Asymptotic Scaling in the Two-Dimensional O(3) σ Model at Correlation Length 10^5

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We carry out a high-precision Monte Carlo simulation of the two-dimensional O(3)-invariant σ model at correlation lengths ξ up to $\sim 10^5$. Our work employs a powerful method for extrapolating finite-volume Monte Carlo data to infinite volume, based on finite-size-scaling theory. We discuss carefully the systematic and statistical errors in this extrapolation. We then compare the extrapolated data to the renormalization-group predictions. The deviation from asymptotic scaling, which is $\approx 25\%$ at $\xi \sim 10^2$, decreases to $\approx 4\%$ at $\xi \sim 10^5$.

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Two-dimensional nonlinear σ models are important "toy models" in elementary-particle physics because they share with four-dimensional non-Abelian gauge theories the property of perturbative asymptotic freedom [1]. However, the nonperturbative validity of asymptotic freedom has been questioned [2], and numerical tests of asymptotic scaling in the O(3) σ model at correlation length $\xi \sim 100$ have shown discrepancies of order 25% [3,4]. In this Letter we employ a finite-size-scaling extrapolation method due originally to Lüscher, Weisz, and Wolff [5–8] to obtain high-precision estimates (errors $\lesssim 2\%$) in the O(3) σ model at correlation lengths ξ up to $\sim 10^5$. We find that the discrepancy has decreased to $\approx 4\%$, in good agreement with the asymptotic-freedom predictions.

We study the lattice σ model taking values in the unit sphere $S^{N-1} \subset \mathbb{R}^N$, with nearest-neighbor action $\mathcal{H}(\boldsymbol{\sigma}) = -\beta \sum \boldsymbol{\sigma}_x \cdot \boldsymbol{\sigma}_y$. Perturbative renormalization-group computations predict that the (infinite-volume) correlation lengths $\xi^{(\exp)}$ and $\xi^{(2)}$ [10] behave as

$$\xi^{\#}(\beta) = C_{\xi^{\#}} e^{2\pi\beta/(N-2)} \left(\frac{2\pi\beta}{N-2}\right)^{-1/(N-2)} \times \left[1 + \frac{a_1}{\beta} + \frac{a_2}{\beta^2} + \cdots\right] \quad (1)$$

as $\beta \to \infty$. Three-loop perturbation theory yields [12,13]

$$a_1 = -0.014127 + (\tfrac{1}{4} - 5\pi/48)/(N-2). \quad (2)$$

The nonperturbative constant $C_{\xi^{(\exp)}}$ has been computed recently using the thermodynamic Bethe ansatz [14]:

$$C_{\xi^{(\exp)}} = 2^{-5/2} \left(\frac{e^{1-\pi/2}}{8}\right)^{1/(N-2)} \Gamma\left(1 + \frac{1}{N-2}\right). \quad (3)$$

The remaining nonperturbative constant is known analytically only at large N [15]:

$$C_{\xi^{(2)}}/C_{\xi^{(\exp)}} = 1 - 0.003\,225/N + O(1/N^2). \quad (4)$$

Previous Monte Carlo studies up to $\xi \sim 100$ agree with these predictions to within about (20–25)% for $N = 3$, 6% for $N = 4$, and 2% for $N = 8$ [4,16].

The extrapolation method [7] is based on the finite-size-scaling ansatz

$$\frac{\mathcal{O}(\beta, sL)}{\mathcal{O}(\beta, L)} = F_{\mathcal{O}}(\xi(\beta, L)/L; s) + O(\xi^{-\omega}, L^{-\omega}), \quad (5)$$

where $\mathcal{O}$ is any long-distance observable, s is a fixed scale factor (usually $s = 2$), L is the linear lattice size, $F_{\mathcal{O}}$ is a universal function, and ω is a correction-to-scaling exponent. We make Monte Carlo runs at numerous pairs (β, L) and (β, sL); we then plot $\mathcal{O}(\beta, sL)/\mathcal{O}(\beta, L)$ vs $\xi(\beta, L)/L$, using those points satisfying both $\xi(\beta, L) \geq$ some value $\xi_{\min}$ and $L \geq$ some value $L_{\min}$. If all these points fall with good accuracy on a single curve, we choose a smooth fitting function $F_{\mathcal{O}}$. Then, using the functions F_ξ and $F_{\mathcal{O}}$, we extrapolate the pair $(\xi, \mathcal{O})$ successively from $L \to sL \to s^2L \to \cdots \to \infty$. See [7] for how to calculate statistical error bars on the extrapolated values.

We have chosen to use functions $F_{\mathcal{O}}$ of the form

$$F_{\mathcal{O}}(x) = 1 + a_1 e^{-1/x} + \cdots + a_n e^{-n/x}. \quad (6)$$

Typically a fit of order $3 \leq n \leq 12$ is sufficient; we increase n until the χ^2 of the fit becomes essentially constant. The resulting χ^2 value provides a check on the systematic errors arising from corrections to scaling and/or from inadequacies of the form (6). The discrepancies between the extrapolated values from different L at the same β can also be subjected to a χ^2 test. Further details on the method can be found in [7].

We simulated the two-dimensional O(3) σ model, using the Wolff embedding algorithm with standard Swendsen-Wang updates [11,17,18]; critical slowing down appears to be completely eliminated. We ran on lattices $L = 32$, 48, 64, 96, 128, 192, 256, 384, 512 at 180 different pairs (β, L) in the range $1.65 \leq \beta \leq 3.00$ (corresponding to $20 \lesssim \xi_\infty \lesssim 10^5$). Each run was between 10^5 and 5×10^6 iterations, and the total CPU time was 7 yr on an IBM RS-6000/370. The raw data will appear in [19].

Our data cover the range $0.15 \lesssim \xi(L)/L \lesssim 1.0$, and we found tentatively that a tenth-order fit (6) is indicated; see Table I. Next we took $\xi_{\min} = 20$ and sought to

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TABLE I. χ^2 and confidence level for the fit (6) of $\xi(\beta,2L)/\xi(\beta,L)$ vs $\xi(\beta,L)/L$. DF is the number of degrees of freedom. The first (second) $L_{\min}$ value applies for $\xi(L)/L \le 0.7$ (>0.7). In all cases $\xi_{\min} = 20$.

$L_{\min}$	DF	$n = 7$	$n = 8$	$n = 9$	$n = 10$	$n = 11$	$n = 12$
(64,64)	$108 - n$	278.38	183.80	144.34	137.82	135.77	135.01
		0.0%	0.0%	0.2%	0.5%	0.6%	0.5%
(96,32)	$107 - n$	228.85	164.46	120.38	124.87	122.15	120.48
		0.0%	0.0%	1.9%	3.0%	3.7%	4.0%
(96,64)	$97 - n$	207.32	137.18	108.23	103.13	102.02	101.59
		0.0%	0.1%	7.1%	11.4%	11.5%	10.6%
(96,96)	$87 - n$	190.61	115.05	100.99	93.90	93.89	93.73
		0.0%	0.5%	4.1%	9.2%	8.0%	7.1%
(128,32)	$93 - n$	160.17	121.29	99.35	94.82	94.20	86.65
		0.0%	0.6%	12.1%	17.7%	16.8%	31.3%
(128,64)	$83 - n$	139.60	95.94	78.23	72.91	72.89	68.43
		0.0%	5.2%	34.6%	48.1%	44.9%	56.4%
(128,96)	$73 - n$	126.20	79.03	71.12	64.33	63.29	59.72
		0.0%	11.3%	25.3%	43.0%	43.1%	52.2%
(128,128)	$64 - n$	101.05	63.45	61.96	59.70	59.28	52.89
		0.0%	23.1%	24.2%	27.6%	25.7%	43.9%
(192,32)	$75 - n$	110.42	93.41	76.13	70.61	65.15	62.16
		0.1%	1.8%	18.5%	29.6%	43.6%	50.6%
(192,64)	$65 - n$	90.60	69.57	55.03	47.60	45.12	43.74
		0.4%	12.3%	51.1%	75.0%	80.0%	81.4%
(192,96)	$57 - n$	82.54	55.94	49.49	38.90	38.67	37.53
		0.3%	23.0%	41.4%	79.4%	77.0%	77.8%

choose $L_{\min}$ to avoid any detectable systematic error from corrections to scaling. There appear to be weak corrections to scaling ($\lesssim 1.5\%$) in the region $0.3 \lesssim \xi(L)/L \lesssim 0.7$ for lattices with $L \lesssim 64-96$; see the deviations plotted in Fig. 1. We therefore investigated systematically the χ^2 of the fits, allowing a different $L_{\min}$ for $\xi(L)/L \le 0.7$ and >0.7; see Table I. A reasonable χ^2 is obtained when $n \ge 9$ and $L_{\min} \gtrsim (128,64)$. Our preferred fit is $n = 10$ and $L_{\min} = (128,64)$; see Fig. 2, where we compare also with the perturbative prediction

$$F_\xi(x;s) = s\left[1 - \frac{a w_0 \ln s}{2} x^{-2} - a^2\left(\frac{w_1 \ln s}{2} + \frac{w_0^2 \ln^2 s}{8}\right) x^{-4} + O(x^{-6})\right] \quad (7)$$

valid for $x \gg 1$, where $a = 1/(N-1)$, $w_0 = (N-2)/2\pi$, and $w_1 = (N-2)/(2\pi)^2$.

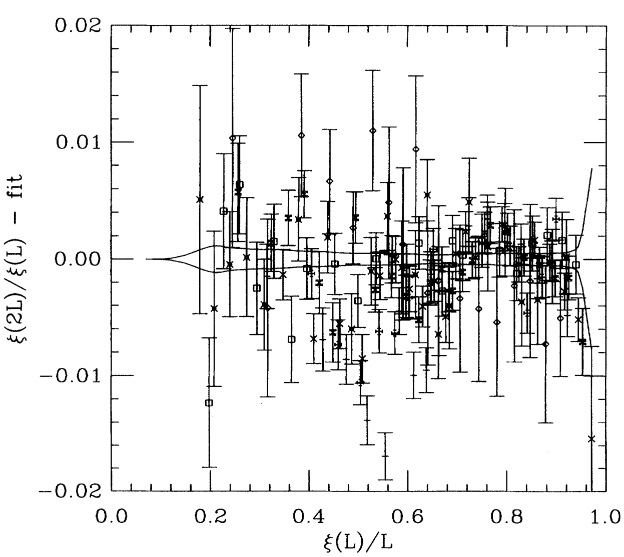

FIG. 1. Deviation of points from fit to F_ξ with $s = 2$, $\xi_{\min} = 20$, $L_{\min} = 128$, and $n = 10$. Symbols indicate $L = 32$ (+), 48 (⊹), 64 (×), 96 (⊠), 128 (□), 192 (⌑), and 256 (◇). Error bars are 1 standard deviation. Curves near zero indicate statistical error bars (±1 standard deviation) on the function $F_\xi(x)$.

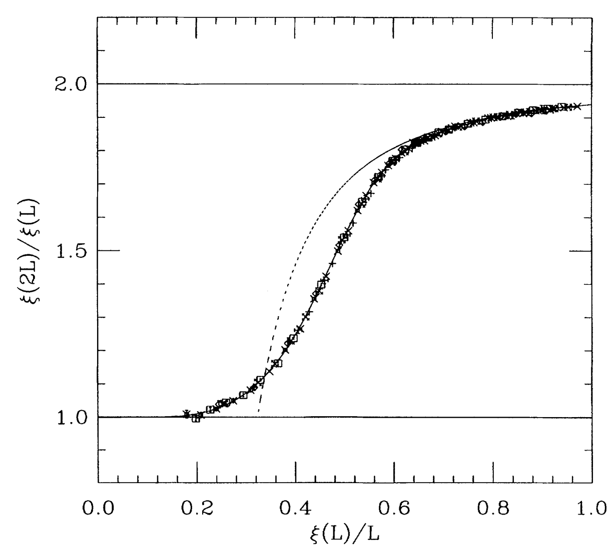

FIG. 2. $\xi(\beta,2L)/\xi(\beta,L)$ vs $\xi(\beta,L)/L$. Symbols indicate $L = 32$ (+), 48 (⊹), 64 (×), 96 (⊠), 128 (□), 192 (⌑), and 256 (◇). Error bars are 1 standard deviation. Solid curve is tenth-order fit in (6), with $\xi_{\min} = 20$ and $L_{\min} = 128$ (64) for $\xi(L)/L \le 0.7$ (>0.7). Dashed curve is the perturbative prediction (7).

The extrapolated values $\xi_\infty^{(2)}$ from different lattice sizes at the same β are consistent within statistical errors: only one of the 24 β values has a χ^2 too large at the 5% level, and summing all β values we have $\chi^2 = 86.56$ (106 degrees of freedom, level = 92%).

In Table II we show the extrapolated values $\xi_\infty^{(2)}$ from our preferred fit and some alternative fits. The discrepancies between these values (if larger than the statistical errors) can serve as a rough estimate of the remaining systematic errors due to corrections to scaling. The statistical errors in our preferred fit are of order 0.2% (0.7%, 1.1%, 1.6%) at $\xi_\infty \approx 10^2$ (10^3, 10^4, 10^5), and the systematic errors are of the same order or smaller. The statistical errors at different β are strongly positively correlated.

In Fig. 3 (points + and $\times$) we plot $\xi^{(2)}_{\infty,\mathrm{estimate}(128,64)}$ divided by the two-loop and three-loop predictions (1)–(4). The discrepancy from three-loop asymptotic scaling, which is $\approx$16% at $\beta = 2.0$ ($\xi \approx 200$), decreases to $\approx$4% at $\beta = 3.0$ ($\xi \approx 10^5$). This is roughly consistent with the expected $1/\beta^2$ corrections. The slight bump at $2.3 \lesssim \beta \lesssim 2.6$ is probably spurious, arising from correlated statistical or systematic errors.

We can also try an "improved expansion parameter" [4,13,19,20] based on the energy $E = \langle \boldsymbol{\sigma}_0 \cdot \boldsymbol{\sigma}_1 \rangle$. First we invert the perturbative expansion [13,21]

$$E(\beta) = 1 - \frac{N-1}{4\beta} - \frac{N-1}{32\beta^2} - \frac{0.005\,993(N-1)^2 + 0.007\,270(N-1)}{\beta^3} + O(1/\beta^4) \tag{8}$$

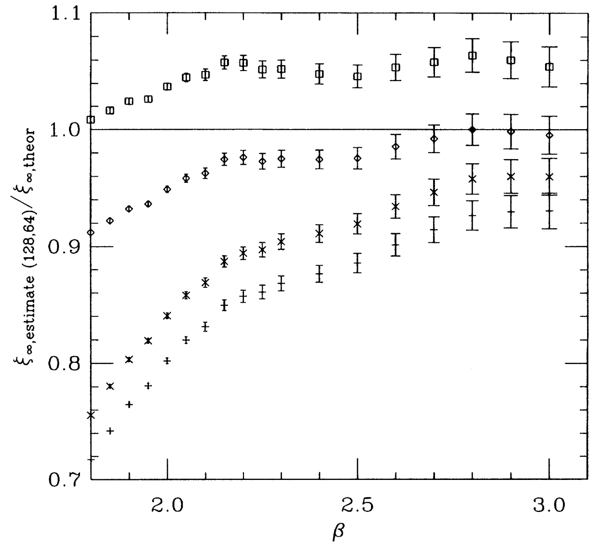

FIG. 3. $\xi^{(2)}_{\infty,\mathrm{estimate}(128,64)}/\xi^{(2)}_{\infty,\mathrm{theor}}$ vs β. Error bars are 1 standard deviation (statistical error only). There are four versions of $\xi^{(2)}_{\infty,\mathrm{theor}}$: standard perturbation theory in $1/\beta$ gives points + (2-loop) and $\times$ (3-loop); "improved" perturbation theory in $1 - E$ gives points $\square$ (2-loop) and $\diamond$ (3-loop).

and substitute into (1); this gives a prediction for ξ as a function of $1 - E$. For E we use the value measured on the largest lattice; the statistical errors and finite-size corrections on E are less than 5×10^{-5}, and therefore induce a negligible error (less than 0.5%) on the predicted ξ. The corresponding observed/predicted ratios are also shown in Fig. 3 (points $\square$ and $\diamond$). The "improved" 3-loop prediction is in excellent agreement with the data.

TABLE II. Estimated correlation lengths $\xi_\infty^{(2)}$ as a function of β, from various extrapolations. Error bar is 1 standard deviation (statistical errors only). All extrapolations use $s = 2$, $\xi_{\min} = 20$, and $n = 10$. The first (second) $L_{\min}$ value applies for $\xi(L)/L \le 0.7$ (>0.7). Our preferred fit is $L_{\min} = (128, 64)$, shown in italics. Kim is the estimate from Ref. [6(c)].

$L_{\min}$	1.90	1.95	2.00	2.05	2.10	2.15	2.20	2.25
(96,64)	122.43 (0.25)	166.79 (0.36)	228.37 (0.55)	311.54 (0.93)	420.52 (1.59)	574.16 (2.51)	774.24 (3.69)	1039.1 (5.7)
(96,96)	122.55 (0.25)	166.95 (0.37)	228.93 (0.57)	312.29 (0.93)	421.61 (1.63)	574.96 (2.51)	776.03 (3.73)	1038.2 (5.5)
(128,32)	122.34 (0.29)	166.68 (0.42)	228.50 (0.66)	311.84 (1.09)	422.67 (1.94)	577.41 (3.13)	779.33 (4.80)	1048.9 (7.3)
(128,64)	*122.34 (0.29)*	*166.66 (0.43)*	*228.54 (0.67)*	*311.99 (1.10)*	*422.73 (1.97)*	*577.73 (3.12)*	*780.04 (4.76)*	*1048.7 (7.3)*
(128,96)	122.25 (0.29)	166.54 (0.43)	228.11 (0.66)	311.59 (1.10)	421.71 (1.90)	576.52 (3.06)	778.40 (4.58)	1045.9 (7.3)
(128,128)	122.36 (0.29)	166.68 (0.43)	228.59 (0.69)	312.06 (1.13)	422.89 (2.00)	577.94 (3.09)	781.23 (4.79)	1046.7 (7.3)
(192,32)	122.40 (0.40)	166.95 (0.60)	229.05 (0.93)	312.94 (1.49)	424.90 (2.69)	580.40 (4.39)	784.04 (7.14)	1057.7 (11.4)
(192,64)	122.41 (0.38)	166.94 (0.57)	229.15 (0.90)	312.86 (1.44)	425.42 (2.62)	580.91 (4.41)	785.39 (7.11)	1057.3 (11.2)
(192,96)	122.43 (0.39)	167.02 (0.58	229.30 (0.90)	313.23 (1.45)	426.08 (2.70)	581.91 (4.44)	787.63 (7.18)	1057.9 (11.2)
Kim	122.0 (2.7)	—	227.8 (3.2)	306.6 (3.9)	419 (5)	574 (8)	766 (7)	—

$L_{\min}$	2.30	2.40	2.50	2.60	2.70	2.80	2.90	3.00
(96,64)	1403.4 (8.3)	2539.1 (17.9)	4619.7 (38.6)	8460.1 (81.7)	15499 (172)	28413 (362)	51624 (746)	93601 (1475)
(96,96)	1402.0 (8.4)	2541.5 (19.2)	4605.9 (44.5)	8450.7 (101.2)	15401 (218)	28119 (455)	51356 (934)	93641 (1923)
(128,32)	1416.7 (10.6)	2566.2 (20.8)	4687.7 (41.3)	8559.0 (81.1)	15594 (161)	28622 (322)	51955 (651)	94133 (1345)
(128,64)	*1416.8 (10.5)*	*2568.8 (21.2)*	*4671.7 (43.9)*	*8569.0 (91.6)*	*15690 (189)*	*28737 (389)*	*52189 (779)*	*94643 (1554)*
(128,96)	1414.1 (10.8)	2558.1 (22.8)	4628.6 (48.4)	8478.0 (104.3)	15507 (226)	28360 (470)	51695 (961)	94033 (1930)
(128,128)	1415.5 (11.2)	2572.1 (26.2)	4637.7 (62.0)	8437.2 (143.2)	15336 (311)	27947 (666)	51319 (1392)	94627 (2922)
(192,32)	1425.3 (17.0)	2584.4 (32.8)	4716.9 (62.6)	8622.7 (118.4)	15638 (225)	28820 (432)	52345 (843)	94724 (1660)
(192,64)	1427.6 (17.0)	2582.2 (32.9)	4702.7 (62.7)	8625.0 (123.1)	15802 (244)	28952 (482)	52502 (934)	95266 (1819)
(192,96)	1427.0 (17.0)	2584.2 (33.4)	4688.2 (65.4)	8599.8 (133.7)	15660 (269)	28663 (542)	52314 (1082)	95304 (2163)
Kim	1402 (22)	2499 (41)	4696 (128)	8022 (234)	15209 (449)	—	—	—

Let us summarize the conceptual basis of our analysis. The main assumption is that if the ansatz (5) with a given function F_ξ is well satisfied by our data for $L_{\min} \leq L \leq 256$ and $1.65 \leq \beta \leq 3$, then it will continue to be well satisfied for $L > 256$ and $\beta > 3$. Obviously this assumption could fail, e.g., if [2] at some large correlation length ($\gtrsim 10^3$) the model crosses over to a new universality class associated with a finite-β critical point. In this respect our work is subject to the same caveats as any other Monte Carlo work on a finite lattice. However, it should be emphasized that our approach does *not* assume asymptotic scaling [Eq. (1)], as β plays no role in our extrapolation method. Thus, we can make an unbiased *test* of asymptotic scaling. The good agreement of our data at large x with the perturbative prediction (7) guarantees that our extrapolated values $\xi_\infty(\beta)$ will scale roughly as in (1), but it does not determine the constant C_ξ. The fact that we confirm (1) *with the correct nonperturbative constant* (3)/(4) is, we believe, good evidence in favor of the asymptotic-freedom picture.

Details of this work, including an analysis of the susceptibility χ, will appear elsewhere [19].

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[8] Our method [7] is essentially identical to that of Lüscher, Weisz, and Wolff [5]. The principal difference is that Lüscher *et al.* choose carefully their runs (β, L) so as to produce only a few distinct values of $x \equiv \xi(L)/L$, while we attempt to cover an entire interval of x. Moreover, we have used the method to obtain extrapolations to $L = \infty$ at each fixed β. The method of Kim [6] is also closely related, but he compares lattice size L to ∞ rather than to sL; this is a disadvantage. Nevertheless, Kim has obtained extremely accurate estimates of $\xi_\infty(\beta)$ in the O(3) σ model; see Table II above. Similar ideas were used also by Flyvbjerg and Larsen [9] in the context of the $1/N$ expansion. It should be emphasized that all these methods are completely general; they are *not* restricted to asymptotically free theories. Also, all these methods work only with observable quantities (ξ, $\mathcal{O}$, and L) and not with bare quantities (β). Therefore, they rely only on "scaling" and not on "asymptotic scaling;" and they differ from other finite-size-scaling-based methods such as phenomenological renormalization.

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[10] Here $\xi^{(\exp)}$ is the exponential correlation length (the inverse mass gap), and $\xi^{(2)}$ is the second-moment correlation length defined by (4.11)–(4.13) of Ref. [11]. Note that $\xi^{(2)}$ is well defined in finite volume as well as in infinite volume; where necessary we write $\xi^{(2)}(L)$ and $\xi_\infty^{(2)}$, respectively. In this paper, ξ without a superscript denotes $\xi^{(2)}$.

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[16] Steffen Meyer (private communication) has kindly supplied us with a high-precision Monte Carlo estimate of the universal ratio $C_{\xi^{(2)}}/C_{\xi^{(\exp)}}$ in the $N = 3$ model: it is 0.9994 ± 0.0008 at $\beta = 1.7$ ($\xi_\infty \approx 35$), $L = 256$; and 0.9991 ± 0.0009 at $\beta = 1.8$ ($\xi_\infty \approx 65$), $L = 512$. This is in excellent agreement with the value 0.9989 obtained from the $1/N$ expansion, and is only marginally different from 1.

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