Domain walls and shape dependence of finite-size correction terms in the two-dimensional Ising-model critical region

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(Received 28 February 1983)

Ferdinand and Fisher have analyzed the finite-size behavior of the two-dimensional Ising model with periodic boundary conditions for T near T_c. In the thermodynamic limit, the leading correction term to the specific heat has an unusual and unexpected behavior as the shape of the $m \times n$ lattice is changed. For shape parameter $s=m/n=1$, the peak in the specific-heat correction term occurs at a reduced temperature $\tau_{\max}=2K_c n(T-T_c)/T_c>0$. With increasing s the peak moves to negative τ values and then increases to 0. We show that this effect may be understood by keeping only the two largest eigenvalues of the transfer matrix. To this approximation, which is good for $s=1$ and improves exponentially with increasing s, all the shape dependence of the free energy is due to a factor that can be expressed entirely in terms of a domain-wall energy. Furthermore, the functional form of this factor is the same as that of the finite-length correction to the one-dimensional Ising model. Thus the dependence of $\tau_{\max}$ on s is qualitatively similar to the dependence of $T_{\max}^1$, the location of the one-dimensional Ising-model specific-heat peak on N, the number of spins. We also argue that the two-dimensional partition function is expressible at least for $s>1$ as a factor due to domains, and another due to a one-dimensional Ising array of domain walls. Approximate expressions are obtained for the effective number of spins and the effective coupling of the array. We also point out that there is reason to believe the one-dimensional Ising array of domain walls at fixed τ connects smoothly with a similar array for $T<T_c$.

I. INTRODUCTION

Ferdinand and Fisher[1] have provided an exhaustive and rigorous analysis of finite-size corrections to the thermodynamics of the two-dimensional Ising model in the critical region. They consider a square lattice of $m \times n$ spins with periodic boundary conditions in the limit $n \to \infty$ with $s=m/n$ fixed. One of their results is that for fixed reduced temperature

$$\tau=2K_c n(T-T_c)/T_c \ , \tag{1}$$

the specific heat per spin is given by

$$C(T)/k_B mn = A_0 \ln n + B(\tau,s) + O(\ln n/n) \ , \tag{2}$$

where $A_0=(8/\pi)K_c^2=0.494\,358\ldots$, and B is given explicitly [see Eq. (18)]. The behavior of B, the leading correction term to the specific heat, is such that for large but finite lattices the maximum in $C(T)$ is at $\tau=\tau_{\max}(s)$, i.e., the shift in the specific-heat peak depends on the lattice shape parameter s. For $s=1$, $\tau_{\max}>0$ so the peak is at $T=T_{\max}>T_c$. This, as pointed out by Ferdinand and Fisher,[1] is to be expected due to periodic boundary conditions strengthening the effective interaction between spins. As s increases (or decreases—the results in Ref. 1 are invariant if $s \to 1/s$, consistent with the symmetry of the problem), $\tau_{\max}$ displays some unusual and intriguing behavior. At first it decreases, passing through $\tau=0$ for $s=s_0 \cong 3$ and continuing to decrease until $s \approx 7$. With a further increase of s it reverses direction, increasing monotonically to an asymptotic value $\tau_{\max}=0$ as $s \to \infty$. The shape dependence of $\tau_{\max}$ is an exact result. However, no explanation for it is offered in Ref. 1 or (as far as we are aware) elsewhere.

In this paper we approximate the thermodynamics of the problem by keeping only the largest two eigenvalues of the transfer matrix. It turns out that in the critical region, i.e., for fixed τ, this gives very accurate expressions for the thermodynamic functions to the order of interest when $s>1$. In particular, B, the leading finite-size correction term to the specific heat, is well approximated. The two-eigenvalue approximation for B is already good for $s=1$ ($m=n$) and improves exponentially with increasing s. Further, simplified analytic expressions for the partition function, energy, and specific heat and their finite-size correction terms result from this approximation. The partition function may then be factored as $Z=Z_0 Z_\sigma$, where in the two-eigenvalue approximation Z_σ contains all the shape dependence. We further show that (the exact form of) Z_σ may be expressed in terms of domain-wall energies, and that the approximate Z_σ has the form of the finite-length correction to the one-dimensional Ising model. Thus we argue that Z may be factored into a product of single-domain partition functions and a partition function for a one-dimensional Ising array of domain walls. The curious behavior of $\tau_{\max}$ as a function of shape s is, therefore, a domain-wall effect that may be understood in terms of the temperature $T_{\max}^1$ of the specific-heat peak of the one-dimensional Ising model with periodic boundary conditions, which, in fact, displays the same qualitative behavior as a function of N, the number of spins (or length).

In Sec. II we first recapitulate the relevant part of the analysis of Ferdinand and Fisher.[1] We then identify the part of the specific-heat correction term B responsible for the s dependence of the peak location $\tau_{\max}$, and give a very accurate and relatively simple approximate closed-form expression for it. This approximation results from keeping only the two leading eigenvalues of the transfer matrix. In Sec. III the general expressions for domain-wall energies are displayed and evaluated for fixed τ using the results of Ref. 1. Here we show that the correction term responsible for the shape dependence of B can be expressed entirely in terms of a domain-wall energy.

Section IV further explores the identification of the domain-wall contribution to B. First we review some results for the one-dimensional Ising model, in particular, the length dependence of the specific-heat peak $T^1_{\max}(N)$, which is qualitatively the same as the s dependence of $\tau_{\max}$ in the two-dimensional Ising model. Next we show that the domain-wall part of B has the form expected for a one-dimensional Ising array of domain walls, thus providing a mechanism for the shape dependence of the finite-size corrections to the Ising model in the critical region. Finally we make an approximate calculation of the effective number of spins and coupling in the Ising array. In Sec. V we present some evidence that the effects of this array extend naturally into the one-dimensional array of domain walls present for $T<T_c$ and sufficiently large s.

II. FINITE-SIZE CORRECTIONS IN THE CRITICAL REGION

In this section we review some results of the asymptotic analysis of Ferdinand and Fisher[1] for the thermodynamic functions of the Ising model (at zero external field) in the critical region. Next we identify the part of the leading specific-heat correction term B [Eq. (2)] responsible for the shape dependence of $\tau_{\max}$, the (reduced) temperature of the specific-heat maximum for large but finite lattices, and give a very accurate approximate analytic expression for it which results from retaining only the two leading eigenvalues of the transfer matrix.

The partition function Z for an Ising model with periodic boundary conditions on an $m\times n$ lattice has been expressed in a convenient form by Kaufman,[2]

$$Z=\tfrac{1}{2}(2\sinh 2K)^{mn/2}\sum_{i=1}^{4}Z_i(K)\ , \tag{3}$$

where the dimensionless coupling is

$$K=J/k_BT\ , \tag{4}$$

and $J=J_x=J_y>0$ is the nearest-neighbor coupling energy. Here we let the n columns define the y direction; the m rows are then in the x direction. In Eq. (3),

$$\begin{aligned}
Z_1&=\prod_{r=0}^{n-1}2\cosh(m/2)\gamma_{2r+1}\ ,\\
Z_2&=\prod_{r=0}^{n-1}2\sinh(m/2)\gamma_{2r+1}\ ,\\
Z_3&=\prod_{r=0}^{n-1}2\cosh(m/2)\gamma_{2r}\ ,\\
Z_4&=\prod_{r=0}^{n-1}2\sinh(m/2)\gamma_{2r}\ ,
\end{aligned}\tag{5}$$

where

$$\cosh\gamma_l=\cosh 2K\coth 2K-\cos(l\pi/n)\ . \tag{6}$$

Note that

$$\gamma_0=2K+\ln\tanh K\ . \tag{7}$$

The critical point of the (infinite) Ising model is given by[3]

$$\sinh^2 2K_c=1,\quad K_c=\tfrac{1}{2}\ln(1+\sqrt{2})=0.440\,68\ldots\ . \tag{8}$$

For fixed temperatures $T\neq T_c$, the free energy per spin derived from Eq. (3) approaches its infinite lattice limit exponentially fast in m and n. However, in accordance with finite-size scaling theory,[4] the critical point is spread over a region about T_c of order $1/n$. In this region, convergence to the thermodynamic limit does not occur. Accordingly, Ferdinand and Fisher introduce a reduced temperature variable τ by

$$\tau^2/n^2=\tfrac{1}{2}(\sinh 2K+1/\sinh 2K)-1\ , \tag{9}$$

which reduces to Eq. (1) for large n or T near T_c. Defining

$$R_i=Z_i/Z_1\ , \tag{10}$$

one has from Eq. (3),

$$\begin{aligned}
Z&=\tfrac{1}{2}(2\sinh 2K)^{mn/2}Z_1(1+R_2+R_3+R_4)\\
&=Z_0Z_\sigma\ ,
\end{aligned}\tag{11a}$$

where

$$Z_\sigma=\tfrac{1}{2}(1+R_2+R_3+R_4)\ . \tag{11b}$$

The factor Z_0 gives rise to the extensive part of the thermodynamics in the limit $n\to\infty, s=m/n$ fixed. In addition, it contains part of the finite-size corrections. Z_σ contains the rest of the finite-size effects, and we will show below that it is responsible for essentially all of the shape dependence of these correction terms.

Ferdinand and Fisher show that to leading order as $n\to\infty$ with the shape parameter $s=m/n$ fixed,

$$\begin{aligned}
Z_1&=\Pi_1\exp\left[\frac{m}{2}\sum_{r=0}^{n-1}\gamma_{2r+1}\right],\\
R_2&=\Pi_2(\tau,s)/\Pi_1(\tau,s)\ ,\\
R_3&=2\cosh[(m/2)\gamma_0]P_0\Pi_3(\tau,s)/\Pi_1(\tau,s)\ ,\\
R_4&=2\sinh[(m/2)\gamma_0]P_0\Pi_4(\tau,s)/\Pi_1(\tau,s)\ ,
\end{aligned}\tag{12}$$

where

$$\begin{aligned}
\Pi_1&=\prod_{r=1}^{\infty}\{1+\exp[-2s\phi(\tau,r-\tfrac{1}{2})]\}^2\ ,\\
\Pi_2&=\prod_{r=1}^{\infty}\{1-\exp[-2s\phi(\tau,r-\tfrac{1}{2})]\}^2\ ,\\
\Pi_3&=\prod_{r=1}^{\infty}\{1+\exp[-2s\phi(\tau,r)]\}^2\ ,\\
\Pi_4&=\prod_{r=1}^{\infty}\{1-\exp[-2s\phi(\tau,r)]\}^2\ ,\\
\phi(\tau,q)&=(\tau^2+\pi^2q^2)^{1/2}\ .
\end{aligned}\tag{13}$$

The function $\phi(\tau,q)$ in Eq. (13) arises from the expansion of $\gamma_l(\tau)$ for $l\neq 0$ as $n\to\infty$. From Eqs. (7) and (9),

$$(m/2)\gamma_0=-s\tau+O(1/n)\ . \tag{14}$$

The function P_0 is defined as

$$\ln P_0=\tfrac{1}{2}m\left[\sum_{r=1}^{n-1}\gamma_{2r}(\tau)-\sum_{r=0}^{n-1}\gamma_{2r+1}(\tau)\right]. \tag{15}$$

Careful analysis shows[1]

$$\ln P_0=-\tfrac{1}{4}\pi s-(\ln 4/\pi)s\tau^2-s\Sigma_0(\tau)+O(\ln n/n^2)\ , \tag{16}$$

where for $|\tau|<\pi/2$,

$$\Sigma_0(\tau)=(\pi/2)\sum_{i=2}^{\infty}\begin{bmatrix}\frac{1}{2}\\ i\end{bmatrix}(2\tau/\pi)^{2i}(1-2^{-2i+2})\,\zeta(2i-1)$$
$$=b\tau^4+O(\tau^6)\ , \tag{17}$$

in which $\zeta(s)$ is the Riemann ζ function. Z_1, Z_0, or Z_σ may be expanded similarly using the results of Ref. 1.

Ferdinand and Fisher[1] then consider the exact expressions for the total energy U and specific heat C, obtained by differentiating Eq. (3) with respect to K. The energy does not concern us here. Evaluating the terms that appear in the specific heat asymptotically as $n\to\infty$, they find [Eq. (2)]

$$C/k_Bmn=A_0\ln n+B(\tau,s)+O(\ln n/n)\ ,$$

where $A_0=(8/\pi)K_c^2=0.494\,358\ldots$, and

$$B(\tau,s)=B_0(\tau,s)+B_\sigma(\tau,s)\ , \tag{18a}$$

$$B_0(\tau,s)/K_c^2=(8/\pi)[\ln(2^{5/2}/\pi)+C_E-\pi/4]+4(\Sigma_2-\tau^2Q_{3,-})-\{4(Q_{1,1}-Q_{3,1}\tau^2-sQ_{2,1}\tau^2)\}\ , \tag{18b}$$

$$\begin{aligned}B_\sigma/K_c^2=&(4/R)(R_3+R_4)\Sigma_3-(4\tau^2/R)(R_3+R_4)(Q_{3,+}-Q_{3,-})\\&+(4s/R^2)[(R_1+R_2)(R_3+R_4)(1+\tau^2\Sigma_3^2)+2\tau(R_3\tanh\tau s+R_4\coth\tau s)(R_1+R_2)\Sigma_3]\\&+\Bigg\{-(4/R)\sum_{i=1}^{4}R_i(Q_{1,i}-Q_{1,1})-(8\tau s/R)(R_3Q_{1,3}\tanh\tau s+R_4Q_{1,4}\coth\tau s)\\&+(4\tau^2/R)\sum_{i=1}^{4}R_i[(Q_{3,i}-Q_{3,1})+s(Q_{2,i}-Q_{2,1})+sQ_{1,i}^2]\\&+(4s/R^2)\Bigg[R_3^2\operatorname{sech}^2\tau s-R_4^2\operatorname{csch}^2\tau s+2\tau(R_2\tanh\tau s+R_4\coth\tau s)\sum_{i=1}^{4}R_iQ_{1,i}\\&-2\tau^2\Sigma_3[(R_1+R_2)(R_3Q_{1,3}+R_4Q_{1,4})-(R_3+R_4)(R_1Q_{1,1}+R_2Q_{1,2})]\\&-\tau^2\left[\sum_{i=1}^{4}R_iQ_{1,i}\right]^2\Bigg]\Bigg\}\ .\end{aligned} \tag{18c}$$

Explicit expressions for the $Q_{i,\pm}$, $Q_{t,i}$, and Σ_i are given in Ref. 1. The functions $\Sigma_i=\Sigma_i(\tau)$ and $Q_{i,\pm}=Q_{i,\pm}(\tau)$, i.e., they are independent of the shape parameter s. The shape dependence of B_0 and B_σ arises entirely from the functions R_i, $Q_{t,i}$, and the explicit s dependence in Eqs. (18b) and (18c). Numerical results for B vs τ at two s values and $\tau_{\max}$ vs s are shown in Figs. 1 and 2. In writing Eq. (18), we have rearranged some of the terms appearing in the corresponding expression given by Ferdinand and Fisher [their Eq. (4.18)].

Now the term $B_0(\tau,s)$ in Eq. (18) arises from differentiation of the factor Z_0 in the partition function [Eq. (11a)], likewise $B_\sigma(\tau,s)$ is due to Z_σ. For $s\geq 1$ (Ref. 5) B_0 depends significantly on the shape parameter s only for s close to 1 as illustrated in Fig. 1. For instance, $B_0(\tau,s=1)$ differs from $B_0(\tau,s=\infty)$ by as much as 75% for $|\tau|<\pi/2$,[6] however, this maximum percentage deviation diminishes exponentially as s grows. For instance, it is less than 2% for $s=2$. Thus, except for shape dependence of B_0 very near $s=1$, the entire dependence of $B(\tau,s)$ on s is contained in $B_\sigma(\tau,s)$. This fact is central to our analysis.

Equation (18) can equally well be obtained exactly by using Eqs. (12) and (16) for the R_i and the corresponding expansion for Z_1, differentiating the logarithm of the partition function [Eq. (11)] with respect to K and using Eq. (9) to expand K in terms of τ. This derivation also shows that all the functions $Q_{t,i}$, $i=1,2,3,4$ in Eq. (18) arise from derivatives of the Π_i [Eq. (13)]. The exponential dependence of these functions on the shape parameter s leads one to suspect that their contribution vanishes rapidly with increasing s. In fact, for $s\geq 1$ and arbitrary $|\tau|<\pi/2$ (Ref. 6), the terms in B involving $Q_{t,i}$, $i=1,2,3,4$ (which arise from the Π_i) contribute at most 1.8% of the total value of $B(\tau,s)$. This maximum contribution is largest at $s=1$ ($m\times m$ lattice)[7] and diminishes very rapidly as s increases. For instance, these terms affect $B(\tau,2)$ in the sixth decimal place at most for the range of τ values of interest. The Π_i themselves are also well approximated by $\pi_i(\tau,s)=1$ for $s\geq 1$,[5] e.g., $\pi_2(\tau=0,s=1)=0.9154$, $\pi_2(0,2)=0.9963$. Furthermore, one can see easily from Eq. (13) that for a given s the deviation

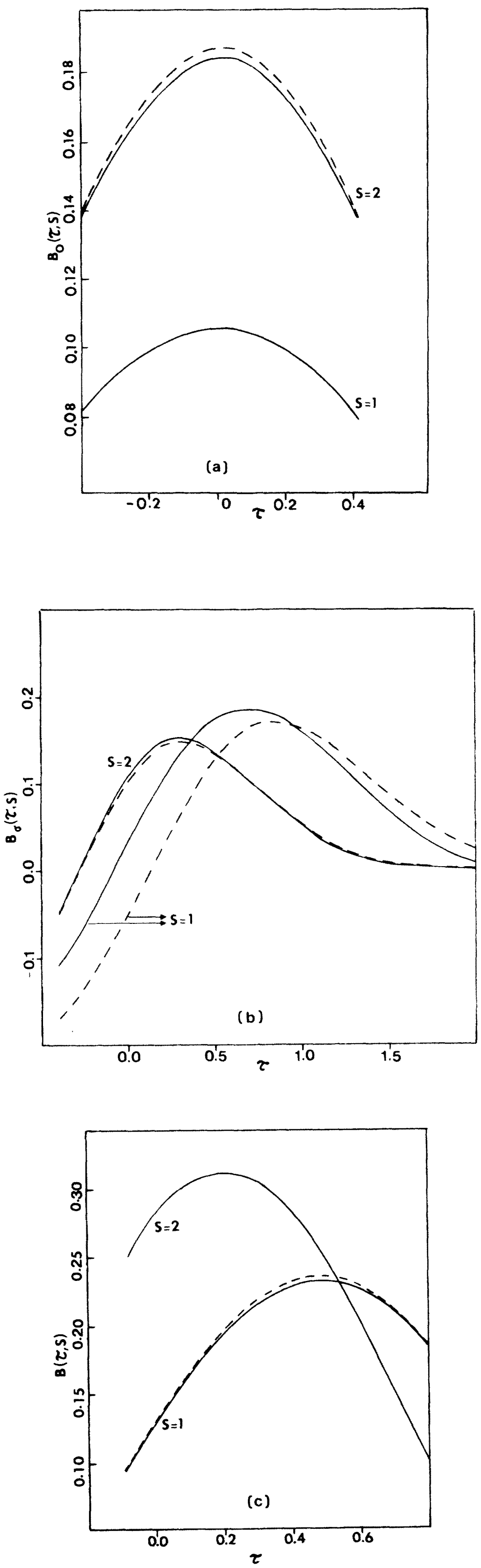

FIG. 1. Finite-size specific-heat correction terms $B_0(a)$, $B_\sigma(b)$, and $B(c)$ defined in Eq. (18) as functions of τ for shape parameter $s=m/n=1,2$. Solid curves: exact values; dotted curves: two-eigenvalue approximation. The exact and approximate values approach exponentially as s increases. Note that the approximate B_0 equals the exact $B_0(\tau,s=\infty)$.

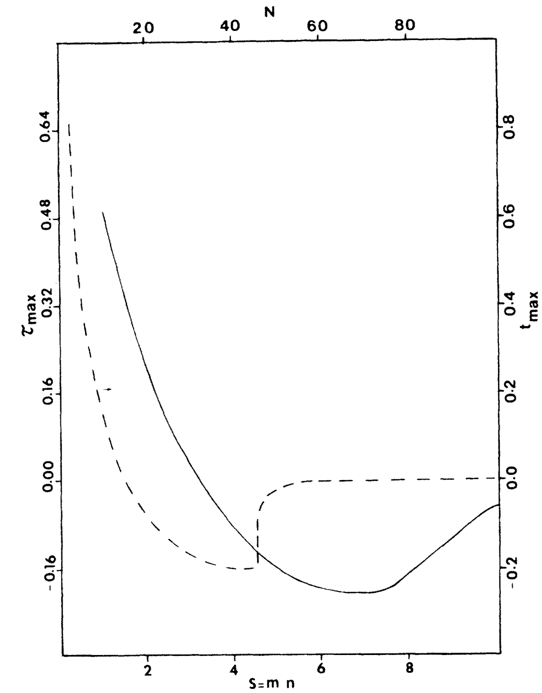

FIG. 2. Solid curve: reduced temperature τ_{max} of the peak in the (two-dimensional) specific-heat correction term B vs shape parameter $s=m/n$. The exact and two-eigenvalue approximation values already coincide to four figures at $s=1$ and become exponentially closer as s increases. Dashed curve: reduced temperature $t_{max}=[T_{max}-T_{max}(N=\infty)],T_{max}(\infty)$, of the specific-heat peak for a one-dimensional periodic Ising chain vs the number of spins N. The fairly abrupt jump in t_{max} between $N=44$ and 44.5 occurs because the specific heat near the maximum is almost constant in T.

of Π_i from 1 is largest at $\tau=0$, since each factor in the product defining a given Π_i is furthest from 1 at $\tau=0$ and approaches it monotonically with increasing $|\tau|$. The almost total lack of shape dependence in $B_0(s,\tau)$ described above is also due to the closeness of the Π_1 to 1; it is easy to see from Eq. (18) and Ref. 1 that the only shape-dependent part of $B_0(\tau,s)$ arises from derivatives of Π_1.

Hence by using Eqs. (12)–(17), we find to good approximation for the factor Z_σ in the partition function [Eq. (11a)],

$$Z_\sigma=\tfrac{1}{2}(1+R_2+R_3+R_4)=1+P_0e^{(m/2)\gamma_0}$$
$$=(1+e^{-sf(\tau)}) , \tag{19}$$

where

$$f(\tau)=\pi/4+\tau+(\ln 4/\pi)\tau^2+b\tau^4+O(\tau^6)$$
$$=0.7854+\tau+0.4413\tau^2-0.02908\tau^4+O(\tau^6) . \tag{20}$$

Note that in the region of the peak in $B(\tau,s)$, $-0.2\lesssim\tau\lesssim0.5$, $f(\tau)$ does not depend strongly on τ.

Within this approximation one therefore finds a free energy F,

$$-\beta F=[(mn/2)\ln(2\sinh 2K)+\ln Z_1]$$
$$+\ln(1+e^{-sf(\tau)})$$
$$=\ln Z_0+\ln Z_\sigma=-\beta F_0-\beta F_\sigma . \tag{21}$$

We may summarize the discussion following Eq. (18) in this way. The first term on the right-hand side of Eq. (21) includes the leading terms in the free energy as $n \to \infty$ as well as part of the finite-size correction terms. If one differentiates twice to obtain the specific heat, this term gives rise to the terms $A_0 \ln n$ and $B(\tau,\infty) \cong B_0(\tau,s)$ in B [Eq. (18)]. The entire shape dependence of B, i.e., $B_\sigma(\tau,s)$ and hence that of $\tau_{\max}$ therefore arises to this approximation from the second term in Eq. (21), i.e., $-\beta F_\sigma \cong \ln(1+e^{-sf(\tau)})$.

We now consider further the meaning of the approximation $\Pi_i = 1$. From Eqs. (10), (12), and (15) it follows that

$$\begin{aligned} Z_{1,2} &= \exp\left[(m/2)\sum_{r=0}^{n-1}\gamma_{2r+1}\right], \\ Z_{3,4} &= \exp\left[(m/2)\sum_{r=0}^{n-1}\gamma_{2r}\right][1 \pm \exp(-m\gamma_0)] . \end{aligned} \tag{22}$$

Substituting in Eq. (11) gives simply

$$Z = (2\sinh 2K)^{mn/2}\left[\exp(m/2)\sum_{r=0}^{n-1}\gamma_{2r+1} + \exp(m/2)\sum_{r=0}^{n-1}\gamma_{2r}\right] = \lambda_0^m + \lambda_1^m . \tag{23}$$

Thus this approximation amounts to keeping only the two largest eigenvalues λ_0 and λ_1 of the transfer matrix.[3] We argue further in Sec. IV that one may write Eq. (23) as a product of a factor attributable to a one-dimensional Ising array of domain walls and another attributable to the partition function of a single domain. In the critical region, Eq. (23) becomes

$$\begin{aligned} Z = \exp s\{&n^2(\ln 2/2 + 2G/\pi) - n\tau/\sqrt{2} + (\ln n)\tau^2/\pi \\ &+ \pi/12 + \tau^2[\ln(2^{5/2}/\pi)/\pi + C_E/\pi] \\ &- \tau^4 b_1\}\{1+\exp[-sf(\tau)]\} , \end{aligned} \tag{24}$$

where $G = 1^{-2} - 3^{-2} + 5^{-2} = 0.9159\ldots$ is Catalan's constant, Euler's constant is $C_E = 0.5772\ldots$, $b_1 = 7b/6$, and use has been made of Eqs. (9), (11), (17), and (19) as well as several related results from Ref. 1. Equation (24) and its derivatives give the thermodynamics of the Ising model in the critical region in the two-eigenvalue approximation ($\Pi_i = 1$) to the order we are working—terms through $O(1)$ in $\ln Z$, $O(n)$ in the total energy U, and $O(n^2)$ in the total specific heat C. The terms in B_0 and B_σ that vanish in the two-eigenvalue approximation are displayed in curly braces in Eqs. (18b) and (18c); these are just the parts of B involving the $Q_{t,i}$ which arise from the derivatives of the π_i. The approximation to the internal energy U is likewise obtained by setting $Q_{t,i} = 0$ in Eq. (4.13) of Ref. 1.

III. DOMAIN-WALL ENERGIES IN THE CRITICAL REGION

Now we consider domain-wall energies (surface tensions) in the critical region. These may be defined by the Onsager method[3] which considers a lattice with antiferromagnetic coupling ($J<0$) and an odd number of layers in the appropriate direction. The latter condition gives rise to an additional domain wall. Since the free energy is an even function of J, the free energy of one extra wall can be obtained by subtraction.

If we set $J_x < 0$ and m odd, the wall is in the y (column) direction, and the partition function is expressible as[8]

$$Z_{\pm} = \tfrac{1}{2}(2\sinh 2K)^{mn/2}(Z_1 + Z_2 - Z_3 - Z_4) . \tag{25}$$

If σ is the wall free energy per spin, using Eqs. (2) and (11) gives

$$-\beta n\sigma = \ln\left[\frac{1+R_2-R_3-R_4}{1+R_2+R_3+R_4}\right] . \tag{26}$$

For a wall in the x (row) direction, one finds similarly[8]

$$-\beta m\sigma_x = \ln\left[\frac{1-R_2+R_3-R_4}{1+R_2+R_3+R_4}\right] . \tag{27}$$

Setting *both* $J_x = J_y < 0$ and m and n odd, one obtains[8] a diagonal wall

$$-\beta m\sigma_{xy} = \ln\left[\frac{-1+R_2+R_3-R_4}{1+R_2+R_3+R_4}\right] . \tag{28}$$

Wall energies for boundaries in the x or y direction in the thermodynamic limit at *fixed* T were evaluated by Onsager[3] with the exact result

$$\beta\sigma = \beta\sigma_x = \begin{cases}\gamma_0, & T \le T_c \\ 0, & T \ge T_c\end{cases} \tag{29}$$

where γ_0 is given in Eq. (7). σ_{xy} has been similarly calculated by Fisher and Ferdinand[9] who find

$$\beta\sigma_{xy} = 2\ln\operatorname{csch}2K . \tag{30}$$

We are now in a position to evaluate the surface-tension expressions in the critical region as a function of the shape parameter s. From Eqs. (12), (14), and (16), we obtain [in the approximation $\Pi_i(\tau,s) = 1$]

$$\begin{aligned} -\beta n\sigma &= \ln\left[\frac{1-P_0 e^{(m/2)\gamma_0}}{1+P_0 e^{(m/2)\gamma_0}}\right] \\ &= \ln\frac{1-e^{-sf(\tau)}}{1+e^{-sf(\tau)}} , \end{aligned} \tag{31}$$

where $f(\tau)$ is defined in Eq. (20). This expression implies several results of interest. It shows that for fixed τ the domain-wall (free) energy σ per spin vanishes as $1/n$ in the thermodynamic limit. Since Eq. (31) is also valid at $\tau = 0$ and $f(0)$ is finite, we see that this slow convergence also holds at the critical point, with the possible exception of an $\infty \times n$ lattice ($s = \infty$), the case considered by Onsager.[3] In addition, Eq. (31) implies that the *total* domain-wall free energy $n\sigma$ is constant for fixed τ. Hence one expects a significant contribution to the thermodynamics from domain walls, at least for sufficiently large s. This is to be contrasted with the situation at fixed $T < T_c$, where Eq. (29) implies a growing total domain-wall energy, hence an exponentially small free-energy contribution.

Considering Eqs. (27) and (28), we similarly obtain

$$-\beta_c m\sigma_{xy} = -\beta_c m\sigma_x = \ln\left[\frac{e^{-sf'(\tau)}}{1+e^{-sf(\tau)}}\right], \tag{32}$$

where

$$f'(\tau) = \pi/4 - \tau + (\ln 4/\pi)\tau^2 + b\tau^4 + O(\tau^6) . \tag{33}$$

Comparing Eqs. (31)—(33) shows that the domain-wall energy is anisotropic at fixed τ.[10] Further, the x direction (σ_x) or diagonal (σ_{xy}) walls have considerably larger free energies than those in the y direction (σ) as $s \to \infty$. For instance, when $\tau=0$, $\beta_c m\sigma_{xy}$ is already 2.3 times $\beta_c n\sigma$ for $s=2$, and the difference grows approximately linearly with s. Thus, for $s>1$,[5] one expects arrays of y direction walls of free energy per spin σ to be thermodynamically favored.

Recall the factorization of the partition function $Z=Z_0 Z_\sigma$ of Eq. (11). The factor Z_σ was shown above, to excellent approximation, to account for the shape dependence of the finite-size correction B to the specific heat in the critical region. Now if one solves Eqs. (26)—(28) for the R_i and substitutes the result in Eq. (11a), one has, quite generally,

$$Z_\sigma^{-1} = [1+\exp(-\beta n\sigma)+\exp(-\beta m\sigma_x) - \exp(-\beta m\sigma_{xy})]/2 . \tag{34}$$

In the present case, $\pi_i=1$ implies $\sigma_x=\sigma_{xy}$ (Ref. 10) (and $\sigma_x \gg \sigma$ as $s\to\infty$) so that

$$Z_\sigma = 1+\tanh(\beta n\sigma/2) . \tag{35}$$

Hence part of the thermodynamics and, in particular, the shape dependence of B, is due to domain walls in the y direction. The two-eigenvalue approximation that we are using here is reminiscent of the one-dimensional Ising model. We argue in Sec. IV that Z_σ may indeed be interpreted as the finite-length correction factor of a one-dimensional Ising array of y-direction domain walls.

Ferdinand and Fisher[1] note that the shape dependence of $\tau_{\max}$ seems to arise from an interplay between the Z_i of Eq. (3) and the cross terms that arise when the partition function is differentiated to calculate the specific heat. It follows from our results [Eqs. (10), (11a), (11b), (18), and (35)] that in the two-eigenvalue approximation this mathematical origin of the effect is attributable to the domain-wall energy $n\sigma$.

IV. FINITE-SIZE CORRECTIONS, DOMAIN WALLS, AND THE ONE-DIMENSIONAL ISING MODEL

This section begins by examining the finite-size behavior of the one-dimensional Ising model. We show, in particular, that for periodic boundary conditions the temperature $T^1_{\max}$ of the specific-heat peak first decreases then increases as the number of spins (or length) $N\to\infty$. This behavior is qualitatively the same as that of $\tau_{\max}$, the peak temperature of the finite-size correction term B to the specific heat of the two-dimensional Ising model, as the lattice shape is varied. Then we show that to very good approximation the shape-dependent part of B is due to a term that has the form of the free energy of a one-dimensional Ising array of domain walls. This provides a mechanism for the behavior of $\tau_{\max}$. We conclude with an approximate calculation of the effective number of degrees of freedom and effective coupling of this array.

The partition function of a one-dimensional Ising model of N spins with periodic boundary conditions and coupling constant $J>0$ is simply

$$\begin{aligned} Z_1(N) &= 2^N(\cosh^N K + \sinh^N K) \\ &= 2^N \cosh^N K(1+\tanh^N K) \\ &= Z_{10} Z_{1\sigma} , \end{aligned} \tag{36}$$

where $K=J/k_B T$ as in Eq. (4) and $Z_{1\sigma}$ refers to the factor in parentheses in the second line of Eq. (36). Thus the free energy F_1 is

$$\begin{aligned} -\beta F_1 &= \ln Z_1 = N\ln(2\cosh K) + \ln(1+\tanh^N K) \\ &= \beta N f_\infty - \beta\delta F_1(n) , \end{aligned} \tag{37}$$

where f_∞ is the free energy per spin of the infinite system and δF_1 is the finite-length free-energy correction. Note that δF_1 arises from the factor $Z_{1\sigma}$ in Eq. (36). Differentiating Eq. (37) gives for the specific heat per spin,

$$C_1/Nk_B = c_\infty + \delta c , \tag{38}$$

where

$$c_\infty = K^2(1-\tanh^2 K) \tag{39}$$

and

$$\begin{aligned} \delta c = c_\infty[&(N-1)(\tanh^{N-2}K - \tanh^N K) - 2\tanh^N K \\ &- \tanh^{2N-2}K - \tanh^{2N}K]/(1+\tanh^N K)^2 . \end{aligned} \tag{40}$$

The function C_∞ has a single peak at temperature $T^a_{\max} = J/k_B K_{\max} = 0.8335$ independent of N.

The correction term δc_1 has a more complicated structure, with both positive and negative extrema $\delta c_\pm$ at temperatures $T^b_\pm, T^b_- < T^b_+$. As N increases, the peak locations $T^b_\pm$ and peak magnitudes $|\delta c_\pm|$ both decrease except for a relatively small increase in δc_{1+} for $N \lesssim 8$. Since $T^b_\pm$ are near or above $T^a_{\max}$ for small N, the net effect on C_1 is a specific-heat peak temperature $T^1_{\max}$ that first decreases and then increases as the length of the chain of spin approaches infinity.[11] This behavior as well as the decrease in $|\delta c\pm|$ is clearly a result of periodic boundary conditions,[12] which act to strengthen the spin coupling K by an amount that decreases with N. The peak temperature $T^1_{\max} - T^a_{\max}$ of C_1 is displayed as a function of N in Fig. 2. What we have seen is that the decrease and increase of $T^1_{\max}$ with N is a result of the interplay of a length-dependent finite-size term due to the factor $Z_{1\sigma}$ in Eq. (36) and a length-independent term due to Z_{10}.

In Sec. II we showed that the shape (s) dependence of the peak in the specific-heat correction term B for the two-dimensional Ising model arises from a similar mathematical mechanism. In that case $B=B_0+B_\sigma$, where B_0 is due to an (essentially) shape-independent factor Z_0 in the partition function, and B_σ arises from the factor Z_σ that does depend significantly on s. As s increases from 1, there is a positive peak in B_σ that moves to lower τ values and B_σ itself decreases, giving rise to a peak position $\tau_{\max}$ vs s that is qualitatively similar to $T^1_{\max}$ vs N, as shown in Fig. 2.

In Sec. II we demonstrated that Z_σ may be expressed in terms of a domain-wall energy. We now go on to show that it is possible to identify Z_σ as the contribution of a one-dimensional Ising array of domain walls.

First we consider the connection between the finite-size correction and domain-wall energies. In the one-dimensional Ising model, we can define a surface-tension or domain-wall energy σ_1 by the Onsager procedure[3] described in Sec. IV. This gives

$$-\beta\sigma_1=\ln\left[\frac{1-\tanh^N K}{1+\tanh^N K}\right] . \tag{41}$$

For $K>0$, taking the limit $N\rightarrow\infty$ gives

$$\beta\sigma_1=2\tanh^N K\rightarrow 0,\quad N\rightarrow\infty \tag{42}$$

so that the surface tension vanishes in the thermodynamic limit when the coupling is finite. If one solves Eq. (41) and substitutes in Eq. (36), the result is

$$Z_{1\sigma}=1+\tanh(\beta\sigma_1/2) . \tag{43}$$

This should be compared with Eq. (35) for the two-dimensional case,

$$Z_\sigma=1+\tanh(\beta n\sigma/2) .$$

Now $n\sigma$ is constant at fixed τ and s in the thermodynamic limit. Hence, in the critical region of the two-dimensional Ising model, the part of the finite-size corrections arising from Z_σ depends on the domain-wall energy in exactly the same way as the entire finite-size correction in the one-dimensional case. This correspondence was used in Sec. III to establish that the dependence of $\tau_{\max}$ on s is a domain-wall effect. It also suggests that the effect is due to an array of domain walls that can be modeled by a one-dimensional Ising chain with an effective number of spins N (that increases with s) and an effective coupling K. Since the Ising chain transfer matrix is two dimensional, the accuracy of the two-eigenvalue approximation (see Sec. III) also supports this picture.

Consider first a one-dimensional Ising model of length m with periodic boundary conditions divided up into $\mathscr{N}$ blocks or domains of length l_0, so $\mathscr{N}=m/l_0$. If we assume that the assembly of blocks itself acts as a one-dimensional array, we have

$$\mathscr{Z}_1=Z_d^{\mathscr{N}}(e^{-\mathscr{N}K'}/2)2^{\mathscr{N}}(\cosh^{\mathscr{N}}K'+\sinh^{\mathscr{N}}K')m , \tag{44}$$

where K' is the coupling between blocks, Z_d is the partition function due to fluctuations in a single domain (of the minimal size), the factor m allows us to start the first domain anywhere along the chain, and the factor $e^{-\mathscr{N}K'}/2$ enforces $\mathscr{Z}_1$ to be independent of K' for large coupling, when all domains should be aligned. We also assume that a periodic form is appropriate for the domain-wall part of the partition function. If we now require that the domain-wall energy in the original model be preserved in the block model, i.e., $\tanh^m K=\tanh^{\mathscr{N}}K'$, it follows from Eqs. (36), (41), (43), and (44) that

$$Z_d=(2/m)^{1/m}(\tfrac{1}{2})\mathscr{Z}_1(l_0) . \tag{45}$$

Hence, aside from some factors independent of coupling, the partition function of the spins in one block or domain of length l_0 is just the partition function of a one-dimensional Ising model of that length. This indicates that the factorization introduced in Eq. (44) is reasonable, at least in one dimension. Of course, one only expects it to be of physical interest when the domain size l_0 is of the order of the correlation length ξ.

A similar picture may be expected in the critical region of the two-dimensional Ising model. Here, for $s>1$, we assume that the important configurations are composed of domains of (minimum) length l_0 (including the width of one neighboring domain wall) in the x direction and width n in the y direction, separated by domain walls running in the y direction. Since, as shown in Sec. IV, x direction (or diagonal) walls have larger energy than y direction walls for $s>1$, a one-dimensional array of this sort is to be expected as long as $l_0\gtrsim n$. In the approximate calculation given below, l_0 in fact satisfies this condition.

The partition function, by analogy with Eq. (45), will then be given by

$$Z=Z_D^N(e^{-NK}/2)2^N(\cosh^N K+\sinh^N K)m , \tag{46}$$

where $N=m/l_0$ is the number of possible domains or walls, K is the domain coupling, and Z_D is the partition function of a single (minimal) two-dimensional domain. Now, in the critical region,

$$Z=Z_0(1+\tanh\beta n\sigma/2) , \tag{47}$$

where we have employed Eqs. (11) and (35). Requiring that the wall energy given by Eqs. (46) and (47) be the same,

$$\tanh^N K=\tanh\beta n\sigma/2 \tag{48}$$

results in

$$Z_D=(2/m)^{1/N}[2/(1+\tanh^{1/N}\beta n\sigma/2)]Z_0^{1/N} . \tag{49}$$

Explicit expressions for $\tanh\beta n\sigma/2$ and Z_0 on terms of s and τ in the two-eigenvalue approximations can be obtained from Eqs. (11), (19), (20), (24), and (31). It is immediately clear from Eq. (48) that since $\beta n\sigma$ is constant and finite as $n\rightarrow\infty$ for fixed s and τ, N and K must also remain fixed (except in the case N, $K\rightarrow\infty$, $N\alpha e^{2K}$). But in order to find N and K separately as functions of s and τ, another equation independent of Eq. (48) is necessary. More generally, to fully establish the one-dimensional domain-wall model that has been assumed here, one apparently needs a detailed microscopic theory of domains and domain walls in the critical region. That is a difficult problem beyond the scope of this paper. In the following we confine ourselves to an approximate calculation of $N=m/l_0$ that gives reasonable results, and then present, in Sec. V, some further support of the model in the form of evidence that it extends naturally into the fixed $T<T_c$ regime.

In the critical region we expect l_0 to be proportional to ξ, the correlation length in the x direction. Since the $m\times n$ lattice is finite in this direction, we use the formula

$$\xi^2=\tfrac{1}{2}\int_0^{m/2}g(x)x^2dx\bigg/\int_0^{m/2}g(x)dx . \tag{50}$$

In Eq. (50), $g(x)$ is the two-spin correlation function, we integrate only to $m/2$ to avoid periodic boundary condition effects, and the factor $\frac{1}{2}$ ensures that Eq. (50) reduces to the usual formula $\xi_\infty=1/\ln(\lambda_0/\lambda_1)$ for $s\rightarrow\infty$ where λ_0 and λ_1 are the two largest eigenvalues of the transfer matrix. When only two eigenvalues are important (e.g., for the one-dimensional Ising model or the two-dimensional case with $\pi_i=1$—see Sec. II), Eq. (50) yields

$$\xi^2=\xi_\infty^2\left[1-\frac{m/2\xi_\infty}{\sinh(m/2\xi_\infty)}\right]. \tag{51}$$

In the critical region we have

$$\xi_\infty=1/\ln(\lambda_0/\lambda_1)=n/f(\tau), \tag{52}$$

where $f(\tau)$ is given by Eq. (20). Thus the correlation length ξ diverges proportionally to n in the thermodynamic limit. An approximate measure of the number of possible domains N or the number of possible domain walls is therefore

$$N=m/\xi=sf\left[1-\frac{sf/2}{\sinh(sf/2)}\right]^{-1/2}. \tag{53}$$

Hence, as expected, N is constant for fixed s and τ as $n\to\infty$, and Eq. (48) implies that the coupling K is constant as well.

A typical value of f for the range of τ of interest here is $f=0.7$. For s near 1, $sf/2$ is thus sufficiently small that we may expand the sinh in Eq. (53) giving $N=2\sqrt{6}+O(s^2)$. Equation (48) then results in $\tanh K=e^{-sf/2\sqrt{6}}$. Hence, in this limit, N is of the order of 1 and the coupling depends on both s and τ. Of course, our evaluation of N (via $l_0=\xi$) is, at best, only semiquantitatively correct. The fact that it indicates N is close to 1 as $s\to 1$ may therefore be taken as evidence in favor of the general validity of the one-dimensional model, since one does not expect more than at most a few domains for $m=n$.

For increasing values of s, one finds N growing monotonically, with limiting behavior $N=sf$ and $\tanh K=1/e$. This constant coupling regime does not occur, for typical f values, until $s\cong 10(N\cong 8)$, which is beyond the range of s values for which the shape dependence of the finite-size correction term B is an important effect (cf. Fig. 2). It is also of interest to note that for large s, $\xi/n\to 1/f>1$, while for $s\to 1$, ξ/n decreases to a minimum of $1/2\sqrt{6}$. However, already for $s=2$ one has $\xi/n=0.4$. So the assumption that the correlation length in the y direction is n or larger is reasonable, since as pointed out above this quantity should exceed the x-direction correlation length ξ for $s>1$.

One may also attempt to evaluate Z_D using Eqs. (49), (51), and (52). We believe there are too many approximations in this treatment [especially Eq. (51)] for the detailed result to be meaningful. It is, however, perhaps worth noting that the s dependence of N from Eq. (53) is such that Z_D depends only weakly on s and approaches a constant as $s\to\infty$. A domain free energy more or less independent of s is what one would expect in an exact theory.

V. FINITE-SIZE CORRECTIONS FOR $T<T_c$

In the two-dimensional Ising model for $T<T_c$, domain walls will still be present. However, here the wall energy per spin σ (or σ_x or σ_{xy}) remains finite in the thermodynamic limit. Hence its contribution to the thermodynamics must be exponentially small, as is evident from Eqs. (11) and (34). For an $m\times n$ lattice with s sufficiently larger than 1, walls in the y direction will dominate since they will be shortest and thus have the smallest total energy. In this case one will again have a one-dimensional array of domain walls, but the average distance l_0 between walls (average domain length) will grow exponentially according to[3,13]

$$l_0=e^{\beta n\sigma}. \tag{54}$$

Hence, as in the critical region, the walls make up at least part of the finite-size correction to the thermodynamics. (Note that the free energy converges exponentially for $T<T_c^3$, so the wall contribution cannot be dominated by some less rapidly vanishing term.)

Now Barber[4] has shown, by an analysis of the $|\tau|\to\infty$ behavior of the critical region correction terms, that

$$B(\tau,s)\underset{\tau\to\infty}{\longrightarrow}-A_0\ln\tau+A_1+O(e^{-\tau}), \tag{55}$$

where

$$A_1=-A_0[\pi/4+\ln(K_c/\sqrt{2})]. \tag{56}$$

Thus the shape dependence of the *leading* specific-heat correction term vanishes [i.e., $B(\tau,s)\to_{\tau\to\infty}B(\tau)$ in Eq. (18)], so that $B_\sigma=0$ in the two-eigenvalue approximation as one moves out of the critical region. Further, substituting Eq. (55) in Eq. (2) gives[4]

$$C/k_Bmn=A_0\ln|(T-T_c)/T_c|^{-1}+A_1+O(1), \tag{57}$$

which is the correct form for the specific heat per spin in the thermodynamic limit for fixed T near T_c. Thus the large-τ behavior of B merges smoothly with the fixed-T specific heat. Presumably, the shape dependence of B vanishes in this limit since it is due to domain walls which have large energies and make a lower-order (exponentially vanishing) contribution to the thermodynamics. This suggests that at least part of the $O(e^{-\tau})$ correction term in Eq. (55) is due to domain walls and therefore depends on shape. Note that

$$\tau\propto n(T-T_c)\propto n\sigma, \tag{58}$$

for T near T_c [see Eqs. (1), (14), and (29)]. These remarks suggest that, at least for s sufficiently greater than 1, a one-dimensional array of domain walls contributes to the partition function both for $T<T_c$ and in the critical region, and these contributions merge smoothly with each other as one passes from the fixed-τ to fixed-T regime.

Note added

We believe there is a minor quantitative correction necessary to a few of the formulas in Ref. 1. In particular, the expressions for Σ_0 and Σ_{00} given should be divided by 2. Differentiating the partition function to find the internal energy and specific heat shows that this correction also applies to the definitions of Σ_1, Σ_2, and $Q_{3,\pm}$. Making these changes does not affect the qualitative results of Ref. 1 (or this work) in any way. The only differences are small and quantitative; e.g., the minimum value of $\tau_{\max}$ is at s approximately 7 rather than 6.

All the results reported here, including error estimates and figures, reflect this change. This alteration reduces the size of the τ^2 term in $B_0(\tau)$ so that it depends less strongly on τ near its maximum. This makes $\tau_{\max}(s)$, the position of the peak in $B(\tau,s)$, more sensitive to the asymmetries in $B_\sigma(\tau,s)$, which are themselves slightly increased in magnitude. One result is that the value of $\tau_{\max}(1)$ given in Ref. 1, from which the temperature of the specific-heat maximum in an $m\times m$ system can be deduced, is about 33% too small. This suggests that the convergence of the specific-heat peak to $\tau_{\max}(1)$ is slower than what is implied by Fig. 3 of Ref. 1 [see also D. P. Landau, Phys. Rev. B 13, 2997 (1976)]. Another possibility is that there are further corrections necessary in the parts of $B(\tau,s)$ that vanish in the two-eigenvalue approximation, which could be important for $s=1$. We do not believe the latter to be the case, but ruling it out definitely would require some very tedious calculations.

We have very recently become aware of the work of A. D. Bruce [J. Phys. C 14, 3667 (1981)] on block spin distributions in Ising models. The mechanisms determining the fixed-point distribution in two dimensions suggested in this work bear some striking similarities with our conclusions, especially the proposal that one-dimensional behavior is important. Note that our results imply this fixed-point distribution must be strongly shape dependent, and approach a Gaussian as s increases.

ACKNOWLEDGMENTS

We would like to thank M. E. Fisher for several stimulating discussions and J. Grinstein for a helpful remark. Thanks are also due to V. Privman for bringing the work of Bruce (see *Note added*) to our attention. This work was supported in part by the Office of Naval Research.

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[1]A. E. Ferdinand and M. E. Fisher, Phys. Rev. 185, 832 (1969). We believe a few of the formulas reported here require minor correction. See *Note Added.*

[2]B. Kaufman, Phys. Rev. 76, 1232 (1949).

[3]L. Onsager, Phys. Rev. 65, 117 (1944).

[4]M. N. Barber, in Phase Transitions and Critical Phenomena, edited by C. Domb and J. L. Lebowitz (Academic, New York, in press), Vol. 7; M. E. Fisher, in *Critical Phenomena, Proceedings of the International School of Physics, "Enrico Fermi,"* Course 51, edited by M. S. Green (Academic, New York, 1971); M. E. Fisher and M. N. Barber, Phys. Rev. Lett. 28, 1516 (1972).

[5]In what follows, we consider $s\geq 1$ only. By symmetry, the same results hold for $s'=1/s\leq 1$. To demonstrate this explicitly would require a determination of the behavior of the $\pi_i(\tau,s)$ for small s, which we have not performed.

[6]This range of τ values includes the peak in $B(s,\tau)$ for all s.

[7]Actually, there is some cancellation of terms in B involving different $Q_{t,i}$ at $s=1$.

[8]P. Stancioff, M. S. thesis, University of Maine, 1983 (unpublished). In terms of the formulation of the Onsager (Ref. 3) solution give by T. D. Schultz, D. C. Mattis, and E. H. Lieb, Rev. Mod. Phys. 36, 856 (1964), the changes of sign from Eq. (11) to Eq. (25) and for the other surface tensions arise from either an exchange of odd and even sets of q values between the operators $V^{\pm}$, or a change of sign of V^- or both.

[9]M. E. Fisher and A. E. Ferdinand, Phys. Rev. Lett. 19, 169 (1967) (this calculation applies for $m=n$ only, but no shape effects are to be expected in σ_{xy} at fixed $T<T_c$).

[10]For $s=1$, one must have $\sigma=\sigma_x$ by symmetry. Equations (31) and (32) do not quite satisfy this since they are obtained using the approximation $\pi_i=1$, which is slightly in error for $s=1$.

[11]J. Bonner, unpublished homework problem.

[12]For free boundary conditions, $T^1_{\max}$ is independent of N and δc_1 has a single minimum at $T^1_{\max}$ that goes to zero at $1/N$.

[13]M. E. Fisher, J. Phys. Soc. Jpn. Suppl. 26, 87 (1969).