

## High-temperature critical behavior of two-dimensional planar models: A series investigation

M. Ferer and M. J. Velgakis

*West Virginia University, Morgantown, West Virginia 26506*

(Received 18 August 1982)

We have analyzed new twelfth-order high-temperature series for the susceptibility and correlation length of classical planar models on the triangular lattice using an  $n$ -fit method of analysis tailored to the form of the singularity  $A \exp(bt^{-\nu})$  predicted by Kosterlitz and Thouless. Test-function analysis shows that the  $n$ -fit method is significantly more reliable in treating a number of possible corrections to the leading singularity than is the  $D \log$  Padé analysis of the logarithm and logarithmic derivative used in earlier series work on tenth-order series. Our  $n$ -fit analysis leads to the results  $\nu=0.5 \pm 0.1$  and  $\eta=0.27 \pm 0.03$  in good agreement with the Kosterlitz-Thouless predictions  $\nu = \frac{1}{2}$  and  $\eta = \frac{1}{4}$ .

### I. INTRODUCTION

We consider the high-temperature behavior of two-dimensional ( $d=2$ ) magnetic models with planar spin coupling ( $n=2$ ) which consist of "spins,"  $\vec{S}_i$ , at sites  $i$  of a two-dimensional lattice interacting with their nearest neighbors through the Hamiltonian

$$-\beta\mathcal{H} = K \sum_{\langle i,j \rangle} (S_i^x S_j^x + S_i^y S_j^y), \quad (1.1)$$

where  $K = \beta J$  and  $\langle i,j \rangle$  restricts the sum to nearest-neighbor pairs. The plane-rotator model is the  $n=2$  Heisenberg model with two-component spins of magnitude  $\sqrt{2}$ ; the classical  $XY$  model has classical three-component spins of magnitude  $\sqrt{3}$ .

In spite of the proven absence of a spontaneous magnetization in these models,<sup>1</sup> early series work indicated a divergent susceptibility and correlation length; at the same time, the series work suggested difficulties with assuming the standard power-law singularities.<sup>2,3</sup> Kosterlitz and Thouless used an approximate renormalization-group scheme to show the existence of a phase transition with a topological order parameter.<sup>4,5</sup> At high temperatures, they predicted exponentially decaying spin-spin correlations with a correlation length  $\xi$  of the form

$$\xi^2 = A_{\xi^2} \exp(b_{\xi^2} t^{-\nu}) \quad (1.2)$$

with  $t = 1 - KT_c$ ,  $T_c \equiv K_c^{-1} \simeq \pi$ , and  $\nu = \frac{1}{2}$ , and a susceptibility of the form

$$\chi = A_{\chi} \exp(b_{\chi} t^{-\nu}), \quad (1.3)$$

where  $b_{\chi} = (2 - \eta)b_{\xi^2}/2$  with  $\eta = \frac{1}{4}$ .

Camp and Van Dyke performed standard  $D \log$  Padé analysis on tenth-order series for the logarithm of the susceptibility  $\ln \chi$ . This analysis produced Padé tables for the index  $\nu$  which were quite irregular and which had a significant number of defects, especially in higher orders. On the basis of this analysis, they asserted  $\nu \simeq 0.7$ .<sup>6</sup>

A similar analysis was performed by Guttmann who performed standard  $D \log$  Padé analysis of the  $D \log$  (the logarithmic derivative) of the susceptibility.<sup>7</sup> The Padé analysis of these series is also irregular with a number of defects leading to the assertion  $\nu \simeq 0.4$  for the plane-rotator model and  $\nu \simeq 0.6$  for the classical  $XY$  model.

Monte Carlo work produced results which were somewhat more consistent with  $\nu \simeq 0.7$  than  $\nu \simeq 0.5$ ; i.e., the "best fits fall between"  $\nu \simeq 0.70$  and  $\nu \simeq 0.50$  with the "most consistent fit being"  $\nu \simeq 0.70$ , with uncertainties "pointing to slightly smaller values of  $\nu$ ."<sup>8</sup> Thus Monte Carlo work and early series work indicate what must be only a slight preference for  $\nu \simeq 0.7$  over the Kosterlitz-Thouless prediction  $\nu = \frac{1}{2}$ . On the other hand, Monte Carlo work predicts  $\eta = 0.243 - 0.254$  in striking agreement with the Kosterlitz-Thouless prediction  $\eta = \frac{1}{4}$ .

To address the sizable disagreement over the value of the index  $\nu$ , we have derived twelfth-order, high-temperature series for the spin-spin correlation function of the classical planar models by extending the same computer programs which Moore used to derive the tenth-order series<sup>3,9</sup> and by developing a new method of series analysis (4 fits) tailored to determining the parameters in Eqs. (1.2) and (1.3). The series for the susceptibility  $\chi$  and for the correlation length  $\xi^2 = \mu_2/2 d\chi$ , where  $\mu_2$  is the second moment of the correlations, are presented in Table I.

TABLE I. Twelfth-order series for the susceptibility  $\chi$  and for the correlation length  $\xi^2 = \mu_2/2d\chi$  for the spin-infinity XY model with  $D=3$  spin components and for the plane-rotator model with  $D=2$  spin components on the triangular lattice. Note our spin normalization  $=D^{1/2}$  is the same as that of Ref. 3; to compare with Ref. 6 one needs to multiply our  $n$ th series coefficient by  $D^{-n-1}$  and our transition temperature by  $D^{-1}$ .

XY model		Plane-rotator model	
$2d\xi^2 = \mu_2/\chi$	$\chi$	$2d\xi^2 = \mu_2/\chi$	$\chi$
6.0K	1+6.0K	6.0K	1+6.0K
+36.0K <sup>2</sup>	+31.2K <sup>2</sup>	+36.0K <sup>2</sup>	+30.0K <sup>2</sup>
+189.12K <sup>2</sup>	+150.72K <sup>3</sup>	+183.0K <sup>3</sup>	+135.0K <sup>3</sup>
+927.36K <sup>4</sup>	+694.08K <sup>4</sup>	+846.0K <sup>4</sup>	+570.0K <sup>4</sup>
+4338.4633469387K <sup>5</sup>	+3086.1296326531K <sup>5</sup>	+3674.0K <sup>5</sup>	+2306.0K <sup>5</sup>
+19611.064946939K <sup>6</sup>	+13359.869387755K <sup>6</sup>	+15269.0K <sup>6</sup>	+9041.5K <sup>6</sup>
+86320.725159182K <sup>7</sup>	+56616.566595918K <sup>7</sup>	+61385.125K <sup>7</sup>	+34582.125K <sup>7</sup>
+372013.02778776K <sup>8</sup>	+235802.09336485K <sup>8</sup>	+240508.91666666K <sup>8</sup>	+129634.16666666K <sup>8</sup>
+1575623.1830223K <sup>9</sup>	+968006.61405210K <sup>9</sup>	+922905.86666638K <sup>9</sup>	+477988.03333333K <sup>9</sup>
+6576564.1514358K <sup>10</sup>	+3925503.2208896K <sup>10</sup>	+3480222.9999904K <sup>10</sup>	+1738252.3916576K <sup>10</sup>
+27109736.166148K <sup>11</sup>	+15752404.879275K <sup>11</sup>	+12930470.159491K <sup>11</sup>	+6246941.2428646K <sup>11</sup>
+110550319.79906K <sup>12</sup>	+62636620.793426K <sup>12</sup>	+47434983.642942K <sup>12</sup>	+22220235.302532K <sup>12</sup>

Our 4-fit method of analysis is presented in Sec. II of this paper. The 4-fit method works directly with the series coefficients in a way which is akin to the ratio method in that estimates of the parameters from higher-order series terms are independent of lower-order terms. We believe that this is an improvement over the earlier series analysis because low-order corrections to the leading singularity, which can be sizeable, will be propagated to high orders in the process of taking the double logarithm. Test-function analysis in Sec. III supports this conclusion that low-order corrections, which have no effect on the 4-fit analysis, can easily disrupt the  $D \log$  Padé analysis of the logarithm of the series. We have studied test functions which include both analytic and confluent corrections to the Kosterlitz-Thouless singularity. The  $D \log$  Padé analysis of the logarithm and logarithmic derivative of these test functions shows the same sort of irregularity and number of defects as the analysis of Refs. 6 and 7, whereas, the 4-fit analysis of the test functions is much smoother and more reliable. Our 4-fit analysis of the model series, presented in Sec. IV, provides evidence which favors the Kosterlitz-Thouless prediction  $\nu = \frac{1}{2}$  and which strongly opposes a value as large as 0.7. This analysis suggests  $\nu = 0.5 \pm 0.1$  where we have tried to err on the side of significantly overestimating the uncertainty. More optimistically, we expect that  $\nu = 0.50 \pm 0.05$  is still quite realistic. Our analysis favors values for  $\eta$  a bit larger than  $\frac{1}{4}$ , e.g., 0.26–0.30, but consistent

downward trends lead us to believe that this preference for larger values of  $\eta$  is an artifact of short and fairly irregular series.

## II. 4-FIT METHOD OF ANALYSIS

The logic behind our 4-fit analysis for this singularity is the same as that behind the 5-fit analysis for confluent singularities<sup>10,11</sup> and even the ratio analysis for standard leading singularities.<sup>12</sup> One takes a parametrization of what one hopes to be the dominant part of the singular function under investigation. Then, one expands this parametrization as a power series in inverse temperature, i.e., the interaction strength  $K = J/kT$ , where the coefficients  $b_j$  are known as functions of  $q$  undetermined parameters. One then takes  $q$  of these coefficients and equates each to the corresponding coefficient  $a_j$  in the exact enumeration series. Thus one has  $q$  equations  $b_j = a_j$ , the solution of which provides values for the  $q$  unknown parameters, hence the name  $q$  fits.

To realize this approach, we expand the predicted leading singularity as a power series in  $K$ , e.g., for the square of the correlation length,

$$\xi^2 \simeq A \exp(bt^{-\nu}) = \sum_{j=0}^{\infty} A e^{bT_c^j} B_j(b\nu, \nu) K^j, \quad (2.1)$$

where  $t = 1 - KT_c$ ,  $T_c \equiv kT_c/J$ , and where the form of these coefficients is determined by first expanding  $bt^{-\nu}$  in powers of  $K$ ,

$$b\sigma = b(t^{-\nu} - 1) = b\nu(T_c K) + b\nu \left[ \frac{\nu+1}{2} \right] (T_c K)^2 + b\nu \left[ \frac{\nu+1}{2} \right] \left[ \frac{\nu+2}{3} \right] (T_c K)^3 + \cdots = b\nu \sum_{j=1}^{\infty} \left[ \sum_{i=0}^{j-1} S_{ij} \nu^i \right] (KT_c)^j, \quad (2.2)$$

and then by expanding the exponential in powers of  $b\sigma$ ,

$$\begin{aligned}\xi^2 &\sim Ae^b e^{b\sigma} = Ae^b \sum_{j=0}^{\infty} \frac{(b\sigma)^j}{j!} = Ae^{b(1+b\nu(KT_c))} + \left[ b\nu \left[ \frac{\nu+1}{2} \right] + \frac{(b\nu)^2}{2} \right] (KT_c)^2 + \dots \\ &= Ae^b + \sum_{j=1}^{\infty} Ae^{bT_c^j} \left[ \sum_{i=1}^j \sum_{k=0}^{i-1} f_{jik}(b\nu)^i \nu^k \right] K^j.\end{aligned}\quad (2.3)$$

To determine values for the four parameters  $\nu$ ,  $b$ ,  $T_c$ , and  $A$  or equivalently  $\nu$ ,  $b\nu$ ,  $T_c$ , and  $Ae^b$ , we equate four consecutive coefficients in Eq. (2.3) with the corresponding coefficients in the exact enumeration series  $\xi^2 = \sum_{j=0}^{\infty} a_j K^j$ , i.e.,

$$a_j = Ae^{bT_c^j} B_j(b\nu, \nu) \quad (2.4)$$

for  $j=n, n-1, n-2$ , and  $n-3$ , so that we have four equations in the four unknowns. If we divide the  $j$ th equation by the  $(j-1)$ st equation, we have

$$(a_j/a_{j-1})B_{j-1}(b\nu, \nu) = T_c B_j(b\nu, \nu) \quad (2.5)$$

for  $j=n, n-1$ , and  $n-2$  eliminating the unknown  $Ae^b$  so that we have three equations in three remaining unknowns. If we then divide this equation by the corresponding  $(j-1)$ st equation, we have eliminated the unknown  $T_c$  and are left with two equations in two remaining unknowns which can be written as

$$\begin{aligned}[(a_{j-1})^2/(a_j a_{j-2})]B_{j-2}(b\nu, \nu)B_j(b\nu, \nu) \\ - B_{j-1}^2(b\nu, \nu) = 0\end{aligned}\quad (2.6)$$

with  $j=n$  and  $n-1$ . Since the  $B_j$ 's are finite polynomials in  $b\nu$  and  $\nu$  with known coefficients, determining the values of  $b\nu$  and  $\nu$  which solve these equations is equivalent to finding the common roots of the  $j=n$  and the  $j=n-1$  polynomials. This is done using standard numerical methods to locate the common physical root in the expected ranges of  $\nu$  and  $b\nu$ . Once these values denoted  $\nu_n$  and  $b_n$  are determined, they can be used in Eq. (2.5) to determine  $T_{c,n}$ . Finally,  $A_n e^{b_n}$  can be determined using these values in Eq. (2.4). Therefore, we have determined the  $n$ th element in each of the four sequences whose limit is the value of the corresponding parameter in Eq. (2.1), e.g.,  $\lim_{n \rightarrow \infty} \nu_n = \nu$ .

### III. TEST-FUNCTION ANALYSIS

We have performed standard Padé analysis and 4-fit analysis for a number of test functions which incorporate the expected leading singularity,

$$Y = A \exp(bt^{-\nu}), \quad (3.1)$$

$t=1-K/K_c$ , various types of analytic corrections, as well as various types of less-singular, confluent corrections. Standard log-derivative Padé analysis was performed on  $\ln Y$  (Ref. 6) and on  $Y'/Y$  (Ref. 7) both of which should yield  $\nu$  and  $K_c$  in Eq. (3.1) as the location and residue of a simple pole:

$$Z_1 = \ln Y, \quad \frac{d}{dK} \ln Z_1 = \frac{\nu}{K_c - K}, \quad (3.2a)$$

$$Z_2 = \frac{Y'}{Y}, \quad \frac{d}{dK} \ln Z_2 = \frac{1+\nu}{K_c - K}. \quad (3.2b)$$

Since both approaches are similar, the reliability of both approaches should also be similar. As borne out by the test-function analysis, it seems likely that any sizeable, low-order analytic corrections could significantly affect the reliability of these Padé methods because low-order deviations are telescoped to higher order in taking the logarithmic derivative on top of the logarithm in  $Z_1$  and on top of the logarithmic derivative in  $Z_2$ , e.g.,  $\ln \ln(Y+1) \approx \ln Y$  only when  $Y \gg 1$ . We developed and applied our 4-fit method in the belief that the effect of these analytic corrections would decrease rapidly with increasing order.

In comparing the results from the Padé analysis with the results from the 4-fit analysis for the test functions which we have analyzed, we find the following:

(i) that the 4-fit analysis is significantly better behaved and more reliable than the  $D \log$  Padé analysis of  $Z_1$  and  $Z_2$ ,

(ii) that sufficiently large low-order analytic corrections can easily confound the  $D \log$  Padé analysis of  $Z_1$  and  $Z_2$  although little effect is observed in the 4-fit analysis, and

(iii) that confluent corrections lead to errors in the 4-fit predictions of a few percent (similar to the effect observed in the spin- $s$  Ising model<sup>10,11</sup>) but that even relatively weak confluent corrections seriously disrupt the Padé analysis of  $Z_1$  and  $Z_2$ .

To demonstrate these effects we will discuss the

TABLE II. Test-function analysis: Results for  $\nu$  from Padé analysis of fifteenth-order series and from 4-fit analysis of twelfth-order series for the test functions in Eq. (3.3). An asterisk denotes a Padé approximant with a nearby or intervening pole.

$N$	$[N/N+1]$	$[N/N]$	$[N+1/N]$	$N$	$[N/N+1]$	$[N/N]$	$[N+1/N]$	$n$	$\nu_n$
$\ln Y_A$									
2	*	*	0.546	2	0.618	0.772	*	3	
								4	0.5773
3	0.482	0.481	0.482	3	0.268	0.492	0.377	5	
								6	
4	0.464	0.481	0.452	4	0.414	0.385	*	7	0.5600
								8	0.5144
5	0.464	0.463	0.464	5	0.654	0.500	0.597	9	0.5028
								10	0.5005
6	0.478	*	0.487	6	0.543	0.575	*	11	0.5001
								12	0.5000
7		0.486							
$Y'_A/Y_A$									
2	0.579	*	0.503	2	0.590	0.688	0.679	3	
								4	0.5488
3	0.449	0.430	0.447	3	0.320	0.526	0.450	5	
								6	0.6543
4	0.448	0.447	0.448	4	0.466	0.449	0.450	7	0.5574
								8	0.5243
5	*	*	*	5	*	0.508	0.594	9	0.5160
								10	0.5146
6	0.456	*	*	6	0.567	0.586	*	11	0.5148
								12	0.5151
7		*							
$Y'_B/Y_B$									
$\ln Y_C$									
2	0.509	0.454	0.490	2	0.579	*	0.627	3	0.5053
								4	0.5652
3	0.510	0.512	0.506	3	0.323	0.562	0.540	5	0.5390
								6	0.5277
4	0.480	0.468	0.480	4	0.418	0.421	0.417	7	0.5208
								8	0.5162
5	0.465	0.478	*	5	*	0.419	*	9	0.5129
								10	0.5104
6	0.472	0.472	0.472	6	0.572	0.452	0.562	11	0.5085
								12	0.5071
7		0.474							
$Y'_C/Y_C$									
$\ln Y_D$									
2	0.460	0.456	0.459	2	0.480	*	0.456	3	0.4782
								4	0.4765
3	0.467	0.461	0.463	3	*	0.484	0.490	5	0.4962
								6	0.5079
4	*	*	*	4	0.562	*	0.570	7	0.5149
								8	0.5189
5	0.467	*	0.462	5	0.485	0.553	0.540	9	0.5209
								10	0.5218
6	0.489	0.484	0.490	6	0.365	0.339	0.374	11	0.5219
								12	0.5215
7		0.489							
$Y'_D/Y_D$									

analysis of the following four test functions:

$$Y_A = 2 \exp(3t^{-1/2}) + \exp(3K), \quad (3.3a)$$

$$Y_B = 2 \exp(3t^{-1/2}) + \exp(3K) + 2 \exp(2.5t^{-1/2}), \quad (3.3b)$$

$$Y_C = 2 \exp(3t^{-1/2}) + t^{-1.25}, \quad (3.3c)$$

$$Y_D = 2 \exp(3t^{-1/2}) + 0.1t^{-2.5}, \quad (3.3d)$$

where  $t = 1 - 3K$ .

Table II shows that values of  $\nu$  from the  $[N, D]$  Padé approximants to  $D \log Z_1$  and  $Z_2$  as well as the 4-fit sequence for  $\nu$ . From this table, it is clear that even a simple analytic correction like  $e^{3K}$  in  $Y_A$  introduces defects and irregularities in the  $D \log$  Padé analysis of  $Z_1$  and  $Z_2$  so that one might estimate  $\nu = 0.485 \pm 0.030$ , an error in the "best value" of 3% and uncertainties of 6%. However, the 4-fit sequence has converged to within 0.1% by the tenth-order term. Introducing confluent corrections, as in  $Y_B$ ,  $Y_C$ , and  $Y_D$ , produces smooth 4-fit sequences which, to the orders studied here, lead to errors of no more than 4% depending on the strength

of the confluent correction, affected by both its amplitude and power of divergence. This is similar to the effect observed in ratio studies, which are essentially 3 fits to the standard critical singularity, of the spin- $s$  Ising model where confluent corrections cause ratio estimates of the leading indices to be in error by a few percent.<sup>10,11</sup> The Padé analysis of these functions shows behavior similar to that caused by the analytic correction, i.e., defects, irregularities of 10% or more, and consistent errors of a few percent which is usually greater than the error from the 4-fit sequence. The one exception to this is for the test function  $Y_D$  which has no analytic corrections but which has a strongly divergent confluent correction with a weak amplitude so that low-order corrections are small. The smallness of the low-order corrections suggests that the Padé tables may be smoother, which they are; the strength of the divergent confluent singularity makes the 4-fit analysis a bit less reliable.

In conclusion, the test-function studies show that the 4-fit analysis is not only better behaved but also more reliable in the presence of low-order corrections which will certainly contribute to the actual series.

TABLE III. Sequences from a 4-fit analysis of the series for the spin-infinity  $XY$  model on the triangular lattice.

$n$	$\nu_n$	$T_{c,n}$	$b_n$	$(b_n \nu_n)$	$A_n$	$[A_n \exp(b_n)]$
$\mu_2/KX$						
3						
4	0.494	3.338	3.348	1.654	0.229	6.52
5	0.519	3.313	3.182	1.651	0.273	6.58
6	0.588	3.256	2.774	1.630	0.424	6.80
7	0.463	3.351	3.640	1.686	0.166	6.33
8	0.549	3.291	2.981	1.636	0.341	6.71
9	0.540	3.296	3.038	1.641	0.320	6.67
10	0.504	3.318	3.316	1.670	0.235	6.46
11	0.483	3.330	3.497	1.689	0.192	6.33
$(X-1)/K$						
3						
4	0.454	3.400	3.054	1.388	0.312	6.61
5	0.571	3.298	2.372	1.354	0.653	7.00
6	0.681	3.221	1.919	1.307	1.092	7.44
7	0.627	3.255	2.128	1.335	0.857	7.19
8	0.590	3.277	2.299	1.357	0.704	7.01
9	0.560	3.294	2.459	1.378	0.585	6.84
10	0.530	3.310	2.646	1.403	0.472	6.65
11	0.503	3.324	2.838	1.428	0.379	6.47

## IV. SERIES ANALYSIS

In Tables III and IV, we present the sequences resulting from the application of 4-fit analysis to the correlation-length series  $\xi^2 = \mu_2/K\chi$  and to the susceptibility series  $(\chi-1)/K$   $n$ -shifted by one for the spin-infinity  $XY$  model and for the plane-rotator model. We present the analysis for the  $n$ -shifted susceptibility because this analysis is significantly better behaved than that of the unshifted susceptibility series  $\chi$ , e.g., using the unshifted series there are no 4-fit solutions for  $n=7, 8, 9, 10$ , and  $11$ , the highest orders, and there are significant monotonic trends in the 3-fit sequences as will be discussed later. In these tables, we also present the sequences for  $b_n\nu_n$  and  $A_n \exp(b_n)$  not only because these are the naturally occurring quantities in the 4-fit equations, Eq. (2.4), i.e.,  $b$  always appears in the form  $b\nu$  and  $A$  always appears in the form  $Ae^b$ , but also because these sequences are obviously smoother than the sequences for  $A_n$  and  $b_n$  independently.

We will first focus our attention on a determination of the index  $\nu$ . Recalling the Kosterlitz-Thouless prediction of  $\nu=0.5$  (Refs. 4 and 5) and the Monte Carlo<sup>8</sup> and early series work<sup>6</sup> favoring  $\nu=0.7$ , we observe that almost none of the elements  $\nu_n$  presented in Tables III and IV and shown in Fig.

1 are larger than 0.6 and that most trends are downwards. In trying to estimate the limiting value of  $\nu$ , we must attempt to determine to what extent the convergence of the sequences is oscillatory and to what extent we can reliably extrapolate apparent trends. These sequences are clearly more irregular than any of the sequences from the test functions; perhaps this is due to low-temperature antiferromagnetic behavior similar to the zero-temperature transition in the triangular Ising antiferromagnet for which short series indicate a finite-temperature transition. Because of this irregularity, it is difficult to determine whether trends in the higher-order terms in the  $\nu_n$  sequences can be assumed to be monotonic to  $n = \infty$  or whether they are just a continuation of the low-order oscillations. If one considers the sequence for the correlation length of the  $XY$  model, the low-order terms are clearly oscillatory, but even the last three terms (see Fig. 1), which are monotonically decreasing, indicate a curvature, suggestive of a continuation of the oscillatory behavior. Similarly, the very irregular sequences for the plane-rotator model are more consistent with oscillatory convergence than with consistent upwards or downwards trends. The most consistent trend is to be found in the sequence for the  $XY$  susceptibility, which is monotonic downwards for the last six terms. We do

TABLE IV. Sequences from a 4-fit analysis of the series for the plane-rotator model on the triangular lattice.

$n$	$\nu_n$	$T_{c,n}$	$b_n$	$(b_n\nu_n)$	$A_n$	$[A_n \exp(b_n)]$
$\mu_2/K\chi$						
3						
4	0.590	2.776	3.514	2.073	0.186	6.26
5	0.418	2.942	4.908	2.050	0.044	5.95
6	0.475	2.891	4.300	2.043	0.083	6.09
7						
8						
9	0.560	2.857	3.477	1.946	0.206	6.66
10	0.489	2.898	4.088	1.998	0.106	6.30
11						
$(\chi-1)/K$						
3						
4						
5	0.474	2.966	3.280	1.554	0.245	6.52
6						
7						
8	0.477	2.934	3.374	1.611	0.214	6.26
9	0.452	2.948	3.604	1.630	0.167	6.13
10	0.535	2.905	2.917	1.561	0.358	6.61
11	0.566	2.890	2.709	1.534	0.454	6.81

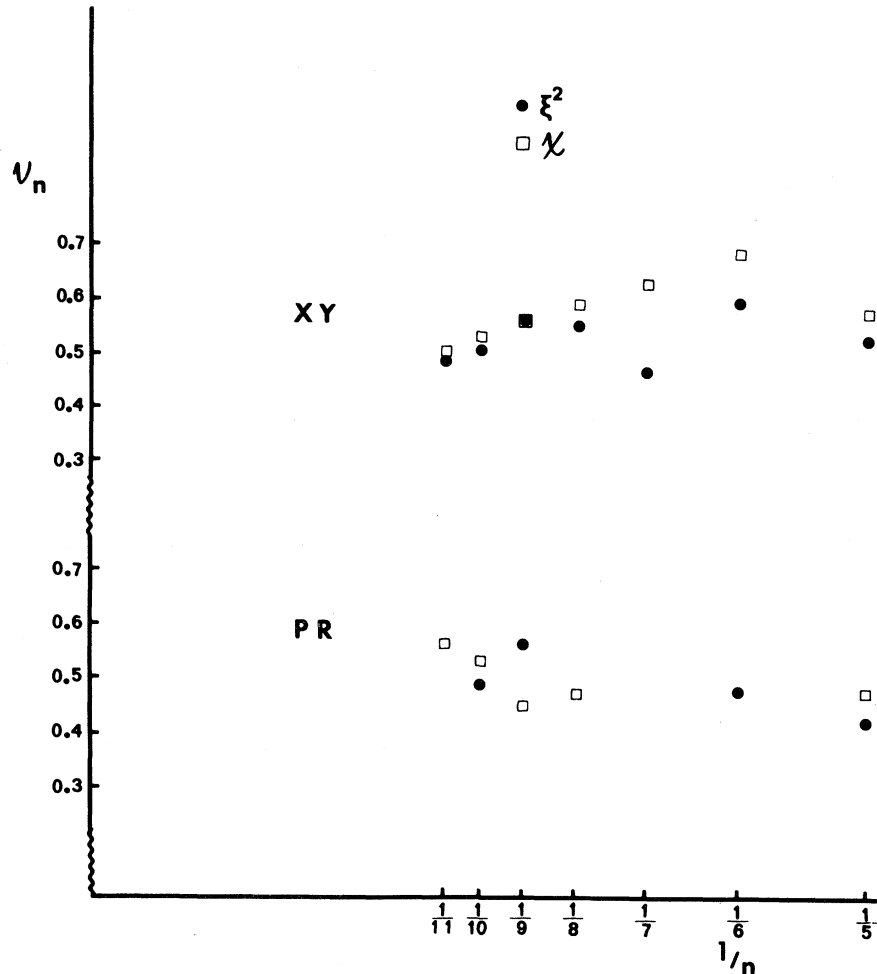


FIG. 1.  $1/n$  plot of the sequences for  $\nu_n$  from the 4-fit analysis of the correlation length  $\xi^2$  and susceptibility  $\chi$  series for the spin-infinity XY and plane-rotator (PR) models. Closed square indicates overlap of  $\xi^2$  and  $\chi$  data points.

not believe this is a real trend since a naive linear extrapolation to  $n = \infty$  predicts  $\nu = 0.2$  which is inconsistent not only with the other sequences but also with the previous work.<sup>4-8</sup> Thus it seems likely that these sequences are converging in an oscillatory fashion. The existing terms "oscillate" about 0.5, and all but a few low-order terms are within 0.1 of 0.5. For these reasons,  $\nu = 0.5 \pm 0.1$  seems to be a conservative estimate of our real uncertainty; it seems unlikely that any monotonic trends camouflaged by the oscillatory behavior would lead to a value outside this range. Given the evidence, it does not seem overly optimistic to suggest smaller uncertainties  $\nu = 0.50 \pm 0.05$ . However, our main assertion is that the results agree with the Kosterlitz-Thouless predictions<sup>4,5</sup> to within our uncertainties and that they are strikingly inconsistent with the

preference of  $\nu \approx 0.7$  from Monte Carlo<sup>8</sup> and early series work<sup>6</sup> using shorter series and seemingly less reliable methods of series analysis, because no terms in our sequences are near 0.7, and any apparent trends are in the opposite direction. They are consistent with the conclusions of Ref. 7 ( $0.4 < \nu < 0.6$ ), but we find our results more convincing and model independent. In Table V, we present, for completeness, the results for  $\nu$  from a Padé analysis, as in Refs. 6 and 7, of the XY series. These Padé tables show the same number of defects and irregularities observed in the test-function analysis. Even this analysis of both the correlation length and  $n$ -shifted susceptibility is not consistent with  $\nu \approx 0.7$ ; recall that Ref. 6 analyzed only the unshifted susceptibility series.

We have used the relation  $b_\chi = (2 - \eta)b_{\xi^2}/2$  to

TABLE V. Values for  $\nu$  from the near-diagonal elements of a Padé table from the Padé analysis as in Refs. 6 and 7 of the series for the susceptibility and correlation length for the spin-infinity  $XY$  model on the triangular lattice. An asterisk indicates a Padé approximant with a nearby or intervening pole. It is our experience from the test-function analysis that the Padé analysis of  $\ln Y$  is somewhat more reliable than the Padé analysis of  $Y'/Y=d(\ln Y)/dK$  for the test functions considered.

$N$	$ N/N+1 $	$ N/N $	$ N+1/N $	$N$	$ N/N+1 $	$ N/N $	$ N+1/N $
$\ln[(\chi-1)/K]$				$\ln(\xi^2/K)$			
2	*	0.524	0.549	2	*	0.517	0.537
3	0.597	0.646	0.605	3	0.549	0.541	*
4	*	0.584	*	4	0.582	*	*
5		*		5		0.555	
$\frac{d}{dK} \ln[(\chi-1)/K]$				$\frac{d}{dK} \ln(\xi^2/K)$			
2	1.151	*	0.799	2	0.728	*	0.667
3	0.609	0.738	*	3	0.648	0.631	0.644
4	*	*	*	4	0.649	0.665	0.646

TABLE VI. Sequences from a 3-fit analysis of the series for the spin-infinity  $XY$  model on the triangular lattice, using the fixed values of  $\nu$  shown.

$n$	$\mu_2/K\chi$			$(\chi-1)/K$		
	$b_n$	$T_{c,n}$	$A_n$	$b_n$	$T_{c,n}$	$A_n$
$\nu=0.5$						
2	3.9941	3.0044	0.111	3.4966	2.9744	0.182
3	3.3093	3.3305	0.239	2.7682	3.3499	0.422
4	3.3063	3.3317	0.240	2.7498	3.3581	0.432
5	3.3133	3.3294	0.237	2.7689	3.3511	0.422
6	3.3383	3.3221	0.230	2.8053	3.3395	0.401
7	3.3280	3.3247	0.233	2.8299	3.3327	0.387
8	3.3389	3.3222	0.229	2.8460	3.3286	0.378
9	3.3470	3.3204	0.227	2.8561	3.3263	0.372
10	3.3477	3.3203	0.226	2.8608	3.3253	0.369
11	3.3447	3.3209	0.227	2.8612	3.3252	0.369
$\nu=0.7$						
2	3.2333	2.6510	0.237	2.8305	2.6244	0.354
3	2.3782	3.1225	0.642	1.9218	3.1727	1.070
4	2.3222	3.1516	0.691	1.8748	3.2000	1.142
5	2.2815	3.1698	0.731	1.8563	3.2092	1.174
6	2.2618	3.1776	0.752	1.8542	3.2101	1.178
7	2.2206	3.1925	0.801	1.8460	3.2134	1.194
8	2.1997	3.1994	0.828	1.8343	3.2176	1.218
9	2.1800	3.2056	0.856	1.8204	3.2224	1.248
10	2.1574	3.2122	0.890	1.8046	3.2274	1.284
11	2.1344	3.2186	0.926	1.7876	3.2325	1.326



TABLE VII. Sequences from a 3-fit analysis of the series for the plane-rotator model on the triangular lattice, using the fixed value  $\nu=0.5$ .

$n$	$\nu=0.5$			$(\chi-1)/K$		
	$b_n$	$\mu_2/K\chi$ $T_{c,n}$	$A_n$	$b_n$	$T_{c,n}$	$A_n$
2	4.3200	2.7778	0.080	3.7500	2.6667	0.141
3	4.0737	2.8745	0.105	3.1702	2.9172	0.272
4	4.1234	2.8589	0.099	3.0993	2.9432	0.297
5	4.0809	2.8701	0.104	3.0898	2.9461	0.301
6	4.0712	2.8723	0.105	3.1523	2.9295	0.277
7	3.9991	2.8872	0.116	3.1938	2.9198	0.261
8	3.9652	2.8937	0.121	3.1887	2.9209	0.263
9	3.9791	2.8913	0.119	3.1787	2.9229	0.267
10	2.9766	2.8917	0.119	3.1848	2.9218	0.264
11	3.9447	2.8966	0.125	3.1949	2.9201	0.260

determine sequences

$$(2-\eta)_n = 2b_{n,\chi}/b_{n,\xi^2}$$

using the 4-fit analysis already discussed as well as 3-fit analysis. In the 3-fit analysis, we fix the value of  $\nu$  at a particular value in Eqs. (2.4)–(2.6); we then solve Eq. (2.6) with  $j=n$  for  $b_n$ , Eq. (2.5) with  $j=n$  for  $T_{c,n}$ , and Eq. (2.4) with  $j=n$  for  $A_n$ . Tables VI and VII show the sequences resulting from the 3-fit analysis of these series. In Table VIII, we present the sequences for  $2-\eta$ . Figure 2 shows a  $1/n$  plot of these sequences. Note that in the sequence from the 4-fit analysis we have used  $b_n\nu_n$  because this sequence is smoother than the sequences for  $b_n$ .

When one considers the convergence of these sequences, the presence of consistent upward trends seems clearly indicated; superimposed on the upwards trends are small oscillations. Naive linear extrapolations shown in the figure lead to values of  $2-\eta$  between 1.69 and 1.73 from all sequences; the authors do not feel that a more complicated extrapolation procedure is warranted given the irregularity of the sequences. Apparently, the best behaved sequences are for the XY model; for the plane-rotator model, a significant number of terms in the 4-fit sequences are absent (no solution) and the 3-fit sequences are more irregular with larger trends. For the XY model, both the 4 fits and the  $\nu=0.5$  3 fits suggest the largest values,  $2-\eta \approx 1.73$ , closest to the

TABLE VIII. Various sequences for  $2-\eta=2b_\chi/b_{\xi^2}$  from 4-fit and 3-fit analysis.

$n$	$2-\eta$			
	4-fit XY model	XY model	3-fit XY model	plane-rotator model
	$2 \frac{(b_n\nu_n)_\chi}{(b_n\nu_n)_{\xi^2}}$	$\nu=0.5$	$2(b_{n,\chi}/b_{n,\xi^2})$ $\nu=0.7$	$\nu=0.5$
2		1.7509	1.7509	1.7361
3		1.6730	1.6161	1.5564
4	1.6781	1.6634	1.6147	1.5033
5	1.6403	1.6714	1.6273	1.5143
6	1.6038	1.6807	1.6396	1.5486
7	1.5833	1.7006	1.6626	1.5973
8	1.6594	1.7048	1.6677	1.6083
9	1.6795	1.7067	1.6701	1.5977
10	1.6796	1.7091	1.6730	1.6018
11	1.6902	1.7109	1.6750	1.6199

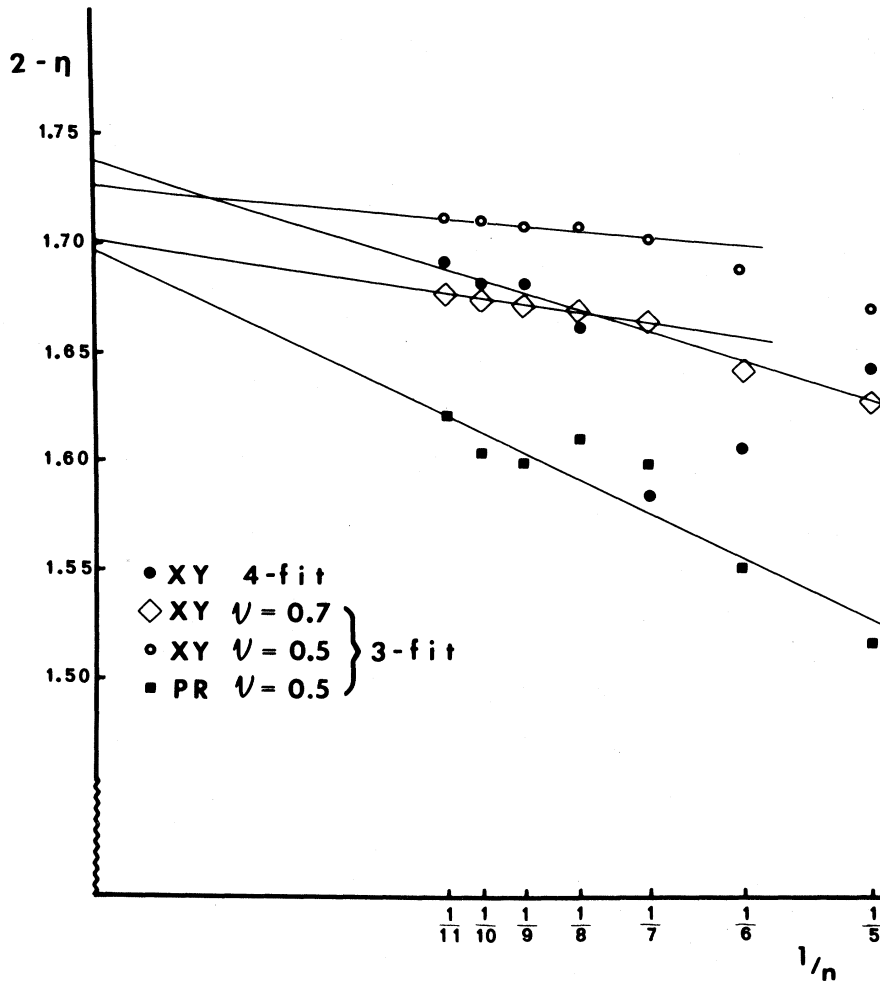


FIG. 2.  $1/n$  plot of sequences for  $2-\eta=2b_x/b_{\xi_2}$  from 3- and 4-fit analyses of the series for the spin-infinity XY model and the PR model on the triangular lattice. The values of  $\nu$  used in the 3-fit analysis are shown. Approximate linear extrapolants are drawn through the points.

Kosterlitz-Thouless prediction  $\eta = \frac{1}{4}$ .<sup>4,5</sup> However, even the 3 fits with  $\nu=0.7$ , which, as we have seen, is clearly inconsistent with 4-fit analysis, leads to the prediction  $2-\eta \simeq 1.70$ . On the basis of the evidence, we estimate  $2-\eta = 1.73 \pm 0.03$  in agreement with the prediction  $\eta = \frac{1}{4}$ .<sup>4,5</sup> We expect that the obvious preference of our results for values of  $2-\eta$  less than 1.75 is an artifact of the short series not correctly representing the limiting upwards trends.

Lastly, Fig. 3 shows the  $1/n$  plots of  $T_{c,n}$ . Of the sequences shown, the  $\nu=0.5$  3-fit sequences are nearly independent of  $n$ , and the 4-fit sequences show what we believe to be primarily oscillatory behavior. On the basis of these sequences, we assert  $T_c = 3.32 \pm 0.03$  for the XY model and

$T_c = 2.91 \pm 0.04$  for the plane-rotator model. It should be added that these estimates for  $T_c$  do not seem to sensitively depend on the value assumed for  $\nu$  because even the  $\nu=0.7$  3-fit sequences for  $T_c$  from the XY model extrapolate to the value quoted within uncertainties.

At the beginning of this section, we mentioned that the behavior of the analysis of the unshifted susceptibility series was significantly worse than the analysis of the series  $n$  shifted by 1. In addition to the absence of the higher-order 4-fit solutions, the 3-fit sequences formed from the unshifted series show much larger trends, e.g., compare the  $\nu=0.5$  3-fit sequence for  $T_c$  from the  $n$ -shifted XY series shown in Table VI with the last six terms ( $n=6 \rightarrow 11$ ) in the  $\nu=0.5$  3-fit sequence from the

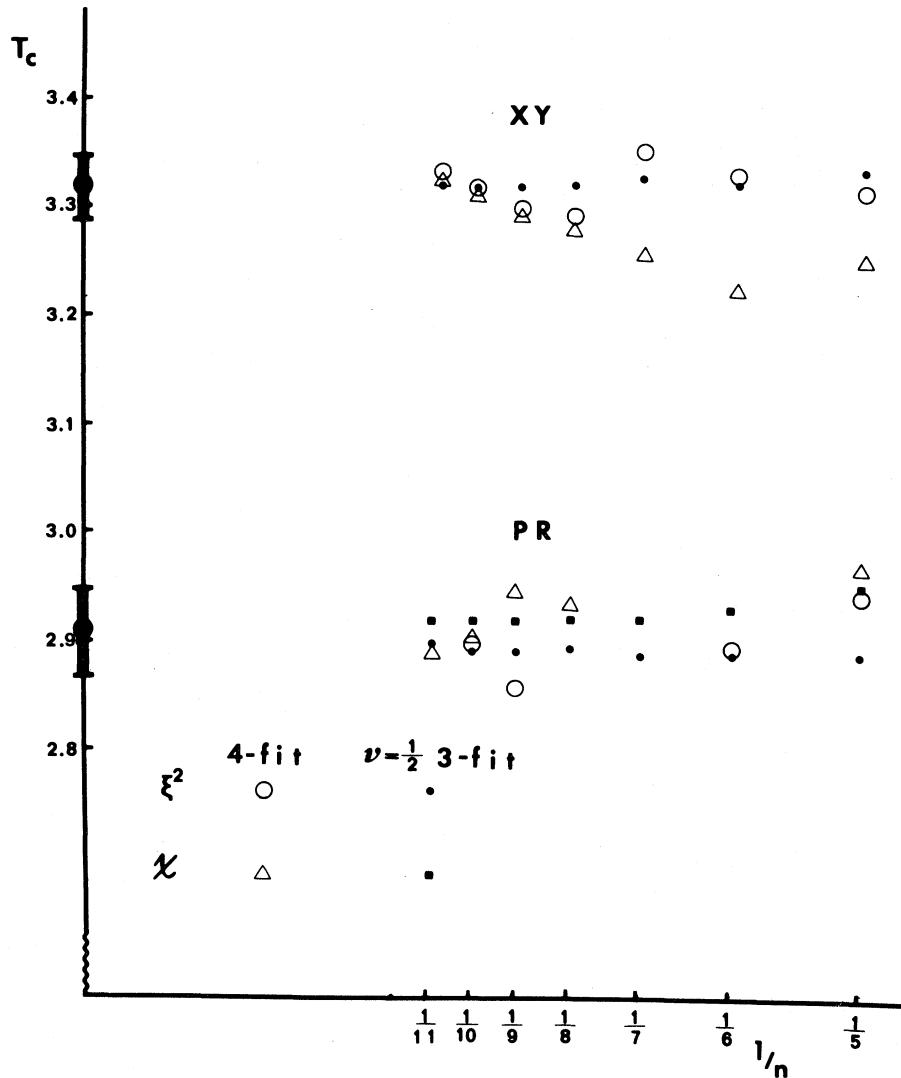


FIG. 3.  $1/n$  plots of the sequences for  $T_c$  from 4-fit analysis and  $\nu = \frac{1}{2}$  3-fit analysis of the correlation length  $\xi^2$  and susceptibility  $\chi$  series for the spin-infinity XY and PR models on the triangular lattice. Our conjectured "best" values plus uncertainties are shown on the vertical axis. The high-order terms in the  $\nu = 0.5$  3-fit sequence for the XY susceptibility are nearly indistinguishable from the terms in the correlation-length sequence.

unshifted XY series: 3.2632, 3.2637, 3.2679, 3.2729, 3.2780, 3.2831, and 3.2880. This is reasonably convincing evidence that the Kosterlitz-Thouless singularity more closely mimics the  $n$ -shifted susceptibility series than the unshifted series.

We have not determined "best" values for  $b$  and  $A$  because they do not seem central to the issues in question and because their determination would depend sensitively on the value chosen for  $\nu$ , whereas the determinations of  $2-\eta$  and  $T_c$  seem relatively insensitive to this choice.

We have also considered the series for the fluctuation of the transverse magnetization of the spin- $\frac{1}{2}$

XY model.<sup>13</sup> Rogiers performed the Padé analysis of Ref. 6 and found some evidence supporting  $\nu = 1.0$ .<sup>14</sup> The results from our application of our 3- and 4-fit methods to these series are disappointing. Allowing  $b$  to range from  $-3.0$  to  $+20$ , there are only three 4-fit solutions for  $n = 3$  with  $\nu = 0.650$  and  $b = 4.65$ , for  $n = 6$  with  $\nu = 0.503$  and  $B = -1.07$ , and for  $n = 7$  with  $\nu = 0.461$  and  $b = -1.23$ . Of the  $\nu = 0.5$  3-fit solutions, those with positive  $b$  from 0 to 20 are very irregular while those with negative  $b$  from  $-3$  to 0 are fairly regular with  $b \approx -1.0$ . Obviously negative  $b$  is not consistent with a divergent susceptibility or the Kosterlitz-

Thouless theory. The extremely bad fit observed for the  $s = \frac{1}{2}$  susceptibility may only mean that corrections are much more important in the quantum  $s = \frac{1}{2}$  model than in the classical models. On the other hand, it may mean that the  $s = \frac{1}{2}$  XY model belongs to a different universality class than the classical models.

### V. CONCLUSION

We have analyzed new, twelfth-order series for the susceptibility and correlation length of classical planar models on the triangular lattice using a 4-fit method of analysis tailored to the form of the singularity predicted by Kosterlitz and Thouless.<sup>4,5</sup> Test-function analysis shows that the 4-fit method used here is significantly more reliable in treating a number of typical corrections to the leading singularity than is the Padé analysis used in earlier series

work.<sup>6,7</sup> This 4-fit analysis of our new longer series predicts  $\nu = 0.5 \pm 0.1$  in good agreement with the Kosterlitz-Thouless prediction  $\nu = \frac{1}{2}$  and in striking disagreement with the preference for  $\nu = 0.7$  of Monte Carlo work<sup>8</sup> and some of the earlier series work.<sup>6</sup> Further, our  $n$ -fit analysis predicts that  $\eta = 0.27 \pm 0.03$  in agreement with the Kosterlitz-Thouless prediction  $\eta = \frac{1}{4}$  and the Monte Carlo work  $\eta = 0.243 - 0.254$ .<sup>8</sup>

The surprising goodness of fit for the classical models<sup>15</sup> lends additional credence to the form of the singularity predicted by Kosterlitz and Thouless.

### ACKNOWLEDGMENT

We are grateful for the support of the National Science Foundation—Experimental Program to Stimulate Competitive Research Grant No. PRM8011453-18.

<sup>1</sup>N. D. Mermin and H. Wagner, Phys. Rev. Lett. **17**, 1133 (1966); N. D. Mermin, Phys. Rev. **176**, 250 (1968); P. C. Hohenberg, *ibid.* **158**, 383 (1967).

<sup>2</sup>H. E. Stanley, Phys. Rev. Lett. **20**, 589 (1968).

<sup>3</sup>M. A. Moore, Phys. Rev. Lett. **23**, 861 (1969).

<sup>4</sup>J. M. Kosterlitz and D. J. Thouless, J. Phys. C **6**, 1181 (1973).

<sup>5</sup>J. M. Kosterlitz, J. Phys. C **7**, 1046 (1974).

<sup>6</sup>W. J. Camp and J. P. Van Dyke, J. Phys. C **8**, 336 (1975).

<sup>7</sup>A. J. Guttmann, J. Phys. A **11**, 545 (1978).

<sup>8</sup>Jan Tobochnik and G. V. Chester, Phys. Rev. B **20**, 3761 (1979).

<sup>9</sup>This program correctly reproduces the twelfth order susceptibility series for the nearest-neighbor  $s = \frac{1}{2}$  Ising model for the fcc lattice [M. F. Sykes, D. S. Gaunt, P. D. Roberts, and J. A. Wyles, J. Phys. A **5**, 640 (1972)] which shows that all "elementary" diagrams have been correctly included. Changes of lattice and coupling dimensionality  $n$  are performed in a routine fashion which is unchanged from the original program. For  $n = 2$ , the only checks of which we are aware are first, that the on-site correlation function for the plane-rotator model must be  $\frac{1}{2}$ , which it is within round-off errors (e.g., the twelfth-order contribution to the on-site correlation function is  $-0.00075K^{12}$  to be compared

with the nearest-neighbor site contribution  $-6477.85132K^{12}$ ) and second, that the eleventh term in the nearest-neighbor site correlation function correctly reproduces the twelfth term in the free energy of the plane-rotator model on the fcc lattice to within round-off [P. S. English, D. L. Hunter, and C. Domb, J. Phys. A **12**, 2111 (1979)].

<sup>10</sup>D. Saul, Michael Wortis, and D. Jasnow, Phys. Rev. B **11**, 2571 (1975).

<sup>11</sup>M. Ferer and M. J. Velgakis (unpublished).

<sup>12</sup>D. L. Hunter and G. A. Baker Jr., Phys. Rev. B **7**, 3346 (1977).

<sup>13</sup>The spin- $\frac{1}{2}$  series are derived in J. Rogiers, T. Lookman, D. D. Betts, and C. J. Elliot, Can. J. Phys. **56**, 409 (1978).

<sup>14</sup>J. Rogiers (unpublished).

<sup>15</sup>Various authors, e.g., W. J. Camp, in *Phase Transitions Cargese 1980*, edited by M. Levy, J. C. LeGuillou, and J. Zinn-Justin (Plenum, New York, 1982), p. 153; D. S. Gaunt, *ibid.*, p. 217, have stated that, usually, unbiased  $n$  fits (our 4 fits) do not provide sensible fits and that biased  $n$  fits (our 3 fits) need to be used to determine sensible fits. That is not the case for the classical models; our unbiased 4 fits do provide sensible fits indicative of a surprising goodness of fit.