Critical Indices and Amplitudes of Classical Planar Models in Finite Field for Temperatures Greater than T_c

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Using renormalization techniques on the Englert linked-cluster expansion we have derived high-temperature series for the spin-spin correlation function of the three-dimensional, plane-rotator, and spin-infinity XY models with nearest-neighbor interactions. Analysis of our zero-field series, which are two terms longer than earlier series for these models, gives results in basic agreement with earlier work. Our finite-field series, to eighth order in the interaction and second order in the field, allow a determination of the gap index Δ ; we assert $2\Delta = 3.33 + 0.02$. The indices are compared with scaling predictions and experimental results. Accessible critical amplitudes are determined. These are used to test predictions of two-scale-factor universality; good agreement is observed.

I. INTRODUCTION

The determination of the critical behavior of model systems via series expansions has proven useful in predicting experimental results and in testing scaling theory and the universality hypothe- \sinh^{-3} In this paper, we present series result for several nearest-neighbor planar models, specifically the spin-infinity XY and the plane-rotator models for the fcc, bcc, and sc lattices. These models consist of spins \overline{S} ; at all sites \overline{r} of the lattice interacting with their nearest neighbors and an external field H through a Hamiltonian of the form

$$
-\beta \mathcal{K} = K \sum_{\langle \vec{x}, \vec{r}^{\,\prime} \rangle} (S^x_{\vec{r}} S^x_{\vec{r}} + S^y_{\vec{r}} S^y_{\vec{r}}) / s^2 + h \sum_{\vec{r}} S^x_{\vec{r}} / s ,
$$
\n(1.1)

where $K = \beta J$, J being the interaction strength, where $K \equiv \beta J$, J being the interaction strength,
 $h \equiv \beta g \mu_B H$, s is the spin quantum number, and the second sum is over all lattice sites and the first is over all nearest-neighbor pairs. For the spininfinity XY model \bar{S}_z/s is a three-dimensional classical rotor of unit length, while, for the planerotator model, \overline{S}_7 /s is again a classical rotor of unit length but now it is constrained to two dimensions, having no z component.

Via computer codes, which have also generated high-temperature series for the Ising and Heisenberg models, 4,5 which agree with presently extant series, we have generated high-temperature series for the correlation function

$$
\Gamma(\vec{\mathbf{r}}, \epsilon, h) = \frac{\langle S_0^z S_1^z \rangle}{s^2} - \frac{\langle S^x \rangle^2}{s^2}
$$

$$
= \sum_{i,j=0}^{\infty} Q(\vec{\mathbf{r}}, i, j) K^i h^{2j} . \qquad (1.2)
$$

All coefficients $Q(\vec{r}, i, 0)$ have been determined for $i \leq 10$ for the fcc lattice and for $i \leq 11$ for the bcc and sc lattices; all coefficients $Q(\mathbf{\vec{r}},\ i,\ 1)$ have been determined for $i \leq 8$. ⁶ From these series, Eq. (1.2), we are able to construct the series for the various correlation-function moments

$$
\mu_{n,2m} = \sum_{i=0}^{\infty} \left[\sum_{\vec{r}} |\vec{r}|^n Q(\vec{r}, i, m) \right] K^i , \qquad (1.3)
$$

where distances $|\mathbf{\ddot{r}}|$ are measured in units of the nearest-neighbor distance. These moments are expected to have a leading singularity of the form²

$$
\mu_{n,2m} \simeq U_{n,2m} \epsilon^{-\gamma - m - 2m\Delta}, \quad \epsilon \equiv 1 - K/K_c. \tag{1.4}
$$

The analysis of these series and of the energydensity series determined from the nearest-neighbor correlation function

$$
E = -J\sum_{\vec{\delta}}\Gamma(\vec{\delta}, \epsilon, h) \simeq -JU_c + \left(\frac{JA}{K_c k_B (1-\alpha)}\right)\epsilon^{-\alpha},
$$
\n(1.5)

where A is the specific-heat amplitude, allows the determination of the critical indices γ , ν , η , 2Δ , and α and of the critical amplitudes U_c , A , and the $U_{n,m}$, 1,2 We present the series for the energy density and several correlation-function moments in Table I. We discuss analysis determining values of T_c , γ , ν , and η from our zero-field series which are two terms longer than previous series.^{7,8} These values presented in Table II are in good agreement with results from shorter series. We present and discuss analysis for determining values of α and 2Δ . This is the first reporting of a value of 2Δ for these classical systems.

lt is consistent with the universality hypothesis

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 $\overline{8}$

		Plane-rotator models	
	fcc	bcc	sc
$\mu_{0,0}$	0.5	0.5	0.5
	3.0K	2.0K	1.5K
	$16.5K^2$	$7.0K^2$	$3.75K^2$
	$87.375K^3$	$24.25K^3$	$9.1875K^3$
	453.0K ⁴	81.0K ⁴	21.75K ⁴
	2317.09375K ⁵	$269.2291666666K^5$	$51.171875K^5$
	11742.6796875K ⁶	881.58854166666K6	118.52734375K6
	59 110, 856 445312 K^7	2878.516 276 0416K7	$273.47314453125K$ ⁷
	296 031.611 65364K8	9323.8951822916K ⁸	626.00244140624K8
	1476 556.3897949K ⁹	30142.589941405K ⁹	1429.4087646482K ⁹
	7340722.3167912K ¹⁰	96 965.248 920 352K ¹⁰	3248.0757039377K10
		311 485.772 423 55K11	7367.6873206967K11
$\mu_{0,2}$	-0.1875	-0.1875	-0.1875
	$-4.5K$	$-3.0K$	$-2.25K$
	$-63.84375K^2$	$-27.5625K^2$	$-15.046875K^2$
	$-700.875K^3$	$-196.5K^3$	$-77.0625K^3$
	$-6585.83203125K4$	$-1196.6796875K4$	$-335.326171875K4$
	$-55703.34375K^5$	$-6561.3125K^5$	$-1309.8515625K^5$
	$-436585.10083007K^6$	$-33319.651855469K^6$	$-4730.1529541015K^6$
	$-3229669.8232421K^7$	$-159703.63671875K^{7}$	$-16100.564941406K^{7}$
	$-22831488.242724K^8$	$-731363.48489582K^8$	$-52310.525903319K^8$
		$-3228774.9643065K^0$	
$\mu_{2,0}$	3.0K	2.0K	1.5K
	$36.0K^2$	$16.0K^2$	$9.0K^2$
	$306.375K^3$	$88.25K^3$	$36.1875K^3$
	2243.25K ⁴	420.0K ⁴	123.75K ⁴
	$15068.96875K^5$	1829.2291666667K ⁵	$385.296875K^5$
	$95688.15625K^6$	7532.9791666667K ⁶	$1130.671875K^6$
	583 946, 856 445 $31K^7$	$29792.016276042K^{7}$	$3180.3325195312K^{7}$
	3459 600.292 3177K ⁸	114 389.177 083 33K ⁸	8671.888 671 8750K ⁸
	$20031441.019026K^9$	$429115.89202473K^9$	23 079.210 522 461K ⁹
	113878974.70668K ¹⁰	1580 539.358 8758K ¹⁰	60 257.659 651 689K ¹⁰
		5734 156, 830 1925 K^{11}	154 873.212 516 00K ¹¹

TABLE I. (Continued)

TABLE II. Values of the indices for several planar systems.

System	Ref.	γ	ν	η	$\pmb{\alpha}$	2Δ
spin- ∞XY	$\mathbf 7$	1.312 ± 0.006			$0 \leq \alpha \leq \frac{1}{22}$	
spin- ∞XY and plane rotator	8	1.32 ± 0.01	0.670 ± 0.007		0.0 ± 0.1	
	this work	1.318 ± 0.010	0.670 ± 0.006	0.04 ± 0.01	-0.02 ± 0.03	3.33 ± 0.02
spin- $1/2 XY$	10	1.35 ± 0.02				
	11					3.3 ± 0.1
Superfluid transition	13		0.674 ± 0.001			
	14				-0.01 ± 0.01	
	15				$-0.06 \le \alpha \le 0.0$	
Renormalization group $n=2$	16	1.30		0.039		
Lieb model	12	1.31 ± 0.03			0.00 ± 0.05	

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XY model	$T_c = K_c^{-1}$	γ	ν	$nv = 2v - \gamma$
fcc	3.3417 ± 0.0007	1.318 ± 0.010	0.669 ± 0.005	0.025 ± 0.005
bcc	2.175 ± 0.003	1.32 ± 0.03	0.668 ± 0.010	0.027 ± 0.008
sc.	1.552 ± 0.003	1.32 ± 0.04	0.668 ± 0.010	0.025 ± 0.012
Plane-rotator model				
fcc	4.820 ± 0.003	1.323 ± 0.015	0.670 ± 0.007	0.028 ± 0.005
bec	3.121 ± 0.005	1.32 ± 0.03	0.673 ± 0.010	0.027 ± 0.010
8C.	2.203 ± 0.006	1.32 ± 0.05	0.675 ± 0.015	0.03 ± 0.02

TABLE III. Values of K_c^{-1} and several indices for the planar models considered here.

to expect that all planar systems, those with a two-dimensional order parameter, mill have the same critical properties. This includes the planar models discussed here and elsewhere and the superfluid transition in liquid helium. 9 Comparing our results with those from other planar systems, we find negligible differences consistent with universality. $\sqrt{7}$, 8, 10–16 We also find good agreement with the predictions of scaling theory for the indices.²

Va1ues for the common correlation-function amplitudes, consistent with our values for the indices and the critical temperature, are presented and discussed within the framework of two-scalefactor universality. $17-21$ These investigations are especially interesting since most previous tests involved lattice dependence only.

II. CRITICAL INDICES

A. Determination of K_t^1 , γ , ν , and $\nu\nu$

Using straight ratio and log-derivative ratio methods, we determined sequences for T_c from the moment series $\mu_{n,0}$, $-1 \le n \le 2$. We then used a Neville table to extrapolate these sequences. We feel the index-independent tests, especially the log-derivative tests, are the most reliable in finding the value of K_c^{-1} , in that they do not contain the obvious built-in bias of the index-dependent ing the value of K_c^* , in that they do not contain the
obvious built-in bias of the index-dependent
tests.^{4,5,24} Our analysis indicates the values show: in Table III. These values are identical, to well within the quoted uncertainty, with the results of index-dependent tests using previously determined values of γ and ν .

The values we find for γ , ν , and $\eta \nu = 2\nu - \gamma$, shown in Table III, are consistent with earlier results^{7,8}, but because our series are longer, we feel our results are more reliable. Straight ratio and log-derivative ratio methods enabled us to form sequences for γ , ν , and $\eta\nu$ from moment series and various products of moment series using the above values for K_c^{-1} . Neville table extrapolations of these sequences indicate the values presented in Table III; the quoted uncertainties reflect

both our uncertainty in reading the Neville table and the uncertainty in K_c^{-1} . We also formed ratio series which allowed a K_c -independent determina tion of ν and $\eta \nu$: The values indicated by this analysis are consistent with the values from the K_{c} dependent analysis. The values of each of the indices γ , ν , and $\eta\nu$ for all these planar systems are identical to within the uncertainties suggesting the universal values presented in Table II.

B. Determination of α

Using the energy-density series in Table I, we formed specific-heat series

$$
C = \frac{\partial E}{\partial T} = \sum_{n=2}^{\infty} a_n K^n \simeq A \epsilon^{-\alpha} + a \,. \tag{2.1}
$$

From these and the values of K_c^{-1} , we formed the standard ratio sequence for the index, in this case α , ²²

$$
l_n^0 = nK_c a_n / a_{n-1} - n + 1.
$$
 (2.2)

Knowing only the first few terms in this sequence, we attempted the extrapolate to its limit using the Neville table, the two-dimensional array²³

$$
l_n^i = [nl_n^{i-1} - (n-1) l_{n-1}^{i-1}]/i . \qquad (2.3)
$$

In this array, the l_n^1 are the linear extrapolants of l_n^0 , the l_π^2 the quadratic extrapolants, and so forth. The Neville table for the series (2. 1) is presented in Table IV. Although these extrapolations are not particularly smooth or well behaved, they are better behaved than specific-heat extrapolations for particularly smooth or well behaved, they are be
ter behaved than specific-heat extrapolations for
other models.^{5,10} Also presented in Table IV are those values for α which feel are indicated by these extrapolations. The uncertainties quoted reflect our estimated uncertainty in reading these tables; the effect of the uncertainty in K_c is negligible due to the irregularity of these tables. Other methods of analysis give consistent results. It should be noted that these tables favor a slightly negative value for α and that the values of the index for all these planar systems are identical to within the uncertainties suggesting the universal value $\alpha = -0.02 \pm 0.03$.

XY model				Plane-rotator model				
	fee, $\alpha = -0.02 \pm 0.03$				fcc, $\alpha = -0.02 \pm 0.04$			
n/i	Ω		$\overline{2}$	$\mathbf 0$		2		
5	0.6641			0.5089				
6	0.5167	-0.0727		0.3647	-0.2121			
7	0.4351	0.0269	0.2262	0.2949	-0.0545	0.2607		
8	0.3683	-0.0322	-0.1800	0.2638	0.0776	0.4079		
9	0.3200	-0.0185	0.0227	0.2392	0.0670	0.0353		
10	0,2831	-0.0116	0.0124	0.2150	0.0209	-0.1407		
11	0.2534	-0.0142	-0.0248	0.1925	-0.0092	-0.1294		
		bcc. $\alpha = -0.02 \pm 0.04$	bcc. $\alpha = -0.04 \pm 0.07$					
n/i	$\bf{0}$		$\overline{2}$	$\bf{0}$		$\mathbf 2$		
6	0.5511			0.3862				
8	0.3683	-0.1803		0.2616	-0.1124			
10	0.2779	-0.0836	0.0615	0.2125	0.0165	0.2097		
12	0.2232	-0.0505	0.0157	0.1724	-0.0281	-0.1172		
		sc. $\alpha = 0.0 \pm 0.3$	sc, $\alpha = 0.0 \pm 0.2$					
n/i	$\bf{0}$	1	$\mathbf{2}$	$\bf{0}$	ı	$\mathbf{2}$		
6	0.4924			0.5870				
8	0.3141	-0.2207		0.1351	$-1,2206$			
10	0.2014	-0.2495	-0.2927	0.1836	0.3777	2.7752		
12	0.1660	-0.0109	0.4663	0.1635	0.0630	-0.5665		

TABLE IV. Neville table extrapolations of specific-heat series for the index α .

TABLE V. Neville table extrapolations of μ_{02}/μ_{00} for the index 2 Δ .

	XY model					Plane-rotator model		
	fcc. $2\Delta = 3.33 \pm 0.01$					fcc, $2\Delta = 3.34 \pm 0.02$		
n/i	$\bf{0}$	1	$\mathbf{2}$	3	$\bf{0}$	1	$\boldsymbol{2}$	3
3	3.433				3.529			
4	3.408	3.305			3.488	3.324		
5	3,391	3.308	3.314		3.461	3.326	3.329	
6	3.380	3.312	3.320	3.328	3.442	3.330	3.340	3.353
7	3.372	3.315	3.324	3.331	3.429	3.334	3.347	3.360
8	3.366	3.317	3.325	3.327	3.419	3.337	3.346	3.344
		bcc, $2\Delta = 3.33 \pm 0.03$				bcc. $2\Delta = 3.34 \pm 0.04$		
n/i	0	1	2		0	1	$\mathbf 2$	
$\mathbf{1}$	3.678				3.845			
3	3.457	3.237			3.558	3.271		
5	3,403	3.295	3.324		3,473	3.302	3.317	
7	3.380	3.310	3.325		3.435	3.323	3.344	
9					3,415	3.332	3.347	
$\bf 2$	3.431				3.539			
$\overline{\mathbf{4}}$	3.396	3.343			3.473	3.373		
6	3.376	3.327	3.314		3.436	3.343	3.320	
8	3.365	3.327	3.328		3.415	3,344	3.347	
		sc. $2\Delta = 3.33 \pm 0.03$			sc. $2\Delta = 3.33 \pm 0.04$			
n/r	0	1	$\boldsymbol{2}$		$\bf{0}$	$\mathbf{1}$	$\boldsymbol{2}$	
$\mathbf{1}$	3.865				4.086			
3	3.492	3.119			3.593	3.101		
5	3.431	3.310	3,406		3.504	3.326	3.438	
7	3.403	3.318	3,326		3.460	3.326	3.325	
$\boldsymbol{2}$	3.491				3.616			
$\overline{\mathbf{4}}$	3.424	3.325			3.504	3.335		
6	3.401	3.342	3.356		3.463	3.363	3.383	
8	3.386	3.335	3.326		3.438	3.350	3,335	

C. Determination of 2Δ

Using the series

$$
\frac{\mu_{n,2}}{\mu_{n,0}} = \sum_{j=0}^{\infty} C_{j,n} K^j \simeq \frac{U_{n,2}}{U_{n,0}} \epsilon^{-2\Delta},
$$
\n(2.4)

we employed standard ratio methods to determine the index 2Δ . Presented in Table V are the Neville table extrapolations, Eq. (2.3) , of sequence (2.2) using the series $\mu_{0,2}/\mu_{0,0}$ as well as the values for 2Δ which we feel are indicated by the analysis. The uncertainties quoted here reflect not only our uncertainty in reading these extrapolations but also the effect of the uncertainty in K_c on these extrapolations. Other analyses, the results of which are consistent with those presented here, include logderivative tests and K_c -independent ratio-series tests. Consistently with our analysis, we suggest the universal value $2\Delta = 3.33 \pm 0.02$ for all these planar systems.

D. Scaling, Universality, and the Superfluid Transition

How do the values we have determined for the indices agree with scaling predictions, and what predictions does scaling enable us to make about undetermined indices? According to scaling the following quantities should be zero²; using our values of the indices, as presented in Table II, we find

$$
2 - \alpha - 3\nu = 0.01 \pm 0.05,
$$

\n
$$
3\nu + \gamma - 2\Delta = 0.01 \pm 0.05,
$$
 (2.5)

so that scaling predictions are obeyed to within sizable uncertainties, which are large enough to mask violations greater than the apparent violations observed for the Ising model. $4, 24, 25$ Because the indices obey scaling to well within the uncertainties in the indices, we can use scaling relations to predict values for undetermined indices such as β and δ :

$$
\beta = \Delta - \gamma = 0.347 \pm 0.020, \qquad \delta = \frac{\Delta}{\Delta - \gamma} = 4.8 \pm 0.3 ;
$$
\n
$$
\beta = \frac{1}{2}(3\nu - \gamma) = 0.346 \pm 0.014, \quad \delta = \frac{6\nu}{3\nu - \gamma} = 4.8 \pm 0.3 ;
$$
\n(2.6)

having confidence that the true values will agree with these to within the uncertainties.

It is the contention of the universality hypothesis that all systems with the same symmetry, in this case all planar systems, should have the same set of indices.³ The values presented in Tables II-V support this contention to within the uncertainties with which the indices have been determined.

The attractive fractional values $\gamma = \frac{4}{3}$, $\nu = \frac{2}{3}$, α = 0, and η = 0 have been suggested as the universal values for these planar systems. $8,17$ These fractional values are not excluded by the data, but the series analysis prefers the somewhat different values shown in Table II. Even recent experimental results for the superfluid transition in liquid helium opt for a higher value of ν and a slightly negative value of α . ¹³⁻¹⁵

III. UNIVERSALITY OF THE CRITICAL AMPLITUDES

In investigations of critical phenomena, most attention has been paid to the indices. In part, this is due to the relatively clear universality of the indices. In the past few years, it has become increasingly evident that the amplitudes should also be universal, in a somewhat restricted sense.^{17,26} The most explicit formulation of the universality of the critical amplitudes is two-scale-factor universality. 18,21 It asserts that, near the critical point of any system, the free energy per site $F(\epsilon, h)$ and the correlation function can be written in scaling form² as follows:

$$
F(\epsilon, h) = (g\epsilon)^{dv} f(hh/(g\epsilon)^{\Delta})/n,
$$

\n
$$
\Gamma(\vec{r}, \epsilon, h) = \frac{D((g\epsilon)^{v}r/l, nh/(g\epsilon)^{\Delta})}{(r/l)^{d-2+\eta}},
$$
\n(3.1)

where $\rho^{s}l^{d}/n$ is universal.²⁷ In these expression the indices as well as the functions f and D are universal, i.e., the same for all systems with the same symmetry, while n , l , and g are systemdependent (nonuniversal) scale factors, and ρ^s is the particle density (in the case of lattice systems the site density). Equations (3. 1) make an explicit separation between the universal and nonuniversal parts of these functions; they also allow us to make explicit predictions regarding the critical amplitudes. Specifically, within a given symmetry class-in our case the set of all planar systemsthey allow us to write the amplitudes for any member of the class in terms of the amplitudes of some reference system in the class, the scale factors for the member in question, and ρ^s and ρ^s , the particle density for the member and the reference system, respectively. Several examples follow¹⁸: for the susceptibility

$$
\mu_{0,0} \simeq U_{0,0} \epsilon^{-\gamma},
$$

\n
$$
\mu_{0,0} = n g^{-\gamma} (U_{0,0})_r ;
$$
\n(3.2a)

for the correlation length

$$
\xi = \kappa^{-1} \approx 1/\kappa_0 \epsilon^{\nu},
$$

\n
$$
\kappa_0 = (\kappa_0)_r g^{\nu}/l;
$$
\n(3.2b)

for the specific heat

$$
C \simeq A \epsilon^{-\alpha} + a,
$$

\n
$$
A = (g)^{d\nu} (A)_r / n;
$$
\n(3.2c)

for the $d = 3$, $h = 0$ correlation function in the Orn-

stein-Zernike limit $\Gamma(r, \epsilon, 0) = \alpha_K e^{-\kappa r}/r$

$$
\mathbf{a} = l^{1+\eta}(\mathbf{a})_{r} ; \qquad (3.2d)
$$

for the $d=3$, $\epsilon=0$, $h=0$ correlation function $\Gamma(r, 0)$, 0) = $D_c / r^{d-2+\eta}$

$$
D_c = l^{1+\eta}(D_c)_r \tag{3.2e}
$$

Our values for the amplitude D_c were determined using the "lattice Green's-function" result of Ref. 28, $D_c = \Gamma(\overline{\delta}, 0, 0) (1 - \epsilon')$, where $\overline{\delta}$ is the nearest neighbor displacement and ϵ' is 0.020, 0.065, and 0. 075 for the fcc, bcc, and sc lattices, respectively. Values for $\Gamma(\overline{\delta}, 0, 0)$ and the other amplitudes for our planar systems were determined using standard ratio analysis for the critical amplitudes as discussed at length in Ref. 18. The results of this analysis is shown in Table VI. The uncertainties quoted here reflect only our uncertainty in reading the appropriate Neville table extrapolations and do not reflect our uncertainty in the indices and in K_c . We quote these uncertainties because we believe it is most important to know the amplitudes associated with a given set of indices and a

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given K_c . However, it is also important to have some idea how the amplitudes vary with values of K_c^{-1} and the index within the range of our uncertainty. We find, for these series, that an increase of 0.01 in the index effects a decrease of roughly 3% in the amplitude and that an increase of 0.1% in K_c^{-1} effects a decrease of roughly 2% in the amplitude. These estimates are only approximate because of the unsatisfactory behavior of the Neville table extrapolations for these extreme values of the parameters.

Using the amplitudes shown in Table VI, we test predictions of two-scale-factor universality, Eqs. (3. 1) and (3. 2). First, we evaluate $100\alpha \rho^s A/\kappa_0^3$, which is postulated to be universal. $18-20$ The values, presented in Table VII, are universal to within our uncertainty in the amplitudes. Second, we have used Egs. (3. 2) to make three independent determinations of the scale factors l and g . As shown in Table VII, these independent determinations give the same value for each scale factor to within the inherent uncertainty. This is the first determination of the scale factor relating systems which differ in more than their lattice structure.

presented in Table II were determined by evaluating the second-order ϵ expansion for $n = 2$ and $\epsilon = 1$. Because these series in ϵ are asymptotic rather than convergent, there is some question as to how seriously the actual numerical values should be taken.

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