Susceptibility scaling functions for ferromagnetic Ising films

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The susceptibility of simple-cubic-lattice ferromagnetic Ising films of n two-dimensional lattice layers is studied by extrapolation of high-temperature series expansions (to eleventh and twelfth orders) for $n = 3,4,\ldots,14$ layers with periodic boundary conditions, and $n = 3,4,\ldots,10$ layers with free-surface conditions. The corresponding surface susceptibility series for sc, bcc, and fcc lattices are analyzed in the light of universality hypotheses. On the basis of finite-size scaling theory explicit scaling functions are constructed describing the crossover from two-dimensional to three-dimensional critical behavior in terms of the ratio $n/\xi(T)$, where $\xi \sim \Delta T^{-\nu}$ is the bulk correlation length.

I. INTRODUCTION

The effect of the dimensionality d on the critical behavior of a system is well established[1-3]: for a given Hamiltonian, the critical exponents depend strongly on d (for $d \leq 4$). The characteristic dimensionality of a system as it approaches a critical point is determined by the number of spatial dimensions in which the system has *infinite* extent. Accordingly, both purely two-dimensional or planar ($\infty \times \infty$) systems and films of finite thickness L ($\infty \times \infty \times L$) must exhibit the same critical exponent values typical of $d = 2$. In the present work, which represents part of a general study[4-14] of the effects of finite size on critical-point behavior,[15-23] the susceptibilities of ferromagnetic films are studied theoretically on the basis of exact high-temperature series expansions.

We consider films formed of magnetic spins localized on the sites of a cubic (sc, bcc, or fcc) lattice with nearest-neighbor distance a and cubic cell edge a'. The films are infinite in two dimensions and of finite thickness $L = na'$ in the third, orthogonal dimension (taken parallel to a cubic lattice axis). Two types of boundary conditions are studied (i) *periodic* (denoted by $\tau = 0$) where the first and nth layers are regarded as adjacent neighboring layers; and (ii) *free-surface conditions* (denoted by $\tau = 1$) where the lattice is simply truncated so that there are no spins in the zeroth and $(n+1)$th layers. The magnetic spins are taken to have spin value $S = \frac{1}{2}$ and to interact through the standard, nearest-neighbor ferromagnetic Ising-model Hamiltonian

$$\mathcal{H} = -J \sum_{(ij)} s_i s_j - mH \sum_i s_i \,, \qquad (1.1)$$

where $s_i = \pm 1$ is the spin at the ith lattice site, (i,j) denotes nearest-neighbor pairs, $J > 0$ is the exchange parameter, m is the magnetic moment per spin, and H is the external magnetic field.

In earlier work by Allan,[7] series expansions for the zero-field reduced susceptibility, $\chi_T(n, T)$, of an n-layer film were derived to ninth order for $n = 2$, 3, 4, and 5 (and analyzed to estimate critical temperatures). Later (see Ref. 8) Allan extended these series to eleventh order for up to $n = 7$ layers. By using the results of Sykes, Gaunt, Roberts, and Wyles[24] for the bulk sc lattice, further series for thicker layers have now been obtained. These sc series are reported in Table I for periodic conditions [to eleventh order for $n = 3$, twelfth order for $n = 4$ to 9, and $(n+3)$rd order up to $n = 14$] and in Table II for free-surface conditions (to eleventh order up to $n = 10$). These susceptibility series are extrapolated to study the crossover from the two-dimensional behavior of $\chi_T(n; T)$, which diverges as $[T - T_c(n)]^{-\dot{\gamma}}$, with[25] $\dot{\gamma} = 1\frac{3}{4}$ as T approaches the critical temperature $T_c(n)$ in a "thin" film, to three-dimensional behavior, namely, $\chi_T \sim [T - T_c(\infty)]^{-\gamma}$, with $\gamma = 1\frac{1}{4}$, in a "thick" ($n \to \infty$) film. In particular, the shift in critical temperature $\epsilon(n) \propto [T_c(n) - T_c(\infty)]$ is found to vary as $n^{-1/\nu}$ for large n, where $\nu \simeq \frac{9}{14}$ is the correlation length exponent. Our estimates of $T_c(n)$ are corroborated fairly well in recent Monte Carlo work by Binder and co-workers.[21,22]

The surface susceptibilities $\chi_T^{\times}(T)$ for the sc lattice (obtained by Allan) and for the bcc and fcc lattices (calculated by Watson[15,16]) are analyzed in the light of the universality hypothesis which relates the amplitude of divergence of $\chi_T^{\times}(T)$ on a particular lattice to the corresponding amplitudes for the bulk susceptibility $\chi_T(T)$ and the bulk correlation length $\xi(T)$.

Finally in the light of finite-size scaling theory,[8,9,12,15,17] which relates the asymptotic crossover behavior to the scaled thickness variable $y = L/\xi(T)$, the extrapolated series for films of different thickness are examined as a family. This leads to numerical determination of the universal scaling functions (differing for free-surface

TABLE I. Susceptibility expansion coefficients $a_l(n)$ for periodic ($\tau=0$), simple cubic, n-layer Ising films. Note: $a_0=1$ and blank entries in a row represent the same figure as in the nearest column.

l	$n=2$	$n=3$	$n=4$	$n=5$	$n=6$	$n=7$	$n=8$
1	6	6					
2	28	30	30				
3	130	148	150	150			
4	564	706	724	726	726		
5	2438	3322	3490	3508	3510	3510	
6	10 132	15 364	16 490	16 690	16 708	16 710	16 710
7	41 794	70 222	77 826	79 234	79 474	79 492	79 494
8	169 652	317 574	362 356	373 106	374 866	375 154	375 172
9	682 870	1 424 652	1 684 966	1 751 810	1 767 138	1 769 322	1 769 666
10	···	6 348 234	7 758 846	8 182 156	8 281 978	8 303 754	8 306 434
11	···	28 129 922	35 693 078	38 100 350	38 793 234	38 940 962	38 971 538
12	···	···	163 033 352	176 751 774	180 872 492	182 004 234	182 219 074

l	$n=9$	$n=10$	$n=11$	$n=12$	$n=13$	$n=14$	$n=\infty$
7	79 494						
8	375 174	375 174					
9	1 769 684	1 769 686	1 769 686				
10	8 306 842	8 306 860	8 306 862	8 306 862			
11	38 974 786	38 975 266	38 975 284	38 975 286	38 975 286		
12	182 261 354	182 265 242	182 265 802	182 265 820	182 265 822	182 265 822	
13	···	852 058 290	852 062 890	852 063 538	852 063 556	852 063 558	852 063 558
14	···	···	3 973 778 738	3 973 784 122	3 973 784 866	3 973 784 884	3 973 784 886
15	···	···	···	18 527 525 202	18 527 531 442	18 527 532 290	18 527 532 310
16	···	···	···	···	86 228 659 746	86 228 666 914	86 228 667 894
17	···	···	···	···	···	401 225 381 954	401 225 391 222

and periodic conditions) which describe the crossover quantitatively.[8,9] Simple analytic approximants are constructed for the scaling functions; these should be useful in the interpretation of data on real ferromagnetic films of sufficient uniformity and controlled thickness.

The layout of the remainder of this paper is as follows. The scaling theory for films is recapitulated briefly in Sec. II, and the new consequences of the universality hypothesis are exhibited. In Sec. III the series expansions are presented. The analysis of the series for $\chi_T(n;T)$ is described in Sec. IV while the surface susceptibilities are analyzed in Sec. V, and used to test the universality hypothesis. Finally, in Sec. VI the construction of the scaling functions is undertaken.

II. SCALING THEORY FOR FILMS

To summarize finite-size scaling theory[8,9,12,17] as applicable to films we introduce the thickness in the form

$$L=na', \tag{2.1}$$

where a' is the distance between corresponding neighboring layers, and refer to n as the "number of layers." It is convenient also to introduce the nearest-neighbor distance a; for a simple cubic lattice one has $a'=a$ but for the bcc and fcc the relation is $a'/a=2/\sqrt{3}$ and $\sqrt{2}$, respectively.

If $T_c(n)$ denotes the critical temperature of the finite-thickness, n-layer film, so that $T_c(\infty)$ is the bulk (three-dimensional) critical temperature, the reduced critical point shift is defined[5,8] by

$$\epsilon(n)=[T_c(n)-T_c(\infty)]/T_c(\infty). \tag{2.2}$$

The critical-point shift exponent λ is then introduced via

$$\epsilon(n)\approx b/n^{\lambda} \quad \text{as } n\to\infty. \tag{2.3}$$

Of course, for finite n a correction factor of the form $[1+b_1/n+\cdots]$ must be anticipated and, indeed, nonintegral inverse powers of n could, in principle, also appear in this factor. The reduced temperature deviation from the bulk critical temperature is measured by

$$t=[T-T_c(\infty)]/T_c(\infty), \tag{2.4}$$

and the bulk correlation length may then be written in the asymptotic form[26]

$$\xi(T)\approx fat^{-\nu} \quad \text{as } t\to 0+. \tag{2.5}$$

If the order of magnitude of the shift in critical temperature can be determined by the criterion[8] $\xi(T_c(n))\approx L$, one obtains the prediction

$$\lambda=1/\nu, \tag{2.6}$$

which is expected to apply at least for free bound-

TABLE II. Susceptibility expansion coefficients $a_l(n)$ for free-surface ($\tau=1$), simple cubic, n-layer Ising films. Note $a_0=1$, all n.

l	$n=2$	$n=3$	$n=4$	$n=5$	$n=6$
1	5	5$\frac{1}{3}$	5$\frac{1}{2}$	5$\frac{3}{5}$	5$\frac{2}{3}$
2	20	23$\frac{1}{3}$	25	26	26$\frac{2}{3}$
3	80	102$\frac{2}{3}$	114$\frac{1}{2}$	121$\frac{3}{5}$	126$\frac{1}{3}$
4	304	433$\frac{1}{3}$	506	550	579$\frac{1}{3}$
5	1152	1822$\frac{2}{3}$	2234	2488$\frac{4}{5}$	2659
6	4236	7478$\frac{2}{3}$	9660	11 060	12 001$\frac{1}{3}$
7	15 528	30 569$\frac{1}{3}$	41 648	49 077$\frac{3}{5}$	54 137$\frac{1}{3}$
8	55 924	123 224	177 290	215 424$\frac{4}{5}$	241 896
9	200 808	494 888	752 728	943 786$\frac{2}{5}$	1 079 657$\frac{1}{3}$
10	712 868	1 968 724	3 168 544	410 368$\frac{2}{5}$	4 787 396
11	2 523 560	7 819 188	13 317 507	18 811 367$\frac{1}{5}$	21 200 632
12	8 865 304				

l	$n=7$	$n=8$	$n=9$	$n=10$
1	5$\frac{5}{7}$	5$\frac{3}{4}$	5$\frac{7}{9}$	5$\frac{4}{5}$
2	27$\frac{1}{7}$	27$\frac{1}{2}$	27$\frac{7}{9}$	28
3	129$\frac{5}{7}$	132$\frac{1}{4}$	134$\frac{2}{9}$	135$\frac{4}{5}$
4	600$\frac{2}{7}$	616	628$\frac{2}{9}$	638
5	2780$\frac{4}{7}$	2871$\frac{3}{4}$	2942$\frac{6}{9}$	299$\frac{2}{5}$
6	12 674	13 156	13 550$\frac{8}{9}$	13 866$\frac{4}{5}$
7	57 759$\frac{3}{7}$	60 476$\frac{1}{4}$	62 589$\frac{3}{9}$	64 279$\frac{4}{5}$
8	260 926$\frac{2}{7}$	275 207	286 314$\frac{4}{9}$	295 200$\frac{2}{5}$
9	1 178 064$\frac{4}{7}$	1 252 008	1 309 527$\frac{5}{9}$	1 355 543$\frac{2}{5}$
10	5 288 015$\frac{3}{7}$	5 665 177$\frac{1}{2}$	5 958 698$\frac{2}{9}$	6 193 514$\frac{2}{5}$
11	23 717 504$\frac{4}{7}$	25 621 904$\frac{1}{4}$	27 105 613$\frac{3}{9}$	28 292 580$\frac{4}{5}$

ary conditions ($\tau=1$). However, exact analysis of Ising and spherical models[4-6,9-11] shows that the value of λ may be different for periodic boundary conditions ($\tau=0$).

To allow for this later possibility we introduce the reduced temperature deviation $\dot{t}$ for the n-layer film by

$$\dot{t}=[T-T_c(n)]/T_c(\infty). \tag{2.7}$$

The bulk ($n\to\infty$) correlation length can then be rewritten

$$\xi(T)\approx fa\dot{t}^{-\nu}. \tag{2.8}$$

The scaling hypothesis[8,9] now asserts that the basic physical variable controlling the behavior for small $\dot{t}$ and large n is the scaled thickness

$$y=L/\xi\approx cn\dot{t}^{\nu}, \quad \text{with } c=a'/fa. \tag{2.9}$$

The crossover from two- to three-dimensional critical behavior should occur when y is of order unity.

To develop this idea systematically for the isothermal, zero-field susceptibility $\chi_T(n;T)$, it is convenient first to define the reduced susceptibility

$$\chi_n(T)=(k_BT/m^2)\chi_T(n;T). \tag{2.10}$$

For a paramagnet obeying Curie's law, we have $\chi_n(T)\equiv 1$. For the bulk system the susceptibility will diverge as

$$\chi_\infty(T)\approx Ct^{-\gamma} \quad \text{as } T\to T_c(\infty)+, \tag{2.11}$$

but for any finite n we expect the exponent of divergence to be $\dot{\gamma}$, corresponding to a system of dimensionality $d-1$. Thus we should have

$$\chi_n(T) \approx \dot{C}(n)\dot{t}^{-\dot{\gamma}} \quad \text{as } T \to T_c(n)+. \tag{2.12}$$

In place of the scaling variable y it is somewhat more convenient, in practice, to use the variable

$$x = n^{\theta}\dot{t} \quad \text{with } \theta = 1/\nu. \tag{2.13}$$

The crossover of behavior from (2.11) to (2.12) may then be described by the scaling hypothesis[8,9]

$$\chi_n(T) \approx n^{\omega} X(n^{\theta}\dot{t}) = n^{\omega} X(x) \quad \text{as } n \to \infty, \dot{t} \to 0. \tag{2.14}$$

To determine the exponent ω one considers the limit $n \to \infty$. Then (2.11) must be reproduced which requires

$$X(x) \approx X_\infty x^{-\gamma} = n^{-\omega} C t^{-\gamma} \quad \text{as } x \to \infty, \tag{2.15}$$

and, since $\chi_n(T)$ must become independent of n in this limit, we also find[8]

$$\omega = \gamma\theta = \gamma/\nu \quad \text{and} \quad X_\infty = C. \tag{2.16}$$

For fixed n as $\dot{t}$ approaches zero, the form (2.12) must be generated so implying

$$X(x) \approx X_0 x^{-\dot{\gamma}} = n^{-\omega}\dot{C}(n)\dot{t}^{-\dot{\gamma}} \quad \text{as } x \to 0. \tag{2.17}$$

This can be satisfied only if

$$\dot{C}(n) \approx X_0 n^{(\gamma - \dot{\gamma})\theta} \quad \text{as } n \to \infty, \tag{2.18}$$

which is a prediction for the behavior of the amplitudes $\dot{C}(n)$ in the finite films.

The leading asymptotic forms for the susceptibility scaling function $X(x)$ are evidently independent of the nature of the boundary conditions, (although X_0 should depend on the conditions). In order to extract explicit information concerning the effect of the boundary conditions on the susceptibility, it is necessary to investigate the approach to the asymptotic forms. For an n-layer system with free surfaces ($\tau = 1$) a decomposition of the free energy per spin into bulk and surface contributions can be made if the range of forces is finite and provided $T \neq T_c$.[8] Then for the susceptibility we can correspondingly write

$$\chi_n(T) \approx \chi_\infty(T) + (2\sigma^{\times}/n)\chi^{\times}(T) \quad \text{as } n \to \infty, \tag{2.19}$$

where $\chi^{\times}(T)$ is the reduced surface susceptibility per surface spin (for one of the two surfaces of the film) and $2\sigma^{\times}/n$ is the number of surface spins per total spin in the film of n layers. This decomposition should certainly be valid for the n-layer Ising model with nearest-neighbor interaction which we consider below.

We now extend the scaling hypothesis[8] by assuming that in the limit $n \to \infty$ with fixed $\dot{t} \ll 1$, the decomposition may be written in a scaled form

$$X(x) \approx X_\infty x^{-\gamma} + Y_\infty n^{-\phi} \quad \text{as } x \to \infty (\tau = 1), \tag{2.20}$$

where ϕ is to be determined by the requirement that (2.19) be matched. Using the definition of the scaling function and the identity

$$\dot{t} = t + \epsilon(n) \approx t + b/n^{\lambda}, \tag{2.21}$$

which follows from (2.2)–(2.4) and (2.7), this implies

$$\chi_n(T) \approx X_\infty t^{-\gamma}(1 - b\gamma t^{-1} n^{-\lambda} + \cdots) + Y_\infty n^{\omega - \theta\phi} t^{-\phi}. \tag{2.22}$$

If $\lambda > 1$, as expected by the earlier scaling argument when $\nu < 1$ (as is the case for three dimensions[26]) the form (2.19) can be matched only if $\omega - \theta\phi = -1$ so that

$$\phi = \gamma + \nu. \tag{2.23}$$

The surface susceptibility is thus predicted to vary as

$$\chi^{\times}(T) \approx C^{\times} t^{-(\gamma+\nu)} \quad \text{with } C^{\times} = Y_\infty/2\sigma^{\times}. \tag{2.24}$$

The possibilities $\lambda \leq 1$ are discussed further in Ref. 8 but need not concern us here since the series evidence indicates $\lambda > 1$ unequivocally for $d = 3$ (see Sec. IV).

In films under periodic boundary conditions ($\tau = 0$) the decomposition (2.19) is not valid since there is no proper surface. The effect of the boundary conditions may be viewed as requiring site l and the corresponding site $(l + n)$ in a column of an infinite system to have the same spin value. When $\dot{t} \neq 0$ it is known that the two-point or spin-spin correlation function decays exponentially fast[1,2] so that

$$\Gamma(T, \vec{r}) = \langle s_{\vec{0}} s_{\vec{r}} \rangle \approx D(r) e^{-r/\xi(t)}, \tag{2.25}$$

where $\xi(T)$ is the appropriate correlation length and $D(r)$ has a power-law dependence. Now for the periodic boundary conditions the distance around the torus is $r = L = na'$. Thus we expect[8] the effect of the boundary conditions on the total susceptibility to decay as

$$\Gamma(T, na') \sim e^{-y} = e^{-cnt^{\nu}} = e^{-cx^{\nu}} \tag{2.26}$$

for $n \gg 1$ and $\dot{t} \neq 0$ [where c is defined in (2.9)]. If this is so, then we should have

$$X(x) - X_\infty x^{-\gamma} = O(e^{-cx^{\nu}}) \quad \text{as } x \to \infty (\tau = 0). \tag{2.27}$$

This prediction is confirmed by exact calculations on the planar Ising model,[5,6,8] and the spherical and ideal Bose models.[9-11]

For free-surface boundary conditions there is no geometrical structure in the film beyond the two surfaces. Hence it is reasonable to expect that the next term in the asymptotic form (2.19) will also be of order $e^{-cx^{\nu}}$.

Finally at *low* values of x, corresponding to $\dot{t} \to 0$ at fixed n, it is plausible to expect corrections to (2.18) to involve integral powers of x which in turn means analytic corrections in t to the form (2.12). This conclusion could, however, well be subject to modification if exponents characteristic of "irrelevant" variables, in the renormalization groups sense,[3,27] can enter (as they certainly do in the leading "corrections to scaling").

As a matter of convenience a superscript label τ will be included in the definition of the reduced susceptibility and in the scaling hypothesis,

$$\chi_n^\tau(T) \approx n^{\gamma\theta} X^\tau(n^\theta \dot{t}) \quad (n \gg 1, \dot{t} \ll 1) \tag{2.28}$$

to denote, as mentioned in Sec. I, the particular boundary conditions which are being considered: for periodic boundary conditions we put $\tau = 0$, for free-surface boundary conditions $\tau = 1$. The expected asymptotic behavior of the scaling functions are then summarized by

$$X^\tau(x) \approx x^{-\dot{\gamma}}(X_0^\tau + X_1^\tau x + X_2^\tau x^2 + \cdots) \tag{2.29}$$

as $x \to 0$ and

$$X^\tau(x) \approx X_\infty x^{-\gamma} + \tau Y_\infty x^{-\gamma-\nu} + O(e^{-cx^\nu}) \tag{2.30}$$

as $x \to \infty$, with

$$c = a'/fa, \quad X_\infty = C, \quad \text{and } Y_\infty = 2\sigma^\times C^\times . \tag{2.31}$$

The scaling functions $X^\tau(x)$, as introduced here, must have an explicit dependence on the lattice structure considered. Thus $X_\infty = C$ is the amplitude of the bulk susceptibility per spin, which is known to be "nonuniversal," i.e., to vary from lattice to lattice (see, e.g., Ref. 26 for explicit estimates). Similarly the variable $x = n^\theta t$ will not have a universal significance since there is an arbitrariness in what is considered "one layer." However, if the amplitude variation of the bulk susceptibility is factored out and if the universal scaled thickness $y = L/\xi$ of (2.9) is used, one may indeed expect[28,29] universality of the corresponding scaling function. Thus, if we rewrite the scaling hypothesis as

$$\chi_n^\tau(T) \approx C W^\tau(cn\dot{t}^\nu)/\dot{t}^\gamma , \tag{2.32}$$

we may postulate that $W^\tau(y)$ is a universal function with, in particular, $W^\tau(\infty) = 1$ in order to reproduce the bulk susceptibility when $n \to \infty$. Comparisons with (2.28) yields the identification

$$X^\tau(x) = C W^\tau(cx^\nu)/x^\gamma , \tag{2.33}$$

which shows how the nonuniversal amplitudes C and c enter into the original scaling functions $X^\tau(x)$ as metrical or scale factors.

By using (2.32) and the universality of $W(y)$ various universal ratios of lattice-dependent amplitudes may be constructed. Thus, in order to reproduce the asymptotic form (2.30) one must have

$$W^\tau(y) = 1 + 2\tau W^\times/y + \cdots \quad \text{as } y \to \infty. \tag{2.34}$$

This then leads via (2.31) to the prediction that the ratio

$$c\sigma^\times C^\times/C = W^\times , \tag{2.35}$$

involving the surface and bulk susceptibility amplitudes, should be universal. We shall test this new prediction in Sec. V using the numerical estimates of $C^\times$ obtained there.

III. HIGH-TEMPERATURE EXPANSIONS

In terms of the standard high-temperature Ising-model variable

$$v = \tanh(J/k_BT), \tag{3.1}$$

the susceptibilities per spin of the n-layer films can be expanded as

$$\chi_n(T) = 1 + \sum_{l=1} a_l(n) v^l , \tag{3.2}$$

where the expansion coefficients $a_l(n)$ have a well-known graphical interpretation in terms of a chain and polygons of l bonds embedded on the lattice.[1,30] The calculation of the coefficients for periodic ($\tau = 0$) films to eleventh order for $n = 3$ and to twelfth order for $n = 4$ to 8, and for free-surface ($\tau = 1$) films to eleventh order for $n = 3$ to 7, was achieved by Allan[31] using a computer program for lattice counting developed by Martin (of King's College, London).[32] The further terms for $n > 8$ and 7, respectively, were obtained later as will be explained.

Allan's calculations[31] for the periodic films employ the Sykes susceptibility counting theorem.[33] The problem falls into two parts: (i) enumeration of all allowable graphs of l bonds; (ii) counting the number of embeddings of each graph in the lattice. The latter task was executed entirely by the Martin counting program which, given a particular graph, will generate and count all embeddings with an assigned "first" or rooted bond on a specified lattice structure. For a periodic film one must distinguish between parallel (or in-layer) and perpendicular root bonds. Adding the corresponding partial lattice constants[1,30] for a graph, with appropriate weights, yields the total lattice constant of the graph in the film.

For free-surface films the calculation likewise falls into two parts. However, owing to the lack of translational invariance perpendicular to the layers the Sykes theorem cannot be employed (at least not in its standard simple form). Accordingly recourse was had to the original methods[1,30] which involve enumerating all possible "magnetic graphs" (with two vertices of odd degree) now both *open* and *closed*; open graphs, having vertices of degree or valence unity, are *not* required when using the Sykes theorem.[33] (Closed graphs have vertices only of degree 2 or higher.) For both sets of boundary conditions it is also necessary to count disconnected configurations by enumerating all possible overlap graphs. Happily, no more than three disconnected components need be considered up to twelfth order.

For free-surface films the computer calculation of the lattice constants must be subdivided both by the orientation of the root bond and by the layer in which it is placed. For n even only $\frac{1}{2}n$ in-layer bonds need be considered by symmetry; for odd n one must use for $\frac{1}{2}(n+1)$ distinct in-layer bonds. Similarly $\frac{1}{2}(n-1)$ different perpendicular root bonds must be considered for n odd, etc.

The enumeration of closed graphs of l bonds proceeded by listing possible graphical topologies through the star topologies (polygon, theta, delta, etc.), and linked stars (dumbbells, etc.). These topologies suffice for periodic films. Open-graph topologies were generated systematically by adding "tails" or chains to the closed graphs at odd vertices or even vertices. This generates all the required possibilities although some may appear more than once. Certain topologies may not be realizable as embedded graphs with 12 or fewer bonds on the simple cubic lattice but, in doubtful cases, the lattice constants were explicitly calculated (and found to be zero). The process used to enumerate the overlap of the disconnected graphs was to consider all overlaps (i) of only one vertex; (ii) of only two vertices; (iii) of only three vertices ...; (iv) of one bond; (v) of one bond and one distinct vertex ...; (vi) of two adjacent bonds; (vii) of two adjacent bonds and one distinct vertex ...; and to continue until all possibilities were exhausted.

These procedures require as many checks as possible. However, the main overall check, which is fairly stringent, is that the previously published[24,30] bulk sc susceptibility series could be generated precisely by both techniques to eleventh or twelfth orders, respectively. The expansion coefficients obtained by Allan are presented in Tables I and II. The series for $n=2$ are included for completeness; the short length for periodic conditions arises from lack of provision for counting "polygons" of length two! However, this feature will not hinder our main purpose which is to study large n.

To extend the series to larger n let us examine the n-layer coefficients for periodic boundary conditions. On comparing them with the bulk, $n=\infty$ series, one finds

$$a_l(n)=a_l(\infty) \quad \text{for } l<n. \tag{3.3}$$

The origin of this result is simply that all graphs of fewer than n bonds or lines have the same lattice constant on the n-layer periodic films as in the bulk lattice since none of them can encircle the $n\times\infty\times\infty$ torus. However, with n lines there is one graph, namely, the straight chain of n bonds, which reaches *around* the torus and interfers with itself (by forming a polygon). This "ghost" configuration must be subtracted off the bulk contribution and leads to

$$a_n(n)=a_n(\infty)-2 \quad (l=n). \tag{3.4}$$

At the next stage, $l=n+1$, similar interfering graphs must be subtracted but, in addition, the disconnected graph of a one-step chain and a polygon that loops the torus, must be accounted for. This yields

$$a_{n+1}(n)=a_{n+1}(\infty)-20 \quad (l=n+1), \tag{3.5}$$

which, like (3.4), is easily checked against the explicit data. At the next stage a two-step chain and a separated polygon must be considered. In addition, an $(n+2)$-step polygon with two kinks can be formed which still loops the torus. The possible locations of the kinks leads to a factor $\frac{1}{2}n(n+1)$ and to the final relation

$$a_{n+2}(n)=a_{n+2}(\infty)-4n(n+1)-140 \quad (l=n+2). \tag{3.6}$$

When $l=n+3$ the configurational argument is more involved but clearly again involves a quadratic (but not cubic) expression in n. Granted this fact, the easiest procedure is to form the differences $a_l(n)-a_l(n-1)$ and take successive differences on l. This yields the expression

$$a_{n+3}(n)=a_{n+3}(\infty)-40n(n+1)-868 \quad (l=n+3). \tag{3.7}$$

Using these relations and the extended series for the bulk susceptibility obtained by Sykes *et al.*,[24] the reduced susceptibility series has been calculated to the $(n+3)$rd term for $9\le n\le 14$ (see Table I).

The search for corresponding recursion relations for the free-surface series coefficients is facilitated by the introduction of the *effective reduced surface susceptibility* of an n-layer system through the definition

$$-\sigma^\times\chi_n^\times(T)\equiv\tfrac{1}{2}n[\chi_\infty(T)-\chi_n(T)]$$
$$=\tfrac{1}{2}n\sum_{l=0}^{\infty}[a_l(\infty)-a_l(n)]v^l=\sum_{l=0}^{\infty}b_l(n)v^l. \tag{3.8}$$

The factor $\sigma^\times$ is included here, as in (2.19), to provide the appropriate normalization between surface and bulk spins. The values of $\sigma^\times$ for sc, bcc, and fcc lattices with surfaces parallel to the cubic lattice planes are presented in Table III.

TABLE III. Properties of the bulk cubic lattices used in the series and scaling function analyses. (From Refs. 24 and 26, and see text; the values of $C^\times$ follow from Table VII below.)

Lattice	sc	bcc	fcc
q	6	8	12
a'/a	1	$2/\sqrt{3}$	$\sqrt{2}$
$\sigma^\times$	1	$\frac{1}{2}$	$\frac{1}{2}$
$v_c(\infty)$	0.218 13 ± 1	0.156 12 ± 2	0.101 740 ± 5
K_∞	0.967 97	0.983 67	0.993 08
$C=C^+$	1.0585 ± 10	0.9868 ± 30	0.971 ± 2
$f=f_0^+$	0.478 26	0.444 56	0.433 66
$C^\times$	0.4334 ± 26	0.642 ± 10	0.512 ± 8

The effective n-layer surface susceptibility can be compared to the reduced surface susceptibility $\chi^\times(T)$, for a semi-infinite system with a surface which may be defined through the limit

$$\sigma^\times\chi^\times(T)=\sigma^\times\chi^\times_\infty = -\lim_{n\to\infty}\tfrac{1}{2}n[\chi_\infty(T)-\chi_n(T)] = -\sum_{l=1}^{\infty} b_l v^l . \tag{3.9}$$

The coefficients $b_l = \lim b_l(n)$ $[n\to\infty]$, are in fact, the number of allowed distinct graphs of l bonds which intersect or lie outside the film. The values of the b_l have been calculated by Allan[31] for the sc lattice to order 11 and by Watson[16] for the bcc and fcc lattices to orders 8 and 7, respectively; they have been published in Ref. 15 (p. 136; but notice that b_l is equal to one-half the coefficient c_l listed there).

Now by construction of the table of deviations $[b_l(\infty)-b_l(n)]$ and differencing one discovers the following recursion relations hold:

$$b_l(n)=b_l(\infty) \qquad (l\le n), \tag{3.10}$$

$$b_{n+1}(n)=b_{n+1}(\infty)-1 \qquad (l=n+1), \tag{3.11}$$

$$b_{n+2}(n)=b_{n+2}(\infty)-4n-10 \qquad (l=n+2), \tag{3.12}$$

$$b_{n+3}(n)=b_{n+2}(\infty)-8n^2-44n-75 \qquad (l=n+3), \tag{3.13}$$

$$b_{n+4}(n)=b_{n+4}(\infty)-10\tfrac{2}{3}n^3-96n^2-349\tfrac{1}{3}n-484 \qquad (l=n+4). \tag{3.14}$$

The first three relations here may be easily checked generally by exact graphical considerations since they involve no disconnected graphs. For $l\le n$ there are no overlapping graphs which intersect both surfaces and the equality of $b_l(n)$ and $b_l(\infty)$ follows. When $l=n+1$ there is a single symmetric overlapping graph, namely a chain of $n+1$ bonds. This yields (3.11). The last simple case is $l=n+2$ where are overlaps resulting from a chain with one kink. For higher order, just the existence of the graphical technique suffices since it, at once, determines the order of the polynomial appearing in the recursion relation. By using the relations (3.10)–(3.14) Allan's results have been extended to obtain the free-surface series for $8\le n\le 11$ to eleventh order as presented in Table II.

IV. SERIES ANALYSIS

The high-temperature expansions (3.2) must be analyzed to estimate the critical temperatures $T_c(n)$ and susceptibility amplitudes $\dot{C}(n)$ and $C^\times$ [see (2.12) and (2.24)]. In terms of the variable v we anticipate the behavior

$$\chi_n(T)=\dot{A}_n(v)[1-v/v_c(n)]^{-\dot\gamma}, \tag{4.1}$$

with

$$v_c(n)=\tanh[J/k_BT_c(n)], \tag{4.2}$$

where $\dot{A}_n(v)$ approaches a finite limit $\dot{A}(n)$ as $v\to v_c-$. Since the variable v features in all the numerical analysis it is convenient to introduce

$$\tilde{t}(n)=1-v/v_c(n) \tag{4.3}$$

to measure deviations from criticality. As $T\to T_c(n)$ this variable is related to the more general $\dot{t}(n)$ introduced in (2.7) by

$$\tilde{t}(n)\approx K_n\dot{t}(n), \tag{4.4}$$

with proportionality factor

$$K_n=2JT_c(\infty)/k_BT_c^2(n)\sinh[2J/k_BT_c(n)]. \tag{4.5}$$

Evidently the critical amplitude $\dot{A}(n)$ in terms of $\tilde{t}$, corresponds to $\dot{C}(n)$ in terms of $\dot{t}$; likewise we will use A and $A^\times$ with $\tilde{t}$, corresponding to C and $C^\times$ with $\dot{t}$. We will also use $\tilde{x}=n^\theta\tilde{t}$ in place of x, as convenient. It may be observed from Table III, however, that K_n is within a few percent of unity for large n.

A. Bulk critical behavior

The susceptibility series for the bulk ($n=\infty$) Ising model on the sc, bcc, and fcc have been obtained to greatest length by Sykes *et al.*[24] and analyzed by them in detail. Their estimates for $v_c(\infty)$, which we adopt, are listed in Table III together with the corresponding values of the conversion factors K_∞ defined in (4.5), and the critical amplitudes C. (But note that the values of C appearing in the journal version of Ref. 24 are slightly in error; the corrected values of $C\equiv C^+$ are taken from Ref. 26.) Sykes *et al.*, also concluded that $\gamma=1.250\pm3$; accordingly we adopt the value

$$\gamma=1\tfrac{1}{4} \tag{4.6}$$

in all our work without further question.

The correlation length $\xi(T)$ has been studied by Fisher and Burford[34] who concluded that the exponent ν lay in the range 0.643 ± 0.0025. Moore, Jasnow, and Wortis[35] using somewhat longer series, especially for the fcc lattice, concluded that ν should be closer to 0.640 or lower. However, these differences will not be significant for our purposes. Accordingly we follow Tarko and Fisher[26] and adopt the simple fractional value

$$\nu = 1/\theta = \tfrac{9}{14} \simeq 0.6428\cdots . \tag{4.7}$$

The correlation length most appropriate to finite-size scaling theory is the "true" or exponential range of correlation[1,26] in the bulk lattice, defined in accordance with the decay law of the two-spin correlation function displayed in (2.25). In the notation of Tarko and Fisher,[26] therefore, the amplitude parameter f in (2.8) should be called f^+. However, for the three cubic Ising lattices the value of f^+ is very close indeed[26,34] to the value of f_1^+ for the second-moment correlation length[1,26] $\xi_1(T)$ (which enters into low-angle scattering theory). Accordingly, in Table III we quote for f the values of f_1^+ calculated, following Tarko and Fisher,[26] by using the values of the parameter $p_c = (r_1/a)_c^{2-\eta}$ found by Fisher and Burford,[34] and the later values[26] of $C \equiv C^+$, in the relation $(f_1^+)^{2-\eta} = p_c C^+$. Multiplying these values of f_1^+ by 1.0003 (see Table XIV of Ref. 26) will give somewhat better estimates of $f \equiv f^+$ but this degree of accuracy is not needed in the present study.

B. Layer critical temperatures

Estimation of the critical points $v_c(n)$ and exponents $\dot{\gamma}$ for finite n may be attempted by standard ratio and Padé approximant methods.[1] For $n \leq 4$ one finds $\dot{\gamma} \simeq 1\frac{3}{4}$, in accord with the expected two-dimensional value which is exactly[1,2,25]

$$\dot{\gamma} = 1\tfrac{3}{4} . \tag{4.8}$$

For larger values of n the crossover to three-dimensionality affects the series analysis, and it is appropriate to *assume* the result (4.8) for all $n < \infty$ in order to obtain the best possible estimates for $v_c(n)$. Accordingly the function $E(v)$ with expansion coefficients $e_r(n)$ defined by

$$E_n(v) = \sum_{r=1} e_r(n) v^r = [\chi_n(T)]^{1/\dot{\gamma}} = \left(\sum_{l=1} a_l(n) v^l\right)^{1/\dot{\gamma}} , \tag{4.9}$$

is calculated.[8] This function must diverge as a *simple pole* at $v = v_c(n)$, so that the ratios $\mu_r(E_n) = e_r(n)/e_{r-1}(n)$ should approach the values $1/v_c(n)$ with *zero slope* on the standard plot[1,30] versus $1/r$. Indeed, as can be seen from Fig. 1, where the ratios $\mu_r(E_n)$ for periodic boundary conditions are plotted versus $(1/r)^2$ in place of $1/r$, this expectation is well borne out for large enough r. The same behavior is observed for free-surface films. The resulting critical point estimates for $n \leq 8$ ($\tau = 1$) are listed in Table IV.

A perusal of the estimates for $v_c(n)$ reveals that the periodic layer critical points approach the bulk value $v_c(\infty) \simeq 0.218\,13$ much more rapidly then do the free-surface values. To determine the shift exponent λ the deviations

$$\Delta v_c(n) = v_c(n) - v_c(\infty) \tag{4.10}$$

were calculated and plots of $[\Delta v_c(n)]^{1/\lambda}$ vs n evaluated[8] for various trial values of λ. Such a plot for free-surface films was presented in Ref. 8 (Fig. 12). The scaling expectation

$$\lambda_{\tau=1} = \theta = 1/\nu \simeq 1.56 \tag{4.11}$$

yields a good linear fit in the range $n = 1-7$. Trial values of λ differing by ± 0.15 clearly display curvature in opposite senses. Furthermore, the approximate representation

$$v_c(n) \simeq v_c(\infty) + 0.350/(n + \tfrac{1}{2})^{1/\nu} \quad (\tau = 1) \tag{4.12}$$

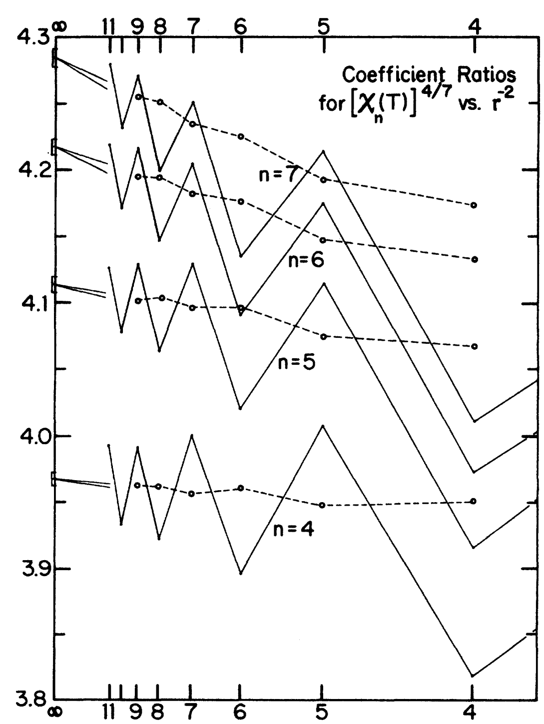

FIG. 1. Estimation of $v_c(n)$ from ratio plots vs $(1/r)^2$ for periodic lattices for $n = 4, 5, 6,$ and 7. The value $\dot{\gamma} = \frac{7}{4}$ is assumed.

TABLE IV. Estimates of the critical temperatures $v_c(n) = \tanh[J/k_B T_c(n)]$ for the n-layer sc lattice.

n	$v_c(n)$ $(\tau=0)$	$v_c(n)$ $(\tau=1)$
2	0.2692 ± 11	0.3020 ± 6
3	0.2401 ± 1	0.2675 ± 3.5
4	0.2305 ± 1	0.2520 ± 3
5	0.2261 ± 1.5	0.2430 ± 3
6	0.2235 ± 2.5	0.2371 ± 3.5
7	0.2220 ± 3	0.2334 ± 4
8	0.2211 ± 4.5	

is found to fit $\Delta v_c(n)$ to within 1% down to $n=2$. The estimate (4.11) is also supported by more recent Monte Carlo calculations by Binder and co-workers[21,22] and by Landau.[23]

For periodic boundary conditions, on the other hand, the larger value

$$\lambda_{\tau=0} = 2.0 \pm 0.1 , \tag{4.13}$$

not equal to $1/\nu$, is clearly indicated.[8] The corresponding formula

$$v_c(n) \simeq v_c(\infty) + 0.177/(n - \tfrac{1}{4})^2 \quad (\tau = 0) \tag{4.14}$$

is found to fit $\Delta v_c(n)$ to within 2% down to $n=4$ and to within 6% for $n=3$. (This representation of the results is an improvement for larger n values over the slightly simpler fit advanced in Ref. 8.) As commented in Sec. II, the difference between $\lambda_{\tau=1}$ and $\lambda_{\tau=0}$ is not unexpected.

C. Critical amplitudes

On adopting the critical-point estimates in Table IV, and using the fitting expressions (4.12) and (4.14) to extrapolate $v_c(n)$ to larger values of n, the n-layer critical amplitudes $\dot{A}^\tau(n)$ may be estimated by standard Padé approximant and ratio techniques. Thus, direct $[L/M]$ Padé approximants were formed to the amplitude functions $\dot{A}_n(v)$ defined through (4.1); evaluation at $v = v_c(n)$ yields estimates for $\dot{A}^\tau(n)$. As an example, the series for free-surface ($n=5$)-layer films yields $[4/4] = 0.3924$, $[4/5] = 0.3928$, $[5/4] = 0.3929$, $[5/5] = 0.3426$, $[5/6] = 0.3930$, and $[6/5] = 0.3938$.

The ratio technique used is based on extrapolation versus $1/r$ of the sequences of estimators[1,30]

$$(\dot{A}_n^\tau)_{r,m} = a_r^\tau(n)/c_{r+m}^{\dot{\gamma}}(n) , \tag{4.15}$$

where the $c_l^{\dot{\gamma}}(n)$ are the expansion coefficients of the binomial $[1 - v/v_c(n)]^{-\dot{\gamma}}$. Some of these plots for particular values of the "shift" m, chosen to reduce the curvature, are shown in Fig. 2. Although the residual curvature allows some latitude of extrapolation the corresponding sequences of pairwise linear intercepts[1,30] extrapolate quite

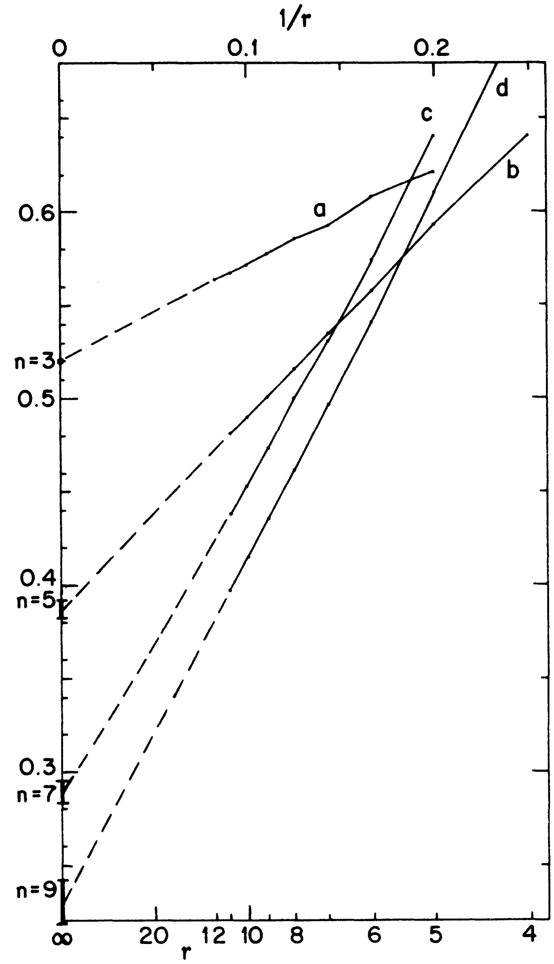

FIG. 2. Plot of the estimators $(\dot{A}_n^1)_{r,m}$ for free-surface boundary conditions [see (4.15)] vs $1/r$ with (a) $n=3$, $m=-1$; (b) $n=5$, $m=-1$; (c) $n=7$, $m=-2$; and (d) $n=9$, $m=-2$.

well and reveal trends to which, as in other cases, the Padé approximants seem unresponsive. Thus, in the case $\tau=1$, $n=5$, mentioned above, the ratios indicate somewhat lower values than the Padé table and the over-all estimate made is $\dot{A}^1(5) = 0.387 \pm 5$. Generally the series-based values are preferred although the uncertainty limits overlap to a considerable degree. As might be expected, the curvature increases for larger n and the Padé tables likewise become less consistent so that the final uncertainties are larger, reaching 5 or 6% at $n \simeq 14$ for $\tau=0$ and at $n \simeq 9$ for $\tau=1$. The over-all estimates made are listed in Tables V and VI.

If the scaling prediction (2.18) for the $\dot{C}(n)$ and, equivalently, for the $\dot{A}(n)$ is valid, the second columns in Tables V and VI, which display $\dot{A}(n) n^{\theta(\dot{\gamma}-\gamma)}$, should approach constant values $\tilde{X}_0^\tau$, directly related to the scaling function amplitudes

TABLE V. Finite-size susceptibility amplitudes $\dot{A}(n)$ for periodic boundary conditions ($\tau=0$) and their analysis.

n	$\dot{A}(n)$	$\dot{A}(n)n^{\theta(\dot{\gamma}-\gamma)}$
2	0.836	1.433
3	0.590 ±1	1.387±2
4	0.4515±10	1.327±3
5	0.366 ±1	1.280±3
6	0.299 ±2	1.205±8
7	0.249 ±3	1.131±13
8	0.220 ±4	1.109±20
9	0.203 ±4	1.121±22
10	0.184 ±5	1.103±30
11	0.169 ±6	1.091±39
12	0.157 ±6	1.085±41
13	0.146 ±7	1.073±54
14	0.137 ±7	1.067±55

X_0^τ. Clearly the expected asymptotic behavior is not well approximated in the range of n displayed, so that allowance for correction factors must be made. Since the values in each table show a downward trend as n increases, a small downward shift in the n values is indicated. Investigation of various shifts suggests $m=-\frac{3}{2}$ for periodic films and $m=-\frac{2}{3}$ for free-surface films as appropriate choices. The corresponding sequence of estimators, namely, $(\tilde{X}_0^\tau)_n=\dot{A}^\tau(n)(n+m^\tau)^{7/9}$, is plotted versus $1/n$ in Fig. 3. From these data the final estimates for the periodically connected films are

$$\tilde{X}_0^0=0.93\pm0.02 \quad \text{or} \quad X_0^0=0.98\pm0.02\,, \qquad (4.16)$$

where the tilde applies with use of the variable $\tilde{t}$, and for the free-surface films

$$\tilde{X}_0^1=1.20\pm0.02 \quad \text{or} \quad X_0^1=1.27\pm0.02\,, \qquad (4.17)$$

since $\tilde{X}_0^\tau=\dot{K}_\infty^{\dot{\gamma}}X_0^\tau$. Combined with the value $\dot{\gamma}=1\frac{3}{4}$ this determines the limiting behavior of the scaling functions $X^\tau(x)$ as $x=n\dot{t}^{\,\theta}\to 0$ [see (2.29)]. The behavior for large x required analysis of the surface susceptibilities to which we now turn.

TABLE VI. Finite-size susceptibility amplitudes $A(n)$ and their analysis for free-surface boundary conditions ($\tau=1$).

n	$\dot{A}(n)$	$\dot{A}(n)n^{\theta(\dot{\gamma}-\gamma)}$
2	0.6863±10	1.177±2
3	0.5200±15	1.222±3
4	0.449 ±4	1.320±12
5	0.387 ±5	1.353±17
6	0.323 ±6	1.301±24
7	0.290 ±7	1.317±32
8	0.255 ±10	1.285±50
9	0.230 ±12	1.270±66
10	0.213 ±12	1.277±72
11	0.197 ±11	1.270±71

D. Surface susceptibilities

The surface susceptibility $\chi^\times(T)$ must (unless the surface interactions are enhanced in some way[22]) diverge only at the bulk critical point $v_c(\infty)$ with an exponent which may be called $\gamma^\times$. The scaling theory makes the unequivocal prediction[8] $\gamma^\times=\gamma+\nu$ [see (2.24)]. However in contrast to the value $\gamma+\nu\simeq1.89$, direct ratio and Padé estimates of $\gamma^\times$ for all three cubic lattices yield[8] distinctly higher values, around 1.95, with uncertainties which *could* be as large as 0.08, owing to curvature of the ratio plots.

If, on the other hand, a scaling value $\gamma^\times\simeq1.89$ is adopted, one can attempt to estimate the corresponding critical amplitude $A^\times$ by studying the sequences $(A^\times)_{r,m}$ defined in analogy to (4.15). The corresponding plots are, however, likewise found to be strongly curved, and the curvature cannot be removed by any value of the shift m (see Capehart[36] for illustrations). This difficulty precludes straightforward estimation of $A^\times$ and $C^\times$. If the asymptotic scaling prediction is valid, this behavior implies that the corrections to the leading critical behavior must be considerably

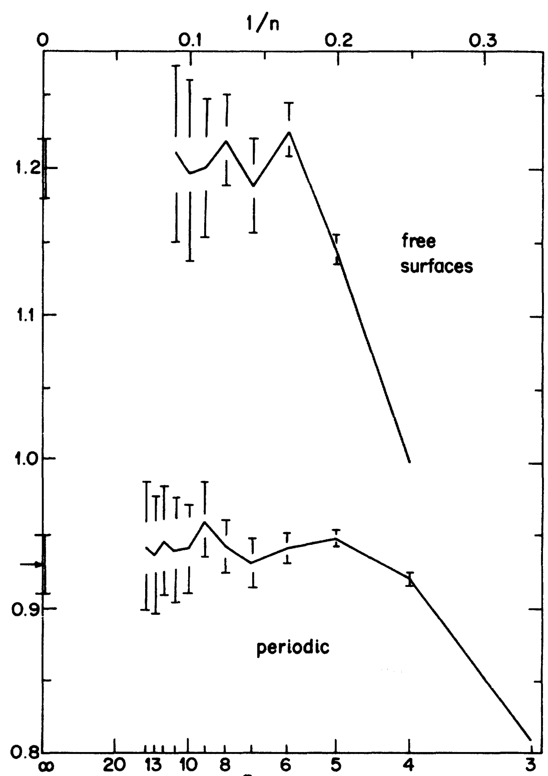

FIG. 3. Extrapolation of the amplitude estimates $\dot{A}^\tau(n)\times(n+m^\tau)^{7/9}$ for $\tilde{X}_0^\tau$ for periodic ($\tau=0$) and free-surface ($\tau=1$) boundary conditions with shifts $m^0=-\frac{3}{2}$ and $m^1=-\frac{2}{3}$.

more singular than in the bulk susceptibility series. To understand this we pause to examine theoretically the likely character of the coincident critical singularities in $\chi^{\times}(T)$ as $T \rightarrow T_c(\infty)$.

First observe that for a film of n layers and thickness $L = na'$ the decomposition of the *total* susceptibility (per unit spin *area* of film) satisfies

$$\chi_n^{\text{tot}}(T) = n\chi_n(T) \approx n\chi_\infty(T) + 2\sigma^{\times}\chi^{\times}(T). \tag{4.18}$$

In this specification, the "surface" of the film nominally ends at a distance $\frac{1}{2}a'$ beyond the final layer of spin sites. Suppose now that "by convention" the surface is considered to extend to $(\frac{1}{2}+b)a'$ beyond the final spin layer. This amounts to a redefinition of the "thickness" as

$$\bar{L} = L + 2ba' = \bar{n}a', \quad \text{with } \bar{n} = n + 2b. \tag{4.19}$$

In terms of this we obtain a new decomposition of the total susceptibility with, in (4.18), n replaced by $\bar{n}$ and $\chi^{\times}(T)$ replaced by

$$\chi^{\times}(T) = \chi^{\times}(T) - (b/\sigma^{\times})\chi_\infty(T). \tag{4.20}$$

Since our original definition of n is really just as arbitrary as the new one, we conclude that $\chi^{\times}(T)$ will, *in general*, have a correction term diverging like the bulk susceptibility $\chi_\infty(T) \sim t^{-\gamma}$. We thus expect the surface susceptibility to have the asymptotic form

$$\chi^{\times}(T) \approx C^{\times}t^{-(\gamma+\nu)} + C_1^{\times}t^{-\gamma} + C_2^{\times}t^{-\psi} + \cdots. \tag{4.21}$$

One may check[36] this conclusion using the Landau-Ginzburg model of a film[14,17] which yields

$$\chi^{\times}(\xi) \approx \xi^3[1 + (\Lambda/\xi) + (\Lambda/\xi)^2 \cdots], \tag{4.22}$$

where Λ is the temperature-independent "extrapolation length" which represents the boundary conditions. Since one has $\gamma = 2\nu = 1$ (with $\eta \equiv 0$) in the Landau-Ginzburg model, the first two terms here confirm those in (4.21). However, the third term is ambiguous: one could conclude $\psi = \nu \simeq 0.64$ or $\psi = \gamma - \nu \simeq 0.61$ or $\psi = \gamma + \nu - 1 \simeq 0.89$. Since one must at least expect *analytic correction factors* to the leading $t^{-(\gamma+\nu)}$ dependence one must certainly have $\psi \leq \gamma + \nu - 1$. However, the standard correction-to-scaling exponent $|\phi_u|$ studied in renormalization-group theory[3] could also be playing a dominant role.

Now it is well known that straightforward extrapolation methods fail when a singular correction term with a small "exponent gap," as in (4.21), has an amplitude comparable to the dominant term. Supposing this to be the case in hand, we have reanalyzed the surface susceptibility series for the three cubic lattices using the ratio technique developed by Wortis and co-workers.[37] In this method one assumes a truncated representation of the form (4.21) with assigned exponents. If t is replaced by $\tilde{t} = [1 - v/v_c(n)]$ and the resulting form expanded about $v = 0$, a sequence of the expansion coefficients b_l of $\chi^{\times}(T)$ may be matched to determine corresponding amplitudes $A^{\times}$, $A_1^{\times}$, and $A_2^{\times}$. As higher-order terms are matched in this manner an asymptotic approach to the values of the amplitudes should be observed. To obtain distinct estimating sequences a set of shifts m, m_1, and m_2 may be introduced as in the extrapolation methods already discussed.

This method was employed to study $\chi^{\times}(T)$ for the sc, bcc, and fcc lattices under the alternative assumptions $\psi = \gamma - \nu$ and $\psi = \gamma + \nu - 1$. For the sc and bcc lattices, where strong oscillations between successive ratios often occur, alternative coefficients were used; for the shorter fcc series where oscillations are insignificant, successive coefficients were used. The solutions to the matching equations may be labeled by the highest-order term involved: for example, the amplitude estimates obtained from the coefficients b_7, b_6, and b_5 for the fcc lattice were labeled $(A^{\times})_7$, $(A_1^{\times})_7$, and $(A_2^{\times})_7$.

Plots of these amplitudes versus $1/r$ for the sc and fcc lattices using $\psi = \gamma - \nu$ are shown in Figs. 4 and 5. The notations (0, 0, 0) and (0, 1, 1) in Fig. 5 denote alternate choices of the shifts m_i. The

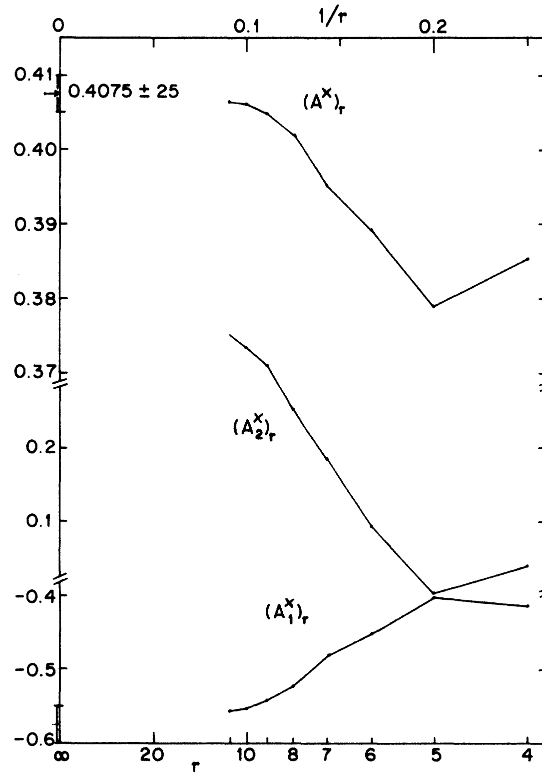

FIG. 4. Results of applying the Wortis technique to the sc surface susceptibility series assuming $\psi = \gamma - \nu$ and zero shifts m_i.

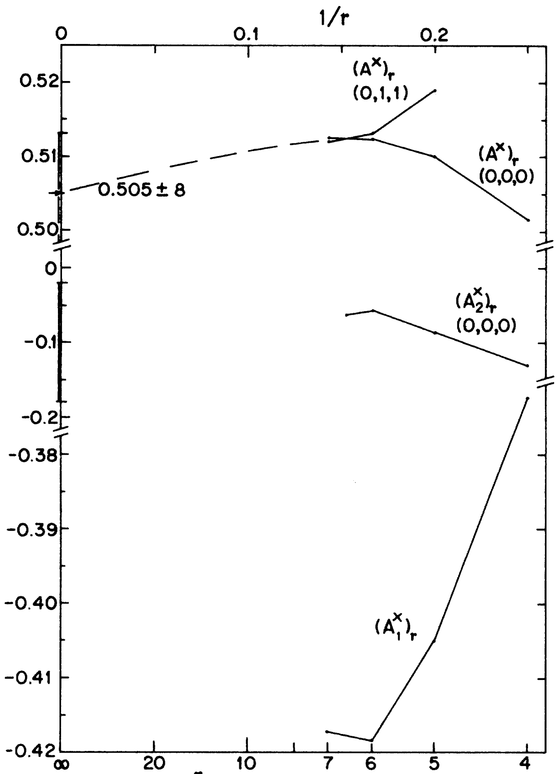

FIG. 5. Application of the Wortis technique to the fcc surface susceptibility series assuming $\psi = \gamma - \nu$ for two sets of shifts m_i (see text).

final amplitude estimates also using $\psi = \gamma + \nu - 1$ for each lattice, are given in Table VII. The amplitudes of interest to scaling theory are the $A^\times$ which are found to be insensitive, to within less than 1%, to the choice of ψ adopted for the analysis. This technique is quite different from the previously described methods and was adopted owing to the failure of the normal techniques. However, there is no strong basis for linear extrapolation versus $1/r$ in estimating the asymptotic amplitude. In an attempt to check this procedure the Wortis method was applied to the bulk sc series by assuming

$$\chi_\infty(T) = \sum_{r=0}^{\infty} a_r v^r \approx A_{-1}\tilde{t}^{-(\gamma+\nu)} + A\tilde{t}^{-\gamma} + A_1\tilde{t}^{-\gamma+1}. \quad (4.23)$$

The sequence of approximants $(A_{-1})_r$ and $(A)_r$ for $r > 8$ alternate regularly about almost constant mean values. The sequence $(A)_r$ linearly extrapolates to a value of $A_\infty \simeq 1.017 \pm 2$, which is in excellent accord with the Sykes *et al.*[24] estimate $A = 1.0163 \pm 10$. The method also gave $A_{-1} \simeq 0.0001 \pm 2$, which is consistent with $A_{-1} \equiv 0$, as expected, and $A_1 \simeq -0.01 \pm 1$. In addition the Wortis technique was applied to various n-layer series and found to yield amplitude estimates which are quite consistent with the other methods used. Thus we have reasonable confidence in the estimates for $A^\times$ presented in Table VII.

TABLE VII. Estimates of the leading and correction amplitudes in the surface susceptibilities for the cubic lattices (see text).

	sc	bcc	fcc
$A^\times$	0.4075 ± 25	0.622 ± 10	0.505 ± 8
$A_1^\times$	−0.575 ± 25	−0.35 ± 8	−0.41 ± 4
$A_2^\times$	0.51 ± 8	−0.27 ± 8	−0.10 ± 8

E. Universality and scaling function

If the scaling function $W(w)$ introduced in Sec. II is universal, the ratio

$$W^\times = c\sigma^\times C^\times / C \quad (4.24)$$

should be the same for all Ising lattices [see (2.35)]. Using the estimates for $C^\times$ following from Table VII and the other data also embodied in Table III, the results for the sc, bcc, and fcc lattices are

$$W^\times = 0.856 \pm 5, \quad 0.845 \pm 14, \quad 0.859 \pm 13, \quad (4.25)$$

respectively. The sc range of uncertainty is included totally within the fcc range and almost entirely within the bcc range. (The bcc sequences are, however, less regular than for the sc and fcc lattices.) A universal value of $W^\times \simeq 0.855$ is strongly suggested by the data (to a precision of ±1.3% or better). We conclude that the evidence for the universality of the scaling function $W(y)$ is good.

Finally the behavior of the original scaling function $X^\tau(x)$ for large values of its argument may be determined [see (2.31)]. Using the data of Tables III and VII we find for the simple cubic lattice

$$c \simeq 2.091, \quad X_0 = 1.0585 \pm 10, \quad Y_\infty = 0.867 \pm 5. \quad (4.26)$$

These results specify the scaling function asymptotically. We now turn to the question of approximating $X^\tau(x)$ over intermediate values of x.

V. SCALING FUNCTIONS

The existence of the scaling function, i.e., the validity of the scaling hypothesis, may be checked by plotting appropriately scaled Padé approximants for $\tilde{x}^{\dot{\gamma}}\chi_n(T)$ vs $\tilde{x} = n^\theta \tilde{t}$ for all the n-layer films. The validity of scaling is then indicated if the deviations between the various approximants appear to decrease as n increases. Explicitly, by constructing Padé approximants[38] to the amplitude function $\dot{A}_n(v) = \tilde{t}^{\dot{\gamma}}\chi_n(T)$ we may evaluate the modified scaling function

$$Z_n^\tau(\tilde{x}) = n^{\theta(\dot{\gamma}-\gamma)}[\tilde{t}^{\dot{\gamma}}\chi_n(T)] \approx Z^\tau(\tilde{x}) = \tilde{x}^{\dot{\gamma}}\tilde{X}^\tau(\tilde{x}) \tag{5.1}$$

as a function of $\tilde{x} = n^\theta \tilde{t}$ for each of the n-layer films. The form of $Z(\tilde{x})$ allows a convenient graphical representation since, on a log-log scale, $Z(\tilde{x})$ is required to have zero slope as $\tilde{x} \to 0$ (i.e., $\ln\tilde{x} \to -\infty$) while for large $\tilde{x}$ it behaves as

$$\ln Z^\tau(\tilde{x}) \approx (\dot{\gamma} - \gamma)\ln\tilde{x} + \ln\tilde{X}_\infty + \ln[1 + \tau(\tilde{Y}_\infty/\tilde{X}_\infty)\tilde{x}^{-\nu}] + O(e^{-\tilde{c}\tilde{x}^\nu}), \tag{5.2}$$

yielding a linear asymptote of slope $(\dot{\gamma} - \gamma) = \frac{1}{2}$.

A. Numerical estimation

The most direct way of testing for the existence of a scaling function would be to plot $Z_n^\tau(\tilde{x})$ vs $\ln\tilde{x}$ for each of the n-layer films with given boundary conditions. However, in these plots, the behavior at small $\tilde{x}$ is not monotonic in n. This merely reflects the previous amplitude analysis where shifts in the value of n were required to extrapolate for the scaling amplitude $\tilde{X}_0$ (see Fig. 3). Further, the curves for different n frequently cross one another making a convincing extrapolation of the trends very hard. Following the philosophy adopted throughout our study of using the central estimate of a quantity in all subsequent calculations, we have, instead, introduced an individual n shift m^* for each approximant for an n-layer film chosen to exactly satisfy the relation

$$(n + m^*)^{(\dot{\gamma}-\gamma)\theta}[\dot{A}_n] = \tilde{X}_0^\tau, \tag{5.3}$$

where the square brackets denote a particular approximant to $\dot{A}_n$. We call the resulting approximants $Z_n^\tau{*}(\tilde{x})$. This normalization simply has the effect of making all the $Z_n^\tau{*}$ approach the same asymptote as $\tilde{x} \to 0$. Some of the corresponding curves are shown in Figs. 6 and 7. While the variation is not entirely monotonic in n, Padé approximants which have been normalized in this manner, and which have no poles in the region $0 \leq v \leq v_c(n)$, have relatively few intersections for different values of n.

With this normalization then, a more detailed study is worthwhile. For each value of n and selected values of $\tilde{x}$, with $\ln\tilde{x}$ in the range -6 to $+3$, various near-diagonal approximants to $Z_n^\tau{*}(\tilde{x})$ have been tabulated. Examination of the values of $\ln Z_n^\tau{*}(\tilde{x})$ vs $1/n$ reveals definite linear trends. In view of the normalization imposed and the fact that the values X_0^τ were estimated by linear extrapolation of $1/n$ plots, this behavior is really to be expected.

In the case of *periodic boundary conditions* ($\tau = 0$) approximants up to $n = 6$ seem very well converged; for $n = 7-12$ there is more fluctuation, but a central value is fairly well identifiable; for $n \geq 13$

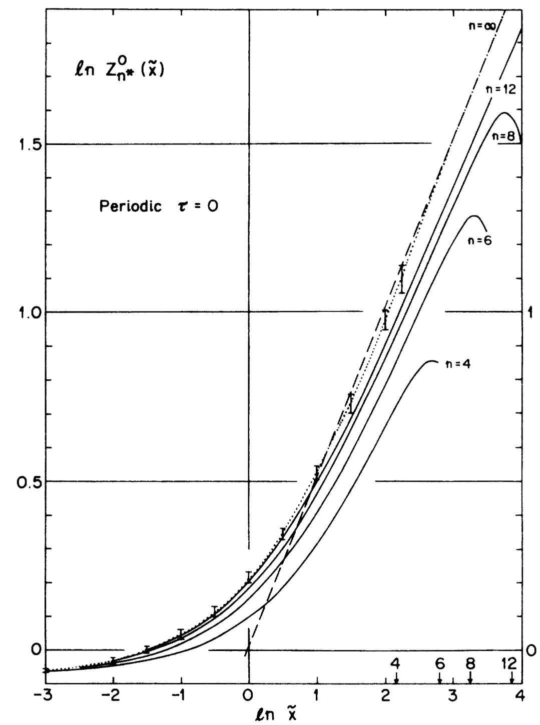

FIG. 6. Plots of the modified scaling function $\ln[Z_n^0{*}(\tilde{x})]$ vs $\ln\tilde{x}$ with $n = 4, 6, 8, 12$, and ∞ for periodic films. The numbered arrows on the lower right-hand side correspond to $\tilde{x} = n^\theta$ or $T = \infty$, for a particular n-layer film. The dotted curve and the uncertainty bars indicate the extrapolated limit.

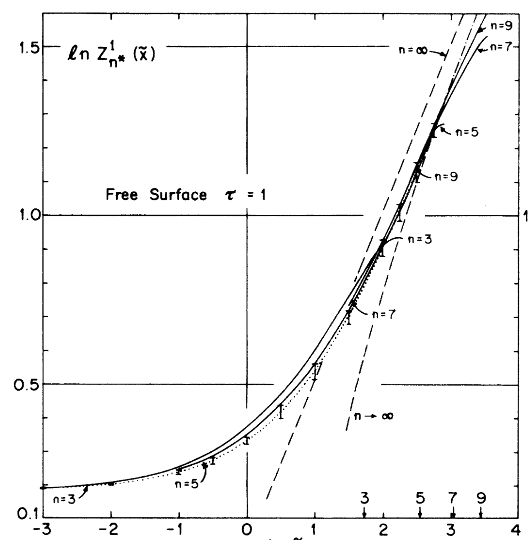

FIG. 7. Plots of the modified scaling function $\ln[Z_n^1{*}(\tilde{x})]$ vs $\ln\tilde{x}$ with $n = 3, 5, 7, 9$, and ∞ for free-surface films. The numbered arrows on the lower right-hand side again correspond to $\tilde{x} = n^\theta$ or $T = \infty$. The dotted curve and uncertainty bars indicate the extrapolated limits. The broken curve labeled $n \to \infty$ corresponds to the surface asymptote.

the variation between different approximants is too large to aid extrapolation, although the results are quite consistent with the extrapolations adopted. Figure 8 shows the behavior for $\ln\tilde{x} = -1$ and 1. By linear extrapolation of the clear upward trend we have prepared the set of estimates $Z^0(\tilde{x})$ presented in the second column of Table VIII and shown by the uncertainty bars in Fig. 6. The nominal uncertainty in $\tilde{x}$ rises from less than $\pm\frac{1}{2}\%$ for $\tilde{x} \leqslant 0.15$ ($\ln\tilde{x} \leqslant -2$), to about $\pm 2\%$ for $\tilde{x} \simeq 1$, and $\pm 4\%$ for $\tilde{x} \geqslant 9$ ($\ln\tilde{x} \geqslant 2.2$). Of course, these uncertainties rest on the validity of the linear extrapolation. The values shown in parentheses for $\ln\tilde{x} > 0$ represent the large $\tilde{x}$ asymptote, namely, $\ln Z^0 \approx (\dot{\gamma} - \gamma)\ln\tilde{x} + \ln\tilde{X}_\infty$. For $\tilde{x} \geqslant 4$ this asymptote is evidently approached from below (as is to be expected). Although the magnitudes of the uncertainties preclude a precise judgement, it appears that $Z^0(\tilde{x})$ merges with the asymptote to within 1% for $\tilde{x} > 16$ ($\ln\tilde{x} > 2.8$). It should be noted that for given n the significant values of $\tilde{x}$ are restricted by $\tilde{x} < n^\theta$, since the value $\tilde{x} = n^\theta$ corresponds to $\tilde{t} = 1$ or $v = 0$, and hence to $T = \infty$! Larger values of $\tilde{x}$ then correspond to antiferromagnetic coupling. These limits are indicated by arrows on the $\ln\tilde{x}$ axes in Figs. 6 and 7. It is however, surprising that the plots for different n remain close to one another, even as the limits are approached and passed.

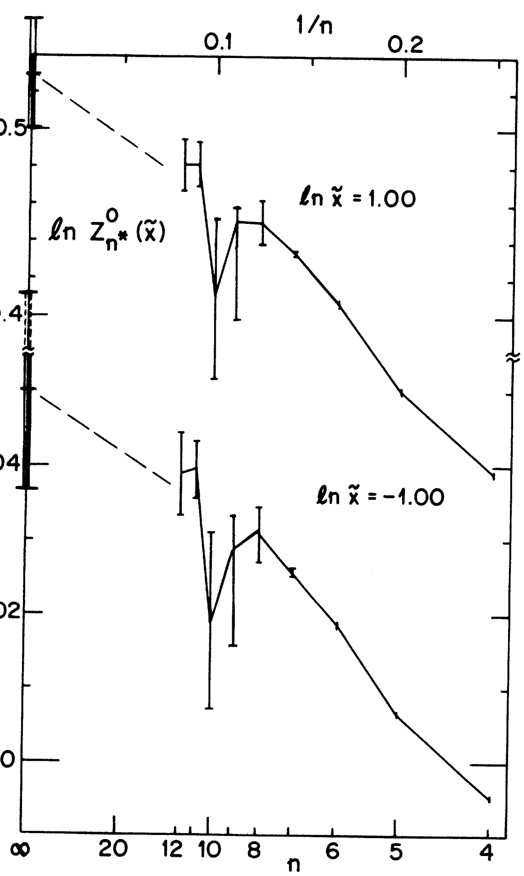

FIG. 8. Representative extrapolations for the periodic scaling function $\ln Z^0(\tilde{x})$ at fixed $\tilde{x}$.

TABLE VIII. Extrapolated values of the scaling functions $Z^0(\tilde{x})$ for periodic boundary conditions, $Z^1(\tilde{x})$ for free surfaces, and the logarithm of the bulk asymptotes (in parentheses) as a function of $\ln\tilde{x} = \ln\{n^{1/\nu}[1 - v/v_c(n)]\}$.

$\ln\tilde{x}$	$\ln Z^0(\tilde{x})$	$\ln Z^1(\tilde{x})$
$-\infty$	-0.0726	0.1823
-6.0	-0.0713	0.1827
-4.0	-0.066 ± 1	0.1853 ± 5
-3.0	-0.055 ± 3	0.1914 ± 20
-2.0	-0.024 ± 5	0.2045 ± 25
-1.5	$+0.005 \pm 10$	
-1.0	0.050 ± 13	0.243 ± 7
-0.5	0.120 ± 15	0.278 ± 10
0.0	0.220 ± 5 (0.0166)	0.336 ± 10
0.5	0.350 ± 18 (0.2662)	0.415 ± 15
1.0	0.530 ± 20 (0.5162)	0.540 ± 22
1.5	0.730 ± 25 (0.7762)	0.700 ± 20 (0.4012)
2.0	0.98 ± 3 (1.016)	0.905 ± 25 (0.7655)
2.25	1.10 ± 4 (1.141)	1.1010 ± 25 (0.9319)
2.5	1.24 (1.266)	1.13 ± 3 (1.091)
2.75	(1.391)	1.255 ± 20 (1.244)
3.0	(1.516)	1.40 ± 2 (1.392)
3.5	(1.766)	(1.678)
4.0	(2.016)	(1.953)

The behavior of the data for *free surfaces* ($\tau = 1$) is significantly different. In the first place, different approximants for fixed n agree closely with one another up to $n = 9$; for $n \geqslant 10$ the agreement deteriorates abruptly and the data are of no aid to the extrapolation. (The $n = 4$ approximants show significant but not disturbing dispersion for reasons not elucidated.) Second, there is a clear odd-even alternation. Third, there is still a well-defined linear trend versus $1/n$, but it is downwards for $\tilde{x} \lesssim 12$ ($\ln\tilde{x} \lesssim 2.5$), although it becomes upwards for larger $\tilde{x}$. The apparent precision of the linear extrapolants can be seen in the last column of Table VIII. It is better than $\pm\frac{1}{2}\%$ up to $\tilde{x} \simeq 0.3$, but rises to $\pm 2\%$ around $\tilde{x} = 3$, and to $\pm 3\%$ for $\tilde{x} \gtrsim 12$. The values in parentheses again represent the asymptote but this time in the form appropriate for free surfaces. It appears from plots of the tabular values, as shown in Fig. 7, that $Z^1(\tilde{x})$ approaches the asymptote from *above* and merges with it to within 1% for $\tilde{x}>17$ ($\ln\tilde{x}\gtrsim 2.85$). The quoted uncertainties of the Z^τ estimates do not, of course, include the ±2% uncertainty in the normalizing values of $\tilde{X}_0^\tau$.

In summary, we believe on the basis of the evidence discussed that the existence of asymptotic scaling functions for both periodic and free-surface conditions can be asserted with reasonable confidence. The numerical values of the scaling functions should be close to the estimates presented in Table VIII and shown as dotted curves in Figs. 6 and 7; for values of $\tilde{x}$ larger than those shown in Table VIII the asymptotic expressions apply to within the precision available. It is striking that over the whole range of finite $\tilde{x}$ the scaling functions for periodic and free-surface conditions exhibit significant quantitative differences. [The plots of Z^0 and Z^1 cross around $\tilde{x}=3.3$ ($\ln\tilde{x}=1.2$).] These differences are, of course, just an indication of the importance of boundary conditions in finite-size phenomena. (See also Ref. 23.)

B. Piecewise analytic approximants

As stated, the numerical evidence indicates that for large $\tilde{x}$ (specifically $\tilde{x}\geqslant 17$) the scaling functions may be represented analytically by their asymptotic forms already determined in terms of X_∞ and Y_∞ [see (2.31) and (5.2)]. For convenience we quote here the necessary values

$$\tilde{X}_\infty=1.0163, \quad \tilde{Y}_\infty=-0.815\pm 5\,. \tag{5.4}$$

From (2.30) and (5.1) we see that

$$Z^\tau(\tilde{x})=\tilde{X}_0^\tau+\tilde{X}_1^\tau\tilde{x}+\tilde{X}_2\tilde{x}^2+\cdots \tag{5.5}$$

should represent the behavior of the modified scaling functions as $\tilde{x}\to 0$. It is straightforward to estimate the initial slopes $\tilde{X}_1^\tau$ from the data shown in Table VIII. By adopting the *central value* of the estimate one can then form rough estimates for the quadratic coefficient $\tilde{X}_2^\tau$. In this way we find for periodic boundary conditions

$$\tilde{X}_0^0=0.93\pm 2,\quad \tilde{X}_1^0=0.34\pm 3,\quad \tilde{X}_2^0\simeq -0.025\,, \tag{5.6}$$

$$X_0^0=0.98\pm 2,\quad X_1^0=0.35\pm 3,\quad X_2^0\simeq -0.025\,, \tag{5.7}$$

respectively, for $\tilde{x}$ and x, while for free-surface films we obtain

$$\tilde{X}_0^1=1.20\pm 2,\quad \tilde{X}_1^1=0.20\pm 2,\quad \tilde{X}_2^1\simeq -0.0038\,, \tag{5.8}$$

$$X_0^1=1.27\pm 2,\quad X_1^1=0.20\pm 2,\quad X_2^1\simeq -0.0038\,. \tag{5.9}$$

Numerically, the linear region extends to about $\tilde{x}=0.4$ for $\tau=0$ and $\tilde{x}=1$ for $\tau=1$. The truncated quadratic expressions then fit well up to $\tilde{x}=3$ and $\tilde{x}=10$, respectively.

Alternate two parameter fits (not counting $\tilde{X}_0^\tau$ which is "given") can be found for the scaling functions by using the [1/1] Padé approximant

$$Z^\tau(\tilde{x})=(\tilde{X}_0^\tau+\tilde{p}^\tau\tilde{x})/(1+\tilde{q}^\tau\tilde{x})\,. \tag{5.10}$$

At the cost of slight deviation from the central estimates of Table VIII, one can choose values of $\tilde{p}^\tau$ and $\tilde{q}^\tau$ which yield agreement within the quoted uncertainties for all the values in Table VIII for which reasonable extrapolations can be made. Specifically, for periodic conditions we find that

$$\tilde{p}^0=0.364,\quad \tilde{q}^0=0.047 \tag{5.11}$$

yield a good fit up to $\tilde{x}\simeq 10$ ($\ln\tilde{x}\simeq 2.3$). However, at $\tilde{x}\simeq 16$ ($\ln\tilde{x}\simeq 2.8$) the fits fall about 5% below the asymptotic values. As mentioned, the asymptote probably represents the correct result to within 1% at that point. Effectively then, (5.2) and (5.4) combined with (5.10) and (5.11) provide analytic fits over the whole range of $\tilde{x}$. However, the values of $\tilde{p}^0$ and $\tilde{q}^0$ chosen in (5.11) yield a slope $\tilde{X}_1^0\simeq 0.32$ which falls somewhat below the central estimate in (5.6), although within the range of uncertainty. Correspondingly, it implies $\tilde{X}_2^0\simeq -0.0015$.

A similar study for free-surface conditions reveals that the choice

$$\tilde{p}^1=0.228,\quad \tilde{q}^1=0.023 \tag{5.12}$$

is consistent with the estimate $\tilde{X}_1^1=0.200$ and agrees well with the central estimates up to $\tilde{x}\simeq 17$–18 ($\ln\tilde{x}=2.85$); indeed, the fit in this region matches the value of the asymptote to within $\frac{1}{2}$%. For higher values of $\tilde{x}$ the asymptote itself should be accurate as mentioned. The quadratic coefficient $\tilde{X}_2^1$ implied by (5.10) and (5.12) has the value -0.0046, which may be compared with (5.8).

While the simplicity and accuracy of the fits just found are very satisfying, and should meet the needs of a comparison with experiment, it would clearly be desirable to find *single* analytic functions which provide good fits over the whole range of x. In addition, the fitting functions should exhibit the correct asymptotic behavior (including appropriate exponential approach to this behavior) at both ends of the range.

C. Approximants with correct analytic form

The search for a functional form which satisfies the analytic requirements discussed in Sec. II and which fits the numerical extrapolations turns out to be a surprisingly tricky problem. The analytic requirements immediately eliminate an approximant of the simple form

$$Z^\tau(\tilde{x})=Z_0^\tau(1+b\,\tilde{x}^{\,\nu})^{(\dot{\gamma}-\gamma)\theta}, \tag{5.13}$$

since for small $\tilde{x}$ it has an expansion in powers of

$\tilde{x}^{\nu}$ instead of in powers of $\tilde{x}$. Again, for large $\tilde{x}$ the leading power expansion is in powers of $\tilde{x}^{-\nu}$, which does not satisfy (5.2) for $\tau=0$. This leads to consideration of functions of the form

$$Z^{\tau}(\tilde{x}) = Z_0^{\tau}[\ln(b + e^{\tilde{c}\,\tilde{x}^{\nu}})]^{(\dot{\gamma}-\gamma)\theta}, \tag{5.14}$$

which exhibit the required exponential approach to the asymptote for $\tau=0$ at large $\tilde{x}$ but have the same difficulty as (5.13) for small $\tilde{x}$.

To overcome these difficulties let us introduce the function

$$L^{\psi}(u,v) = [\ln(u+e^{v})]^{\psi}, \tag{5.15}$$

with limiting behavior

$$\begin{aligned} L^{\psi}(u,v) &= [\ln(1+u)]^{\psi} + \frac{\psi[\ln(1+u)]^{\psi-1}}{1+u}\,v \\ &\qquad + O(v^2) \quad \text{as } v\to 0, \\ &= v^{\psi} + \psi u e^{-v}/v + O(e^{-2v}) \quad \text{as } v\to\infty. \end{aligned} \tag{5.16}$$

In terms of this function the form

$$Z^{\tau}(\tilde{x}) = Z_u^{\tau} L^{(\dot{\gamma}-\gamma)\theta}(a, L^{\nu}(b,\tilde{c}\,\tilde{x})) \tag{5.17}$$

is found to satisfy the requirements for periodic boundary conditions both for small and large $\tilde{x}$. To obtain the additional single power-law corrections required for free-surface boundary conditions ($\tau=1$) a sum of two terms of this form may be used.

Unfortunately, however, these forms contain a very limited number of parameters and so are unsuitable for practical fitting requirements. The function (5.17) may be generalized to the set of approximants

$$Z^{\tau}(\tilde{x}) = Z_0^{\tau}\left[\ln\left(\sum_{m=0}^{N} a_m \exp[mL^{\nu}(b,\tilde{c}\,\tilde{x})]\right)\right]^{(\dot{\gamma}-\gamma)\theta}, \tag{5.18}$$

with $a_N=1$, which has an expansion in powers of $\tilde{x}$ for $\tilde{x}\to 0$, and the desired asymptotic expansion as $\tilde{x}\to\infty$. These approximants are sufficiently complex that the only tractable technique for fitting the numerical estimates seems to be to build in the desired $\tilde{x}\to 0$ and $\tilde{x}\to\infty$ behavior and to use a least-square fitting routine in the intermediate or crossover region.

A second variation of (5.17) is obtained by noting that the parameter b may be replaced by a finite polynomial in $\tilde{x}$, say $B(\tilde{x})$. These approximants again have correct asymptotic forms. Moderately satisfactory fits to the numerical estimates have been obtained using approximants of the form (5.18) [and the replacement of b by $B(\tilde{x})$ has also been explored to some extent]. However, to avoid significant "over swing" or, conversely, unphysical oscillations, in the crossover region, requires use of four or more parameters a_m. In view of the intrinsic complexity of these analytic approximants, which seems hard to avoid, such fits appear of doubtful practical value at this time and will not be quoted. The earlier, piecewise approximants form a simpler numerical synopsis of our results which should be useful (see further below).

D. Summary

For convenience we summarize here our estimates for the asymptotic crossover behavior of the reduced susceptibilities of n-layer ferromagnetic Ising films. In terms of the reduced deviation

$$\dot{t} = [T - T_c(n)]/T_c(\infty) \tag{5.19}$$

from the critical temperature $T_c(n)$ of the film of n layers, and the scaling variable

$$x = n^{1/\nu}\dot{t}, \tag{5.20}$$

where ν is defined via the temperature dependence of the "true" or exponential bulk correlation length[26,34] in the critical region as

$$\xi(T) \approx fa\dot{t}^{-\nu} \quad (n=\infty, \dot{t}\to 0), \tag{5.21}$$

the results are as follows. The n-layer reduced susceptibility per spin may be written asymptotically

$$\begin{aligned} (k_B T/m^2)\chi_T^{\tau}(n;T) &= \chi_n^{\tau}(\dot{t}) \\ &\approx n^{\gamma/\nu} X^{\tau}(x), \quad (n\to\infty,\ \dot{t}\to 0), \end{aligned} \tag{5.22}$$

where $\tau=0,1$ denotes periodic or free-surface boundary conditions, respectively. The exponent γ is defined by the divergence of the bulk ($n=\infty$) susceptibility; for $n<\infty$ the divergence is described by an exponent $\dot{\gamma}$.

For the simple cubic Ising model with nearest-neighbor interactions we estimate the scaling function as

$$\begin{aligned} X^{\tau}(x) &\simeq x^{-\dot{\gamma}}\,\frac{X_0^{\tau}+p^{\tau}x}{1+q^{\tau}x} \qquad \text{for } x \lesssim x_0^{\tau}, \\ &\simeq x^{-\gamma}(X_\infty + \tau Y_\infty x^{-\nu}) \quad \text{for } x \gtrsim x_0^{\tau}, \end{aligned} \tag{5.23}$$

where $\gamma=\frac{5}{4}$, $\dot{\gamma}=\frac{7}{4}$, $\nu=\frac{9}{14}$, $X_\infty=1.0585$, and $Y_\infty=-0.867$. Best estimates for the small x parameters are

$$\begin{aligned} &X_0^0=0.98,\quad p^0=0.373,\quad q^0=0.0455 \ \text{(periodic)}, \\ &X_0^1=1.27,\quad p^1=0.234, \\ &\qquad\qquad q^1=0.0223 \ \text{(free surface)}. \end{aligned} \tag{5.24}$$

The limits of validity of the small-x and large-x forms in (5.26) are specified by

$$x_0^0 \simeq 9 \text{ and } x_0^1 \simeq 18. \qquad (5.25)$$

The over-all precision should be ±2% or better but it should be recalled that for small n (say, $n \lesssim 7$) the corrections to the asymptotic behavior may be larger than this, even when x is small. Indeed, a full crossover from bulk to finite behavior is observable only in films with n significantly larger than 10.

In accordance with universality[3,28,29] concepts, which we have tested to some degree in the study of the surface susceptibility, the form of the scaling functions $X^\tau(x)$ should apply to all Ising-like[3] ferromagnetic films. As explained in Sec. II [see Eq. (2.32)] it is merely necessary (*i*) to multiply the scaling function X^τ by the ratio $C_{(\mathcal{L})}/C_{(\mathrm{sc})}$, where $C_{(\mathcal{L})}$ and $C_{(\mathrm{sc})}$ are the amplitudes of the bulk susceptibility divergence for the system in question and the simple cubic nearest-neighbor Ising model, respectively; and (*ii*) to multiply the scaling variable x by the corresponding ratio $(c_{(\mathcal{L})}/c_{(\mathrm{sc})})^{1/\nu}$, where $c = a'/fa$; the correlation length amplitude f here is defined in (5.21) while a' and a are the interlayer and nearest-neighbor lattice spacings, respectively.

A useful way of displaying the crossover behavior[39,40] is in terms of the *effective critical exponent*

$$\gamma^*(n;T) = -\left[T - T_c(n)\right]\frac{\partial}{\partial T}\ln \chi_T(n;T). \qquad (5.26)$$

In the asymptotic region $n \to \infty$, $T \to T_c(n)$ this should approach the scaled form

$$\gamma^*(n;T) \approx \Gamma(\xi/L) = \Gamma(1/cn\dot{t}^{\nu}) = \Gamma(x^{-\nu}/c), \qquad (5.27)$$

where the universal crossover function $\Gamma(y^{-1})$ can be derived from (5.22) and (5.23). The asymptotic behavior of γ^* with $\xi(T)/L$ and with $x = n^{1/\nu}\dot{t}$ for the sc lattice is shown in Fig. 9 (upper and lower scales, respectively). The effective exponent crosses over from $\gamma = 1.25$ at small ξ/L (large x) to $\dot{\gamma} = 1.75$ at large ξ/L. The crossover for free-surface films commences at much smaller values of ξ/L than for periodically connected films, and initially has a marked under-swing to values of γ^* *lower* than γ. This arises directly from the negative contribution due to the surface susceptibility. In the region $\xi/L \simeq 10^{-2}$, where γ^* already starts to depart strongly from γ, the two approximating analytic forms in (5.23) for x small and large do

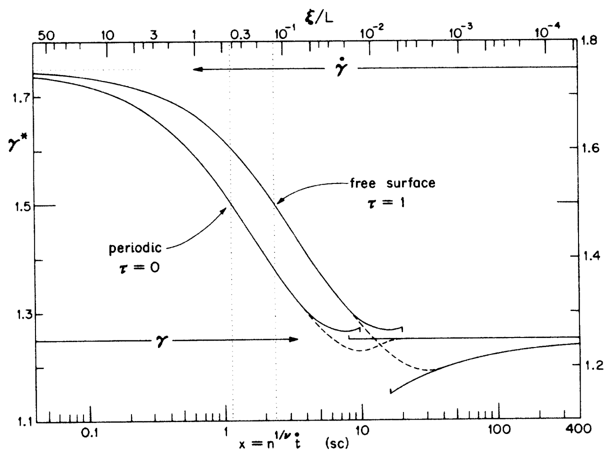

FIG. 9. Asymptotic behavior of the effective critical exponent $\gamma^*(n;T)$ as a function of ξ/L (upper scale) or x for the sc lattice (lower scale) for periodic and free-surface films. The solid lines represent the piecewise analytic approximants developed in the text. The dashed curves represent appropriate interpolating behavior.

not quite meet (see the solid lines in the figure); this, of course, is hardly surprising. The dashed curve which joins the limiting forms smoothly is drawn to recognize that $X^\tau(x)$ itself must be continuous. For this reason γ^* for periodic films also exhibits a small under swing as shown. The *halfway crossover point* $\gamma^* = \frac{1}{2}(\gamma + \dot{\gamma}) = 1.50$ is reached for free-surface films at the surprisingly small value $\xi/L \simeq \frac{1}{8}$; for periodic conditions it occurs at $\xi/L \simeq 0.4$. Finally, in applying these results to real systems, one must remember that correction-to-scaling terms will be present at finite n and $T - T_c(n)$. However, as the complete crossover occurs over about two decades in $T - T_c(n)$ many effects should be experimentally observable.

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