*	1.8865							
9	1.8838	1.8874	1.8884	1.8864	1.8865								
10	1.885*	1.8885	1.888*	1.8865									
11	1.8856	1.8864	1.8867										
12	1.8860	1.8871											
13	1.8863												

$h(z)$, defined after the mapping (14). The convergence is better than in Table III, and the results are quite compatible with the estimate (12). This shows that the 14 and 15 line results agree with those of 13 lines or less, on which Eq. (12) is based.[8]

If there are nonanalytic connections to $h(x)$, i.e.,

$$h(x) \sim (1-x)^{-(1+2\nu)} \times \left[1+\sum_{n=1}^{\infty} f_n (1-x)^n + A(1-x)^{\Delta}\right], \quad (19)$$

with Δ nonintegral, then one expects the Neville table coefficients to behave as

$$q_j^{(0)} = 2\nu + \frac{\alpha_1}{j} + \frac{\alpha_2}{j^2} + \cdots + \frac{\beta}{j^{\Delta+1}} + \cdots , \quad (20)$$

$$q_j^{(1)} = 2\nu + \frac{\alpha'}{j^2} + \frac{\beta'}{j^{\Delta+1}} + \cdots . \quad (21)$$

I have tried to fit $q_j^{(1)}$ to the form (21) in both Tables III and IV for $j=8, 10, 12, 14$. But there are no consistent values for ν, α', β', Δ.

Let us now consider the exponent $\gamma-2\Delta$, where

TABLE VI. Neville table for $2\Delta-\gamma-3\nu$ defined by Eqs. (5), (6), (7), and (27).

	$q_j^{(0)}$	$q_j^{(1)}$	$q_j^{(2)}$	$q_j^{(3)}$	$q_j^{(4)}$	$q_j^{(5)}$
2	0.285 714					
4	0.131 815	−0.022 085				
6	0.081 588	−0.018 864	−0.017 254			
8	0.053 303	−0.031 552	−0.044 239	−0.053 235		
10	0.035 106	−0.037 686	−0.046 886	−0.048 651	−0.047 505	
12	0.022 655	−0.039 595	−0.043 415	−0.039 944	−0.035 590	−0.033 208
14	0.013 665	−0.040 278	−0.041 983	−0.040 074	−0.040 172	−0.042 005
3	0.161 932					
5	0.096 313	−0.002 114				
7	0.063 827	−0.017 388	−0.028 843			
9	0.042 399	−0.032 600	−0.051 614	−0.063 000		
11	0.027 878	−0.037 468	−0.045 986	−0.041 296	−0.033 157	
13	0.017 550	−0.039 252	−0.043 266	−0.040 091	−0.039 338	−0.041 193
15	0.009 888	−0.039 920	−0.041 758	−0.039 497	−0.038 977	−0.038 796

Δ, γ are defined by

$$\frac{\partial^2\chi}{\partial H^2}=-B_+\tau^{-\gamma-2\Delta} \qquad (22)$$

and

$$\chi=A_+\tau^{-\gamma} \ . \qquad (23)$$

Using the 15 term results[9] for $\partial^2\chi/\partial H^2$ as $f(v)$ in Eq. (5), and using χ^2 as $g(v)$, the Padé results for $(2\Delta-\gamma)$ are shown in Table V. The result is

$$2\Delta-\gamma=1.8863\pm0.0006 \ , \qquad (24)$$

again using the Hunter-Baker[6] estimate of the error. According to hyperscaling

$$2\Delta-\gamma-3\nu=0 \ . \qquad (25)$$

Our result, combining Eq. (12) with Eq. (24), is

$$2\Delta-\gamma-3\nu=-0.041\pm0.003 \ , \qquad (26)$$

which shows a violation of hyperscaling even more drastic than Baker's previous estimate[4] of $-0.028 + 0.003$ obtained from the fcc lattice up to ten orders.

One can test hyperscaling directly by using critical-point renormalization with

$$f(v)=\frac{\partial^2\chi}{\partial H^2} \ , \ g(v)=(M_2)^{3/2}(\chi)^{1/2} \ . \qquad (27)$$

The central part of the Padé table is full of defects. The Neville table coefficients for $h(x)$, which should tend to $2\Delta-\gamma-3\nu$, are shown in Table VI. The even and odd terms appear to be two monotonically converging sequences, with limits well within the error bounds of Eq. (26).

Finally, one can repeat the analysis of Nickel and Sharpe,[10] which asks whether the function $\gamma(y)$, analogous to the Callan-Symanzik function of field theory, can have a zero. $\gamma(y)$ is defined by the relations

$$x(v)=M_2(v)/6\chi(v) \ , \qquad (28)$$

$$y(v)=x(v)\left[\frac{\partial^2\chi(v)}{\partial H^2}\frac{1}{\chi^2(v)}\right]^{-2/3} \ , \qquad (29)$$

$$\gamma(y)=x\frac{dy}{dx}=x(v)\frac{dy}{dv}\Big/\frac{dx}{dv} \ , \qquad (30)$$

expressed as a function of y by inverting Eq. (29). Our results add three more terms to the series for $\gamma(y)$ for the sc lattice

TABLE VII. Padé estimates for zero of $\gamma(y)$ (upper number) and slope (lower number), for $\gamma(y)$ defined in Eq. (30).

D \ N	3	4	5	6	7	8	9	10	11
4	0.18340 −0.666	0.175* −0.745		0.19218 −0.492	0.18816 −0.602	0.18918 −0.570	0.191* −0.513	0.18911 −0.575	0.19045 −0.524
5	0.185* −0.639		0.184* −0.678	0.18996 −0.548	0.18907 −0.573	0.186* −0.644	0.190* −0.551	0.190* −0.577	
6	0.190* −0.556	0.19134 −0.521	0.18868 −0.582	0.18939 −0.563	0.18962 −0.557	0.18964 −0.556	0.18965 −0.556		
7	0.19087 −0.531	0.190* −0.544	0.18918 −0.570	0.19023 −0.536	0.18964 −0.556	0.190* −0.556			
8	0.18962 −0.560	0.185* −0.775	0.18943 −0.563	0.18954 −0.560	0.18965 −0.556				
9	0.18869 −0.585	0.18894 −0.578	0.18951 −0.561	0.189* −0.566					
10	0.18903 −0.575	0.188* −0.591	0.18961 −0.557						
11	0.190* −0.550	0.190* −0.530							
12	0.190* −0.539								

$$\gamma(y) = y - 8y^2 + 24y^3 - 112y^4 + 469\tfrac{1}{3}y^5 - 896y^6 - 2880y^7 + 46\,563\tfrac{5}{9}y^8 - 159\,466\tfrac{2}{3}y^9 - 512\,960y^{10} + 5\,772\,583\tfrac{41}{81}y^{11} - 16\,377\,353\tfrac{13}{27}y^{12} - 53\,100\,416y^{13} + 755\,196\,452\tfrac{212}{243}y^{14} - 2\,561\,217\,461\tfrac{59}{81}y^{15} - 6\,729\,254\,272y^{16} \quad . \tag{31}$$

Padé results for the zeros of $\gamma(y)$ and the slopes $\gamma'(y)$ there are shown in Table VII. There is a stable zero at

$$y^* = 0.1896 \pm 0.0015 \tag{32}$$

with a slope of

$$\gamma'(y^*) = -0.556 \pm 0.07 \quad . \tag{33}$$

These numbers are quite consistent with the Nickel-Sharpe analysis based on 13 terms

$$y^*_{\rm NS} = 0.189 \pm 0.002 \quad , \tag{34}$$

$$\gamma'(y^*)_{\rm NS} = 0.56 \pm 0.04 \quad , \tag{35}$$

but the Hunter-Baker[6] error estimates are disappointingly large and preclude pinning down the parameters more precisely.

In conclusion, I have added three more terms to the series for M_2 in the Ising model on the simple cubic lattice. The high-temperature series determination of ν is given in Eq. (12), while that of $2\Delta - \gamma$ is given in Eq. (24). These indicate a violation of hyperscaling given in Eq. (26). However, the Nickel-Sharpe analysis yields a zero of $\gamma(y)$, which is evidence for compatibility with hyperscaling.

It is noteworthy that from Nickel's 21-term results for ν and M_2 for the bcc lattice,[3] the estimate for ν drops appreciably for 18 lines or more. His high-temperature estimate of ν becomes compatible with the field-theoretic estimates of 0.630. If the results for $2\Delta - \gamma$ are unchanged to 21 orders, the violation of hyperscaling (from the high-temperature series analysis) will have disappeared. It may be that the defects obtained in our Padé analysis of ν for 14 and 15 lines indicate that a similar shift in the value of ν is imminent.

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[7]See, e.g., D. Jasnow and M. Wortis, Phys. Rev. 176, 739 (1968).

[8]B. Nickel, in his 1980 Cargese lectures has pointed out that an Euler transformation (13) makes the jth coefficient $\tilde{h}_j$ of the series $\tilde{h}(z) = \sum \tilde{h}_j z^j$ primarily sensitive to the (αj)th coefficient h of the series $h(x) = \sum h_j x^j$. Thus the agreement between the 15 term series of Table IV and the 13 term series of Table III is not surprising. Nevertheless even the results from Table III to 15 terms seem compatible with Eq. (12).

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