Helmholtz free energy of electrons scattered in the presence of a strong magnetic field by randomly distributed impurity centers is developed in ascending powers of the scattering potential to terms of fourth order. The free energy is evaluated for impurities represented by a short-range screened Coulomb potential, which gives as expected a result essentially independent of the exact form of the potential function.

For randomly distributed impurities, the first-order correction to the free energy vanishes; this result is independent of the exact form of the impurity potential. The second-order correction to the free energy, which contributes only to the periodic susceptibility, is in essential agreement with an earlier result found by a different and somewhat less general method. The third-order correction to the free energy is found to contain only periodic components involving the magnetic field. The previous conclusion that impurity scattering does not affect the periodic susceptibility, provided $KT \gg \hbar/\tau$, is extended to terms of third order in the scattering potential.

The influence of collisions on the nonperiodic part of the magnetic susceptibility first appears in terms of fourth order, where, as expected, additional contributions to the periodic susceptibility also occur. The influence of collisions on the constant susceptibility is shown to be small when $\eta^{(0)} \gg \hbar/\tau$, as predicted by Peierls; this condition is much less stringent than the condition $KT \gg \hbar/\tau$ that was previously thought to apply.

The steady diamagnetism turns out to be increased in magnitude by collisions, a rather unexpected result. However, as has already been pointed out by Dingle,[6] this appears quite reasonable when it is remembered that the steady diamagnetism actually has its origin in a type of broadening of the energy levels,[17,18] that due to the unquantized motion along the direction of the magnetic field; in a two-dimensional system the nonperiodic term in the susceptibility is entirely absent.[19]

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Bounded and Inhomogeneous Ising Models. I. Specific-Heat Anomaly of a Finite Lattice

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The critical-point anomaly of a plane square $m\times n$ Ising lattice with periodic boundary conditions (a torus) is analyzed asymptotically in the limit $n\rightarrow\infty$ with $\xi=m/n$ fixed. Among other results, it is shown that for fixed $\tau=n(T-T_c)/T_c$, the specific heat per spin of a large lattice is given by

$$C_{mn}(T)/k_B mn = A_0 \ln n + B(\tau,\xi) + B_1(\tau)(\ln n)/n + B_2(\tau,\xi)/n + O[(\ln n)^3/n^2],$$

where explicit expressions can be given for A_0 and for the functions B, B_1, and B_2. It follows that the specific-heat peak of the finite lattice is rounded on a scale $\delta=\Delta T/T_c\sim 1/n$, while the maximum in $C_{mn}(T)$ is displaced from T_c by $\epsilon=(T_c-T_{\max})/T_c\sim 1/n$. For $\xi_0>\xi>\xi_0^{-1}$, where $\xi_0=3.13927\cdots$, the maximum lies *above* T_c; but for $\xi>\xi_0$ or $\xi<\xi_0^{-1}$, the maximum is depressed below T_c; when $\xi=\infty$, ξ_0, or ξ_0^{-1}, the relative shift in the maximum from T_c is only of order $(\ln n)/n^2$. Detailed graphs and numerical data are presented, and the results are compared with some for lattices with free edges. Some heuristic arguments are developed which indicate the possible nature of finite-size critical-point effects in more general systems.

1. INTRODUCTION AND SUMMARY

THE experimental and theoretical study of critical phenomena has made notable advances in the last few years.[1–3] On the theoretical side, however, most attention has been paid to the behavior of infinite, homogeneous systems. Real physical systems, on the other hand, are finite and possess boundaries, surfaces, and interfaces which can make measurable contributions to the observed thermodynamic properties; furthermore, real systems are usually inhomogeneous on some scale containing, for example, impurity atoms, random point defects, grain boundaries, dislocation nets, strains, etc., which might all be expected to "round" or "smear out" in some way a sharp critical point. Indeed, the best measurements of specific-heat anomalies in solid-state systems display a rounding of the specific-heat peaks which is definitely intrinsic to

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the samples studied[4–8] (rather than an instrumental or truncation effect, due to use of finite temperature increments, etc.).

The theoretical problems posed by a serious consideration of boundary and inhomogeneity effects on critical point behavior are extensive and difficult. In this series of articles we make a modest approach to some aspects of these problems by studying in detail the properties of planar Ising models which are finite, have surfaces and interfaces and contain point impurities, grain boundaries, etc.[9–13] The Ising model in its various forms is known to be a good first approximation for studying the critical behavior of many types of systems[1]; our restriction to two-dimensional planar Ising lattices is motivated by a desire for an exact and precise mathematical treatment; we hope that a rigorous knowledge of the two-dimensional behavior will serve as a guide to drawing reliable conclusions about more realistic three-dimensional models.

The present article is mainly devoted to a calculation of the critical properties of a finite Ising model consisting of a square $m\times n$ lattice with periodic boundary conditions (i.e., the lattice is wrapped on a torus). While in a direct comparison with real systems, the periodic boundary conditions are certainly artificial, they have the conceptual advantage of enabling one to separate the effects of finite size *alone* from those associated with a real boundary or edge. (The thermodynamic properties of boundaries will be discussed in a later paper.[9]) As usual, each nearest-neighbor pair of spins, i and j, are coupled with an energy $-4JS_i^zS_j^z$, where S_i^z, $S_j^z=\pm\frac{1}{2}$.

The specific-heat anomaly per spin of an infinite square Ising lattice in zero field has the form[14]

$$\begin{aligned}C(T)/k_B&=\lim_{m,n\to\infty} C_{mn}(T)/k_{\mathrm{B}}mn\\&=A_0\ln|(T/T_c)-1|+A_1\\&\quad+O\{[(T/T_c)-1]\ln|(T/T_c)-1|\},\quad(1.1)\end{aligned}$$

that is, it displays a logarithmically infinite and perfectly sharp singularity as a function of temperature T. Already in his original paper, however, Onsager considered the specific heat of an infinite cylinder ($m=\infty$) of finite width n.[14] He showed that the specific heat of such a finite width cylinder *at* the limiting critical point $T=T_c$ behaved for large n as

$$\begin{aligned}C_n(T)/k_B&=\lim_{m\to\infty} C_{mn}(T_c)/k_{\mathrm{B}}mn\\&=A_0\ln n+B_\infty+o(1),\quad(1.2)\end{aligned}$$

where A_0 is the same constant as in (1.1); he also concluded that the temperature $T_{\max}$ at which $C_n(T)$ had its maximum was removed from the limiting critical point T_c by a term of relative order only $(\ln n)/n^2$. We will show that (1.2) extends into the more general critical point result

$$C_{mn}(T_c)/k_{\mathrm{B}}mn=A_0\ln n+B(0,\xi)+O[(\ln n)^3/n^2]\quad(1.3)$$

as m, $n\to\infty$, where

$$\xi=m/n\quad(1.4)$$

determines the "shape" of the torus and remains fixed fixed as m, $n\to\infty$. It is notable that the coefficient of the divergent part $\ln n$ remains unchanged.

For fixed temperatures $T\neq T_c$ the approach of $C_{mn}(T)/mn$ to its limit (1.1) is, ultimately, exponentially fast in m and n. However, we shall show that asymptotically there is a region of width

$$\Delta T^{\times}(n)\approx a/n\quad(1.5)$$

about T_c, over which the critical point is "spread" and in which convergence to the thermodynamic limit does *not* occur. For temperatures measured on the corresponding reduced scale by

$$\tau\approx(T-T_c)/\Delta T^{\times}(n),\quad(1.6)$$

we find

$$\begin{aligned}C_{mn}(T)/k_{\mathrm{B}}mn&=A_0\ln n+B(\tau,\xi)+B_1(\tau,\xi)(\ln n)/n\\&\quad+B_2(\tau,\xi)/n+O[(\ln n)^3/n^2],\quad(1.7)\end{aligned}$$

where the functions B, B_1, and B_2 can be given explicitly [see the formula (4.17) to (4.22) below]. From this we conclude, in contradistinction to Onsager's special case $\xi=\infty$, that for $0<\xi<\infty$ the "shift" in $T_{\max}$ is

$$\epsilon=(T_c-T_{\max})/T_c\approx a^*(\xi)/n,\quad(n\to\infty).\quad(1.8)$$

For the symmetric case $n=m$, or $\xi=1$, we find

$$a^*(1)\simeq-0.3603,\quad(1.9)$$

so that $T_{\max}>T_c$; this asymptotic result is already evident in the explicit numerical calculations for small $m=n$ displayed in Fig. 1. It might be interpreted as an indication of increased cooperation between nearby spins as a result of extra "communication" via paths that encircle the torus. (By contrast, if boundaries in the shape of "free" edges are present we expect $T_{\max}$

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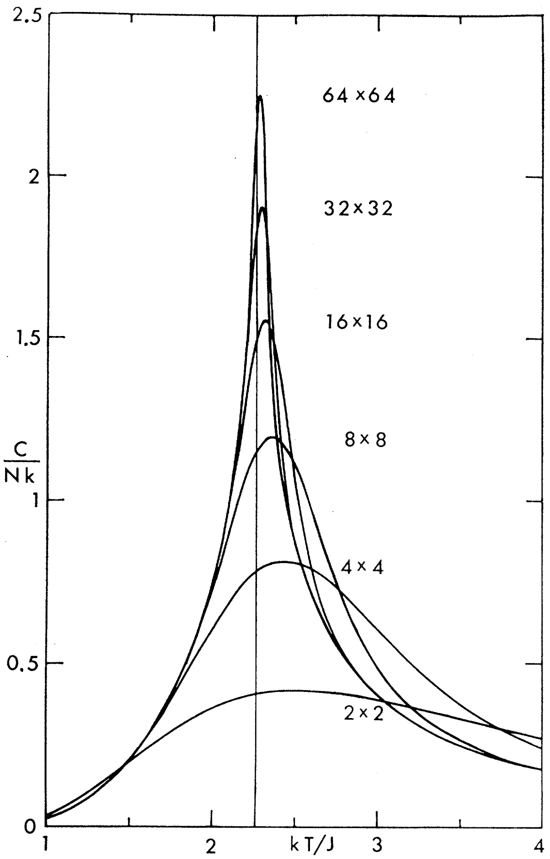

FIG. 1. The specific heat per spin for small Ising lattices; exact results for the $m\times n$ square lattice with periodic boundary conditions are displayed for $m=n=2, 4, 8, 16, 32$, and 64 ($N=mn$). The limiting critical point is marked by a vertical line.

$<T_c$; see Ref. 9 and the concluding section below.) However for an *asymmetric* torus we find, surprisingly, that $T_{\max}$ remains above T_c *only* for $\xi_0>\xi>\xi_0^{-1}$, where $\xi_0\simeq 3.139$; when $\xi>\xi_0$ or $\xi<\xi_0^{-1}$ the maximum is displaced *below* the limiting critical point, (i.e., $a^*(\xi)$ becomes positive). The reason for this change of behavior at $\xi=\xi_0$ is not understood; it illustrates an unexpected subtlty of finite-size behavior.

The main character of our conclusions can be summarized by the approximate formula

$$C_{mn}(T)/k_B mn \simeq \mathcal{A}_0(T)\ln\{[(T/T_c)-1+(a^*/n)]^2+b^2/n^2\}^{-1/2} +\mathcal{B}_0(T), \quad (1.10)$$

in which $\mathcal{A}_0(T)$ and $\mathcal{B}_0(T)$ are slowly varying functions of T with only a weak dependence on n and m (say, relative terms of order $1/n$). The dominant rounding and shift of the specific-heat maximum are evident from this formula.

The calculations leading to the above results are based on Kaufman's exact expressions for the partition function of a square lattice on a finite torus.[15] The necessary analysis is fairly long and intricate; hence the reader interested only in the results is advised to omit Secs. 2, 3, and 4 and to read only the concluding Sec. 5, where the asymptotic results are discussed graphically, and specific results for small finite n and m are exhibited. This review leads to a number of more general heuristic arguments of relevance to three-dimensional and non-Ising systems.

The general nature of the calculation is quite similar to, but more involved than, that employed recently[16] to study finite-size and boundary effects in a plane square lattice filled with rigid dimers.[17] Indeed, the dimer problem is effectively equivalent to that of the Ising model *at* $T=T_c$; in this latter case we find, as in the dimer analysis, that the results can be expressed exactly in terms of elliptic theta functions. For $T\neq T_c$ we have to define an extensive set of generalized theta functions, and related sums and products, etc., which are, however, easily computed numerically.

Of the following sections the first, Sec. 2, sets out the basic formulas for the partition function, energy, and specific heat of a finite torus, and for various auxiliary functions which arise, in particular, the reduced temperature variable $\tau(T)\sim n(T-T_c)/T_c$. In Sec. 3 the main steps of the asymptotic analysis needed to evaluate the partition function for large n at fixed τ and ξ are presented; the final expressions are (3.36) and (3.37). Lastly, in Sec. 4 we sketch the analysis of the range of sums needed for the energy and specific heat; the results are contained in (4.13)–(4.25). As mentioned already, the asymptotic results are discussed and related to calculations for small finite n and more general critical-point considerations in the concluding section.

2. GENERAL EXPRESSIONS

The canonical partition function $Z_{mn}(T)$ of a finite $m\times n$ square Ising lattice wrapped on a torus and in zero magnetic field is[15]

$$Z_{mn}(T)=\tfrac{1}{2}(2\sinh 2K)^{\frac{1}{2}mn}\sum_{i=1}^{4} Z_i(K), \quad (2.1)$$

in which the reciprocal temperature variable is

$$K=J/kT. \quad (2.2)$$

and where J $(=J_x=J_y)$ is the nearest-neighbor spin-coupling energy. The partial partition functions $Z_i(K)$ are defined by

$$Z_1=\prod_{r=0}^{n-1} 2\cosh\tfrac{1}{2}m\gamma_{2r+1}, \quad Z_2=\prod_{r=0}^{n-1} 2\sinh\tfrac{1}{2}m\gamma_{2r+1},$$
$$Z_3=\prod_{r=0}^{n-1} 2\cosh\tfrac{1}{2}m\gamma_{2r}, \quad Z_4=\prod_{r=0}^{n-1} 2\sinh\tfrac{1}{2}m\gamma_{2r}, \quad (2.3)$$

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where

$$\cosh\gamma_l = c_l = \cosh 2K \coth 2K - \cos(l\pi/n) \tag{2.4}$$

so that

$$\begin{aligned}\gamma_0 &= 2K + \ln\tanh K,\\ \gamma_l &= \ln[c_l + (c_l^2-1)^{1/2}], \quad l\neq 0.\end{aligned} \tag{2.5}$$

We note that $\gamma_l = \gamma_{2n-l}$ and that for $0\leq l\leq n$ the function γ_l is monotonically increasing in l.

The internal energy per spin is given by

$$\begin{aligned}\frac{U_{mn}}{mn} &= -(mn)^{-1}J\frac{d}{dK}\ln Z_{mn},\\ &= -J\coth 2K - \frac{J}{mn}[\sum_{i=1}^{4} Z_i'][\sum_{i=1}^{4} Z_i]^{-1},\end{aligned} \tag{2.6}$$

while the specific heat per spin is

$$\begin{aligned}C_{mn}/k_{\mathrm{B}}mn &= (mn)^{-1}K^2(d^2/dK^2)\ln Z_{mn},\\ &= -2K^2\operatorname{csch}^2 2K\\ &\quad + \frac{K^2}{mn}\left\{\frac{\sum_{i=l}^{4} Z_i''}{\sum_{i=1}^{4} Z_i} - \left[\frac{\sum_{i=l}^{4} Z_i'}{\sum_{i=1}^{4} Z_i}\right]^2\right\},\end{aligned} \tag{2.7}$$

where the primes here and below denote differentiation with respect to K. From (2.3) we obtain the more explicit expressions

$$\begin{aligned}Z_1'/Z_1 &= \tfrac{1}{2}m\sum_{r=0}^{n-1}\gamma_{2r+1}'\tanh\tfrac{1}{2}m\gamma_{2r+1},\\ Z_2'/Z_2 &= \tfrac{1}{2}m\sum_{r=0}^{n-1}\gamma_{2r+1}'\coth\tfrac{1}{2}m\gamma_{2r+1},\end{aligned} \tag{2.8}$$

with analogous expressions for Z_3' and Z_4' in terms of γ_{2r}' and γ_{2r}. The second derivatives are given by

$$\begin{aligned}Z_1''/Z_1 = {}&[\tfrac{1}{2}m\sum_{r=0}^{n-1}\gamma_{2r+1}'\tanh\tfrac{1}{2}m\gamma_{2r+1}]^2\\ &+\tfrac{1}{2}m\sum_{r=0}^{n-1}[\gamma_{2r+1}''\tanh\tfrac{1}{2}m\gamma_{2r+1}\\ &+\tfrac{1}{2}m(\gamma_{2r+1}'\operatorname{sech}\tfrac{1}{2}m\gamma_{2r+1})^2],\end{aligned} \tag{2.9}$$

the formula for Z_2'', etc., are obtained from the correspondences:

Z_1'':	$2r+1$,	tanh,	sech
Z_2'':	$2r+1$,	coth,	$i$csch
Z_3'':	$2r$,	tanh,	sech
Z_4'':	$2r$,	coth,	$i$csch.

(The factor $i=\sqrt{(-1)}$ changes the sign of the last term in (2.9) for Z_2'' and Z_4''.)

From these expressions it is clear that our analytical task consists in the asymptotic evaluation of a collection of n-fold products and sums. An obvious first step in view of (2.4), is to introduce the variable $\omega = l\pi/n$ and to convert the sums on r (after taking logarithms of the products) to integrals on ω from 0 to 2π. For real ω the integrands of all the integrals will be analytic and periodic functions of ω unless, for some value of ω the function $\gamma(\omega)$, analogous to γ_l, vanishes. By (2.4) and (2.5) this can occur only for temperatures such that

$$\cosh 2K\coth 2K = \sinh 2K + (\sinh 2K)^{-1} \leq 2. \tag{2.10}$$

This inequality has the unique real positive solution $K = K_c = J/k_{\mathrm{B}}T_c$ ($\omega = 0$) corresponding, in fact, to the critical point at which[14]

$$\sinh^2 2K_c = 1, \quad K_c = \tfrac{1}{2}\ln(1+\sqrt{2}) = 0.44068\cdots. \tag{2.11}$$

Thus, at any temperature $T\neq T_c$ the integrands are analytic periodic functions of ω; under these circumstances the integral approximates the corresponding sum exponentially fast in n, the modulus of the exponential being, in fact, determined by the imaginary part of the root ω_0 of $\gamma(\omega)=0$ which lies nearest to the real axis in the complex ω plane.

Close to T_c, however, convergence will be slow initially since $\mathrm{Im}\{\omega_0\}$ is small and we can expect to find an n-dependent scaling of the temperature deviation from T_c for which the asymptotic behavior will be distinct from that at *fixed* $T\neq T_c$. Consideration of (2.10) and (2.4) suggests introducing the reduced temperature variable τ via

$$\tau^2/n^2 = \tfrac{1}{2}[\sinh 2K + (\sinh 2K)^{-1}] - 1. \tag{2.12}$$

In terms of τ the true temperature is given by [compare with (1.6)]

$$T/T_c = 1 + \tfrac{1}{2}K_c^{-1}(\tau/n) + \tfrac{1}{4}K_c^{-2}(\tau^2/n^2) + \cdots. \tag{2.13}$$

In the remainder of our analysis we will consider only the limit in which $n\to\infty$ with τ and $\xi = m/n$ fixed (with $0<\xi<\infty$).

In terms of the variable τ we have for $l\neq 0$

$$\begin{aligned}\exp\tfrac{1}{2}\gamma_l(\tau) = {}&[1+(\tau/n)^2+\sin^2(l\pi/2n)]^{1/2}\\ &+[(\tau/n)^2+\sin^2(l\pi/2n)]^{1/2},\end{aligned} \tag{2.14}$$

while

$$\begin{aligned}c_l^2 - 1 = {}&4[(\tau/n)^2+\sin^2(l\pi/2n)]\\ &\times[1+(\tau/n)^2+\sin^2(l\pi/2n)].\end{aligned} \tag{2.15}$$

From here and (2.5) we find

$$\gamma_0 = -2(\tau/n) - \tfrac{1}{2}\sqrt{2}(\tau/n)^2 + O[(\tau/n)^3] \tag{2.16a}$$

and for $l\neq 0$ and $l/n\ll 1$

$$\begin{aligned}\gamma_l(\tau) = {}&(2/n)(\tau^2+\tfrac{1}{4}l^2\pi^2)^{1/2}\\ &-(\pi/24)(l^3/n^3)\{[1+(2\tau/\pi l)^2]^{3/2}\\ &+(8/l^2)[1+(2\tau/\pi l)^2]^{-1/2}\}+\cdots,\end{aligned} \tag{2.16b}$$

which displays clearly the pertinence of the variable τ. For later convenience we introduce the notation

$$\varphi(\tau,q)=(\tau^2+\pi^2q^2)^{1/2}, \qquad (2.17)$$

and observe that

$$\varphi(\tau,q)\approx\pi q \quad \text{as} \quad q\to\infty. \qquad (2.18)$$

Lastly, we note that

$$\gamma_0'=2(1+\operatorname{csch}2K)=4+2\sqrt{2}(\tau/n)+O[(\tau/n)^2], \quad \gamma_l'=c'(c_l^2-1)^{-1/2}, \quad (l\neq0), \qquad (2.19)$$

$$\gamma_0''=-4\operatorname{csch}2K\coth2K=-4\sqrt{2}-12(\tau/n)+O[(\tau/n)^2], \qquad (2.20)$$
$$\gamma_l''=c''(c_l^2-1)^{-1/2}-(c')^2c_l(c_l^2-1)^{-3/2}, \quad (l\neq0)$$

where

$$c'=c_l'=2\cosh2K(1-\operatorname{csch}^22K)=-8(\tau/n)+O[(\tau/n)^2], \qquad (2.21)$$

and

$$c''=c_l''=8\operatorname{csch}^32K\cosh^22K+4(\sinh2K-\operatorname{csch}2K)=16+24\sqrt{2}(\tau/n)+O[(\tau/n)^2]. \qquad (2.22)$$

It is evident from (2.19), (2.20), and (2.16) that many of the sums required for Z_i' and Z_i'' will be singular for small r and τ. Our approach will consist of isolating successively the most singular pieces and bounding the remainders as $n\to\infty$.

3. ANALYSIS OF PRODUCTS FOR THE PARTITION FUNCTIONS

From the definition (2.3) we have

$$Z_4=P_4(n)\exp[\tfrac{1}{2}m\sum_{r=0}^{n-1}\gamma_{2r}][1-\exp(-m\gamma_0)], \qquad (3.1)$$

where

$$\ln P_4(n)=\sum_{r=1}^{n-1}\ln[1-\exp(-m\gamma_{2r})], \qquad (3.2)$$

with a similar expression for Z_3; the expressions for Z_1 and Z_2 are analogous except that the factor involving γ_0 does not arise. To evaluate $P_4(n)$ we expand the logarithm, which is justified since γ_{2r} does not vanish for $0<r<n$; this yields

$$\ln P_4(n)=-2\sum_{p=1}^{\infty}p^{-1}\sum_{r=1}^{[\frac{1}{2}n]}\exp(-mp\gamma_{2r}), \qquad (3.3)$$

where $[x]$ denotes the largest integer contained in x. Now the sum on r may be split into two parts as follows:

$$S_p(n)=\sum_{r=1}^{s-1}\exp(-mp\gamma_{2r})+\exp(-mp\gamma_{2s})\sum_{r=s}^{[\frac{1}{2}n]}\exp[-mp(\gamma_{2r}-\gamma_{2s})]. \qquad (3.4)$$

In the second term $\gamma_{2r}-\gamma_{2s}$ is a positive monotonic increasing function for $r>s$. Thus, this sum is bounded by the product of its first term and the number of terms, namely, $([\frac{1}{2}n]-s+1)$; its contribution to $\ln P_4$ is hence bounded as

$$|\ln P_4(n)|_2\leq\tfrac{1}{2}n\ln[1-\exp(-m\gamma_{2s})]^{-1}. \qquad (3.5)$$

Now for $l/n\ll1$ we may use the expression (2.16) for $\gamma_l(\tau)$. For a suitable constant d_1 and $s\gg\tau/\pi$, we can hence obtain a bound

$$|\ln P_4(n)|_2\leq d_1n\exp(-\pi\xi s). \qquad (3.6)$$

This will vanish as $1/n^2$ when $n\to\infty$ provided we choose $s=s(n)$ such that

$$s(n)=[(3/\pi\xi)\ln n]. \qquad (3.7)$$

With this value of s we return to the first sum in (3.4) and note that the expression (2.16) for γ_{2r} may be used throughout the range; in particular, we have

$$m\gamma_{2r}(\tau)=2\xi\phi(\tau,r)+\tfrac{1}{3}\xi\pi(r^3/n^2)+\cdots \qquad (3.8)$$

from which we obtain

$$\Big|S_{p,1}(n)-\sum_{r=1}^{s-1}e^{-2p\xi\varphi(\tau,r)}\Big|\leq d_2\sum_{r=1}^{s-1}(r^3/n^2)e^{-2p\xi\varphi(\tau,r)} \qquad (3.9)$$

for a suitable constant d_2. On the right we may remove the largest value of r^3, namely, $(s-1)^3$ from the summand; on extending the sum to $r=\infty$ a relative error $\exp[-p\xi\varphi(\tau,s)]\sim\exp(-p\pi\xi s)$ is introduced, but by (3.7) this vanishes as $1/n^{3p}$. On substituting these results back into (3.3) and interchanging the sums on p and r once more, we finally obtain

$$\ln P_4(n)=2\sum_{r=1}^{\infty}\ln[1-e^{-2\xi\varphi(\tau,r)}]+O[(\ln n)^3/n^2], \qquad (3.10)$$

or

$$P_4\approx\prod_{r=1}^{\infty}[1-e^{-2\xi\varphi(\tau,r)}]^2=\pi_4(\tau,\xi), \qquad (3.11)$$

where in view of (3.6) and (3.7) the error term arises from the right-hand side of (3.9).

By the same means we obtain the asymptotic formula for the other products

$$P_1(n)=\prod_{r=0}^{n-1}[1+\exp(-m\gamma_{2r+1})]\approx\prod_{r=1}^{\infty}[1+e^{-2\xi\varphi(\tau,r-\frac{1}{2})}]^2=\pi_1(\tau,\xi),$$

$$P_2(n)=\prod_{r=0}^{n-1}[1-\exp(-m\gamma_{2r+1})]\approx\prod_{r=1}^{\infty}[1-e^{-2\xi\varphi(\tau,r-\frac{1}{2})}]^2=\pi_2(\tau,\xi), \qquad (3.12)$$

$$P_3(n)=\prod_{r=1}^{n-1}[1+\exp(-m\gamma_{2r})]\approx\prod_{r=1}^{\infty}[1+e^{-2\xi\varphi(\tau,r)}]^2=\pi_3(\tau,\xi),$$

where, in each case, the errors are of relative order $(\ln n)^3/n^2$. Now, recall that when $\tau=0$, so that $T=T_c$, we have $2\varphi(0,r)=2\pi r$; the products on the right of (3.11) can then be reduced to elliptic theta functions of modulus $q=\exp(-\pi\xi)$. In a notation adapted from Whittaker and Watson[18] we have

$$\theta_0=\prod_{r=1}^{\infty}\left[1-e^{-2r\pi\xi}\right]=e^{\pi\xi/12}(\tfrac{1}{2}\theta_2\theta_3\theta_4)^{\frac{1}{3}}, \qquad (3.13)$$

where

$$\theta_2=\theta_2(0,e^{-\pi\xi})=2\theta_0 e^{-\pi\xi/4}\prod_{r=1}^{\infty}\left[1+e^{-2r\pi\xi}\right]^2,$$

$$\theta_3=\theta_3(0,e^{-\pi\xi})=\theta_0\prod_{r=1}^{\infty}\left[1+e^{-(2r-1)\pi\xi}\right]^2, \qquad (3.14)$$

$$\theta_4=\theta_4(0,e^{-\pi\xi})=\theta_0\prod_{r=1}^{\infty}\left[1-e^{-(2r-1)\pi\xi}\right]^2.$$

Thus, at the critical point itself ($\tau=0$) we find

$$P_1\approx\pi_1(0,\xi)=\theta_3/\theta_0, \qquad P_2\approx\pi_2(0,\xi)=\theta_4/\theta_0,$$
$$P_3\approx\pi_3(0,\xi)=\tfrac{1}{2}\theta_2/\theta_0 e^{-\pi\xi/4}, \quad P_4\approx\pi_4(0,\xi)=\theta_0^2. \qquad (3.15)$$

Similar reductions to elliptic θ functions take place at $T=T_c$ for the other sums and products arising below in the analysis.

Now the sums of Z_i in (2.1), (2.6), and (2.7) are conveniently dealt with by removing Z_1 and considering the ratios

$$R_i(n)=Z_i/Z_1. \qquad (3.16)$$

From (2.3), (3.12), and the formulas analogous to (3.1) we have

$$R_1=1, \quad R_2(n)\approx R_2=\pi_2(\tau,\xi)/\pi_1(\tau,\xi), \qquad (3.17)$$

while

$$R_3(n)\approx R_3=2\cosh(\tfrac{1}{2}m\gamma_0)P_0\pi_3(\tau,\xi)/\pi_1(\tau,\xi),$$
$$R_4(n)\approx R_4=2\sinh(\tfrac{1}{2}m\gamma_0)P_0\pi_4(\tau,\xi)/\pi_1(\tau,\xi), \qquad (3.18)$$

where P_0 denotes the n-independent limit of

$$\ln P_0(n)=\tfrac{1}{2}m\left[\sum_{r=1}^{n-1}\gamma_{2r}(\tau)-\sum_{r=0}^{n-1}\gamma_{2r+1}(\tau)\right]. \qquad (3.19)$$

The errors arising from the factors π_i are, as before, of order $(\ln n)^3/n^2$ for fixed τ and ξ.

We will evaluate $\ln P_0(n)$ as a power series in τ^2 which will be convergent for small enough τ. To this end write

$$\tfrac{1}{2}\gamma_l(\tau)=g(\tau,\theta)=g_0(\theta)+\tau^2 g_1(\theta)+\tau^4 g_2(\theta)+\cdots, \qquad (3.20)$$

with $\theta=l\pi/2n$. Then

$$g_0(\theta)=\ln[\sigma+(1+\sigma^2)^{1/2}], \quad \sigma=\sigma_l=\sin\theta, \qquad (3.21)$$

$$g_1(\theta)=\tfrac{1}{2}n^{-2}\sigma^{-1}(1+\sigma^2)^{-1/2}, \qquad (3.22)$$

$$g_2(\theta)=-\tfrac{1}{8}n^{-4}[\sigma^{-3}(1+\sigma^2)^{-1/2}+\sigma^{-1}(1+\sigma^2)^{-3/2}], \qquad (3.23)$$

while in the expression for $g_i(\theta)$ terms of the form

$$n^{-2i}\sigma^{-2i+1+2k}(1+\sigma^2)^{-k-\frac{1}{2}}, \qquad k=0,1,2,\cdots,i$$

appear. Such a term makes a contribution to $\ln P_0(n)$ in (3.19) equal (essentially) to m times its sum on l; since $(1+\sigma^2)^{-k-\frac{1}{2}}\leq 1$, this sum is bounded by

$$mn^{-2i}\sum_{l=1}^{2n-1}\sigma_l^{-2i+1+2k}$$
$$\sim\xi(\tfrac{1}{2}\pi)^{-2i+1+2k}n^{-2k}\sum_{l=1}^{n}l^{-2i+1+2k}, \qquad (3.24)$$

where for the purposes of estimation we have used the approximation $\sigma_l=\sin\theta_l\approx\theta=l\pi/2n$. For $k=i$ the final sum on l diverges as $\ln n$ but for $k<i$ it converges as $n\to\infty$. Hence, all those terms with $k\geq 1$ give contributions to $g_i(\theta)$ of order at most $(\ln n)/n^2$; furthermore, in view of the prefactor $(\frac{1}{2}\pi)^{-2i+1}$ in (3.2) the coefficient of the corresponding error term in $g(\tau,\theta)$ obtained by summing on i, can be bounded for all $|\tau|<\frac{1}{2}\pi$. This limitation on the range of τ will prove quite acceptable.

Let us then evaluate to leading order the coefficient of τ^{2i} for $i\geq 2$ in the expression for $\ln P_0(n)$: it is

$$mn^{-2i}\binom{\frac{1}{2}}{i}\left[\sum_{r=1}^{n-1}\frac{(1+\sigma_{2r}^2)^{-1/2}}{[\sin(r\pi/n)]^{2i-1}}-\sum_{r=0}^{n-1}\frac{(1+\sigma_{2r+1}^2)^{-1/2}}{[\sin(r+\frac{1}{2})\pi/n]^{2i-1}}\right].$$

Now, as above, we may to leading order replace $\sin(r\pi/n)$ by $(r\pi/n)$ and reduce the sums to Riemann zeta functions; in the term for $i=2$ this again leaves an error term of order $(\ln n)/n^2$, but for $i>2$ the error is only of order $1/n^2$. The total contribution of the terms of order τ^4 and higher is hence $-\xi\Sigma_0(\tau)$, where

$$\Sigma_0(\tau)=\pi\sum_{i=2}^{\infty}\binom{\frac{1}{2}}{i}\left(\frac{2\tau}{\pi}\right)^{2i}[1-2^{-2i+2}]\zeta(2i-1). \qquad (3.25)$$

This sum is convergent for $|\tau|<\frac{1}{2}\pi$ (in accordance with the range of validity of the error estimates). For numerical purposes it is convenient to sum on i explicitly for the first one or two terms in the expansion of the zeta function: $\zeta(s)=1+2^{-s}+3^{-s}+\cdots$.

As the next stage we evaluate the term of order τ^2 which involves the sum

$$S_1(n)=n^{-1}\sum_{r=1}^{n-1}\operatorname{csch}[(r-\tfrac{1}{2})\pi/n][1+\sin^2(r-\tfrac{1}{2})\pi/n]^{-\frac{1}{2}} \qquad (3.26)$$

and a corresponding sum $S_2(n)$ in which $r-\frac{1}{2}$ is replaced by r. We may expand the second factor of the summand to yield

$$\operatorname{csch}[(r-\tfrac{1}{2})\pi/n]+\sum_{k=1}^{\infty}\binom{-\frac{1}{2}}{k}\sin^{2k-1}[(r-\tfrac{1}{2})\pi/n]. \qquad (3.27)$$

[18] E. T. Whittaker and G. N. Watson, *A Course of Modern Analysis* (Cambridge University Press, 1927), 4th ed., Chap. 21.

Because $\sin^{2k-1}\theta$ is a polynomial in $e^{\pm i\theta}$, each term for $k\geq 1$ may be summed explicitly over r to yield

$$\frac{1}{n}\sum_{r=1}^{n}\sin^{2k-1}(r-\tfrac{1}{2})\pi/n=\pi^{-1}\int_0^\pi \sin^{2k-1}\theta d\theta =\frac{2k-2}{2k-1}\frac{2k-4}{2k-3}\cdots\frac{4}{5}\frac{2}{3}\frac{2}{\pi}. \quad (3.28)$$

On substituting into (3.26) one obtains simply

$$S_1(n)=n^{-1}\sum_{r=1}^{n}\operatorname{csch}[(r-\tfrac{1}{2})\pi/n]-\pi^{-1}\ln 2. \quad (3.29)$$

The remaining sum has been evaluated by Onsager[19] correct to order $1/n^2$; using his expression we obtain

$$S_1(n)=(2/\pi)[\ln n+\ln(2^{5/2}/\pi)+C_E]+O(1/n^2), \quad (3.30)$$

where $C_E=0.5772\cdots$ is Euler's constant.

The sum $S_2(n)$ corresponding to (3.26) with r in place of $r-\frac{1}{2}$ is calculated similarly. Following Onsager's method the divergent part is decomposed in the form

$$n^{-1}\sum_{r=1}^{n-1}\operatorname{csch}\left(\frac{r\pi}{n}\right) =\frac{2}{\pi}\left[1+\tfrac{1}{2}+\tfrac{1}{3}+\cdots+\frac{1}{n-1}-\frac{1}{n+1} -\frac{1}{n+3}-\cdots-\frac{1}{2n-1}+\frac{1}{2n+1}+\cdots\right] =\frac{2}{\pi}\sum_{t=0}^{\infty}(-1)^t\{\psi[n(t+1)]-\psi(nt+1)\}, \quad (3.31)$$

where $\psi(z)=(d/dz)\ln\Gamma(z)=\psi(z+1)-(1/z)$, is the digamma function which varies as $\ln z-1/2z+O(z^{-2})$ as $z\to\infty$. This estimate together with $\psi(1)=-C_E$ and Wallis's product

$$\ln\frac{2}{1}\frac{2}{3}\frac{4}{3}\frac{4}{5}\cdots=\ln\frac{\pi}{2},$$

finally yields

$$S_2(n)=(2/\pi)[\ln n+\ln(2^{1/2}/\pi)+C_E]+O(1/n^2). \quad (3.32)$$

Because the forms of $S_1(n)$ and $S_2(n)$ are so similar the only contribution to $\ln P_0(n)$ in leading order is a term $-(2\ln 2/\pi)\xi\tau^2$; the individual expressions for $S_1(n)$ and $S_2(n)$ will, however, be needed later.

Lastly, we must evaluate the contribution independent of τ which arises from (3.21). The corresponding sums in (3.19) can be handled by the use of the Euler-Maclaurin summation formula. Since the identical analysis arises in the dimer problem[16] we quote here only the results, namely, for $T=T_c$:

$$\tfrac{1}{2}m\sum_{r=1}^{n-1}\gamma_{2r}(0)=2mn\left(\frac{G}{\pi}\right)-\frac{\pi}{6}\xi+O\left(\frac{1}{n^2}\right), \quad (3.33)$$

$$\tfrac{1}{2}m\sum_{r=0}^{n-1}\gamma_{2r+1}(0)=2mn\left(\frac{G}{\pi}\right)+\frac{\pi}{12}\xi+O\left(\frac{1}{n^2}\right), \quad (3.34)$$

where

$$G=1^{-2}-3^{-2}+5^{-2}-\cdots\simeq 0.915\,965\,594$$

is Catalan's constant and the order of the error term follows from the boundedness of the corresponding derivatives of $\gamma(\omega)$. Note that by (3.1) these expressions are also needed to evaluate the Z_i. On combining all these results we conclude that

$$\ln P_0(n)=-\tfrac{1}{4}\pi\xi-(\ln 4/\pi)\xi\tau^2 -\xi\Sigma_0(\tau)+O(\ln n/n^2), \quad (3.35)$$

where $\Sigma_0(\tau)=O(\tau^4)$ is defined for $|\tau|<\frac{1}{2}\pi$ by (3.25).

With this result we are already in a position to evaluate the partition function, or free energy, near T_c; we obtain

$$\ln Z_{mn}(T)-mn(\tfrac{1}{2}\ln 2\sinh 2K) =mn(2G/\pi)+(\pi/12)\xi-\ln 2+\ln\pi_1(\tau,\xi) +\ln[1+R_2(n)+R_3(n)+R_4(n)] +\xi\Sigma_{00}(\tau)+O[(\ln n)^3/n^2], \quad (3.36)$$

where, to recapitulate, the functions π_i and $R_i(n)=R_i+O(1/n)$ are defined in (3.11), (3.12), and (3.17), (3.18), and (3.35), while $\Sigma_{00}(\tau)$ has the same form as $\Sigma_0(\tau)$ in (3.25) except that the factor $(1-2^{-2i+2})$ must be replaced by $(1-2^{-2i+1})$. At the critical point this expression reduces to

$$\ln Z_{mn}(T_c)=mn[(2G/\pi)+\tfrac{1}{2}\ln 2]+\ln(\theta_2+\theta_3+\theta_4) -\tfrac{1}{3}\ln(4\theta_2\theta_3\theta_4)+O[(\ln n)^3/n^2]. \quad (3.37)$$

Note that there are no terms proportional to $(m+n)$ in these expressions since the periodic boundary conditions allow no "edges." The results (3.36) and (3.37) should, of course, be invariant under interchange of m and n, or, equivalently, the replacement of ξ by ξ^{-1}. This symmetry may be checked explicitly at $T=T_c$, by using Jacobi's imaginary transformation of the θ functions,[18] namely,

$$\begin{aligned}\theta_2(0,e^{-\pi/\xi})&=\xi^{1/2}\theta_4(0,e^{-\pi\xi}),\\ \theta_3(0,e^{-\pi/\xi})&=\xi^{1/2}\theta_3(0,e^{-\pi\xi}),\\ \theta_4(0,e^{-\pi/\xi})&=\xi^{1/2}\theta_2(0,e^{-\pi\xi}).\end{aligned} \quad (3.38)$$

[Jacobi's transformation plays a similar role in the dimer problem.[16]]

In the symmetric case $m=n$ ($\xi=1$) the $O(1)$ terms in (3.37) reduce to $\ln(2^{1/4}+2^{-1/2})$. We may also note the limiting result

$$\lim_{m\to\infty}(mn)^{-1}\ln Z_{mn}(T_c)=(2G/\pi)+\tfrac{1}{2}\ln 2+\pi/12n^2 +O[(\ln n)^3/n^4], \quad (3.39)$$

although strictly this requires a closer look at the re-

[19] Reference 14, p. 143.

mainder terms to ensure that they remain bounded as $\xi\to\infty$ (or 0).

4. SUMS FOR THE DERIVATIVES

To calculate the energy and specific heat we must evaluate asymptotically the sums appearing in the expressions (2.8) and (2.9) for Z_i' and Z_i''. The analysis follows the same general lines as in the last section, so we will not present all the (fairly lengthy) details. These sums involving $\tanh x$ and $\coth x$ are split by writing $\tanh x=1-(1-\tanh x)$ which leads to the consideration of the typical sum

$$Q_{t,4}(n)=2n^{-t}\sum_{r=1}^{[\frac{1}{2}n]}\frac{1-\coth\frac{1}{2}m\gamma_{2r}}{[(\tau/n)^2+\sin^2(r\pi/n)]^{\frac{1}{2}t}[1+(\tau/n)^2+\sin^2(r\pi/n)]^{\frac{1}{2}t}},\tag{4.1}$$

where $t\geq 1$; we will only require the values $t=1$ and $t=3$ here. By expanding the hyperbolic cotagent into a series in powers of $\exp(-m\gamma_{2r})$ we are lead to consider the sums $Q_{t,4}(n,p)$ of the same form as (4.1), but with $\exp[-pm\gamma_{2r}]$ ($p=1,2,\cdots$) in the numerator. As in the analysis of the sum in (3.3) defining $\ln P_4$, we split the sums over r at $r=s(n)$. The sum for $r\geq s$ can then be bounded, as previously, by a term of order $n\exp(-\pi\zeta s)$ which vanishes as $1/n^2$ with the same choice, (3.7), of $s(n)$. By use of the estimate (3.8) for $m\gamma_{2r}(\tau)$ the numerators of the sums for $r<s$ can again be expressed in terms of $\varphi(\tau,r)$ alone, at the cost of an error of order $s^3/n^2\sim(\ln n)^3/n^2$. To this order, therefore,

$$Q_{t,4}(n,p)\approx 2n^{-t}\sum_{r=1}^{s}\frac{\exp[-2p\xi\varphi(\tau,r)]}{[(\tau/n)^2+\sin^2(r\pi/n)]^{\frac{1}{2}t}[1+(\tau/n)^2+\sin^2(r\pi/n)]^{\frac{1}{2}t}}.\tag{4.2}$$

As in the analysis leading to (3.25), neglect of the second factor in the denominator incurs an error of order no greater than $(\ln n)/n^2$. Similarly, the approximation of $\sin(r\pi/n)$ by $(r\pi/n)$ in the first factor removes the n dependence and is quite easily seen to be correct up to a term of order $s^2/n^2\sim(\ln n)^2/n^2$. Finally, with comparable accuracy the sum on r may be extended to ∞. Substitution back into (4.1) and summation over p then yields

$$Q_{t,4}(n)=2\sum_{r=1}^{\infty}\{1-\coth[\xi\varphi(\tau,r)]\}[\varphi(\tau,r)]^{-t}+O[(\ln n)^3/n^2].\tag{4.3}$$

A set of other sums $Q_{t,i}(n)$ and $Q_{t,\pm}(n)$ may be defined in analogy to $Q_{t,4}(n)$ by the correspondences

$t=1$ or 3

$$\begin{aligned}
&Q_{t,1}(n):\quad r-\tfrac{1}{2}\quad \{1-\tanh\},\\
&Q_{t,2}(n):\quad r-\tfrac{1}{2}\quad \{1-\coth\},\\
&Q_{t,3}(n):\quad r\quad \{1-\tanh\},\\
&Q_{t,4}(n):\quad r\quad \{1-\coth\},\\
&Q_{t,-}(n):\quad r-\tfrac{1}{2}\quad \{1\},\\
&Q_{t,+}(n):\quad r\quad \{1\},
\end{aligned}$$

$t=2$

$$\begin{aligned}
&Q_{2,1}(n):\quad r-\tfrac{1}{2}\quad \{\mathrm{sech}^2\},\\
&Q_{2,2}(n):\quad r-\tfrac{1}{2}\quad \{-\mathrm{csch}^2\},\\
&Q_{2,3}(n):\quad r\quad \{\mathrm{sech}^2\},\\
&Q_{2,4}(n):\quad r\quad \{-\mathrm{csch}^2\}.
\end{aligned}\tag{4.4}$$

With the corresponding replacements, the asymptotic formula (4.3) remains valid for all these sums except for $Q_{1,-}(n)$ and $Q_{1,+}(n)$. We will use the symbols $Q_{t,i}$ and $Q_{t,\pm}$ below to denote the asymptotically approximating sums (which are independent of n).

The special sums $Q_{1,-}(n)$ and $Q_{1,+}(n)$ which arise in (2.8) and (2.9) are logarithmically divergent with n and must be handled separately. Apart from the dependence on τ they are similar to the sums S_1 and S_2 calculated in the previous section [see (3.26)]. In fact, by dealing with the τ dependence via an expansion (valid as before for $|\tau|<\frac{1}{2}\pi$), we obtain

$$Q_{1,+}(n)=S_2(n)+\sum_{k=1}^{\infty}\binom{-\frac{1}{2}}{k}\tau^{2k}\times\left\{n^{-2k-1}\sum_{r=1}^{n-1}\frac{(1+2\sigma_{2r}^2)^k}{[\sigma_{2r}(1+\sigma_{2r}^2)^{1/2}]^{2k+1}}\right\}\tag{4.5}$$

with a similar expression for $Q_{1,-}$ where, as before, $\sigma_l=\sin(l\pi/2n)$. As in the steps leading to (3.25) the term in braces in (4.5) can be reduced to a Riemann zeta function by neglecting the factors $(1+2\sigma^2)$ and $(1+\sigma^2)$ and replacing σ_l by $(l\pi/2n)$. For $k=1$ this introduces an error term of relative order $(\ln n)/n^2$ but for $k>1$ it is only of order $1/n^2$. The prefactor $(2/\pi)^{2k+1}$ enables the leading terms and the error terms to be summed on k for $|\tau|<\frac{1}{2}\pi$, so that by recalling the formulas (3.30) and (3.32) for S_1 and S_2 we finally obtain, correct to order $(\ln n)/n^2$,

$$Q_{1,+}(n)\approx(2/\pi)[\ln n+\ln(2^{1/2}/\pi)+C_{\mathrm{E}}]+\Sigma_1(\tau),\tag{4.6}$$

$$Q_{1,-}(n)\approx(2/\pi)[\ln n+\ln(2^{5/2}/\pi)+C_{\mathrm{E}}]+\Sigma_2(\tau),\tag{4.7}$$

where

$$\Sigma_1(\tau)=\frac{2}{\pi}\sum_{k=1}^{\infty}\binom{-\frac{1}{2}}{k}\left(\frac{\tau}{\pi}\right)^{2k}\zeta(2k+1).\tag{4.8}$$

and

$$\Sigma_2(\tau)=\frac{4}{\pi}\sum_{k=1}^{\infty}\binom{-\frac{1}{2}}{k}\left(\frac{2\tau}{\pi}\right)^{2k}\zeta(2k+1)[1-2^{-2k-1}]. \quad (4.9)$$

We are now in a position to substitute into the formulas (2.6)–(2.9) for the energy and specific heat. For certain of the sums factors γ_0, γ_0', or γ_0'' appear for $l=0$ $(r=0)$; we remove the corresponding terms from the sum and carry them separately; thus we have, for example, to leading order,

$$\sum_{r=0}^{n-1}(\gamma_{2r}'\operatorname{sech}\tfrac{1}{2}m\gamma_{2r})^2 \approx (\gamma_0'\operatorname{sech}\tfrac{1}{2}m\gamma_0)^2+\tfrac{1}{4}(nc')^2Q_{2,3}, \quad (4.10)$$

but

$$\sum_{r=0}^{n-1}(\gamma_{2r+1}'\operatorname{sech}\tfrac{1}{2}m\gamma_{2r})^2\approx\tfrac{1}{4}(nc')^2Q_{2,1}, \quad (4.11)$$

where we recall the definition (2.21) of c'. As an example of another term occurring in the reduction we quote

$$n^{-1}\sum_{r=0}^{n-1}\gamma_{2r+1}''\tanh\tfrac{1}{2}m\gamma_{2r+1} \approx\tfrac{1}{2}c''(Q_{1,-}-Q_{1,1})-\tfrac{1}{8}(nc')^2(Q_{3,-}-Q_{3,1}). \quad (4.12)$$

After further lengthy algebra we find for the energy

$$-U_{mn}(T)/Jmn\approx\sqrt{2}-(4/\pi)\tau(\ln n)/n-(4/\pi)[\ln(2^{5/2}/\pi)+C_E-\tfrac{1}{4}\pi](\tau/n)-[R_3\tanh\tau\xi+R_4\coth\tau\xi](2/Rn)$$
$$+\{\sum_{i=1}^{4}R_iQ_{1,i}-(R_1+R_2)\Sigma_2-(R_3+R_4)[\Sigma_1-(4/\pi)\ln 2]\}(2\tau/Rn)+O(1/n^2), \quad (4.13)$$

where

$$R=\sum_{i=1}^{4}R_i \quad (4.14)$$

and the R_i are defined through (3.17), (3.18), (3.11), (3.12), (3.35) retaining now only leading order terms in each case, and Σ_1 and Σ_2 are defined in (4.8) and (4.9).

At the critical point ($\tau=0$, $T=T_c$) this reduces to

$$-U_{mn}(T_c)/Jmn=\sqrt{2}+\frac{2}{n}\left[\frac{\theta_2\theta_3\theta_4}{\theta_2+\theta_3+\theta_4}\right]+O(1/n^2), \quad (4.15)$$

where the θ functions were defined in (3.14). The leading term agrees, of course, with Onsager's result for an infinite lattice. The invariance of the second term under $n\leftrightarrow m$ in $\xi\leftrightarrow\xi^{-1}$ can again be checked with the aid of Jacobi's transformation (3.38).

Lastly, we can write the specific heat as

$$C_{mn}/k_Bmn=A_0\ln n+B(\tau,\xi)+B_1(\tau,\xi)(\ln n)/n+B_2(\tau,\xi)/n+O[(\ln n)^3/n^2], \quad (4.16)$$

where

$$A_0=(8/\pi)K_c^2=(2/\pi)[\ln(1+2^{1/2})]^2=0.494358\cdots \quad (4.17)$$

and

$$B(\tau,\xi)/K_c^2=\frac{8}{\pi}[\ln(2^{5/2}/\pi)+C_E-\tfrac{1}{4}\pi]-\frac{4}{R}\left[\sum_{i=1}^{4}R_iQ_{1,i}-(R_1+R_2)\Sigma_2-(R_3+R_4)\left(\Sigma_1-\frac{4}{\pi}\ln 2\right)\right]$$
$$-8\frac{\tau\xi}{R}[R_3Q_{1,3}\tanh\tau\xi+R_4Q_{1,4}\coth\tau\xi]-4\frac{\tau^2}{R}[(R_1+R_2)Q_{3,-}+(R_3+R_4)Q_{3,+}-\sum_{i=1}^{4}R_i(Q_{3,i}+\xi Q_{2,i}+\xi Q_{1,i}^2)]$$
$$+4\frac{\xi}{R^2}\{(R_1+R_2)(R_3+R_4)(1+\tau^2\Sigma_3^2)+R_3^2\operatorname{sech}^2\tau\xi-R_4^2\operatorname{csch}^2\tau\xi$$
$$+2\tau(R_3\tanh\tau\xi+R_4\coth\tau\xi)[(R_1+R_2)\Sigma_3+\sum_{i=1}^{4}R_iQ_{1,i}]$$
$$-2\tau^2\Sigma_3[(R_1+R_2)(R_3Q_{1,3}+R_4Q_{1,4})-(R_3+R_4)(R_1Q_{1,1}+R_2Q_{1,2})]-\tau^2[\sum_{i=1}^{4}R_iQ_{1,i}]^2\}, \quad (4.18)$$

$$B_1(\tau,\xi)=\tfrac{3}{2}\sqrt{2}A_0\tau, \quad (4.19)$$

where

$$\Sigma_3=\Sigma_1-\Sigma_2-(4/\pi)\ln 2\,, \tag{4.20}$$

and where the sums $Q_{t,i}$, etc., are defined via (4.3) and (4.4).

At the critical point $T=T_c$ only the first two terms and part of the last term in (4.18) survive; these reduce to

$$B(0,\xi)=\frac{2}{\pi}[\ln(1+2^{1/2})]^2[\ln(2^{5/2}/\pi)+C_{\rm E}-\tfrac{1}{4}\pi]$$
$$-\frac{[\ln(1+2^{1/2})]^2}{\theta_2+\theta_3+\theta_4}\left[\frac{4}{\pi}\sum_{i=2}^{4}\theta_i\ln\theta_i+\frac{\xi\theta_2{}^2\theta_3{}^2\theta_4{}^2}{\theta_2+\theta_3+\theta_4}\right], \tag{4.21}$$

which takes the value $0.138149\cdots$ at $\xi=1$. If we allow $\xi\to\infty$ (when $\theta_3,\ \theta_4\to 1,\ \theta_2\to 0$), we obtain

$$B(0,\infty)=(2/\pi)[\ln(1+2^{1/2})]^2[\ln(2^{5/2}/\pi)+C_{\rm E}-\tfrac{1}{4}\pi]$$
$$=0.187902\cdots. \tag{4.22}$$

As observed before, both $\xi=0$ and $\xi=\infty$ correspond to a torus (or cylinder) infinitely long compared to its width; as expected the value (4.22) agrees with Onsager's result[14] for this special case. When we let $\xi\to\infty$ for general τ, we find $Q_{1,i}$, $Q_{2,i}$, $Q_{3,i}$, ξR_3, ξR_4, $\xi Q_{1,i}$, $\xi Q_{2,i}\to 0$ ($i=1,\ 2,\ 3,\ 4$), R_1, $R_2\to 2$, and the formula (4.18) for $B(\tau,\xi)$ reduces to

$$B(\tau,\infty)/K_c{}^2=(8/\pi)[\ln(2^{5/2}/\pi)+C_{\rm E}-\tfrac{1}{4}\pi]$$
$$+4(\Sigma_2-\tau^2Q_{3,-})\,. \tag{4.23}$$

Since both $\Sigma_2(\tau)$ and $Q_{3,-}(\tau)$ are symmetric about the point $\tau=0$, $B(\tau,\infty)$ itself is also symmetric about T_c. If we apply Jacobi's transformation $\xi\leftrightarrow\xi^{-1}$ to (4.21), we find the relation

$$B(0,\xi)=B(0,\xi^{-1})+(2/\pi)[\ln(1+2^{1/2})]^2\ln\xi\,. \tag{4.24}$$

More generally it follows from the definition of τ and the symmetry of $C_{mn}(\tau)$ in m and n that we must, in fact, have the relation

$$B(\tau,\xi)=B(\xi\tau,\xi^{-1})+A_0\ln\xi\,. \tag{4.25}$$

Although we have not verified this analytically from (4.18) it has been checked numerically; indeed this provides a very stringent test on the correctness of the formula. We may hence write (4.16) in the manifestly symmetric form

$$C_{mn}(T)/k_{\rm B}mn=A_0\ln(m^{-2}+n^{-2})^{1/2}$$
$$+\bar{B}(\tau,\xi)+O[(\ln n)/n]\,, \tag{4.26}$$

where

$$\bar{B}(\tau,\xi)=\tfrac{1}{2}[B(\tau,\xi)+B(\xi\tau,\xi^{-1})+A_0\ln(\xi+\xi^{-1})]\,. \tag{4.27}$$

It is clear from this expression that the magnitude of $C(T)$ near T_c is limited primarily by the *smaller* of m and n. Incidentally, one may usefully introduce a new temperature variable, say,

$$\tau^*=2\tau\xi/(1+\xi)\sim[2nm/(n+m)](\Delta T/T_c)\,, \tag{4.28}$$

which is invariant under $\xi\leftrightarrow\xi^{-1}$.

Lastly, we remark that an explicit expression for $B_2(\tau,\xi)$ may be found by straightforward but tedious algebra; it derives from the higher order τ/n dependence of γ_0', γ_0'', c', and c'' [see (2.21) and (2.22)] entering through expressions like (4.10)–(4.12). Since the general expression is long and unilluminating we do not quote it; at the critical point ($\tau=0$) it reduces to

$$B_2(0,\xi)=-\tfrac{1}{2}\sqrt{2}[\ln(1+2^{1/2})]^2\frac{\theta_2\theta_3\theta_4}{\theta_2+\theta_3+\theta_4}\,. \tag{4.29}$$

The terms of order $(\ln n)^3/n^2$ in (4.16) represent our bounds on the remainder; in fact the next correction term is probably of the slightly higher order $(\ln n)/n^2$.

5. DISCUSSION AND NUMERICAL RESULTS

The general character of the specific heat per spin $C(T)$ of a finite $m\times n$ Ising torus is already evident from Fig. 1, which shows the exact results for a "square torus" ($n=m$) computed for $n=2,\ 3,\ \cdots 64$ by direct evaluation of the formulas (2.3) to (2.9).[20] The nearly equal increments in height of the maximum consequent upon doubling n are indicative of the logarithmic behavior

$$C(T_c)/k_{\rm B}\approx A_0\ln n+O(1)\,, \tag{5.1}$$

which follows from (4.16) for all n and m. The "rounding" of the anomaly clearly decreases with n; in view of the asymptotic result (4.16), we now know that the scale of this rounding is asymptotically set by

$$\tau\approx 2K_cn(T-T_c)/T_c=O(1)\,. \tag{5.2}$$

More explicitly, the deviation $[C(T)-C(T_c)]$ of the specific heat per spin from its value at the limiting critical point T_c approaches a limit $B(\tau,\xi)$, which is independent of n and m [see (4.16) and (4.17)], although it does depend on the ratio $\xi=m/n$. The limiting form of the rounded critical point anomaly is plotted in Fig. 2 for the case $\xi=1$ (solid curve). The broken curves for $n=8$, 16, 32, and 64 are derived from the data of Fig. 1 and indicate that the rate of approach to the limiting form is not so rapid. From Fig. 2 it is clear that the maximum in $C(T)$ lies asymptotically above T_c and varies generally as

$$\epsilon=1-(T_{\max}/T_c)\approx a^*(\xi)/n\,,\quad (n\to\infty) \tag{5.3}$$

[20] We have also compared the exact results for the specific heats of finite tori of sizes 4×4, 8×8, and 12×12 with the interesting Monte Carlo calculations of C. P. Yang, Proc. Symp. Appl. Math. **15**, 351 (1963) [American Mathematical Society]. Away from the maximum the Monte Carlo results are accurate to within their standard deviation of 2 or 3%. In the vicinity of the maximum, however, errors or order 10–15% occur in all three cases. These errors are about 7–12 times the standard deviations and have a somewhat systematic appearance. Yang makes some pertinent comments on the difficulties of the Monte Carlo calculations in the critical region but probably one would still not have anticipated errors as large as our comparisons revealed. [Graphs showing the exact and Monte Carlo results are given by A. E. Ferdinand, Ph.D. thesis, published by the University of London (1967).]

as was mentioned in the Introduction. From the data for Fig. 2 we find

$$B_c(1) = B(0,1) = 0.138149\cdots, \qquad \tau_{\max}(1) = 0.31775\cdots,$$

and (5.4)

$$B_{\max}(1) = 0.201359\cdots,$$

so that

$$-a^*(1) \simeq 0.36029. \tag{5.5}$$

A test of the relation (5.3) [with (5.5)] for finite n is indicated in Fig. 3; the approach to limiting behavior is reasonably rapid and, indeed, by numerical extrapolation (5.3) had originally been conjectured with $-a^*(1) \simeq 0.353$.

The result (5.1) for $C(T_c)$ may clearly be supplemented by

$$C_{\max} = C(T_{\max}) \approx C(T_c) + k_B[B_{\max}(\xi) - B(0,\xi)], \quad (n, m \to \infty). \tag{5.6}$$

The rate of approach of $C(T_c)$ and $C_{\max}$ to their limiting behavior is revealed in Fig. 4. Because of the presence of the $(\ln n)/n$ term at $\tau \simeq \tau_{\max}$ (but not at $\tau = 0$) the approach is slower for $C_{\max}$.

The change of form of the limiting rounded anomaly for an asymmetric torus is illustrated in Fig. 5 which shows the asymptotic deviation of $C_{mn}(T)$ from its critical value $C_{mn}(T_c)$ versus the reduced temperature τ for various values of ξ. As ξ changes, $\tau_{\max}$, the position of the maximum shifts. In terms of the symmetrized

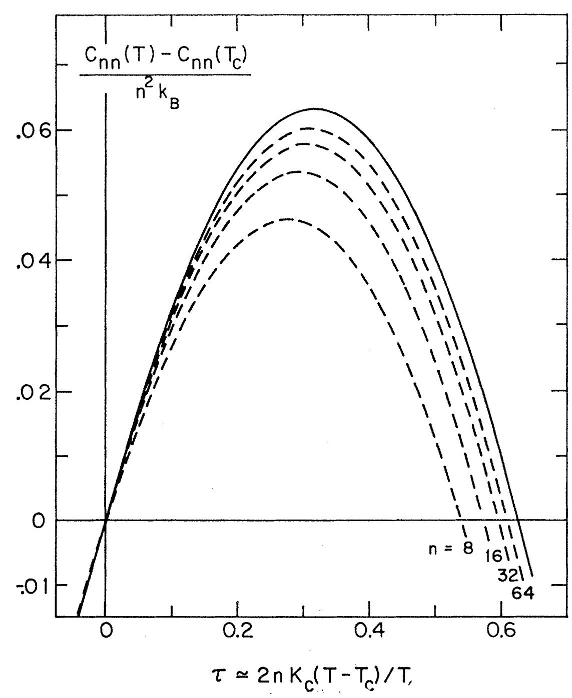

FIG. 2. Plots of the specific heat per spin relative to its critical value versus the reduced temperature variable $\tau \simeq 0.881 n(T - T_c)/T_c$ for $\xi = 1$ $(n = m)$; the limiting behavior for $n \to \infty$ is shown by a solid line, the broken lines show the results for finite $n = 8, 16, 32$, and 64.

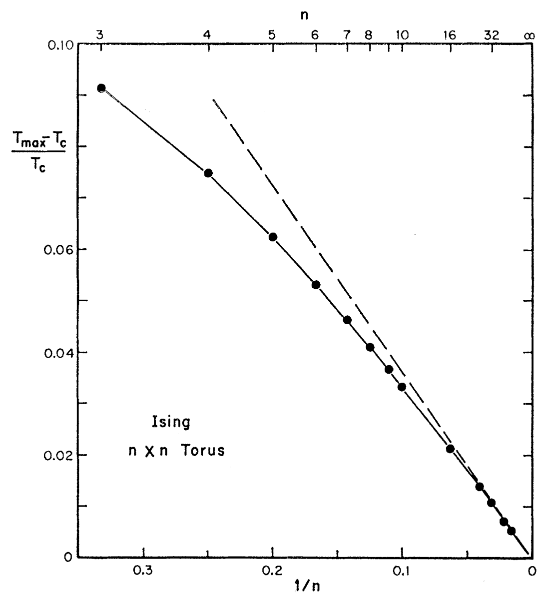

FIG. 3. Variation of $T_{\max} - T_c$ with n for finite tori with $\xi = 1$; the broken curve indicates the limiting behavior as $n \to \infty$.

temperature variable τ^*, defined in (4.28), the shift of the maximum is *downwards* as ξ departs from the symmetric value unity. The variation of $\tau_{\max}^*$ with ξ is shown in Fig. 6; the most striking feature is that for

$$\xi = \xi_0 \simeq 3.139278 \quad \text{or} \quad \xi = \xi_0^{-1} \simeq 0.318544$$

the maximum occurs, asymptotically, *at* $T_{\max} = T_c$. As ξ rises above ξ_0 or falls below ξ_0^{-1}, the maximum moves *below* T_c [see Fig. 5]. The extreme excursion of

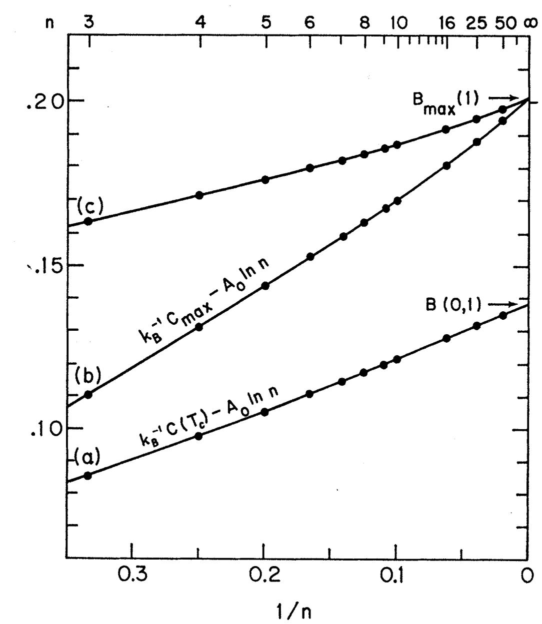

FIG. 4. Approach of $C(T_c)$ and $C_{\max}$ to their limiting behavior for $\xi = 1$: (a) $k_B^{-1}C(T_c) - A_0 \ln n$, (b) $k_B^{-1}C_{\max} - A_0 \ln n$, (c) $k_B^{-1}[C_{\max} - C(T_c)] + B(0,1)$.

the peak below T_c is reached for $\xi \simeq 0.17$ or 6. Ultimately as $\xi \to \infty$ (or 0) the maximum shifts back into asymptotic coincidence with T_c. Notice the limiting curve for $\xi = \infty$ shown by the broken line in Fig. 5. The reason for the nonmonotonic behavior of $\tau_{max}(\xi)$ is not understood; it seems to arise from a subtle interplay between the four different terms making up the exact partition function and the various cross terms brought into existence by differentiating the free energy twice. The value of ξ_0 has been checked by deriving, from (4.18), an explicit expression for the gradient

$$B'(\tau,\xi) = \frac{\partial B}{\partial \tau}(\tau,\xi) = \xi \frac{\partial B}{\partial \tau}(\xi\tau,\xi^{-1}), \qquad (5.7)$$

at $\tau = 0$ in terms of the elliptic theta functions. This gradient must vanish at ξ_0 when the maximum is at $\tau = 0$.

A further impression of the effect of changing ξ may be obtained from the curves in Fig. 6 showing the parameters $\bar{B}_{max}(\xi) = \bar{B}(\tau_{max},\xi)$ (solid line) and $\bar{B}_c(\xi) = \bar{B}(0,\xi) = \bar{B}(0,\xi^{-1})$ (broken line) occuring in the symmetrized formula [see (4.26)]

$$C(T)/k_B = A_0 \ln(m^{-2}+n^{-2})^{-1/2} + \bar{B}(\tau, m/n) + \cdots. \quad (5.8)$$

The over-all variation is not large but both curves display somewhat unexpected maxima around $\xi = 1.4$ and 2.3, respectively. The two curves touch at $\xi = \xi_0$ which is simply a consequence of $\tau_{max}(\xi)$ passing through zero at that point.

In the limiting case $\xi \to \infty$ of an infinitely long tours we have $B_{max} = B(0,\infty) = 0.18790\cdots$, and, as mentioned, $\tau_{max} = 0$. Although to order $1/n$ this implies $T_{max} = T_c$ the actual asymptotic deviation of T_{max} from T_c is now determined by the term of order $(\ln n)/n$ in (4.16); if $B(\tau,\infty) = B(0,\infty) - \frac{1}{2}b_2(\infty)\tau^2 + O(\tau^3)$, we find from (4.19) when $\xi \to \infty$, that

$$[C(T) - C(T_c)]/k_B \approx -\tfrac{1}{2}b_2(\infty)\tau^2 + \tfrac{3}{2}\sqrt{2}A_0\tau(\ln n)/n. \quad (5.9)$$

from which we obtain a maximum at

$$\tau_{max}'(\infty) \approx \tfrac{3}{2}\sqrt{2}[A_0/b_2(\infty)](\ln n)/n,$$

so that

$$(T_{max} - T_c)/T_c \approx a^\dagger (\ln n)/n^2. \qquad (5.10)$$

As expected, this result is of the same form stated by Onsager for the special case $m \to \infty$, n finite. From (4.23) we find $b_2(\infty) = 168 K_c^2 \zeta(3)/\pi^3$, and hence, $a^\dagger = \pi^2\sqrt{2}/28\zeta(3) = 0.414697\cdots$, where $\zeta(3)$ is the Riemann zeta function. A similar analysis could evidently also be carried out for the case $\xi = \xi_0$ or ξ_0^{-1}; the relation (5.10) would remain valid but with some different value of the constant $a^\dagger$.

The results discussed above are, of course, limited to the somewhat unrealistic periodic or toroidal boundary conditions. Another case which may be discussed analytically is that in which periodic boundary conditions are imposed in one direction only, leaving two free edges parallel to, say, the y axis (there might be

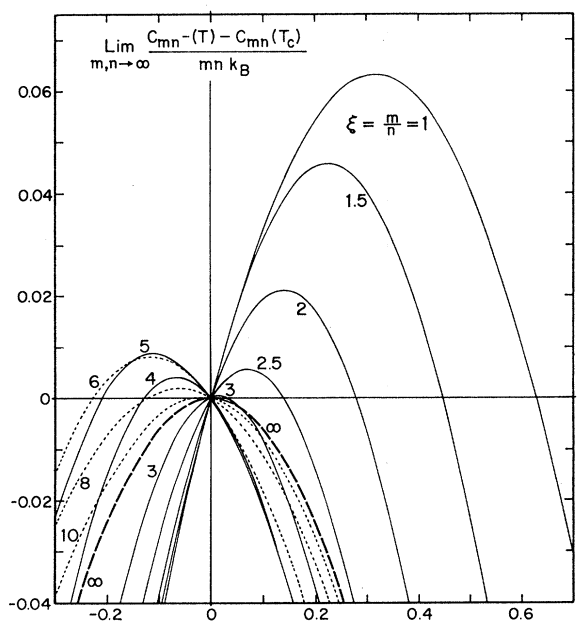

FIG. 5. Dependence of the limiting rounding of the specific-heat anomaly on $\xi = m/n$. Note the broken curve represents the limit $\xi = \infty$ while the curves for $\xi = 6$, 8, and 10 are dotted for carity.

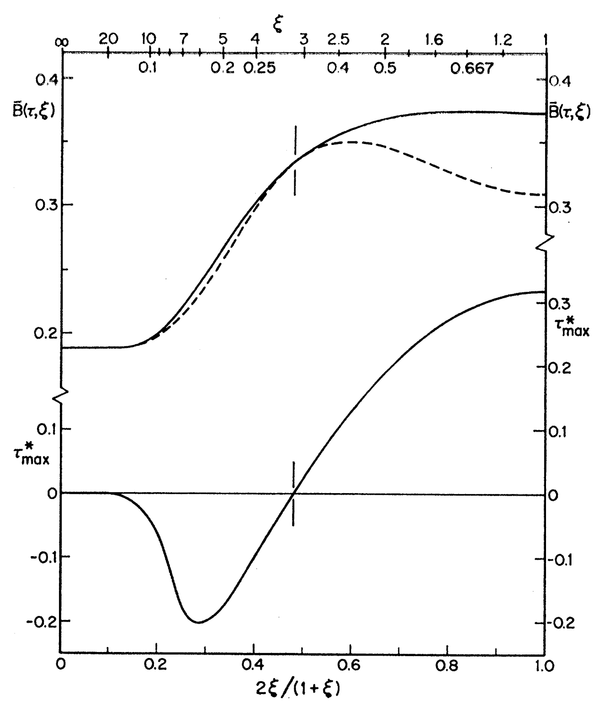

FIG. 6. Variation with $\xi = m/n$ of the symmetrized specific-heat maximum, $\bar{B}_{max} = \bar{B}(\tau_{max},\xi)$, and critical value, $\bar{B}_c = \bar{B}(0,\xi)$ [see Eqs. (4.26) and (4.27)], and of

$$\tau_{max}^* = 2\xi(1+\xi)^{-1}\tau_{max} \approx [2nm/(n+m)](T_{max} - T_c)/T_c.$$

(Note that the top and bottom horizontal scales correspond identically.)

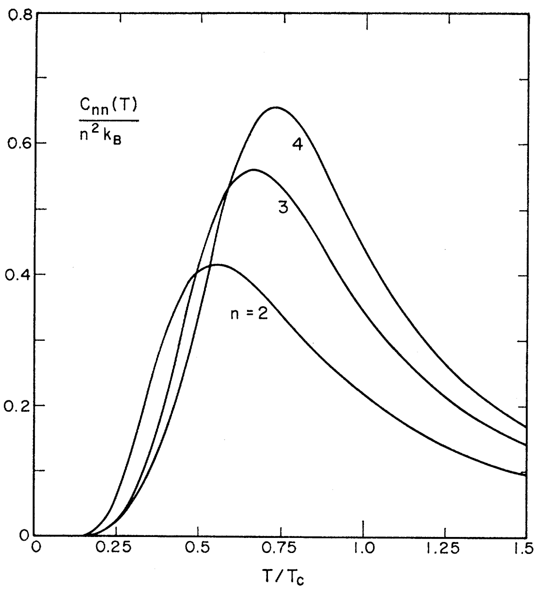

FIG. 7. Specific heats per spin of $n\times n$ Ising lattices with free edges. Note the large depression of the maxima below T_c.

terms cylindrical boundary conditions). This situation will be discussed in a later paper in this series; in particular, results for infinitely long strips of finite width n will be obtained as a limiting case of a uniform lattice which is perturbed by a periodic array of parallel "grain boundaries" constituted by "ladders" of altered J_x interactions. (When $J_x'=0$ one obtains independent finite width strips.) In this case we find the rounded specific-heat maximum is depressed *below* the limiting T_c but the scale of rounding and depression is still of relative order $1/n$.

We have also studied numerically a few small $n\times n$ lattices with four free edges (no periodicity). It is feasible to construct the exact partition functions for $n=2$, 3, and 4 as polynomials in $v=\tanh(J/k_BT)$. Again the maximum is depressed below T_c as evident from Fig. 7. One finds T_{max}/T_c is about 0.5533, for $n=2$, and 0.7305 for $n=4$; the relation (5.3) appears to be valid with $a^*(1)$ close to[9] 1.35, which is of significantly larger magnitude than the toroidal value of -0.36.

A heuristic argument presented previously[9] suggests that if one has any finite d-dimensional Ising lattice (or more general system) of size $n_1\times n_2\times\cdots\times n_d$ with free boundaries one should expect a depression of T_{max} below T_c in accord with (5.3) where n is a suitable average of the n_i. Explicitly, it is reasonable to expect that

$$k_BT_{max}/k_BT_c \simeq E(n_1,\cdots n_d)/n_1n_2\cdots n_dE_0\,, \quad (5.11)$$

where $E(n_1,\cdots n_d)$ is the ground-state energy of the system with boundaries while E_0 is the limiting ground-state energy per spin in an infinite system. Any mean-field argument will lead to this sort of conclusion; for the depression of a *bulk* critical point by regular changes of interaction it amounts to little more than the observation that kT_c must scale with the energies of interaction. Since $E(n_1,\cdots n_d)$ falls below the "bulk" energy $n_1\cdots n_dE_0$ by an amount proportional to the surface area

$$S(n_1,\cdots n_d)=2(n_2\cdots n_d+n_1n_3\cdots n_d+n_1n_2n_4\cdots n_d+\cdots)\,,$$
$$=2n_1\cdots n_d/\tilde{n}\,, \quad (5.12)$$

where

$$1/\tilde{n}=1/n_1+1/n_2+\cdots+1/n_d\,, \quad (5.13)$$

we conclude that (5.3) should hold with the identification $n\Rightarrow\tilde{n}$ (although a^* might still have some residual shape dependence and would certainly depend on the details of the boundary conditions[9]). It would be interesting to check this by calculations on three-dimensional systems.

Our results for the plane Ising model have shown that the scale of the rounding, $\delta=\Delta T/T_c$, is of order $1/n$ (for $\xi=m/n$ fixed). The essential mathematical origin of this rounding can be understood by the following rough argument. The complete expression (2.1) for the partition function involves the sum of the four products (or partial partition functions) Z_1 to Z_4, but to obtain the correct result in the thermodynamic limit n, $m\to\infty$ it is sufficient to retain only the first of these products, Z_1. This product can, in turn, be expressed more symmetrically as a double product[14,21] of the form

$$\prod_{r=0}^{m-1}\prod_{s=0}^{n-1}\left\{f(T)-g(T)\cos\left[(2r+1)\frac{\pi}{m}\right]-g(T)\cos\left[(2s+1)\frac{\pi}{n}\right]\right\} \quad (5.14)$$

which brings out the relationship to the periodic structure of the lattice. Correspondingly, if we ignore the effects of Z_2, Z_3, and Z_4, the free energy per spin can be written *approximately* as

$$-\frac{F_{mn}}{mnk_BT}\simeq\frac{1}{2mn}\sum_{r=0}^{m-1}\sum_{s=0}^{n-1}\ln\left[h^2(T)+2\left(1-\cos\frac{(2r+1)\pi}{m}\right)+2\left(1-\cos\frac{(2s+1)\pi}{n}\right)\right]+e(T)\,, \quad (5.15)$$

where $h(T)$ and $e(T)$ are known analytic functions of T independent of m and n (except for minor terms). In the

[21] See M. Kac and J. C. Ward, Phys. Rev. 88, 1332 (1952); and M. E. Fisher, *Lectures in Theoretical Physics* (University of Colorado Press, Boulder, 1965), Chap. VII c, p. 58.

limit $n, m\rightarrow\infty$ the sums in (5.15) may be replaced by integrals and we obtain correctly Onsager's famous result[15] for the limiting free energy per spin, namely,

$$-\frac{F}{k_BT}=\frac{1}{2}\int_{-\pi}^{\pi}\frac{d\theta}{2\pi}\int_{-\pi}^{\pi}\frac{d\varphi}{2\pi}\ln[h^2(T)+2(1-\cos\theta)+2(1-\cos\varphi)]+e(T). \tag{5.16}$$

On differentiating this expression under the integral sign twice with respect to T one obtains an expression for the specific heat. The critical point is then readily identified by the vanishing of $h(T)$; specifically, we have

$$h(T)= h_0(T-T_c)/T_c\{1+O(T-T_c)\}. \tag{5.17}$$

At the same time the logarithmic divergence is seen to arise from the vanishing of the argument of the logarithm in the integrand which occurs when $\theta=\varphi=0$.

To see the dominant effects more explicitly we may approximate the integral over the Brillouin zone in (5.16) (for that is what it really is) by a spherically symmetric integral over the reduced wave vector $\mathbf{q}=(\theta,\varphi)$. We need an upper cutoff $q=Q\simeq\pi$ independent of n and m, to represent the zone boundary. In the limiting case $m,n\rightarrow\infty$ the lower limit of the q integration should be zero; we may, however, approximate the truncation effects in (5.15) for finite m and n by imposing the natural *lower cutoff*

$$q_0=q_0(n,m)=|(\theta_0,\varphi_0)|=|(\pi/m,\pi/n)|=\pi(m^{-2}+n^{-2})^{1/2}. \tag{5.18}$$

Then we obtain the approximation

$$-\frac{F_{mn}}{mnk_BT}\simeq\pi\int_{q_0}^{Q}\ln[h^2(T)+q^2]qdq+e(T), \tag{5.19}$$

which should reveal some of the dominant finite size effects. From this expression we find by straightforward differentiation that

$$C_{mn}(T)/mnk_B \simeq\mathcal{A}_0(T)\ln[h^2(T)+q_0^2]^{-1/2}+\mathcal{B}(T), \tag{5.20}$$

where

$$\mathcal{A}_0(T)=T^2(h')^2+T^2hh''+2Thh', \tag{5.21}$$

and

$$\mathcal{B}(T)=\pi[T^2(h')^2+T^2hh''+2Thh']\ln[h^2+Q^2]+\pi T^2(h')^2\{h^2/(h^2+Q^2)+h^2/(h^2+q_0^2)\}+2Te'+T^2e'', \tag{5.22}$$

in which the primes denote differentiation with respect to T. Now $\mathcal{B}(T)$ remains a slowly varying and analytic function of T, even when n, $m\rightarrow\infty$, so that $q_0\rightarrow 0$. As $T\rightarrow T_c$ we find from (5.17) that $\mathcal{A}_0(T)$ approaches the constant h_0^2. Finally, therefore, near T_c we can write

$$C_{mn}(T)/mnk_B \simeq A_0\ln\{[(T/T_c)-1]^2+\tfrac{1}{2}b^2(n^{-2}+m^{-2})\}^{-1/2}+B+\cdots, \tag{5.23}$$

where $b=(\pi/h_0)^2$. This displays the expected symmetric logarithmic singularity rounded on a relative scale $\delta=b/\bar{n}$ with

$$\bar{n}^{-2}=\tfrac{1}{2}(m^{-2}+n^{-2}). \tag{5.24}$$

However, it does *not* show the shift ϵ of $T_{\max}$ from T_c [compare with (1.10)]; the shift evidently arises from the "interference" between the different partial-partition functions Z_i in the exact expression (2.1), which correctly represents the detailed form of the boundary conditions.

An interesting feature of the above results for the plane Ising models is that δ, the relative width of the rounding, is of the *same* asymptotic order, namely, $1/n$, as the depression of $T_{\max}$. The heuristic arguments just presented suggest, however, that the "mechanisms" of the two effects may be distinct so that this coincidence is a peculiarity of plane Ising models. As suggested previously[9] it is plausible that the rounding of a sharp specific-heat anomaly sets in when the range of correlation $1/\kappa(T)$ in the corresponding homogeneous infinite system approaches the characteristic dimension of the system $\bar{n}$, defined generally, say, in analogy to (5.24). If[1] $\kappa(T)$ vanishes as $(T-T_c)^\nu$ as $T\rightarrow T_c$, this would imply a width varying as

$$\delta=\Delta T/T_c\approx c/\bar{n}^{-1/\nu}. \tag{5.25}$$

For planar Ising models one knows[1,14] that $\nu=1$ so that (5.25) is consistent with our exact results. More generally, if the specific heat of an ideal infinite system varies[1] as $|T-T_c|^{-\alpha}$ one is lead to conjecture[9] that the formula

$$C_N(T)Nk_B\simeq\mathcal{A}(|t^*|^{-\alpha}-1)/\alpha+\mathcal{B}(T)+\cdots \tag{5.26}$$

with $\mathcal{A}$ and $\mathcal{B}$ relatively slowly varying functions[22] of T and N and

$$t^{*2}=[(T/T_c)+\epsilon]^2+\delta^2, \tag{5.27}$$

might be a reasonable description of the dominant behavior of a finite system of $N=n_1\cdots n_d$ spins near its critical point. [Note that when $\alpha\rightarrow 0$ the singularity becomes logarithmic and (5.26) and (5.27) reduce to (1.10) which characterizes our results.] Since in most three-dimensional systems one has $\nu\simeq\frac{2}{3}<1$ this conjecture suggests that the rounding of the transition, δ, should be smaller, asymptotically, than the shift or

[22] This formula already presupposes exponent symmetry about T_c (i.e., $\alpha=\alpha'$) but in general $B(T)$ would have to contain a more or less sharp step at T_c to account for the residual lack of symmetry above and below T_c observed in most three-dimensional specific heat anomalies. (See also below.)

depression ϵ of $T_{\max}$. There is some experimental evidence in support of this conclusion.[5,6] To test it theoretically, however, calculations must be made on a system for which $\nu \neq 1$. A related consequence of the conjecture is that $C_N(T_c)/N$ varies as $N^{\alpha/d}$ but $C_{N,\max}/N = C_N(T_{\max})/N$ varies as $N^{\alpha/d\nu}$.

As a final speculation we remark that the guess (5.25) for δ leads naturally to the suggestion that for a general finite d-dimensional system the approximation (5.19) for the free energy might be extended to

$$-F_N/Nk_BT \simeq D\int_{q_0}^{Q} \ln[h^2(T)+q^{2/\nu}]q^{d-1}dq + e(T)\,, \quad (5.28)$$

where D is constant, or slowly varying, and as before, we suppose the lower cutoff, q_0 varies as $1/\bar{n}\sim N^{-1/d}$. If to allow for a displaced specific-heat maximum we postulate that $h\sim T-T_{\max}$ and $T_{\max}\sim T_c-(b/\bar{n})$, the specific-heat anomaly will be rounded on the scale set by (5.25) as required. On the other hand, the nature of the specific-heat anomaly in the thermodynamic limit ($N\rightarrow\infty$, $q_0\rightarrow 0$) is now determined by d and ν. A straightforward analysis shows that the exponents of divergence of the specific heat[1] implied by (5.28) are

$$\alpha=\alpha'=\max\{2-d\nu, 0\}\,. \quad (5.29)$$

When $\nu\leq\frac{1}{2}d$ this result is the same as the usual d-dependent correlation homogeneity or scaling conjectures.[23] For $\nu=\frac{1}{2}d$ the singularity is a logarithmic divergence but for $\nu>\frac{1}{2}d$ the limiting specific heat remains finite at $T=T_c$, although it may be cusped there. Among a variety of objections to the conjectural formula (5.28) we mention: (a) that the scaling-law conjecture $\alpha=2-d\nu$ is, like the other dimension-dependent relations, most open to doubt, since, in particular, it seems to be in disagreement with the numerically estimated values $\alpha\simeq\frac{1}{8}$ and $\nu\simeq 9/14$ of the three-dimensional Ising model[23,24]; (b) that the expression in no clear way represents the *asymmetry* about T_c observed in most three-dimensional critical points. Thus, even if there is an equality of the exponents above and below T_c ($\alpha=\alpha'$) some sort of superimposed "step" in the specific heat remains a dominant feature of the transition. One could postulate that this is contained in the $e(T)$ term but its apparently intimate relation to the critical point makes this an artificial assumption.

In conclusion, then, the detailed exact results found for the square Ising lattice do serve as a check on, and a stimulus to, various heuristic, but more general, arguments concerning the distortion of specific-heat anomalies by finite size. One may hope that further accurate, even if less detailed and exact, calculations will extend the checks beyond the present limits.

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[23] See Refs. 1 and 3 and M. E. Fisher, J. Appl. Phys. **38**, 981 (1967).

[24] See M. E. Fisher and R. J. Burford, Phys. Rev. **156**, 583 (1967); M. F. Sykes, J. L. Martin, and D. L. Hunter, Proc. Phys. Soc. (London) **91**, 671 (1967).